

## Supplemental Material-II

### Impact of Conformational Structures on Low-Temperature Oxidation Chemistry for Cyclohexyl Radical: A Theoretical and Kinetic Modeling Study on First Oxygen Addition

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**Table S1.** Geometries and frequencies of major species in this work, they were obtained by self-

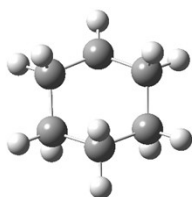
consistent field (SCF) calculations with tight convergence criteria, of which the maximum energy

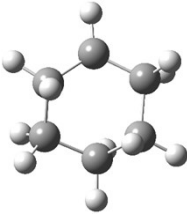
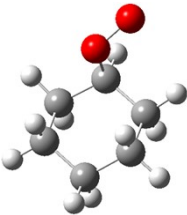
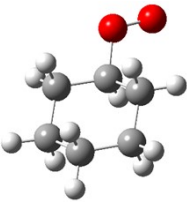
change was less than  $1 \times 10^{-6}$  Hartree. Geometry optimizations were also conducted using tight

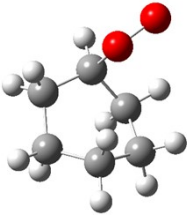
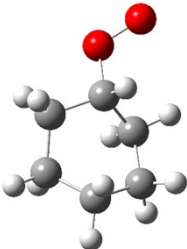
thresholds, including a maximum force of 0.00045 Hartree/Bohr, RMS force of 0.00030

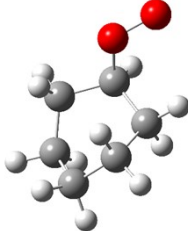
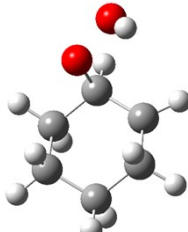
Hartree/Bohr, maximum displacement of 0.0018 Bohr, and RMS displacement of 0.0012 Bohr. Note

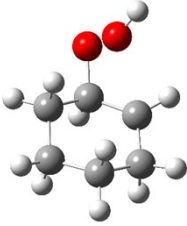
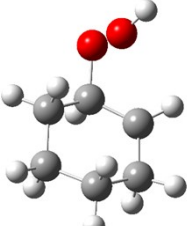
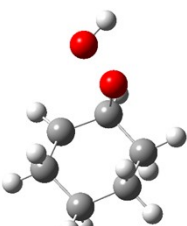
that the frequencies in red indicate the low frequencies relevant to torsional motions.

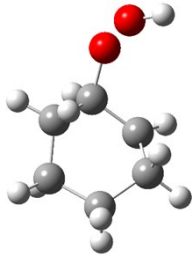
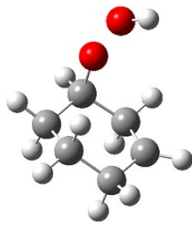
| Reactants                                                                           | Cartesian Coordinates (Å) |           |           |           | Frequencies (cm <sup>-1</sup> ) |            |            |
|-------------------------------------------------------------------------------------|---------------------------|-----------|-----------|-----------|---------------------------------|------------|------------|
|  | C                         | -0.048373 | 0.793125  | 1.287975  | 171.7145,                       | 207.3100,  | 320.8808,  |
|                                                                                     | C                         | -0.539837 | 1.370342  | 0.000000  | 388.4253,                       | 437.2557,  | 456.7276,  |
|                                                                                     | C                         | -0.048373 | 0.793125  | -1.287975 | 605.4736,                       | 778.2984,  | 803.6399,  |
|                                                                                     | C                         | -0.048373 | -0.750060 | -1.268808 | 850.0994,                       | 869.2072,  | 873.5138,  |
|                                                                                     | C                         | 0.621779  | -1.295425 | 0.000000  | 922.6603,                       | 1011.0765, | 1030.6598, |
|                                                                                     | C                         | -0.048373 | -0.750060 | 1.268808  | 1056.3243,                      | 1095.3575, | 1108.6952, |
|                                                                                     | H                         | -0.636703 | 1.166945  | -2.131697 | 1128.3345,                      | 1152.4275, | 1250.6170, |
|                                                                                     | H                         | -1.053209 | 2.325989  | 0.000000  | 1279.9083,                      | 1293.4505, | 1338.2814, |
|                                                                                     | H                         | 0.989200  | 1.130415  | 1.472875  | 1344.4954,                      | 1349.7019, | 1376.0033, |
|                                                                                     | H                         | -0.636703 | 1.166945  | 2.131697  | 1385.4505,                      | 1391.8394, | 1465.5503, |
|                                                                                     | H                         | -1.084113 | -1.107993 | -1.310308 | 1470.7396,                      | 1485.0950, | 1489.2889, |
|                                                                                     | H                         | 0.455480  | -1.133660 | -2.161976 | 1499.7507,                      | 2894.1080, | 2898.9000, |
|                                                                                     | H                         | 0.591319  | -2.389981 | 0.000000  | 2995.5110,                      | 3009.8778, | 3010.7175, |
|                                                                                     | H                         | 1.683461  | -1.013694 | 0.000000  | 3045.0948,                      | 3047.1956, | 3048.9818, |
|                                                                                     | H                         | -1.084113 | -1.107993 | 1.310308  | 3050.0712,                      | 3054.7502, | 3162.3620  |

|                                                                                     |   |           |           |           |            |            |            |
|-------------------------------------------------------------------------------------|---|-----------|-----------|-----------|------------|------------|------------|
|                                                                                     | H | 0.455480  | -1.133660 | 2.161976  |            |            |            |
|                                                                                     | H | 0.989200  | 1.130415  | -1.472875 |            |            |            |
| RTi                                                                                 | C | 1.170909  | 0.837649  | 0.346064  | 66.9325,   | 223.5182,  | 237.5422,  |
|    | C | -0.125921 | 1.490787  | -0.015147 | 334.9474,  | 455.6509,  | 479.4640,  |
|                                                                                     | C | -1.305974 | 0.626533  | -0.332708 | 575.6879,  | 767.3161,  | 801.9495,  |
|                                                                                     | C | -1.177841 | -0.737679 | 0.368270  | 835.0576,  | 872.7402,  | 879.3749,  |
|                                                                                     | C | 0.122223  | -1.481849 | -0.017640 | 947.2566,  | 1008.7130, | 1025.6537, |
|                                                                                     | C | 1.299319  | -0.530530 | -0.350097 | 1051.8924, | 1078.9829, | 1125.2241, |
|                                                                                     | H | -2.239312 | 1.121864  | -0.040840 | 1127.3678, | 1162.0554, | 1218.0608, |
|                                                                                     | H | -0.208971 | 2.571281  | -0.050393 | 1275.8389, | 1291.2962, | 1335.8334, |
|                                                                                     | H | 1.331387  | -0.354921 | -1.430636 | 1348.8656, | 1358.8129, | 1365.0348, |
|                                                                                     | H | 1.246994  | 0.692740  | 1.438991  | 1381.9314, | 1387.9619, | 1469.2356, |
|                                                                                     | H | -1.190915 | -0.563077 | 1.449645  | 1471.3210, | 1489.3141, | 1500.2261, |
|                                                                                     | H | -2.046936 | -1.364224 | 0.146955  | 1513.2686, | 2906.0820, | 2908.6403, |
|                                                                                     | H | -0.064795 | -2.127658 | -0.881601 | 3013.5896, | 3015.8836, | 3023.4230, |
|                                                                                     | H | 0.402191  | -2.149179 | 0.803703  | 3028.3171, | 3034.5299, | 3042.3214, |
|                                                                                     | H | 2.250029  | -1.003347 | -0.086629 | 3058.5796, | 3070.0549, | 3169.0020  |
|                                                                                     | H | 2.016822  | 1.481524  | 0.081110  |            |            |            |
|                                                                                     | H | -1.392794 | 0.465535  | -1.422762 |            |            |            |
| W1Ca                                                                                | C | -2.033236 | 0.357584  | -0.291140 | 82.3286,   | 134.3539,  | 185.8044,  |
|  | C | -0.924107 | 1.419230  | -0.273514 | 290.1923,  | 318.0976,  | 375.0291,  |
|                                                                                     | C | 0.135725  | 1.111777  | 0.794261  | 425.0504,  | 480.2289,  | 537.1648,  |
|                                                                                     | C | 0.689896  | -0.307468 | 0.683594  | 632.7747,  | 780.9337,  | 799.6373,  |
|                                                                                     | C | -0.393627 | -1.376598 | 0.578692  | 810.2303,  | 868.6583,  | 873.0957,  |
|                                                                                     | C | -1.451283 | -1.049325 | -0.487518 | 899.5563,  | 940.2361,  | 1032.1785, |
|                                                                                     | H | 0.967721  | 1.818834  | 0.744948  | 1038.0069, | 1048.2413, | 1089.6450, |
|                                                                                     | H | -0.445582 | 1.460491  | -1.258320 | 1137.0798, | 1141.2005, | 1168.7130, |
|                                                                                     | H | -1.346985 | 2.411719  | -0.091132 | 1198.6605, | 1266.2038, | 1291.1166, |
|                                                                                     | H | -2.588444 | 0.394274  | 0.655750  | 1299.7456, | 1342.6643, | 1348.5963, |
|                                                                                     | H | -2.754733 | 0.579574  | -1.083387 | 1359.8619, | 1378.6610, | 1386.2766, |
|                                                                                     | H | 1.384895  | -0.519234 | 1.499181  | 1391.3460, | 1395.3957, | 1474.9525, |
|                                                                                     | H | 0.072170  | -2.346944 | 0.383940  | 1481.9088, | 1491.1810, | 1494.4665, |
|                                                                                     | H | -0.871012 | -1.447647 | 1.563299  | 1507.0061, | 2998.0513, | 3017.7914, |
|                                                                                     | H | -0.996487 | -1.118928 | -1.481611 | 3022.5853, | 3025.4028, | 3026.4318, |
|                                                                                     | H | -2.245816 | -1.800885 | -0.453997 | 3055.4293, | 3061.4609, | 3064.3270, |
|                                                                                     | H | -0.304597 | 1.208742  | 1.794259  | 3071.2818, | 3073.5779, | 3078.7935  |
|                                                                                     | O | 1.497956  | -0.435449 | -0.552489 |            |            |            |
|                                                                                     | O | 2.625627  | 0.239050  | -0.484907 |            |            |            |
| W1Ce                                                                                | C | -1.330308 | 1.379756  | 0.200860  | 77.6212,   | 126.7568,  | 223.0547,  |
|  | C | 0.115763  | 1.162623  | -0.273809 | 251.4576,  | 321.0939,  | 362.9032,  |
|                                                                                     | C | 0.645859  | -0.174332 | 0.234875  | 438.7243,  | 453.1202,  | 504.1905,  |
|                                                                                     | C | -0.227343 | -1.349680 | -0.184153 | 563.8373,  | 796.1469,  | 805.5444,  |
|                                                                                     | C | -1.676166 | -1.132429 | 0.284832  | 844.9254,  | 894.4489,  | 896.7287,  |
|                                                                                     | C | -2.237271 | 0.209687  | -0.206897 | 913.9209,  | 936.7620,  | 1015.8120, |
|                                                                                     | H | 0.151282  | 1.157190  | -1.369717 | 1042.5922, | 1066.3887, | 1089.5449, |
|                                                                                     | H | 0.770143  | 1.966973  | 0.071080  | 1101.5631, | 1167.2674, | 1182.9539, |

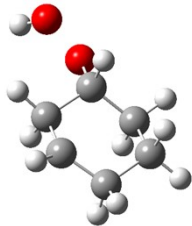
|                                                                                             |   |           |           |           |            |            |            |
|---------------------------------------------------------------------------------------------|---|-----------|-----------|-----------|------------|------------|------------|
|                                                                                             | H | -1.343482 | 1.487498  | 1.292878  | 1212.8051, | 1271.9775, | 1283.9049, |
|                                                                                             | H | -1.711995 | 2.320360  | -0.206821 | 1290.2634, | 1330.4672, | 1335.9793, |
|                                                                                             | H | -0.199137 | -1.436235 | -1.276514 | 1364.2399, | 1375.0155, | 1376.2614, |
|                                                                                             | H | 0.179112  | -2.279181 | 0.223918  | 1380.7152, | 1392.5259, | 1487.1380, |
|                                                                                             | H | -2.300551 | -1.959492 | -0.065258 | 1488.6614, | 1492.1913, | 1498.1362, |
|                                                                                             | H | -1.710833 | -1.160751 | 1.381261  | 1511.3640, | 3003.9225, | 3008.1708, |
|                                                                                             | H | -2.326812 | 0.185620  | -1.300315 | 3013.5074, | 3022.4666, | 3025.8258, |
|                                                                                             | H | -3.247506 | 0.360745  | 0.185832  | 3053.5953, | 3057.7696, | 3060.6564, |
|                                                                                             | H | 0.782676  | -0.148306 | 1.319901  | 3064.2183, | 3076.0974, | 3085.0005  |
|                                                                                             | O | 2.918041  | 0.296166  | 0.252790  |            |            |            |
|                                                                                             | O | 1.983697  | -0.429687 | -0.326603 |            |            |            |
| W1Ta<br>   | C | -1.834153 | -0.756611 | -0.087727 | 70.3397,   | 87.5705,   | 156.7672,  |
|                                                                                             | C | -0.522024 | -1.491783 | 0.251796  | 251.3990,  | 291.6222,  | 339.5508,  |
|                                                                                             | C | 0.630569  | -0.541252 | 0.601437  | 420.6787,  | 468.0009,  | 557.0119,  |
|                                                                                             | C | 0.160134  | 0.828998  | 1.072341  | 673.9627,  | 757.8569,  | 765.8366,  |
|                                                                                             | C | -0.752226 | 1.538813  | 0.043957  | 805.9855,  | 866.9929,  | 872.6871,  |
|                                                                                             | C | -1.549615 | 0.549807  | -0.837307 | 908.6467,  | 932.1639,  | 1008.6694, |
|                                                                                             | H | 1.323523  | -0.988530 | 1.316147  | 1044.3563, | 1061.1596, | 1111.7915, |
|                                                                                             | H | -0.675639 | -2.177249 | 1.090114  | 1128.7350, | 1165.5478, | 1177.3040, |
|                                                                                             | H | -0.201791 | -2.107389 | -0.594662 | 1195.7722, | 1264.4801, | 1271.9955, |
|                                                                                             | H | -0.975587 | 0.318459  | -1.740933 | 1301.7266, | 1329.3563, | 1347.2884, |
|                                                                                             | H | -2.386319 | -0.533521 | 0.833064  | 1359.9483, | 1360.6921, | 1383.4906, |
|                                                                                             | H | -0.380944 | 0.663165  | 2.010671  | 1388.4722, | 1389.7951, | 1476.8062, |
|                                                                                             | H | 1.027483  | 1.445034  | 1.317882  | 1482.0002, | 1494.5188, | 1501.7044, |
|                                                                                             | H | -0.150250 | 2.190350  | -0.594161 | 1512.6720, | 3011.7080, | 3027.5984, |
|                                                                                             | H | -1.441218 | 2.192316  | 0.587646  | 3028.4159, | 3035.8450, | 3037.6092, |
|                                                                                             | H | -2.482061 | 1.013589  | -1.170534 | 3060.4829, | 3062.5833, | 3073.7103, |
|                                                                                             | H | -2.478227 | -1.412339 | -0.679878 | 3075.2933, | 3084.4616, | 3091.4516  |
|                                                                                             | O | 1.427415  | -0.388026 | -0.645993 |            |            |            |
|                                                                                             | O | 2.575701  | 0.216560  | -0.434300 |            |            |            |
| W1Te<br> | C | 0.620957  | -0.142825 | -0.257566 | 62.1670,   | 100.4001,  | 163.2261,  |
|                                                                                             | C | -0.218467 | -1.407389 | -0.028957 | 250.0070,  | 265.0259,  | 365.8036,  |
|                                                                                             | C | -1.689232 | -1.070006 | 0.303718  | 410.9943,  | 473.2943,  | 513.0755,  |
|                                                                                             | C | -2.149217 | 0.188288  | -0.444052 | 596.3028,  | 763.9075,  | 792.6440,  |
|                                                                                             | C | -1.328556 | 1.429961  | -0.013015 | 841.4280,  | 884.8470,  | 890.8587,  |
|                                                                                             | H | -2.325453 | -1.923062 | 0.053854  | 933.7809,  | 935.9374,  | 1011.0434, |
|                                                                                             | H | -0.164443 | -2.042437 | -0.917463 | 1041.8085, | 1082.7692, | 1107.2675, |
|                                                                                             | H | 0.232838  | -1.974186 | 0.790927  | 1123.2251, | 1156.3095, | 1183.3176, |
|                                                                                             | H | 0.729148  | 0.095594  | -1.318174 | 1210.8737, | 1252.1321, | 1278.5871, |
|                                                                                             | H | -2.032615 | 0.020306  | -1.521241 | 1300.0014, | 1327.6466, | 1338.1756, |
|                                                                                             | H | -3.214978 | 0.366297  | -0.277828 | 1360.5479, | 1367.8768, | 1376.2141, |
|                                                                                             | H | -1.242347 | 2.122329  | -0.855564 | 1382.2585, | 1391.2421, | 1487.8233, |
|                                                                                             | H | -1.856174 | 1.971455  | 0.777221  | 1490.6752, | 1498.8456, | 1505.3905, |
|                                                                                             | H | -1.800748 | -0.909264 | 1.381664  | 1519.0694, | 3010.4474, | 3023.6094, |
|                                                                                             | C | 0.081412  | 1.060123  | 0.504348  | 3032.3259, | 3035.4746, | 3038.6650, |
|                                                                                             | H | 0.044654  | 0.807584  | 1.569219  | 3057.6357, | 3061.8707, | 3068.2705, |

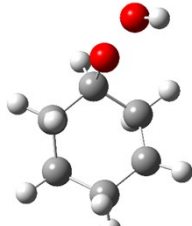
|                                                                                                     |   |           |           |           |                                 |            |            |
|-----------------------------------------------------------------------------------------------------|---|-----------|-----------|-----------|---------------------------------|------------|------------|
|                                                                                                     | H | 0.769394  | 1.900992  | 0.395675  | 3074.3967, 3083.7105, 3095.4858 |            |            |
|                                                                                                     | O | 1.983712  | -0.467675 | 0.204224  |                                 |            |            |
|                                                                                                     | O | 2.886205  | 0.369610  | -0.262368 |                                 |            |            |
| <hr/>                                                                                               |   |           |           |           |                                 |            |            |
| <div>W1Ti</div>    | C | 0.671527  | -0.387685 | 0.446057  | 70.1728,                        | 100.5191,  | 188.9564,  |
|                                                                                                     | C | -0.345130 | -1.361893 | -0.159965 | 226.6481,                       | 309.2912,  | 358.3307,  |
|                                                                                                     | C | -1.775036 | -0.986725 | 0.253631  | 420.5513,                       | 523.0410,  | 537.0361,  |
|                                                                                                     | C | -2.171899 | 0.409249  | -0.279926 | 577.2859,                       | 768.6323,  | 779.8342,  |
|                                                                                                     | C | -0.959509 | 1.367946  | -0.375826 | 819.6922,                       | 871.5706,  | 879.5308,  |
|                                                                                                     | H | -2.476307 | -1.743508 | -0.107114 | 906.0420,                       | 963.8187,  | 1013.8028, |
|                                                                                                     | H | -0.255679 | -1.312487 | -1.250898 | 1032.1415,                      | 1070.1626, | 1107.0550, |
|                                                                                                     | H | -0.103277 | -2.387623 | 0.127614  | 1133.4807,                      | 1149.0439, | 1180.0708, |
|                                                                                                     | H | 1.120550  | -0.771408 | 1.364062  | 1197.1078,                      | 1246.0217, | 1278.4432, |
|                                                                                                     | H | -2.631764 | 0.310053  | -1.267965 | 1299.6911,                      | 1330.9743, | 1343.9321, |
|                                                                                                     | H | -2.937519 | 0.838705  | 0.373462  | 1350.2450,                      | 1370.2988, | 1377.9178, |
|                                                                                                     | H | -0.509763 | 1.305079  | -1.371971 | 1386.7834,                      | 1390.3840, | 1484.7592, |
|                                                                                                     | H | -1.284841 | 2.404295  | -0.254194 | 1490.7478,                      | 1494.3222, | 1506.3750, |
|                                                                                                     | H | -1.847543 | -1.005013 | 1.346949  | 1515.5047,                      | 3015.4926, | 3024.0285, |
|                                                                                                     | C | 0.106291  | 1.019770  | 0.668017  | 3028.6673,                      | 3032.6818, | 3036.2337, |
|                                                                                                     | H | -0.328886 | 1.056866  | 1.673097  | 3053.5323,                      | 3069.5799, | 3070.3245, |
|                                                                                                     | H | 0.935528  | 1.731296  | 0.666235  | 3078.2779,                      | 3082.9555, | 3088.3624  |
|                                                                                                     | O | 2.860187  | 0.240870  | -0.044674 |                                 |            |            |
|                                                                                                     | O | 1.785066  | -0.339648 | -0.531727 |                                 |            |            |
| <hr/>                                                                                               |   |           |           |           |                                 |            |            |
| <div>W2Ca</div>  | C | -2.123092 | 0.364785  | -0.225799 | 79.7706,                        | 132.8335,  | 145.4917,  |
|                                                                                                     | C | -1.043397 | 1.464216  | -0.151456 | 212.7885,                       | 262.2151,  | 285.3711,  |
|                                                                                                     | C | 0.096872  | 1.077272  | 0.733752  | 349.7300,                       | 384.8016,  | 457.7134,  |
|                                                                                                     | C | 0.649338  | -0.307653 | 0.677122  | 513.3402,                       | 577.1152,  | 657.9868,  |
|                                                                                                     | C | -0.445380 | -1.374479 | 0.535440  | 787.4390,                       | 806.1175,  | 853.9231,  |
|                                                                                                     | C | -1.501943 | -1.007038 | -0.516674 | 870.2671,                       | 879.4144,  | 918.4435,  |
|                                                                                                     | H | -0.671556 | 1.646986  | -1.175369 | 930.3548,                       | 1014.4497, | 1038.4957, |
|                                                                                                     | H | -1.478450 | 2.412229  | 0.179278  | 1056.9056,                      | 1089.7747, | 1127.1388, |
|                                                                                                     | H | -2.658711 | 0.325100  | 0.730484  | 1160.7802,                      | 1177.8830, | 1263.3519, |
|                                                                                                     | H | -2.861053 | 0.621865  | -0.991890 | 1294.5545,                      | 1319.2551, | 1341.8154, |
|                                                                                                     | H | 1.278723  | -0.518421 | 1.546180  | 1349.5343,                      | 1358.0676, | 1361.0491, |
|                                                                                                     | H | 0.026289  | -2.333212 | 0.302895  | 1381.2072,                      | 1394.8449, | 1400.1187, |
|                                                                                                     | H | -0.925446 | -1.480038 | 1.514997  | 1465.4320,                      | 1475.1724, | 1491.0437, |
|                                                                                                     | H | -1.042181 | -1.000807 | -1.510996 | 1499.1386,                      | 2920.4367, | 3010.6018, |
|                                                                                                     | H | -2.280474 | -1.776189 | -0.535785 | 3022.6625,                      | 3024.1153, | 3049.6810, |
|                                                                                                     | H | 0.633070  | 1.836090  | 1.292229  | 3052.4474,                      | 3055.4474, | 3062.7675, |
|                                                                                                     | O | 1.491636  | -0.510984 | -0.504566 | 3074.2115,                      | 3173.6126, | 3769.6732  |
|                                                                                                     | O | 2.707922  | 0.262046  | -0.329514 |                                 |            |            |
|                                                                                                     | H | 2.588930  | 0.955282  | -0.993688 |                                 |            |            |

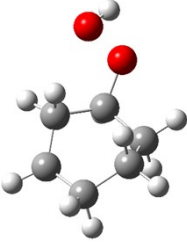
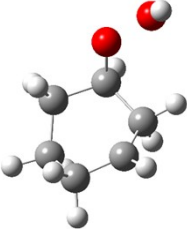
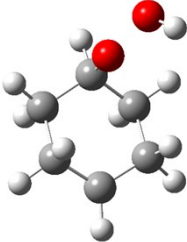
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|-----------------------------------------------------------------------------------------------------|---|-----------|-----------|-----------|------------|------------|------------|
| <div>W2Ce</div>    | C | -1.343440 | 1.439376  | 0.114654  | 90.6648,   | 117.6455,  | 173.6731,  |
|                                                                                                     | C | 0.096863  | 1.124684  | -0.129977 | 187.8853,  | 233.9762,  | 314.1786,  |
|                                                                                                     | C | 0.622425  | -0.215774 | 0.262280  | 355.1111,  | 376.2869,  | 451.3422,  |
|                                                                                                     | C | -0.321649 | -1.355445 | -0.148547 | 487.7212,  | 530.4828,  | 614.5730,  |
|                                                                                                     | C | -1.763221 | -1.056468 | 0.290449  | 791.3590,  | 836.2944,  | 865.1476,  |
|                                                                                                     | C | -2.266157 | 0.272001  | -0.287806 | 896.0437,  | 903.7043,  | 932.3869,  |
|                                                                                                     | H | 0.807551  | 1.921252  | -0.316113 | 959.7995,  | 1035.0582, | 1054.7765, |
|                                                                                                     | H | -1.502119 | 1.647916  | 1.189214  | 1068.6130, | 1097.0275, | 1109.4421, |
|                                                                                                     | H | -1.628470 | 2.357320  | -0.408115 | 1151.1748, | 1202.7749, | 1256.5014, |
|                                                                                                     | H | -0.282116 | -1.459618 | -1.238335 | 1277.1719, | 1304.9273, | 1327.4711, |
|                                                                                                     | H | 0.036669  | -2.293184 | 0.283307  | 1346.4945, | 1351.1395, | 1365.4908, |
|                                                                                                     | H | -2.414678 | -1.877600 | -0.023615 | 1370.7989, | 1379.3804, | 1394.6132, |
|                                                                                                     | H | -1.814291 | -1.021658 | 1.386472  | 1470.2244, | 1488.6659, | 1492.8604, |
|                                                                                                     | H | -2.299437 | 0.200171  | -1.381112 | 1501.6137, | 2903.5035, | 2915.5262, |
|                                                                                                     | H | -3.287969 | 0.471552  | 0.049767  | 3004.4674, | 3016.8200, | 3029.7036, |
|                                                                                                     | H | 0.777434  | -0.263768 | 1.355146  | 3050.8367, | 3056.8098, | 3060.7907, |
|                                                                                                     | O | 1.878836  | -0.535689 | -0.354849 | 3080.5072, | 3181.4921, | 3784.9715  |
|                                                                                                     | O | 2.891616  | 0.332264  | 0.237386  |            |            |            |
|                                                                                                     | H | 3.294890  | 0.694770  | -0.563237 |            |            |            |
| <div>W2Ta</div>  | C | -1.763207 | -1.056460 | 0.290487  | 90.6555,   | 117.6448,  | 173.6158,  |
|                                                                                                     | C | -0.321643 | -1.355460 | -0.148526 | 187.8629,  | 233.9813,  | 314.1712,  |
|                                                                                                     | C | 0.622435  | -0.215784 | 0.262288  | 355.1399,  | 376.3090,  | 451.3424,  |
|                                                                                                     | C | 0.096854  | 1.124691  | -0.129914 | 487.7208,  | 530.4912,  | 614.5938,  |
|                                                                                                     | C | -1.343455 | 1.439386  | 0.114576  | 791.3538,  | 836.2913,  | 865.1491,  |
|                                                                                                     | C | -2.266147 | 0.271977  | -0.287831 | 896.0368,  | 903.7020,  | 932.3794,  |
|                                                                                                     | H | 0.777467  | -0.263814 | 1.355153  | 959.8121,  | 1035.0735, | 1054.7860, |
|                                                                                                     | H | 0.036674  | -2.293194 | 0.283336  | 1068.6169, | 1097.0274, | 1109.4514, |
|                                                                                                     | H | -0.282130 | -1.459646 | -1.238314 | 1151.1828, | 1202.7775, | 1256.5013, |
|                                                                                                     | H | -2.299412 | 0.200089  | -1.381134 | 1277.1778, | 1304.9298, | 1327.4792, |
|                                                                                                     | H | -1.814252 | -1.021598 | 1.386510  | 1346.5085, | 1351.1393, | 1365.4969, |
|                                                                                                     | H | 0.807597  | 1.921246  | -0.315906 | 1370.8063, | 1379.3876, | 1394.6219, |
|                                                                                                     | H | -1.628458 | 2.357276  | -0.408310 | 1470.2194, | 1488.6671, | 1492.8607, |
|                                                                                                     | H | -1.502228 | 1.648064  | 1.189099  | 1501.6142, | 2903.4642, | 2915.4910, |
|                                                                                                     | H | -3.287966 | 0.471536  | 0.049714  | 3004.4647, | 3016.8138, | 3029.7036, |
|                                                                                                     | H | -2.414673 | -1.877605 | -0.023524 | 3050.8012, | 3056.8089, | 3060.7870, |
|                                                                                                     | O | 1.878810  | -0.535655 | -0.354884 | 3080.5108, | 3181.4786, | 3784.9970  |
|                                                                                                     | O | 2.891603  | 0.332274  | 0.237399  |            |            |            |
|                                                                                                     | H | 3.295052  | 0.694585  | -0.563222 |            |            |            |
| <div>W2Te</div>  | C | -0.647537 | -0.302076 | 0.687564  | 77.4129,   | 135.8054,  | 147.4773,  |
|                                                                                                     | C | 0.445505  | -1.372110 | 0.550215  | 192.1959,  | 261.6503,  | 285.8151,  |
|                                                                                                     | C | 1.495160  | -1.013537 | -0.512073 | 356.3182,  | 388.7586,  | 460.2067,  |
|                                                                                                     | C | 2.117852  | 0.361271  | -0.238537 | 514.4386,  | 587.7737,  | 659.7122,  |
|                                                                                                     | C | 1.038842  | 1.460063  | -0.161029 | 788.8377,  | 806.3069,  | 853.1703,  |
|                                                                                                     | H | 2.273263  | -1.783364 | -0.529323 | 873.2968,  | 877.9952,  | 918.6607,  |
|                                                                                                     | H | 0.929737  | -1.467644 | 1.528701  | 930.8117,  | 1016.3337, | 1037.8233, |
|                                                                                                     | H | -0.023839 | -2.335350 | 0.329464  | 1057.0434, | 1088.8942, | 1127.6310, |

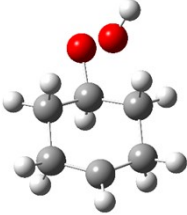
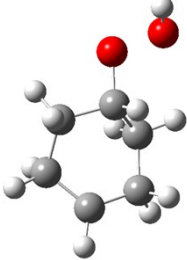
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|-------------------------------------------------------------------------------------|---|-----------|-----------|-----------|------------|------------|------------|
|                                                                                     | H | -1.275803 | -0.503956 | 1.561764  | 1160.3298, | 1179.3613, | 1263.9041, |
|                                                                                     | H | 2.665481  | 0.328919  | 0.711406  | 1294.2534, | 1326.5149, | 1341.0594, |
|                                                                                     | H | 2.846732  | 0.611135  | -1.015647 | 1349.4256, | 1352.0677, | 1365.9527, |
|                                                                                     | H | 1.477255  | 2.410914  | 0.157063  | 1382.0678, | 1395.3325, | 1402.3044, |
|                                                                                     | H | 0.646690  | 1.634464  | -1.178226 | 1465.1349, | 1475.9376, | 1490.8013, |
|                                                                                     | H | 1.026856  | -1.015073 | -1.501994 | 1499.1930, | 2930.5178, | 3008.8091, |
|                                                                                     | C | -0.091203 | 1.081049  | 0.738411  | 3019.3840, | 3024.4797, | 3032.4037, |
|                                                                                     | H | -0.656277 | 1.850029  | 1.251705  | 3049.0665, | 3054.4111, | 3061.3761, |
|                                                                                     | O | -1.480809 | -0.508597 | -0.496892 | 3070.7312, | 3179.2678, | 3776.0516  |
|                                                                                     | O | -2.609299 | 0.409245  | -0.415846 |            |            |            |
|                                                                                     | H | -3.340946 | -0.223221 | -0.400317 |            |            |            |
|    | C | -0.629950 | -0.322024 | -0.353158 | 60.4879,   | 103.4442,  | 138.6888,  |
|                                                                                     | C | 0.376158  | -1.301091 | 0.261227  | 195.1540,  | 204.4231,  | 268.1691,  |
|                                                                                     | C | 1.773521  | -1.030878 | -0.313624 | 353.1421,  | 367.4627,  | 463.1317,  |
|                                                                                     | C | 2.306503  | 0.364012  | 0.086549  | 510.3446,  | 564.9177,  | 634.8462,  |
|                                                                                     | C | 1.165168  | 1.397835  | 0.318654  | 768.1071,  | 803.2326,  | 855.4725,  |
|                                                                                     | H | 2.470239  | -1.807321 | 0.013555  | 893.0202,  | 893.4375,  | 917.0810,  |
|                                                                                     | H | 0.383797  | -1.168035 | 1.349077  | 936.8336,  | 996.0380,  | 1044.5015, |
|                                                                                     | H | 0.055194  | -2.326641 | 0.067988  | 1060.3704, | 1110.4433, | 1125.1713, |
|                                                                                     | H | -0.952540 | -0.673944 | -1.340891 | 1158.8280, | 1214.7576, | 1250.1736, |
|                                                                                     | H | 2.904038  | 0.287217  | 1.000025  | 1286.6318, | 1305.7916, | 1319.8751, |
|                                                                                     | H | 2.978588  | 0.731694  | -0.693623 | 1339.2787, | 1353.6592, | 1368.6283, |
|                                                                                     | H | 0.930899  | 1.414765  | 1.396554  | 1370.4711, | 1379.5319, | 1394.1451, |
|                                                                                     | H | 1.507661  | 2.406948  | 0.077640  | 1471.8010, | 1492.2451, | 1499.9511, |
|                                                                                     | H | 1.720810  | -1.106728 | -1.405819 | 1509.5701, | 2929.0801, | 3007.7661, |
|                                                                                     | C | -0.077199 | 1.061191  | -0.435136 | 3015.5656, | 3029.2116, | 3032.2788, |
|                                                                                     | H | -0.650401 | 1.826476  | -0.945265 | 3056.2358, | 3067.5100, | 3076.5321, |
|                                                                                     | O | -1.799857 | -0.410063 | 0.513417  | 3087.3946, | 3179.2505, | 3776.2440  |
|                                                                                     | O | -2.916151 | 0.215792  | -0.178596 |            |            |            |
|                                                                                     | H | -3.105427 | 0.955472  | 0.415119  |            |            |            |
|  | C | -2.057624 | 0.461011  | -0.386414 | 86.8389,   | 141.0807,  | 167.8325,  |
|                                                                                     | C | -0.950824 | 1.446317  | -0.200836 | 202.8167,  | 237.5960,  | 296.3157,  |
|                                                                                     | C | 0.137763  | 1.138608  | 0.774308  | 348.5589,  | 390.9241,  | 424.3541,  |
|                                                                                     | C | 0.630200  | -0.316699 | 0.683010  | 500.5369,  | 556.6801,  | 695.2073,  |
|                                                                                     | C | -0.533006 | -1.311933 | 0.616054  | 800.5371,  | 824.2264,  | 848.5266,  |
|                                                                                     | C | -1.528448 | -0.983149 | -0.506393 | 876.0568,  | 878.5409,  | 916.0088,  |
|                                                                                     | H | 0.986909  | 1.817054  | 0.664326  | 954.3404,  | 1007.4602, | 1033.6773, |
|                                                                                     | H | -1.042075 | 2.448282  | -0.604983 | 1064.8569, | 1100.3076, | 1119.8440, |
|                                                                                     | H | -2.741562 | 0.504445  | 0.482692  | 1146.7326, | 1193.0136, | 1239.3822, |
|                                                                                     | H | -2.667044 | 0.718653  | -1.257699 | 1282.4224, | 1316.6213, | 1341.5826, |
|                                                                                     | H | 1.275133  | -0.546719 | 1.538398  | 1346.9146, | 1352.3415, | 1374.8161, |
|                                                                                     | H | -0.132597 | -2.322064 | 0.495071  | 1381.5582, | 1393.2085, | 1408.0071, |
|                                                                                     | H | -1.042760 | -1.282862 | 1.586721  | 1463.4295, | 1468.5201, | 1480.4651, |
|                                                                                     | H | -1.034959 | -1.107597 | -1.474424 | 1496.1123, | 2894.0124, | 2905.2436, |
|                                                                                     | H | -2.363012 | -1.690548 | -0.478349 | 3016.5394, | 3031.2668, | 3031.8494, |
|                                                                                     | H | -0.223693 | 1.280383  | 1.810160  | 3052.4120, | 3068.5222, | 3075.6850, |

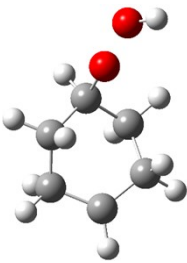
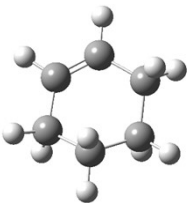
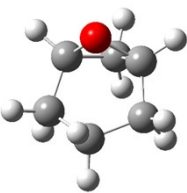
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| O | 1.388372 | -0.566690 | -0.511858 | 3076.9867, 3168.3136, 3781.3803 |
| O | 2.636404 | 0.177756  | -0.413824 |                                 |
| H | 2.599080 | 0.687517  | -1.234826 |                                 |

|                                                                                   |   |           |           |           |            |            |            |
|-----------------------------------------------------------------------------------|---|-----------|-----------|-----------|------------|------------|------------|
|  | C | 1.313474  | 1.418077  | -0.133692 | 99.3630,   | 139.3278,  | 168.3894,  |
|                                                                                   | C | -0.119431 | 1.177189  | 0.218480  | 180.8804,  | 228.0287,  | 280.6256,  |
|                                                                                   | C | -0.583176 | -0.215677 | -0.240578 | 361.4707,  | 384.3022,  | 454.9200,  |
|                                                                                   | C | 0.379578  | -1.310990 | 0.219305  | 461.1536,  | 503.7426,  | 617.4423,  |
|                                                                                   | C | 1.800190  | -1.041326 | -0.299562 | 793.9292,  | 843.5954,  | 860.9450,  |
|                                                                                   | C | 2.314586  | 0.344618  | 0.141572  | 892.8237,  | 913.7188,  | 929.6756,  |
|                                                                                   | H | -0.256051 | 1.213612  | 1.315175  | 951.3464,  | 1035.9307, | 1039.2159, |
|                                                                                   | H | -0.767006 | 1.947006  | -0.206218 | 1089.5492, | 1096.5363, | 1117.1800, |
|                                                                                   | H | 1.641946  | 2.414621  | -0.405192 | 1132.1039, | 1219.4592, | 1245.1132, |
|                                                                                   | H | 0.381038  | -1.343144 | 1.315685  | 1276.0780, | 1303.6162, | 1326.0384, |
|                                                                                   | H | 0.016777  | -2.280772 | -0.131217 | 1345.6062, | 1354.3591, | 1361.7625, |
|                                                                                   | H | 2.476663  | -1.824306 | 0.056084  | 1376.9140, | 1388.9510, | 1395.5536, |
|                                                                                   | H | 1.802134  | -1.094019 | -1.394168 | 1467.8237, | 1474.2983, | 1493.2917, |
|                                                                                   | H | 2.525638  | 0.301391  | 1.226307  | 1501.6114, | 2904.2737, | 2911.2347, |
|                                                                                   | H | 3.270320  | 0.568735  | -0.341128 | 3013.4021, | 3018.5674, | 3025.2054, |
|                                                                                   | H | -0.670966 | -0.235716 | -1.333557 | 3055.4500, | 3061.8253, | 3075.9713, |
|                                                                                   | O | -1.853379 | -0.581544 | 0.311184  | 3080.9967, | 3174.1736, | 3785.2520  |
|                                                                                   | O | -2.865873 | 0.265916  | -0.312321 |            |            |            |
|                                                                                   | H | -3.297806 | 0.626281  | 0.474164  |            |            |            |

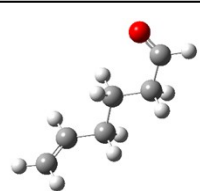
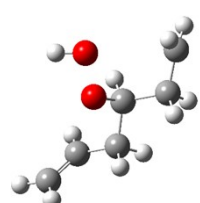
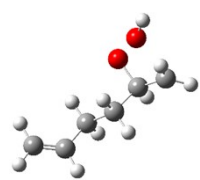
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|-------------------------------------------------------------------------------------|---|-----------|-----------|-----------|------------|------------|------------|
|  | C | -1.891677 | -0.857326 | 0.239977  | 29.8886,   | 133.7692,  | 151.3889,  |
|                                                                                     | C | -0.473163 | -1.368468 | -0.047749 | 184.9497,  | 245.0741,  | 294.0121,  |
|                                                                                     | C | 0.617426  | -0.400838 | 0.458004  | 353.0101,  | 373.9630,  | 419.8604,  |
|                                                                                     | C | 0.096493  | 1.034017  | 0.700565  | 506.3560,  | 535.7345,  | 657.3414,  |
|                                                                                     | C | -0.992969 | 1.428011  | -0.238089 | 787.7407,  | 834.3085,  | 845.3132,  |
|                                                                                     | C | -2.133326 | 0.486888  | -0.465929 | 883.0090,  | 884.8567,  | 917.3358,  |
|                                                                                     | H | 1.079093  | -0.776880 | 1.377133  | 948.8664,  | 1008.5779, | 1040.9100, |
|                                                                                     | H | -0.313475 | -2.360898 | 0.379579  | 1065.9537, | 1082.8327, | 1125.9750, |
|                                                                                     | H | -0.349293 | -1.470587 | -1.131898 | 1163.1604, | 1187.5628, | 1236.2944, |
|                                                                                     | H | -2.268648 | 0.313238  | -1.545145 | 1260.8278, | 1313.4211, | 1328.6803, |
|                                                                                     | H | -2.035375 | -0.742900 | 1.320648  | 1344.1746, | 1360.4572, | 1367.4534, |
|                                                                                     | H | -0.265900 | 1.063755  | 1.743815  | 1379.8118, | 1393.9468, | 1405.4224, |
|                                                                                     | H | 0.940835  | 1.725107  | 0.667789  | 1464.7634, | 1466.4810, | 1490.9196, |
|                                                                                     | H | -1.000952 | 2.409173  | -0.698615 | 1503.5973, | 2913.7326, | 2952.2231, |
|                                                                                     | H | -3.084525 | 0.927538  | -0.127758 | 2958.6402, | 3019.5619, | 3028.1305, |
|                                                                                     | H | -2.625436 | -1.597018 | -0.091635 | 3029.7664, | 3066.8017, | 3081.1727, |
|                                                                                     | O | 1.617264  | -0.453753 | -0.572311 | 3086.7653, | 3173.0308, | 3789.8985  |
|                                                                                     | O | 2.823218  | 0.183855  | -0.048764 |            |            |            |
|                                                                                     | H | 3.063112  | 0.734951  | -0.805983 |            |            |            |

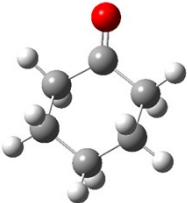
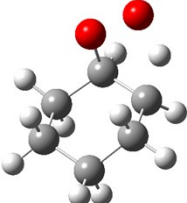
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|-----------------------------------------------------------------------------------------------------|---|-----------|-----------|-----------|------------|------------|------------|
| <div>W3Te</div>    | C | -0.621895 | -0.123662 | 0.488762  | 39.7253,   | 131.6731,  | 173.5956,  |
|                                                                                                     | C | 0.395983  | -1.286274 | 0.454302  | 188.7442,  | 230.7563,  | 289.3311,  |
|                                                                                                     | C | 1.577887  | -1.027091 | -0.487909 | 370.6339,  | 380.8322,  | 428.2138,  |
|                                                                                                     | C | 2.329719  | 0.246910  | -0.068158 | 488.5824,  | 554.2469,  | 614.5398,  |
|                                                                                                     | C | 1.376779  | 1.372056  | 0.184826  | 781.9355,  | 823.9295,  | 852.5818,  |
|                                                                                                     | H | 2.253755  | -1.886826 | -0.483403 | 875.6627,  | 912.7907,  | 925.8333,  |
|                                                                                                     | H | 0.774348  | -1.444341 | 1.469645  | 948.8667,  | 1017.8822, | 1040.5012, |
|                                                                                                     | H | -0.135271 | -2.199928 | 0.173547  | 1071.8024, | 1088.1550, | 1129.4453, |
|                                                                                                     | H | -0.948895 | 0.063833  | 1.517549  | 1146.9629, | 1188.7391, | 1236.0074, |
|                                                                                                     | H | 2.924686  | 0.042366  | 0.836168  | 1273.8594, | 1303.1751, | 1332.7822, |
|                                                                                                     | H | 3.068955  | 0.522064  | -0.836845 | 1344.4725, | 1358.1834, | 1367.6054, |
|                                                                                                     | H | 1.751073  | 2.337564  | 0.504697  | 1378.1548, | 1382.2740, | 1395.9230, |
|                                                                                                     | H | 1.212668  | -0.923526 | -1.514927 | 1465.4222, | 1476.6085, | 1482.6113, |
|                                                                                                     | C | -0.070731 | 1.183880  | -0.126157 | 1505.5354, | 2938.4489, | 2952.3738, |
|                                                                                                     | H | -0.226724 | 1.103841  | -1.215217 | 2958.0567, | 3014.2452, | 3032.6026, |
|                                                                                                     | H | -0.669279 | 2.033379  | 0.204292  | 3035.1641, | 3068.4338, | 3075.6335, |
|                                                                                                     | O | -1.753649 | -0.616832 | -0.248669 | 3096.1798, | 3174.5565, | 3781.7959  |
|                                                                                                     | O | -2.798903 | 0.400379  | -0.194083 |            |            |            |
|                                                                                                     | H | -3.511342 | -0.111716 | 0.212520  |            |            |            |
| <div>W3Ti</div>  | C | 0.617449  | -0.400737 | 0.457899  | 29.8648,   | 133.8205,  | 150.9231,  |
|                                                                                                     | C | -0.473099 | -1.368411 | -0.047852 | 184.8971,  | 245.0731,  | 294.0156,  |
|                                                                                                     | C | -1.891614 | -0.857417 | 0.240130  | 353.0086,  | 373.9567,  | 419.8580,  |
|                                                                                                     | C | -2.133498 | 0.486758  | -0.465773 | 506.3371,  | 535.7341,  | 657.3289,  |
|                                                                                                     | C | -0.993164 | 1.427965  | -0.238180 | 787.7360,  | 834.3256,  | 845.3105,  |
|                                                                                                     | H | -2.625364 | -1.597180 | -0.091342 | 883.0168,  | 884.8499,  | 917.2595,  |
|                                                                                                     | H | -0.349372 | -1.470364 | -1.132035 | 948.8909,  | 1008.5923, | 1040.9043, |
|                                                                                                     | H | -0.313240 | -2.360877 | 0.379326  | 1065.9577, | 1082.8438, | 1125.9809, |
|                                                                                                     | H | 1.078995  | -0.776733 | 1.377113  | 1163.1415, | 1187.5761, | 1236.3021, |
|                                                                                                     | H | -2.268990 | 0.313042  | -1.544959 | 1260.8118, | 1313.4232, | 1328.6783, |
|                                                                                                     | H | -3.084673 | 0.927352  | -0.127465 | 1344.1756, | 1360.4582, | 1367.4650, |
|                                                                                                     | H | -1.001219 | 2.409037  | -0.698895 | 1379.8059, | 1393.9764, | 1405.4278, |
|                                                                                                     | H | -2.035128 | -0.742991 | 1.320826  | 1464.7653, | 1466.4794, | 1490.9212, |
|                                                                                                     | C | 0.096471  | 1.034136  | 0.700336  | 1503.5979, | 2913.7304, | 2952.2449, |
|                                                                                                     | H | -0.265739 | 1.064023  | 1.743645  | 2958.6270, | 3019.5579, | 3028.0840, |
|                                                                                                     | H | 0.940790  | 1.725238  | 0.667280  | 3029.7548, | 3066.7999, | 3081.1857, |
|                                                                                                     | O | 1.617339  | -0.453715 | -0.572307 | 3086.8299, | 3173.0342, | 3789.9297  |
|                                                                                                     | O | 2.823254  | 0.183923  | -0.048522 |            |            |            |
|                                                                                                     | H | 3.063924  | 0.734020  | -0.806220 |            |            |            |
| <div>W4Ca</div>  | C | -1.985075 | 0.486863  | -0.395662 | 87.9230,   | 137.7534,  | 154.0739,  |
|                                                                                                     | C | -0.901598 | 1.496218  | -0.196296 | 175.7315,  | 230.4310,  | 295.1435,  |
|                                                                                                     | C | 0.112293  | 1.057183  | 0.879392  | 363.1748,  | 389.7242,  | 414.7936,  |
|                                                                                                     | C | 0.590041  | -0.383555 | 0.678778  | 530.5534,  | 571.1406,  | 680.2033,  |
|                                                                                                     | C | -0.578198 | -1.368488 | 0.572248  | 763.9334,  | 806.2410,  | 855.6804,  |
|                                                                                                     | C | -1.615292 | -0.957488 | -0.494376 | 875.6141,  | 902.3428,  | 937.0237,  |
|                                                                                                     | H | 0.975223  | 1.727324  | 0.896617  | 950.3492,  | 1007.8600, | 1029.1434, |
|                                                                                                     | H | -0.355839 | 1.643159  | -1.145540 | 1070.5375, | 1091.7151, | 1124.8949, |

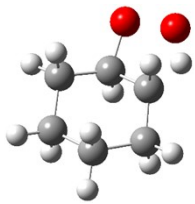
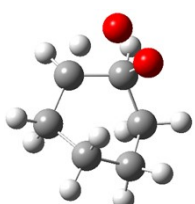
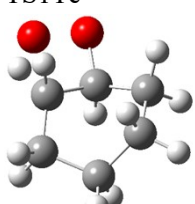
|                                                                                             |   |           |           |           |            |            |            |
|---------------------------------------------------------------------------------------------|---|-----------|-----------|-----------|------------|------------|------------|
|                                                                                             | H | -1.319605 | 2.474047  | 0.060621  | 1158.7038, | 1184.3283, | 1226.1914, |
|                                                                                             | H | -2.968618 | 0.811418  | -0.718074 | 1298.0151, | 1318.7181, | 1326.6148, |
|                                                                                             | H | 1.248348  | -0.679728 | 1.503428  | 1349.7260, | 1354.9710, | 1379.6283, |
|                                                                                             | H | -0.190895 | -2.369894 | 0.366851  | 1383.1023, | 1395.5425, | 1398.8817, |
|                                                                                             | H | -1.060098 | -1.400745 | 1.555101  | 1464.7456, | 1472.6059, | 1476.5602, |
|                                                                                             | H | -1.186731 | -1.164667 | -1.490066 | 1490.3053, | 2916.2081, | 2930.4142, |
|                                                                                             | H | -2.501965 | -1.593412 | -0.412427 | 3019.1113, | 3027.0491, | 3038.1311, |
|                                                                                             | H | -0.355261 | 1.114389  | 1.868981  | 3050.9500, | 3052.7048, | 3077.4709, |
|                                                                                             | O | 1.328114  | -0.555122 | -0.544823 | 3079.1035, | 3163.7304, | 3785.9035  |
|                                                                                             | O | 2.594325  | 0.153637  | -0.396803 |            |            |            |
|                                                                                             | H | 2.602906  | 0.665593  | -1.216991 |            |            |            |
| W4Ce<br>   | C | -1.350639 | 1.442820  | 0.129527  | 101.0709,  | 137.2895,  | 191.6107,  |
|                                                                                             | C | 0.085537  | 1.128785  | -0.340177 | 203.2754,  | 212.4998,  | 267.4051,  |
|                                                                                             | C | 0.552382  | -0.219176 | 0.208466  | 365.9438,  | 395.1636,  | 444.2357,  |
|                                                                                             | C | -0.372162 | -1.354591 | -0.230838 | 470.9769,  | 512.8969,  | 647.6910,  |
|                                                                                             | C | -1.819568 | -1.087599 | 0.233983  | 780.5370,  | 816.0376,  | 868.9926,  |
|                                                                                             | C | -2.280505 | 0.295171  | -0.095068 | 895.3470,  | 923.2606,  | 944.2439,  |
|                                                                                             | H | 0.114732  | 1.084067  | -1.434896 | 955.9695,  | 1019.4192, | 1050.9533, |
|                                                                                             | H | 0.769102  | 1.917848  | -0.018350 | 1082.9287, | 1098.3456, | 1113.8163, |
|                                                                                             | H | -1.315694 | 1.688225  | 1.207531  | 1136.1988, | 1216.0053, | 1245.1640, |
|                                                                                             | H | -1.719291 | 2.346569  | -0.364546 | 1281.0840, | 1306.2704, | 1318.7150, |
|                                                                                             | H | -0.342750 | -1.427995 | -1.323111 | 1340.4374, | 1350.3394, | 1368.7727, |
|                                                                                             | H | -0.007740 | -2.302754 | 0.172466  | 1384.4731, | 1390.9962, | 1398.9579, |
|                                                                                             | H | -2.491158 | -1.835952 | -0.196972 | 1466.6430, | 1473.6671, | 1490.1247, |
|                                                                                             | H | -1.863749 | -1.243627 | 1.327965  | 1505.9724, | 2901.7353, | 2905.6950, |
|                                                                                             | H | -3.337726 | 0.483290  | -0.248021 | 2998.2346, | 3024.2491, | 3032.8914, |
|                                                                                             | H | 0.600516  | -0.184288 | 1.305387  | 3052.7151, | 3053.8779, | 3080.4972, |
|                                                                                             | O | 1.850129  | -0.594137 | -0.273596 | 3084.0794, | 3165.7248, | 3785.1456  |
|                                                                                             | O | 2.827673  | 0.295755  | 0.345801  |            |            |            |
|                                                                                             | H | 3.281069  | 0.629213  | -0.440451 |            |            |            |
| W4Te<br> | C | 0.556093  | -0.167525 | -0.287041 | 51.5164,   | 138.4538,  | 184.8806,  |
|                                                                                             | C | -0.352716 | -1.406413 | -0.142987 | 187.9673,  | 206.3338,  | 262.3347,  |
|                                                                                             | C | -1.806234 | -1.046904 | 0.268179  | 364.4734,  | 383.1743,  | 428.7187,  |
|                                                                                             | C | -2.247076 | 0.273697  | -0.271786 | 500.8148,  | 519.8233,  | 625.7608,  |
|                                                                                             | C | -1.340812 | 1.456013  | -0.126326 | 781.9904,  | 827.3057,  | 849.9487,  |
|                                                                                             | H | -2.484421 | -1.845049 | -0.043824 | 884.5377,  | 908.5984,  | 930.4597,  |
|                                                                                             | H | -0.356623 | -1.956747 | -1.086640 | 955.6944,  | 1025.5498, | 1039.2820, |
|                                                                                             | H | 0.087434  | -2.067386 | 0.609834  | 1079.5607, | 1096.5475, | 1128.0967, |
|                                                                                             | H | 0.679253  | 0.094410  | -1.345485 | 1142.4723, | 1209.9720, | 1242.4220, |
|                                                                                             | H | -3.256670 | 0.408971  | -0.643151 | 1255.3068, | 1322.3685, | 1328.7891, |
|                                                                                             | H | -1.188659 | 1.941963  | -1.102995 | 1332.9764, | 1350.4460, | 1357.1421, |
|                                                                                             | H | -1.802899 | 2.231412  | 0.503692  | 1383.8999, | 1387.7713, | 1404.8611, |
|                                                                                             | H | -1.856653 | -1.031082 | 1.370713  | 1466.7640, | 1473.6899, | 1491.3177, |
|                                                                                             | C | 0.019612  | 1.048645  | 0.464921  | 1506.8770, | 2918.3727, | 2955.9975, |
|                                                                                             | H | -0.083269 | 0.793597  | 1.525211  | 2963.4637, | 3001.8997, | 3037.8702, |
|                                                                                             | H | 0.734786  | 1.869970  | 0.396154  | 3039.0718, | 3063.1617, | 3083.0389, |

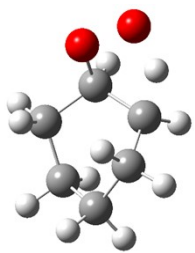
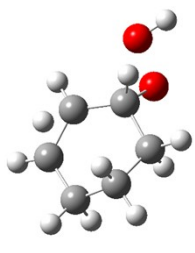
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|-------------------------------------------------------------------------------------------|---|-----------|-----------|-----------|---------------------------------|------------|------------|
|                                                                                           | O | 1.831181  | -0.604787 | 0.208153  | 3098.5744, 3170.8004, 3782.1883 |            |            |
|                                                                                           | O | 2.807651  | 0.440014  | -0.083964 |                                 |            |            |
|                                                                                           | H | 3.443865  | -0.066958 | -0.606782 |                                 |            |            |
| W4Ti<br> | C | 0.583433  | -0.393739 | 0.431066  | 46.8387,                        | 129.4044,  | 141.3467,  |
|                                                                                           | C | -0.471649 | -1.364649 | -0.134712 | 197.2810,                       | 206.1091,  | 284.5472,  |
|                                                                                           | C | -1.911987 | -0.936416 | 0.202201  | 326.7335,                       | 363.4507,  | 441.3468,  |
|                                                                                           | C | -2.182835 | 0.453589  | -0.279578 | 507.5441,                       | 555.3393,  | 594.3573,  |
|                                                                                           | C | -1.045307 | 1.422629  | -0.353595 | 771.8139,                       | 820.1769,  | 867.5705,  |
|                                                                                           | H | -2.619628 | -1.646705 | -0.238066 | 887.9025,                       | 898.4629,  | 932.4170,  |
|                                                                                           | H | -0.359729 | -1.378432 | -1.223935 | 971.0670,                       | 1015.6871, | 1027.1031, |
|                                                                                           | H | -0.268390 | -2.378501 | 0.216783  | 1059.3403,                      | 1082.7469, | 1124.8488, |
|                                                                                           | H | 0.997812  | -0.776621 | 1.369567  | 1161.4852,                      | 1183.6630, | 1207.2537, |
|                                                                                           | H | -3.184522 | 0.751658  | -0.567050 | 1274.0600,                      | 1311.2996, | 1336.4847, |
|                                                                                           | H | -0.614693 | 1.447382  | -1.369668 | 1351.8025,                      | 1356.1737, | 1372.0027, |
|                                                                                           | H | -1.390307 | 2.444972  | -0.162108 | 1376.9504,                      | 1393.0955, | 1398.0178, |
|                                                                                           | H | -2.066769 | -1.013169 | 1.293343  | 1470.7075,                      | 1473.3158, | 1489.2071, |
|                                                                                           | C | 0.054993  | 1.033279  | 0.647021  | 1494.3174,                      | 2912.5490, | 2926.2379, |
|                                                                                           | H | -0.351513 | 1.096821  | 1.662535  | 3019.6973,                      | 3027.6327, | 3031.2429, |
|                                                                                           | H | 0.899333  | 1.725221  | 0.609263  | 3039.7294,                      | 3042.6707, | 3084.3031, |
|                                                                                           | O | 1.636645  | -0.446559 | -0.548252 | 3084.5305, 3173.7819, 3793.3958 |            |            |
|                                                                                           | O | 2.819280  | 0.168154  | 0.053319  |                                 |            |            |
|                                                                                           | H | 3.151127  | 0.666460  | -0.705622 |                                 |            |            |
| P1<br> | C | 1.496988  | 0.047299  | 0.110409  | 164.9786,                       | 277.4402,  | 399.2077,  |
|                                                                                           | C | 0.665815  | 1.304847  | 0.057099  | 457.4410,                       | 501.9485,  | 653.9142,  |
|                                                                                           | C | -0.664133 | 1.305634  | -0.057099 | 730.4464,                       | 820.8572,  | 827.0377,  |
|                                                                                           | C | -1.496927 | 0.049125  | -0.110333 | 879.6995,                       | 908.0926,  | 934.4442,  |
|                                                                                           | C | -0.699316 | -1.192117 | 0.317059  | 1001.0136,                      | 1015.8592, | 1047.1303, |
|                                                                                           | C | 0.697802  | -1.192797 | -0.317061 | 1071.3074,                      | 1097.4411, | 1161.8379, |
|                                                                                           | H | 1.196439  | 2.252122  | 0.113168  | 1163.3047,                      | 1247.7775, | 1269.4494, |
|                                                                                           | H | 2.380910  | 0.164695  | -0.527204 | 1293.3427,                      | 1353.5889, | 1368.9057, |
|                                                                                           | H | 1.887016  | -0.087356 | 1.129378  | 1370.5283,                      | 1382.6504, | 1419.9392, |
|                                                                                           | H | -2.380689 | 0.167772  | 0.527304  | 1474.5225,                      | 1480.6882, | 1493.5318, |
|                                                                                           | H | -1.887064 | -0.085160 | -1.129259 | 1502.0164,                      | 1707.1520, | 2986.7645, |
|                                                                                           | H | -0.596952 | -1.195670 | 1.409040  | 2987.1617,                      | 3007.1426, | 3012.6349, |
|                                                                                           | H | -1.244811 | -2.102232 | 0.049157  | 3030.4497,                      | 3030.5698, | 3055.0793, |
|                                                                                           | H | 1.242352  | -2.103626 | -0.049653 | 3058.5836, 3125.6929, 3149.1798 |            |            |
|                                                                                           | H | 0.595208  | -1.195911 | -1.409063 |                                 |            |            |
|                                                                                           | H | -1.193782 | 2.253429  | -0.113314 |                                 |            |            |
| P2<br> | C | -0.028783 | 0.813029  | 1.296751  | 141.2492,                       | 300.5241,  | 399.5562,  |
|                                                                                           | C | -0.028783 | -0.692991 | 1.014182  | 428.0714,                       | 543.3074,  | 629.2515,  |
|                                                                                           | C | -1.124251 | -1.067987 | 0.000000  | 760.1302,                       | 807.5819,  | 825.9008,  |
|                                                                                           | C | -0.028783 | -0.692991 | -1.014182 | 849.4975,                       | 865.4279,  | 918.0688,  |
|                                                                                           | C | -0.028783 | 0.813029  | -1.296751 | 924.9268,                       | 951.2147,  | 982.0331,  |
|                                                                                           | C | 0.340244  | 1.582223  | 0.000000  | 1024.6537,                      | 1035.7305, | 1087.1077, |
|                                                                                           | H | -1.344005 | -2.136135 | 0.000000  | 1119.1948,                      | 1120.2877, | 1155.6830, |

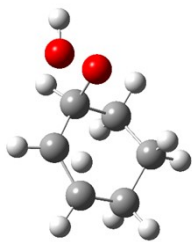
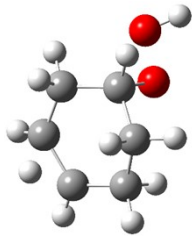
|    |   |           |           |           |            |            |            |
|----|---|-----------|-----------|-----------|------------|------------|------------|
|    | H | 0.099087  | -1.308661 | 1.906104  | 1224.1588, | 1236.7948, | 1259.3342, |
|    | H | -1.016097 | 1.101686  | 1.674945  | 1265.6199, | 1325.0719, | 1329.1852, |
|    | H | 0.694273  | 1.054134  | 2.081200  | 1346.4009, | 1347.6039, | 1377.3321, |
|    | H | 0.099087  | -1.308661 | -1.906104 | 1378.6132, | 1482.5167, | 1492.1807, |
|    | H | 0.694273  | 1.054134  | -2.081200 | 1497.0002, | 1511.7325, | 3021.5952, |
|    | H | -1.016097 | 1.101686  | -1.674945 | 3022.1043, | 3050.6410, | 3055.2668, |
|    | H | 1.421378  | 1.727804  | 0.000000  | 3060.0360, | 3060.3670, | 3077.8148, |
|    | H | -0.108206 | 2.578645  | 0.000000  | 3080.5933, | 3095.6069, | 3115.5288  |
|    | H | -2.049179 | -0.487034 | 0.000000  |            |            |            |
|    | O | 0.990040  | -0.987932 | 0.000000  |            |            |            |
| P3 | C | 0.335846  | 1.517727  | -0.026245 | 139.6450,  | 268.7500,  | 357.7047,  |
|    | C | -0.991068 | 0.830777  | -0.297394 | 374.4336,  | 440.2382,  | 542.2032,  |
|    | C | -1.090840 | -0.635900 | -0.414632 | 646.2417,  | 763.7975,  | 781.6580,  |
|    | C | 0.135312  | -1.510722 | -0.283847 | 826.2105,  | 843.8399,  | 890.4346,  |
|    | C | 1.291707  | -0.800915 | 0.436221  | 900.1253,  | 982.5003,  | 1002.1621, |
|    | C | 1.548748  | 0.582297  | -0.174305 | 1041.7644, | 1050.9150, | 1078.0740, |
|    | H | -1.749735 | 1.434750  | -0.792269 | 1100.4446, | 1167.4347, | 1193.7256, |
|    | H | 0.438698  | 2.370918  | -0.704450 | 1210.0028, | 1276.4156, | 1287.7092, |
|    | H | 0.295970  | 1.929553  | 0.988444  | 1303.1856, | 1354.3153, | 1370.8071, |
|    | H | -0.136525 | -2.435494 | 0.237171  | 1376.8959, | 1388.4320, | 1396.5999, |
|    | H | 0.448828  | -1.800283 | -1.295286 | 1461.2657, | 1479.6646, | 1484.2509, |
|    | H | 1.052296  | -0.698139 | 1.499328  | 1492.1218, | 1501.9449, | 3004.7691, |
|    | H | 2.193298  | -1.417160 | 0.370433  | 3007.7661, | 3022.5954, | 3030.0438, |
|    | H | 2.427801  | 1.045734  | 0.283599  | 3046.2245, | 3053.9735, | 3062.3499, |
|    | H | 1.781601  | 0.459343  | -1.239640 | 3071.5851, | 3090.5807, | 3105.4732  |
|    | H | -1.906372 | -1.051225 | -1.006163 |            |            |            |
|    | O | -1.528011 | 0.032801  | 0.777506  |            |            |            |
| P4 | C | 0.463531  | -0.780294 | 1.265370  | 153.1138,  | 329.0852,  | 400.6323,  |
|    | C | 0.463531  | 0.780194  | 1.265445  | 555.6216,  | 584.8939,  | 762.6653,  |
|    | C | -0.369796 | 1.077420  | 0.000000  | 794.8723,  | 811.2249,  | 828.6308,  |
|    | C | 0.463531  | 0.780194  | -1.265445 | 832.0532,  | 886.7759,  | 909.8037,  |
|    | C | 0.463531  | -0.780294 | -1.265370 | 933.8132,  | 944.9219,  | 980.7870,  |
|    | C | -0.370029 | -1.077296 | 0.000000  | 1008.1180, | 1015.1297, | 1021.7675, |
|    | H | -0.032299 | 1.176379  | 2.153228  | 1096.7635, | 1122.0955, | 1176.3760, |
|    | H | 1.466076  | 1.210739  | 1.215605  | 1218.2529, | 1228.6763, | 1229.9349, |
|    | H | 1.466077  | -1.210825 | 1.215241  | 1274.2396, | 1290.3352, | 1298.7592, |
|    | H | -0.032217 | -1.176560 | 2.153134  | 1303.1743, | 1330.8217, | 1343.9734, |
|    | H | -0.032299 | 1.176379  | -2.153228 | 1352.2477, | 1479.0362, | 1491.9819, |
|    | H | 1.466076  | 1.210739  | -1.215605 | 1500.4446, | 1516.8497, | 3049.6142, |
|    | H | -0.032217 | -1.176560 | -2.153134 | 3053.0734, | 3058.6891, | 3063.3125, |
|    | H | 1.466077  | -1.210825 | -1.215241 | 3086.2165, | 3089.1782, | 3104.3122, |
|    | H | -0.897081 | -2.029694 | 0.000000  | 3109.7498, | 3118.9669, | 3124.4147  |
|    | H | -0.896646 | 2.029934  | 0.000000  |            |            |            |
|    | O | -1.328417 | 0.000093  | 0.000000  |            |            |            |
| P5 | C | -3.413195 | -0.357963 | -0.433516 | 57.1959,   | 85.6861,   | 103.0573,  |
|    | C | -2.372010 | -0.262821 | 0.390310  | 148.3202,  | 174.4170,  | 265.8283,  |

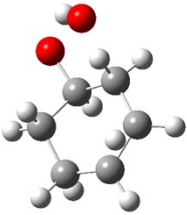
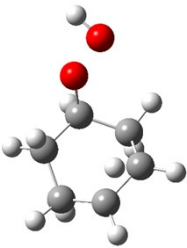
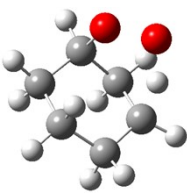
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|-------------------------------------------------------------------------------------------|---|-----------|-----------|-----------|------------|------------|------------|
|          | C | -1.193105 | 0.649434  | 0.199348  | 355.3425,  | 437.4034,  | 632.1079,  |
|                                                                                           | C | 0.140751  | -0.111859 | 0.103860  | 669.0370,  | 714.0857,  | 777.6929,  |
|                                                                                           | C | 1.339552  | 0.822393  | -0.046009 | 885.7935,  | 921.8759,  | 946.4569,  |
|                                                                                           | C | 2.681319  | 0.135992  | -0.121029 | 950.8959,  | 1024.7971, | 1038.0482, |
|                                                                                           | H | -3.485407 | 0.247440  | -1.332504 | 1043.9230, | 1083.2684, | 1157.5718, |
|                                                                                           | H | -4.232080 | -1.041298 | -0.238682 | 1214.7975, | 1266.0668, | 1294.1805, |
|                                                                                           | H | -2.344384 | -0.892891 | 1.278717  | 1319.7291, | 1330.2286, | 1353.4184, |
|                                                                                           | H | -1.140538 | 1.347895  | 1.046059  | 1394.6573, | 1414.2059, | 1447.1586, |
|                                                                                           | H | -1.342570 | 1.258186  | -0.699493 | 1454.3109, | 1482.8879, | 1501.5534, |
|                                                                                           | H | 0.109307  | -0.803819 | -0.742566 | 1701.5642, | 1802.1695, | 2865.6342, |
|                                                                                           | H | 0.278365  | -0.733549 | 0.994154  | 2990.4557, | 2993.0380, | 3011.5177, |
|                                                                                           | H | 1.397363  | 1.539369  | 0.786438  | 3035.2267, | 3041.2567, | 3078.8801, |
|                                                                                           | H | 1.252367  | 1.449187  | -0.945554 | 3115.0810, | 3126.0248, | 3208.7131  |
|                                                                                           | H | 3.547487  | 0.823717  | -0.242307 |            |            |            |
|                                                                                           | O | 2.857528  | -1.055661 | -0.057757 |            |            |            |
| P6<br>  | C | 3.247848  | 0.211566  | -0.167943 | 57.0901,   | 65.7787,   | 94.1931,   |
|                                                                                           | C | 2.220348  | -0.313597 | 0.494125  | 127.5655,  | 179.5911,  | 202.3370,  |
|                                                                                           | C | 1.024442  | -0.967062 | -0.138370 | 257.1346,  | 334.9760,  | 340.9168,  |
|                                                                                           | C | -0.311731 | -0.290405 | 0.213452  | 412.0871,  | 459.0170,  | 508.8056,  |
|                                                                                           | C | -1.525851 | -1.156306 | -0.213036 | 576.4169,  | 670.0631,  | 774.2439,  |
|                                                                                           | C | -2.861277 | -0.598230 | 0.130856  | 836.0745,  | 910.2064,  | 933.2847,  |
|                                                                                           | H | 3.283595  | 0.213441  | -1.253085 | 940.0660,  | 950.5160,  | 1023.5672, |
|                                                                                           | H | 4.088301  | 0.659261  | 0.350506  | 1031.5468, | 1044.7786, | 1069.9873, |
|                                                                                           | H | 2.225168  | -0.288164 | 1.583287  | 1099.3452, | 1163.6143, | 1244.4268, |
|                                                                                           | H | 0.956851  | -2.008331 | 0.199030  | 1267.3059, | 1293.6826, | 1322.5405, |
|                                                                                           | H | 1.133234  | -0.991880 | -1.227349 | 1338.2847, | 1352.8521, | 1364.5041, |
|                                                                                           | H | -0.359997 | -0.080969 | 1.288033  | 1381.2188, | 1449.5267, | 1461.2023, |
|                                                                                           | H | -1.396393 | -2.134021 | 0.267999  | 1470.8711, | 1479.4932, | 1703.7470, |
|                                                                                           | H | -1.441902 | -1.311209 | -1.295022 | 2999.6747, | 3019.0596, | 3025.0347, |
|                                                                                           | H | -3.342388 | 0.123594  | -0.515285 | 3047.6497, | 3066.7889, | 3115.0158, |
|                                                                                           | H | -3.286706 | -0.756221 | 1.114909  | 3129.3392, | 3140.6860, | 3211.3570, |
|                                                                                           | H | -0.626529 | 2.600146  | 0.363128  | 3246.3875, | 3766.1759  |            |
|                                                                                           | O | -0.275713 | 0.959383  | -0.485212 |            |            |            |
|                                                                                           | O | -1.223776 | 1.872936  | 0.136380  |            |            |            |
| P7<br> | C | -3.610105 | -0.507883 | -0.428479 | 58.2843,   | 69.2084,   | 76.9454,   |
|                                                                                           | C | -2.723300 | 0.225824  | 0.240824  | 128.6002,  | 189.8943,  | 219.0562,  |
|                                                                                           | C | -1.304133 | -0.178344 | 0.524958  | 259.2559,  | 305.4328,  | 336.1732,  |
|                                                                                           | C | -0.287312 | 0.797713  | -0.096356 | 438.1337,  | 477.6992,  | 503.6906,  |
|                                                                                           | C | 1.176766  | 0.475948  | 0.252578  | 582.6993,  | 660.1162,  | 760.0392,  |
|                                                                                           | C | 2.133170  | 1.491260  | -0.265432 | 845.8964,  | 921.7604,  | 932.3324,  |
|                                                                                           | H | -3.354826 | -1.487644 | -0.821465 | 942.0274,  | 950.1608,  | 985.8464,  |
|                                                                                           | H | -4.621627 | -0.158633 | -0.603557 | 1026.0086, | 1027.4304, | 1061.2517, |
|                                                                                           | H | -3.025957 | 1.203522  | 0.615509  | 1116.1249, | 1167.9642, | 1233.0798, |
|                                                                                           | H | -1.145450 | -0.200905 | 1.611463  | 1269.9970, | 1307.8072, | 1327.0206, |
|                                                                                           | H | -1.118951 | -1.189172 | 0.156126  | 1333.9357, | 1354.6515, | 1365.5156, |
|                                                                                           | H | -0.488942 | 1.816714  | 0.250493  | 1386.2562, | 1451.2093, | 1453.2759, |

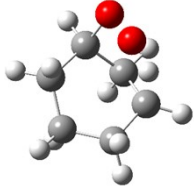
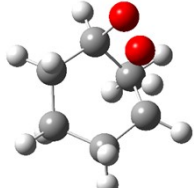
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|-------------------------------------------------------------------------------------|---|-----------|-----------|-----------|-------------|------------|------------|
|                                                                                     | H | -0.395947 | 0.809988  | -1.185905 | 1474.5863,  | 1495.4561, | 1699.2126, |
|                                                                                     | H | 1.281423  | 0.361933  | 1.336909  | 3000.5690,  | 3028.0900, | 3035.4035, |
|                                                                                     | H | 2.220336  | 1.645648  | -1.335546 | 3065.7517,  | 3088.9565, | 3111.8162, |
|                                                                                     | H | 2.730028  | 2.102315  | 0.399141  | 3126.6158,  | 3133.5321, | 3208.9546, |
|                                                                                     | H | 3.243916  | -1.240287 | -0.554132 | 3245.4948,  | 3764.4207  |            |
|                                                                                     | O | 1.405510  | -0.823301 | -0.347020 |             |            |            |
|                                                                                     | O | 2.640176  | -1.363022 | 0.192322  |             |            |            |
| P8                                                                                  | C | -1.015602 | -1.265354 | -0.281233 | 91.2894,    | 178.6672,  | 304.1125,  |
|    | C | 0.394004  | -1.285195 | 0.345333  | 404.4380,   | 414.9570,  | 476.2885,  |
|                                                                                     | C | 1.158962  | 0.000000  | 0.066888  | 491.9481,   | 654.9590,  | 747.5931,  |
|                                                                                     | C | 0.394003  | 1.285196  | 0.345330  | 760.1076,   | 837.9092,  | 876.1905,  |
|                                                                                     | C | -1.015605 | 1.265354  | -0.281230 | 895.3133,   | 916.5632,  | 998.6348,  |
|                                                                                     | C | -1.790586 | -0.000001 | 0.106391  | 1025.1437,  | 1064.3763, | 1079.7934, |
|                                                                                     | H | 0.299418  | -1.377734 | 1.436075  | 1132.9707,  | 1135.5335, | 1240.8026, |
|                                                                                     | H | 0.989793  | -2.128445 | -0.008349 | 1248.9899,  | 1273.7675, | 1289.5219, |
|                                                                                     | H | -0.922322 | -1.313025 | -1.372809 | 1334.9004,  | 1344.7232, | 1368.0414, |
|                                                                                     | H | -1.563637 | -2.161929 | 0.023182  | 1377.7478,  | 1378.4323, | 1462.1357, |
|                                                                                     | H | 0.299424  | 1.377738  | 1.436073  | 1470.9332,  | 1491.4044, | 1492.0905, |
|                                                                                     | H | 0.989790  | 2.128445  | -0.008356 | 1506.8249,  | 1779.9467, | 2999.7796, |
|                                                                                     | H | -1.563641 | 2.161927  | 0.023190  | 3002.5158,  | 3006.5905, | 3016.8451, |
|                                                                                     | H | -0.922329 | 1.313029  | -1.372806 | 3019.1417,  | 3057.2058, | 3059.1619, |
|                                                                                     | H | -1.974872 | -0.000003 | 1.188623  | 3063.7030,  | 3095.2409, | 3096.6958  |
|                                                                                     | H | -2.772508 | -0.000002 | -0.376885 |             |            |            |
|                                                                                     | O | 2.298729  | 0.000001  | -0.347101 |             |            |            |
| TS1Ca                                                                               | C | -1.939985 | 0.643779  | -0.128694 | 2132.6103i, | 138.9380,  | 164.2046,  |
|  | C | -0.652902 | 1.503908  | -0.142916 | 253.0779,   | 295.6253,  | 351.3130,  |
|                                                                                     | C | 0.396649  | 0.913838  | 0.769881  | 429.9744,   | 458.5624,  | 581.7850,  |
|                                                                                     | C | 0.653451  | -0.594282 | 0.609815  | 620.1795,   | 690.5461,  | 776.4871,  |
|                                                                                     | C | -0.606157 | -1.439635 | 0.430797  | 813.7370,   | 832.9475,  | 862.4956,  |
|                                                                                     | C | -1.626990 | -0.804653 | -0.523905 | 888.6658,   | 909.6633,  | 932.2245,  |
|                                                                                     | H | 1.621753  | 1.097004  | 0.222106  | 956.3888,   | 1002.0623, | 1036.1940, |
|                                                                                     | H | -0.277080 | 1.523425  | -1.172058 | 1049.8820,  | 1089.9910, | 1135.6207, |
|                                                                                     | H | -0.872252 | 2.535413  | 0.143600  | 1143.6804,  | 1165.2609, | 1195.8361, |
|                                                                                     | H | -2.391726 | 0.668949  | 0.870823  | 1272.0332,  | 1287.2746, | 1329.9041, |
|                                                                                     | H | -2.670060 | 1.079920  | -0.817317 | 1335.3597,  | 1348.0246, | 1356.6936, |
|                                                                                     | H | 1.258896  | -0.954659 | 1.449400  | 1378.4286,  | 1386.2585, | 1391.9498, |
|                                                                                     | H | -0.314578 | -2.438899 | 0.092186  | 1473.2955,  | 1484.8297, | 1491.6099, |
|                                                                                     | H | -1.057014 | -1.565035 | 1.422445  | 1499.6449,  | 1701.9312, | 3008.4251, |
|                                                                                     | H | -1.234220 | -0.824582 | -1.545649 | 3014.6556,  | 3023.7499, | 3028.1560, |
|                                                                                     | H | -2.543052 | -1.403452 | -0.525740 | 3029.0948,  | 3058.0817, | 3060.6442, |
|                                                                                     | H | 0.398474  | 1.282828  | 1.795644  | 3070.8386,  | 3074.6022, | 3110.8500  |
|                                                                                     | O | 1.444694  | -0.666051 | -0.592607 |             |            |            |
|                                                                                     | O | 2.397364  | 0.373721  | -0.410557 |             |            |            |

|                                                                                              |   |           |           |           |             |            |            |
|----------------------------------------------------------------------------------------------|---|-----------|-----------|-----------|-------------|------------|------------|
| TS1Ce<br>   | C | -0.988550 | 1.509575  | 0.182907  | 2162.9087i, | 155.8214,  | 210.5214,  |
|                                                                                              | C | 0.304689  | 0.937965  | -0.315234 | 286.6184,   | 313.6476,  | 335.7865,  |
|                                                                                              | C | 0.611763  | -0.439554 | 0.260595  | 396.1702,   | 467.0668,  | 507.0595,  |
|                                                                                              | C | -0.424322 | -1.457290 | -0.193916 | 581.8940,   | 658.6263,  | 795.8740,  |
|                                                                                              | C | -1.806657 | -0.941224 | 0.265667  | 819.3197,   | 835.0612,  | 887.1911,  |
|                                                                                              | C | -2.109173 | 0.496221  | -0.203225 | 904.5523,   | 924.1105,  | 944.3533,  |
|                                                                                              | H | 0.414139  | 0.958670  | -1.404619 | 970.2355,   | 1036.9602, | 1051.7381, |
|                                                                                              | H | 1.598388  | 1.242232  | 0.016850  | 1056.7829,  | 1092.6835, | 1146.1676, |
|                                                                                              | H | -0.967419 | 1.629073  | 1.272169  | 1166.5465,  | 1188.4052, | 1200.6499, |
|                                                                                              | H | -1.205523 | 2.487014  | -0.255437 | 1261.1464,  | 1266.1446, | 1304.3804, |
|                                                                                              | H | -0.390833 | -1.555489 | -1.283883 | 1334.0095,  | 1340.2217, | 1359.9906, |
|                                                                                              | H | -0.219025 | -2.441870 | 0.236450  | 1372.0828,  | 1385.7741, | 1395.8980, |
|                                                                                              | H | -2.587744 | -1.615119 | -0.097722 | 1485.3554,  | 1488.3585, | 1495.8967, |
|                                                                                              | H | -1.852531 | -0.979668 | 1.360766  | 1503.3007,  | 1731.1981, | 2988.4979, |
|                                                                                              | H | -2.224963 | 0.505829  | -1.293103 | 3014.3119,  | 3019.0156, | 3022.4644, |
|                                                                                              | H | -3.062087 | 0.831826  | 0.217354  | 3031.6160,  | 3055.0860, | 3061.4971, |
|                                                                                              | H | 0.625360  | -0.380474 | 1.358106  | 3065.6688,  | 3076.7521, | 3080.4833  |
|                                                                                              | O | 2.601379  | 0.519274  | 0.184402  |             |            |            |
|                                                                                              | O | 1.941838  | -0.683795 | -0.197864 |             |            |            |
| TS1Ta<br>  | C | 1.399103  | 0.668171  | -0.827189 | 2157.1648i, | 79.1662,   | 146.7137,  |
|                                                                                              | C | 1.648214  | -0.809065 | -0.440356 | 197.5571,   | 272.1845,  | 314.3087,  |
|                                                                                              | C | 0.667496  | -1.352991 | 0.630111  | 448.4407,   | 467.6962,  | 542.5212,  |
|                                                                                              | C | -0.649325 | -0.590384 | 0.690229  | 652.2223,   | 724.1303,  | 755.1767,  |
|                                                                                              | C | -0.456455 | 0.930972  | 0.849568  | 790.6415,   | 806.4702,  | 846.5176,  |
|                                                                                              | C | 0.850645  | 1.489947  | 0.347009  | 883.0523,   | 899.9286,  | 935.8750,  |
|                                                                                              | H | 0.464765  | -2.414859 | 0.464247  | 953.9276,   | 993.8389,  | 1043.3829, |
|                                                                                              | H | 1.583787  | -1.422212 | -1.341649 | 1055.8832,  | 1112.6210, | 1115.0851, |
|                                                                                              | H | 2.668934  | -0.924024 | -0.062441 | 1151.7368,  | 1172.5224, | 1188.4028, |
|                                                                                              | H | 1.578005  | 1.494001  | 1.175352  | 1258.9468,  | 1292.8213, | 1309.3929, |
|                                                                                              | H | 0.679083  | 0.712407  | -1.648519 | 1336.0899,  | 1346.1526, | 1361.6031, |
|                                                                                              | H | -1.300874 | -0.962872 | 1.489029  | 1377.2919,  | 1382.4348, | 1390.4749, |
|                                                                                              | H | -0.821357 | 1.358161  | 1.783762  | 1460.9910,  | 1478.1847, | 1494.5864, |
|                                                                                              | H | -1.494183 | 1.091674  | -0.005348 | 1508.7471,  | 1691.5700, | 2954.7468, |
|                                                                                              | H | 0.727979  | 2.542685  | 0.067768  | 3017.1257,  | 3027.2865, | 3028.3231, |
|                                                                                              | H | 2.326576  | 1.114052  | -1.196472 | 3037.3244,  | 3045.7602, | 3060.4498, |
|                                                                                              | H | 1.114089  | -1.282291 | 1.628205  | 3074.1780,  | 3088.2078, | 3106.4277i |
|                                                                                              | O | -1.317054 | -0.754999 | -0.579331 |             |            |            |
|                                                                                              | O | -2.218555 | 0.339172  | -0.651939 |             |            |            |
| TS1Te<br> | C | -0.581726 | 0.397943  | -0.323816 | 2160.9938i, | 94.5601,   | 211.6529,  |
|                                                                                              | C | 0.416467  | 1.511245  | -0.000745 | 247.1147,   | 255.7993,  | 331.8189,  |
|                                                                                              | C | 1.807980  | 0.885222  | 0.304468  | 405.4707,   | 465.8918,  | 506.9774,  |
|                                                                                              | C | 2.025724  | -0.463439 | -0.410714 | 591.2943,   | 656.1753,  | 779.1041,  |
|                                                                                              | C | 0.990243  | -1.549890 | 0.042448  | 806.5333,   | 836.5502,  | 885.1957,  |
|                                                                                              | H | 2.596372  | 1.586989  | 0.021119  | 898.1431,   | 924.6032,  | 949.1558,  |
|                                                                                              | H | 0.478785  | 2.205732  | -0.842692 | 972.9951,   | 1028.3289, | 1053.5028, |
|                                                                                              | H | 0.056395  | 2.075030  | 0.864227  | 1084.2115,  | 1105.3947, | 1133.8490, |

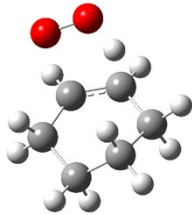
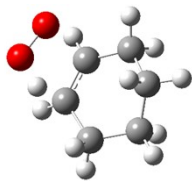
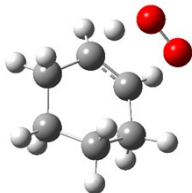
|                                                                                              |   |           |           |           |             |            |            |
|----------------------------------------------------------------------------------------------|---|-----------|-----------|-----------|-------------|------------|------------|
|                                                                                              | H | -0.567472 | 0.155546  | -1.394409 | 1153.4916,  | 1187.1622, | 1204.3960, |
|                                                                                              | H | 1.947075  | -0.314376 | -1.492590 | 1260.3767,  | 1271.1179, | 1309.4097, |
|                                                                                              | H | 3.038666  | -0.828781 | -0.223088 | 1325.4456,  | 1341.0578, | 1360.0802, |
|                                                                                              | H | 0.805339  | -2.232323 | -0.794907 | 1371.1627,  | 1383.1412, | 1398.4912, |
|                                                                                              | H | 1.399236  | -2.149718 | 0.858682  | 1483.5556,  | 1488.3420, | 1499.4264, |
|                                                                                              | H | 1.908389  | 0.730668  | 1.383924  | 1507.7034,  | 1731.7133, | 2998.9961, |
|                                                                                              | C | -0.280585 | -0.863851 | 0.474331  | 3017.7167,  | 3026.1792, | 3033.6991, |
|                                                                                              | H | -0.387759 | -0.707477 | 1.551462  | 3041.3597,  | 3060.0766, | 3069.6201, |
|                                                                                              | H | -1.569069 | -1.222602 | 0.189936  | 3070.0493,  | 3085.2693, | 3090.5209  |
|                                                                                              | O | -1.926869 | 0.703549  | 0.050278  |             |            |            |
|                                                                                              | O | -2.569952 | -0.553808 | -0.129964 |             |            |            |
| TS1Ti<br>   | C | 0.626670  | -0.628380 | 0.426581  | 2158.5864i, | 90.1074,   | 180.3936,  |
|                                                                                              | C | -0.531275 | -1.405263 | -0.210712 | 197.2085,   | 261.0038,  | 349.1992,  |
|                                                                                              | C | -1.873678 | -0.804977 | 0.237486  | 402.6268,   | 494.0164,  | 563.8527,  |
|                                                                                              | C | -2.042238 | 0.662513  | -0.222234 | 586.7772,   | 678.4004,  | 777.2393,  |
|                                                                                              | C | -0.680686 | 1.420378  | -0.339937 | 791.2268,   | 835.3617,  | 869.4396,  |
|                                                                                              | H | -2.700041 | -1.412211 | -0.140545 | 904.3358,   | 916.6130,  | 931.9685,  |
|                                                                                              | H | -0.432346 | -1.335937 | -1.299048 | 971.1142,   | 994.8584,  | 1036.3342, |
|                                                                                              | H | -0.469079 | -2.463870 | 0.051475  | 1061.7941,  | 1094.3257, | 1129.7371, |
|                                                                                              | H | 0.952555  | -1.073101 | 1.373885  | 1146.0016,  | 1152.3466, | 1211.3493, |
|                                                                                              | H | -2.536685 | 0.696296  | -1.197559 | 1266.8863,  | 1276.2928, | 1301.1636, |
|                                                                                              | H | -2.696017 | 1.188854  | 0.478675  | 1315.8453,  | 1341.1810, | 1360.1686, |
|                                                                                              | H | -0.284218 | 1.280754  | -1.350899 | 1370.7356,  | 1376.3345, | 1387.3214, |
|                                                                                              | H | -0.832034 | 2.492539  | -0.197727 | 1486.4080,  | 1492.9498, | 1503.2054, |
|                                                                                              | H | -1.934418 | -0.858423 | 1.330621  | 1511.3996,  | 1697.7020, | 3016.6017, |
|                                                                                              | C | 0.306951  | 0.863678  | 0.646280  | 3020.6120,  | 3027.3224, | 3035.3708, |
|                                                                                              | H | 0.178866  | 1.175877  | 1.683283  | 3037.7540,  | 3061.5709, | 3074.4649, |
|                                                                                              | H | 1.616134  | 1.114676  | 0.347025  | 3083.5123,  | 3085.6651, | 3106.2341  |
|                                                                                              | O | 2.554960  | 0.439898  | -0.039324 |             |            |            |
|                                                                                              | O | 1.732892  | -0.621541 | -0.498672 |             |            |            |
| TS2Ce<br> | C | -1.303613 | 1.430881  | -0.093748 | 1924.7420i, | 45.3633,   | 125.3309,  |
|                                                                                              | C | 0.104736  | 1.129425  | 0.321860  | 186.3072,   | 204.3086,  | 254.6095,  |
|                                                                                              | C | 0.643427  | -0.273845 | 0.397956  | 311.6579,   | 359.7232,  | 433.7578,  |
|                                                                                              | C | -0.357639 | -1.348543 | -0.052101 | 474.1130,   | 524.9384,  | 589.2742,  |
|                                                                                              | C | -1.807303 | -0.994916 | 0.304494  | 651.4342,   | 767.7083,  | 814.8384,  |
|                                                                                              | C | -2.240608 | 0.298236  | -0.402508 | 861.1553,   | 883.3672,  | 895.1611,  |
|                                                                                              | H | 0.825757  | 1.936295  | 0.302474  | 919.1338,   | 922.6895,  | 1006.7410, |
|                                                                                              | H | -0.851929 | 1.449754  | 1.137941  | 1056.3480,  | 1070.4058, | 1084.5946, |
|                                                                                              | H | -1.508196 | 2.426436  | -0.470567 | 1150.6157,  | 1182.6132, | 1202.3408, |
|                                                                                              | H | -0.275685 | -1.438314 | -1.141233 | 1257.5423,  | 1279.4440, | 1329.0224, |
|                                                                                              | H | -0.069310 | -2.313847 | 0.370369  | 1338.8429,  | 1347.0068, | 1359.7296, |
|                                                                                              | H | -2.464787 | -1.817962 | 0.011536  | 1361.0098,  | 1373.6711, | 1383.1069, |
|                                                                                              | H | -1.914953 | -0.881695 | 1.390947  | 1393.7500,  | 1482.6076, | 1493.8340, |
|                                                                                              | H | -2.244168 | 0.108455  | -1.489025 | 1500.4818,  | 2168.6243, | 2934.1334, |
|                                                                                              | H | -3.270106 | 0.558872  | -0.135270 | 2992.8453,  | 3006.0532, | 3028.2516, |
|                                                                                              | H | 1.025202  | -0.495543 | 1.402539  | 3035.4838,  | 3065.0549, | 3080.0356, |

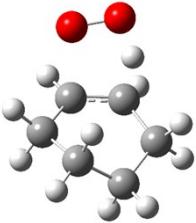
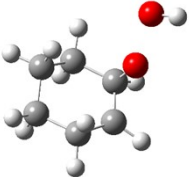
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|----------------------------------------------------------------------------------------------|---|-----------|-----------|-----------|---------------------------------|------------|------------|
|                                                                                              | O | 1.762868  | -0.456998 | -0.511964 | 3161.7125, 3196.1455, 3774.0059 |            |            |
|                                                                                              | O | 2.862436  | 0.373081  | -0.040247 |                                 |            |            |
|                                                                                              | H | 3.511739  | -0.308547 | 0.182268  |                                 |            |            |
| <hr/>                                                                                        |   |           |           |           |                                 |            |            |
| TS2Te<br>   | C | -0.652937 | -0.182923 | 0.645306  | 1856.8359i,                     | 77.6759,   | 132.2287,  |
|                                                                                              | C | 0.407152  | -1.292363 | 0.601566  | 169.4862,                       | 200.1483,  | 263.9781,  |
|                                                                                              | C | 1.459995  | -1.067444 | -0.490365 | 298.6329,                       | 389.8143,  | 442.8373,  |
|                                                                                              | C | 2.222909  | 0.245324  | -0.253941 | 477.7021,                       | 532.8425,  | 621.1192,  |
|                                                                                              | C | 1.293585  | 1.410079  | -0.077312 | 661.2109,                       | 769.5095,  | 808.5268,  |
|                                                                                              | H | 2.162485  | -1.905633 | -0.503827 | 826.0581,                       | 878.5560,  | 889.5377,  |
|                                                                                              | H | 0.897238  | -1.318869 | 1.581459  | 913.8485,                       | 926.3333,  | 1005.9718, |
|                                                                                              | H | -0.095662 | -2.254078 | 0.468823  | 1045.8366,                      | 1056.8941, | 1100.9993, |
|                                                                                              | H | -1.209591 | -0.227549 | 1.588752  | 1129.3966,                      | 1175.3437, | 1213.6364, |
|                                                                                              | H | 2.830550  | 0.129395  | 0.661281  | 1256.3631,                      | 1283.3791, | 1325.9096, |
|                                                                                              | H | 2.931651  | 0.431711  | -1.067113 | 1337.4506,                      | 1345.7745, | 1359.5127, |
|                                                                                              | H | 1.692723  | 2.413177  | 0.011614  | 1361.8092,                      | 1379.2395, | 1384.9494, |
|                                                                                              | H | 0.170970  | 1.436823  | -0.772431 | 1389.5546,                      | 1474.6309, | 1485.1227, |
|                                                                                              | H | 0.973119  | -1.045153 | -1.471106 | 1497.8076,                      | 2183.6522, | 2914.2383, |
|                                                                                              | C | -0.089457 | 1.193954  | 0.460243  | 3008.2173,                      | 3026.1186, | 3029.5527, |
|                                                                                              | H | -0.608973 | 2.039577  | 0.890968  | 3041.8641,                      | 3068.1161, | 3075.2674, |
|                                                                                              | O | -1.589750 | -0.566255 | -0.407933 | 3171.0246,                      | 3193.7558, | 3772.7013  |
|                                                                                              | O | -2.681079 | 0.397885  | -0.402379 |                                 |            |            |
|                                                                                              | H | -3.425361 | -0.192200 | -0.218905 |                                 |            |            |
| <hr/>                                                                                        |   |           |           |           |                                 |            |            |
| TS3Ca<br> | C | -1.923161 | 0.362903  | -0.613149 | 1927.3289i,                     | 86.0723,   | 138.9339,  |
|                                                                                              | C | -1.038118 | 1.471529  | -0.129961 | 151.8438,                       | 185.2549,  | 260.6668,  |
|                                                                                              | C | 0.127202  | 1.173532  | 0.785338  | 292.2523,                       | 357.0436,  | 422.1093,  |
|                                                                                              | C | 0.625172  | -0.275878 | 0.705283  | 522.1568,                       | 553.6449,  | 591.5593,  |
|                                                                                              | C | -0.535861 | -1.275043 | 0.737155  | 698.9072,                       | 788.0488,  | 800.0434,  |
|                                                                                              | C | -1.512372 | -1.072953 | -0.433071 | 853.7192,                       | 877.7627,  | 883.0246,  |
|                                                                                              | H | 0.957823  | 1.845301  | 0.559087  | 911.6591,                       | 951.8242,  | 1001.5308, |
|                                                                                              | H | -1.065197 | 2.409629  | -0.671648 | 1054.3759,                      | 1061.6819, | 1080.5294, |
|                                                                                              | H | -2.182264 | 1.167785  | 0.393494  | 1142.8064,                      | 1196.0010, | 1214.7181, |
|                                                                                              | H | -2.592037 | 0.612465  | -1.428938 | 1259.7971,                      | 1269.2730, | 1322.1650, |
|                                                                                              | H | 1.317176  | -0.472103 | 1.533039  | 1335.7721,                      | 1346.5307, | 1353.7635, |
|                                                                                              | H | -0.146339 | -2.296332 | 0.729532  | 1362.6469,                      | 1385.7421, | 1388.2593, |
|                                                                                              | H | -1.054551 | -1.134234 | 1.692947  | 1399.7764,                      | 1474.8658, | 1482.3437, |
|                                                                                              | H | -1.013729 | -1.409774 | -1.354152 | 1488.7953,                      | 2169.9605, | 2959.5172, |
|                                                                                              | H | -2.385332 | -1.720485 | -0.301574 | 2967.0770,                      | 3011.4440, | 3023.8362, |
|                                                                                              | H | -0.125917 | 1.358790  | 1.840459  | 3039.0286,                      | 3073.4466, | 3081.8509, |
|                                                                                              | O | 1.314113  | -0.552122 | -0.525226 | 3155.3539,                      | 3170.7336, | 3779.4370  |
|                                                                                              | O | 2.516079  | 0.271199  | -0.559937 |                                 |            |            |
|                                                                                              | H | 3.191662  | -0.418212 | -0.620518 |                                 |            |            |

|                                                                                              |   |           |           |           |             |            |            |
|----------------------------------------------------------------------------------------------|---|-----------|-----------|-----------|-------------|------------|------------|
| TS3Ce<br>   | C | 1.347285  | 1.435288  | -0.004195 | 1914.7967i, | 105.0059,  | 128.6160,  |
|                                                                                              | C | -0.116338 | 1.175471  | 0.283094  | 180.1429,   | 186.0766,  | 235.3059,  |
|                                                                                              | C | -0.558818 | -0.212468 | -0.195033 | 302.7799,   | 367.5746,  | 459.6155,  |
|                                                                                              | C | 0.375932  | -1.299387 | 0.335459  | 468.4196,   | 507.1757,  | 577.8412,  |
|                                                                                              | C | 1.784263  | -1.119268 | -0.254698 | 645.0459,   | 773.7369,  | 826.3299,  |
|                                                                                              | C | 2.303657  | 0.286385  | -0.118549 | 842.2693,   | 892.4689,  | 916.5388,  |
|                                                                                              | H | -0.341178 | 1.226609  | 1.357919  | 937.5612,   | 949.7181,  | 1046.0406, |
|                                                                                              | H | -0.727671 | 1.944334  | -0.192533 | 1047.3821,  | 1073.8822, | 1104.0790, |
|                                                                                              | H | 1.659423  | 2.397337  | -0.393120 | 1124.0495,  | 1187.6792, | 1227.5290, |
|                                                                                              | H | 0.407067  | -1.238182 | 1.429404  | 1269.9109,  | 1273.5834, | 1306.2228, |
|                                                                                              | H | -0.016518 | -2.285529 | 0.074832  | 1318.5055,  | 1334.8189, | 1350.6998, |
|                                                                                              | H | 2.472022  | -1.841930 | 0.195121  | 1362.7569,  | 1378.5469, | 1386.4342, |
|                                                                                              | H | 1.736791  | -1.371267 | -1.328449 | 1394.3871,  | 1483.0595, | 1486.1866, |
|                                                                                              | H | 2.109883  | 1.023381  | 0.952925  | 1503.8752,  | 2178.7193, | 2923.1976, |
|                                                                                              | H | 3.285971  | 0.520180  | -0.512634 | 2978.8302,  | 2996.5371, | 3025.7628, |
|                                                                                              | H | -0.582794 | -0.248138 | -1.292843 | 3044.9065,  | 3078.4659, | 3087.7404, |
|                                                                                              | O | -1.857024 | -0.559115 | 0.299096  | 3157.7495,  | 3172.8966, | 3782.7410  |
|                                                                                              | O | -2.818506 | 0.374847  | -0.280336 |             |            |            |
|                                                                                              | H | -3.414635 | -0.248784 | -0.717166 |             |            |            |
| TS3Te<br> | C | -1.911680 | -0.911389 | 0.200850  | 1949.7412i, | 45.8485,   | 145.6837,  |
|                                                                                              | C | -0.461700 | -1.385125 | -0.006310 | 175.5803,   | 214.1199,  | 286.5772,  |
|                                                                                              | C | 0.605921  | -0.372494 | 0.468433  | 306.3355,   | 356.2971,  | 422.6822,  |
|                                                                                              | C | 0.087832  | 1.065111  | 0.669685  | 506.1168,   | 518.8730,  | 605.7069,  |
|                                                                                              | C | -1.049873 | 1.443119  | -0.237463 | 654.9531,   | 774.1957,  | 803.8893,  |
|                                                                                              | C | -2.135228 | 0.435474  | -0.430672 | 850.7845,   | 891.4719,  | 901.8174,  |
|                                                                                              | H | 1.077813  | -0.709473 | 1.397469  | 921.6900,   | 957.1353,  | 1010.5888, |
|                                                                                              | H | -0.296368 | -2.348926 | 0.480738  | 1039.5745,  | 1063.6056, | 1102.3383, |
|                                                                                              | H | -0.303940 | -1.542456 | -1.079166 | 1130.7261,  | 1195.3833, | 1221.9174, |
|                                                                                              | H | -1.248084 | 0.760670  | -1.335204 | 1245.2849,  | 1277.4870, | 1316.9256, |
|                                                                                              | H | -2.130783 | -0.867450 | 1.280751  | 1336.1542,  | 1339.1388, | 1351.6845, |
|                                                                                              | H | -0.245174 | 1.142315  | 1.718585  | 1362.8687,  | 1371.1247, | 1393.5527, |
|                                                                                              | H | 0.931468  | 1.750164  | 0.568847  | 1401.3579,  | 1477.1377, | 1488.8525, |
|                                                                                              | H | -1.286292 | 2.488098  | -0.399443 | 1495.1964,  | 2154.6813, | 2926.2727, |
|                                                                                              | H | -3.137020 | 0.779062  | -0.662890 | 2940.3824,  | 3024.8005, | 3027.8736, |
|                                                                                              | H | -2.593785 | -1.656188 | -0.218249 | 3057.1794,  | 3079.1490, | 3090.4030, |
|                                                                                              | O | 1.602172  | -0.441962 | -0.570246 | 3154.0799,  | 3172.7878, | 3779.9049  |
|                                                                                              | O | 2.770087  | 0.309527  | -0.126311 |             |            |            |
|                                                                                              | H | 3.442461  | -0.384517 | -0.166124 |             |            |            |
| TS4Ca<br> | C | -1.546951 | 0.939572  | -0.304643 | 1913.4133i, | 140.2223,  | 206.6270,  |
|                                                                                              | C | -0.219743 | 1.446739  | 0.217591  | 267.2031,   | 332.9875,  | 403.7835,  |
|                                                                                              | C | 0.413931  | 0.577734  | 1.283510  | 429.9871,   | 488.5242,  | 557.6214,  |
|                                                                                              | C | 0.595115  | -0.822448 | 0.689663  | 580.0058,   | 697.8951,  | 787.4347,  |
|                                                                                              | C | -0.764688 | -1.429274 | 0.321087  | 809.1853,   | 812.1857,  | 863.9168,  |
|                                                                                              | C | -1.502672 | -0.549406 | -0.704625 | 879.0094,   | 893.9873,  | 946.2930,  |
|                                                                                              | H | 1.368342  | 0.990609  | 1.612810  | 962.0904,   | 1025.0613, | 1036.2198, |
|                                                                                              | H | 0.772560  | 1.187207  | -0.680872 | 1052.7277,  | 1078.7775, | 1115.0965, |

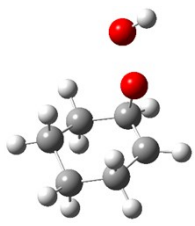
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|----------------------------------------------------------------------------------------------|---|-----------|-----------|-----------|-------------|------------|------------|
|                                                                                              | H | -0.144468 | 2.523579  | 0.371641  | 1139.8218,  | 1168.7111, | 1221.2824, |
|                                                                                              | H | -2.293165 | 1.083282  | 0.494917  | 1226.5499,  | 1277.4753, | 1311.8881, |
|                                                                                              | H | -1.889038 | 1.545761  | -1.148405 | 1326.4448,  | 1346.5387, | 1350.9180, |
|                                                                                              | H | 1.157871  | -1.469725 | 1.368774  | 1373.1996,  | 1385.6691, | 1391.3632, |
|                                                                                              | H | -0.620127 | -2.432861 | -0.088655 | 1463.9819,  | 1473.3038, | 1486.6684, |
|                                                                                              | H | -1.353578 | -1.542834 | 1.239744  | 1497.3363,  | 1559.3523, | 2946.1682, |
|                                                                                              | H | -0.991093 | -0.640716 | -1.666084 | 2999.1827,  | 3017.8182, | 3040.7016, |
|                                                                                              | H | -2.520110 | -0.923014 | -0.851478 | 3045.9656,  | 3057.3731, | 3067.3431, |
|                                                                                              | H | -0.232959 | 0.489296  | 2.166999  | 3082.7270,  | 3092.9347, | 3103.9098  |
|                                                                                              | O | 1.350617  | -0.767543 | -0.567766 |             |            |            |
|                                                                                              | O | 1.761360  | 0.544032  | -0.911594 |             |            |            |
| TS4Ta<br>   | C | 1.632540  | -0.703733 | -0.478115 | 1738.3961i, | 153.0058,  | 203.3774,  |
|                                                                                              | C | 0.465895  | -1.378777 | 0.229328  | 285.8252,   | 357.2516,  | 439.6870,  |
|                                                                                              | C | -0.157124 | -0.560934 | 1.330767  | 446.0931,   | 472.7568,  | 575.7393,  |
|                                                                                              | C | -0.760264 | 0.697839  | 0.662635  | 599.8938,   | 694.8974,  | 765.3717,  |
|                                                                                              | C | 0.285701  | 1.468166  | -0.178932 | 776.4975,   | 836.8432,  | 874.7838,  |
|                                                                                              | C | 1.678103  | 0.808297  | -0.176321 | 882.3325,   | 905.2040,  | 937.7318,  |
|                                                                                              | H | -0.943522 | -1.106054 | 1.856311  | 967.8963,   | 1018.9615, | 1025.6322, |
|                                                                                              | H | -0.555689 | -1.222790 | -0.656058 | 1057.2014,  | 1091.7696, | 1108.0594, |
|                                                                                              | H | 0.537120  | -2.454752 | 0.381770  | 1147.1974,  | 1161.6021, | 1180.8006, |
|                                                                                              | H | 2.144041  | 0.961196  | 0.803642  | 1227.9011,  | 1278.7382, | 1289.9927, |
|                                                                                              | H | 1.558898  | -0.871955 | -1.559157 | 1329.9843,  | 1340.5204, | 1345.8068, |
|                                                                                              | H | -1.245485 | 1.339777  | 1.400763  | 1369.2440,  | 1376.6946, | 1388.0759, |
|                                                                                              | H | 0.368959  | 2.493479  | 0.190821  | 1467.1005,  | 1473.8708, | 1483.6897, |
|                                                                                              | H | -0.095116 | 1.526242  | -1.200797 | 1506.4742,  | 1578.1112, | 2985.8630, |
|                                                                                              | H | 2.325072  | 1.313707  | -0.898283 | 2997.4695,  | 3015.1442, | 3030.5804, |
|                                                                                              | H | 2.578095  | -1.168773 | -0.169592 | 3047.5274,  | 3066.4424, | 3079.2243, |
|                                                                                              | H | 0.587777  | -0.248058 | 2.076377  | 3087.6989,  | 3096.9304, | 3115.2038  |
|                                                                                              | O | -1.876153 | 0.231825  | -0.122133 |             |            |            |
|                                                                                              | O | -1.390004 | -0.550220 | -1.198114 |             |            |            |
| TS4Ti<br> | C | -0.760504 | 0.697410  | 0.662857  | 1738.3805i, | 153.0939,  | 203.3927,  |
|                                                                                              | C | 0.285191  | 1.468309  | -0.178577 | 285.9396,   | 357.2601,  | 439.6786,  |
|                                                                                              | C | 1.677793  | 0.808659  | -0.176337 | 446.0911,   | 472.7771,  | 575.7803,  |
|                                                                                              | C | 1.632718  | -0.703427 | -0.478057 | 599.8433,   | 694.9100,  | 765.3445,  |
|                                                                                              | C | 0.466152  | -1.378757 | 0.229133  | 776.4914,   | 836.8732,  | 874.8022,  |
|                                                                                              | H | 2.324589  | 1.314230  | -0.898341 | 882.3364,   | 905.2038,  | 937.7271,  |
|                                                                                              | H | -0.095762 | 1.526642  | -1.200386 | 967.8951,   | 1018.9723, | 1025.6257, |
|                                                                                              | H | 0.368283  | 2.493493  | 0.191563  | 1057.1688,  | 1091.7767, | 1108.0117, |
|                                                                                              | H | -1.245949 | 1.339040  | 1.401118  | 1147.2909,  | 1161.6133, | 1180.8535, |
|                                                                                              | H | 1.559257  | -0.871717 | -1.559104 | 1227.9676,  | 1278.7855, | 1289.9814, |
|                                                                                              | H | 2.578393  | -1.168179 | -0.169422 | 1330.0249,  | 1340.5696, | 1345.7900, |
|                                                                                              | H | -0.555687 | -1.222827 | -0.656244 | 1369.2696,  | 1376.6870, | 1388.0732, |
|                                                                                              | H | 0.537447  | -2.454778 | 0.381220  | 1467.1158,  | 1473.8686, | 1483.6709, |
|                                                                                              | H | 2.143780  | 0.961735  | 0.803571  | 1506.4734,  | 1578.1139, | 2985.8027, |
|                                                                                              | C | -0.156966 | -0.561214 | 1.330698  | 2997.4164,  | 3015.1239, | 3030.5491, |
|                                                                                              | H | 0.587877  | -0.248173 | 2.076305  | 3047.5259,  | 3066.4429, | 3079.1398, |

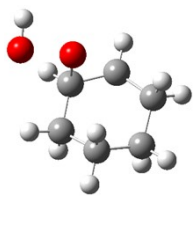
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|-------|---|-----------|-----------|-----------|---------------------------------|------------|------------|
|       | H | -0.943126 | -1.106660 | 1.856269  | 3087.6116, 3096.8753, 3115.1731 |            |            |
|       | O | -1.389468 | -0.549895 | -1.198464 |                                 |            |            |
|       | O | -1.876207 | 0.231309  | -0.122142 |                                 |            |            |
|       |   |           |           |           |                                 |            |            |
| TS5Ti | C | 0.762590  | 0.450832  | 0.842898  | 1857.0239i,                     | 134.6788,  | 192.4718,  |
|       | C | 0.227647  | -0.940693 | 1.204175  | 264.0502,                       | 321.2625,  | 338.7338,  |
|       | C | -1.033100 | -1.319424 | 0.373219  | 436.7700,                       | 489.5221,  | 537.7995,  |
|       | C | -1.149927 | -0.451909 | -0.865210 | 634.1095,                       | 730.7386,  | 764.1862,  |
|       | C | -1.240659 | 1.038075  | -0.603117 | 790.3940,                       | 819.7483,  | 864.4323,  |
|       | H | -1.000635 | -2.376393 | 0.099710  | 887.1810,                       | 901.1028,  | 922.2916,  |
|       | H | 1.020689  | -1.674337 | 1.054938  | 959.6459,                       | 1007.2192, | 1039.2822, |
|       | H | -0.013036 | -0.936678 | 2.270903  | 1059.2251,                      | 1098.4076, | 1107.9557, |
|       | H | 1.440434  | 0.810071  | 1.621659  | 1154.3845,                      | 1163.5724, | 1222.8602, |
|       | H | 0.116540  | -0.582985 | -1.334536 | 1248.4958,                      | 1265.1336, | 1296.6050, |
|       | H | -1.783991 | -0.830228 | -1.667183 | 1332.1993,                      | 1342.2183, | 1347.4286, |
|       | H | -0.908143 | 1.585861  | -1.490136 | 1362.7436,                      | 1376.1450, | 1384.4511, |
|       | H | -2.289277 | 1.327875  | -0.447133 | 1469.0785,                      | 1473.3268, | 1483.2875, |
|       | H | -1.939201 | -1.185982 | 0.982798  | 1498.3184,                      | 1517.4444, | 2972.8938, |
|       | C | -0.385599 | 1.441864  | 0.624800  | 2985.8395,                      | 3024.6556, | 3047.1348, |
|       | H | -0.997985 | 1.453737  | 1.534004  | 3048.7184,                      | 3063.7956, | 3070.3446, |
|       | H | 0.012099  | 2.450823  | 0.497396  | 3084.4453,                      | 3103.0953, | 3106.0933  |
|       | O | 1.303355  | -0.624535 | -1.219312 |                                 |            |            |
|       | O | 1.603745  | 0.455256  | -0.353563 |                                 |            |            |
|       |   |           |           |           |                                 |            |            |
| TS6Ca | C | 2.052107  | -0.342451 | -0.322980 | 962.4358i,                      | 87.8188,   | 123.7773,  |
|       | C | 1.028969  | -1.454546 | -0.047048 | 198.8779,                       | 214.9197,  | 309.7696,  |
|       | C | -0.169124 | -0.970003 | 0.788811  | 375.0393,                       | 444.1258,  | 469.7053,  |
|       | C | -0.354142 | 0.391396  | 1.045898  | 537.6009,                       | 659.1644,  | 713.9964,  |
|       | C | 0.477854  | 1.471971  | 0.427680  | 794.9735,                       | 820.0365,  | 823.0833,  |
|       | C | 1.355758  | 0.964268  | -0.722300 | 882.4056,                       | 905.5081,  | 942.2551,  |
|       | H | -1.214670 | -1.076162 | 0.006679  | 973.4919,                       | 1023.7361, | 1050.9383, |
|       | H | 0.677841  | -1.863946 | -1.001299 | 1073.0426,                      | 1105.8671, | 1149.9640, |
|       | H | 1.512922  | -2.285040 | 0.475055  | 1182.0440,                      | 1234.3700, | 1273.9768, |
|       | H | 2.651552  | -0.164267 | 0.578712  | 1289.3377,                      | 1304.6586, | 1314.0393, |
|       | H | 2.747456  | -0.663509 | -1.103946 | 1351.4732,                      | 1367.3047, | 1375.9287, |
|       | H | -1.006273 | 0.686710  | 1.860734  | 1383.0954,                      | 1403.2631, | 1457.4581, |
|       | H | -0.163117 | 2.299767  | 0.109449  | 1489.9311,                      | 1497.8649, | 1507.2522, |
|       | H | 1.117002  | 1.880455  | 1.226376  | 1553.4963,                      | 1566.7119, | 2972.6078, |
|       | H | 0.736642  | 0.795802  | -1.610802 | 3005.1764,                      | 3015.4223, | 3024.5110, |
|       | H | 2.090365  | 1.728664  | -0.990688 | 3054.0585,                      | 3054.8486, | 3062.9047, |
|       | H | -0.501418 | -1.645982 | 1.577573  | 3067.6920,                      | 3092.9104, | 3171.3654  |
|       | O | -2.139166 | 0.605491  | -0.326410 |                                 |            |            |
|       | O | -2.235438 | -0.612530 | -0.692116 |                                 |            |            |

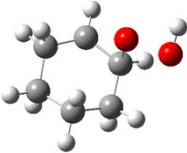
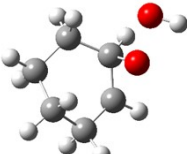
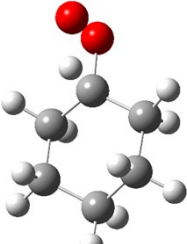
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|----------------------------------------------------------------------------------------------|---|-----------|-----------|-----------|------------|------------|------------|
| TS6Ce<br>   | C | 0.955121  | -1.482481 | 0.269864  | 926.2157i, | 79.2412,   | 128.5342,  |
|                                                                                              | C | -0.230026 | -0.794411 | 0.952133  | 191.8412,  | 214.8925,  | 315.8466,  |
|                                                                                              | C | -0.319751 | 0.601333  | 0.967309  | 347.5699,  | 447.5552,  | 471.9694,  |
|                                                                                              | C | 0.590409  | 1.503686  | 0.179565  | 533.3513,  | 663.7094,  | 677.3641,  |
|                                                                                              | C | 1.863937  | 0.795495  | -0.315474 | 810.2554,  | 814.2850,  | 828.5569,  |
|                                                                                              | C | 1.555147  | -0.611287 | -0.841378 | 880.2157,  | 900.9052,  | 943.3036,  |
|                                                                                              | H | -1.244823 | -0.978152 | 0.156514  | 958.3595,  | 1023.8617, | 1047.7510, |
|                                                                                              | H | -0.623923 | -1.302233 | 1.834445  | 1069.9171, | 1112.2866, | 1149.0250, |
|                                                                                              | H | 1.726194  | -1.696383 | 1.020640  | 1176.1876, | 1237.4552, | 1268.2102, |
|                                                                                              | H | 0.643974  | -2.451477 | -0.132486 | 1293.4190, | 1301.0339, | 1314.5105, |
|                                                                                              | H | 0.031013  | 1.912878  | -0.670156 | 1353.1097, | 1364.6755, | 1369.0495, |
|                                                                                              | H | 0.848236  | 2.368788  | 0.801082  | 1385.0893, | 1407.2031, | 1463.6856, |
|                                                                                              | H | 2.343153  | 1.402709  | -1.088585 | 1491.4091, | 1495.3228, | 1505.9657, |
|                                                                                              | H | 2.581450  | 0.716413  | 0.510075  | 1550.8079, | 1561.1785, | 3006.9296, |
|                                                                                              | H | 0.851375  | -0.543682 | -1.679578 | 3010.5058, | 3015.0262, | 3019.8472, |
|                                                                                              | H | 2.463798  | -1.079723 | -1.231102 | 3040.2039, | 3051.0224, | 3061.9345, |
|                                                                                              | H | -0.978949 | 1.074769  | 1.685242  | 3065.8704, | 3084.1925, | 3181.6453  |
|                                                                                              | O | -2.253785 | -0.595752 | -0.624777 |            |            |            |
|                                                                                              | O | -2.137529 | 0.658512  | -0.434998 |            |            |            |
| TS6Ta<br> | C | -2.052111 | -0.342450 | -0.322951 | 962.4292i, | 87.8195,   | 123.7751,  |
|                                                                                              | C | -1.355762 | 0.964260  | -0.722297 | 198.8769,  | 214.9186,  | 309.7677,  |
|                                                                                              | C | -0.477847 | 1.471976  | 0.427669  | 375.0374,  | 444.1210,  | 469.7047,  |
|                                                                                              | C | 0.354157  | 0.391408  | 1.045889  | 537.6027,  | 659.1619,  | 713.9954,  |
|                                                                                              | C | 0.169134  | -0.969994 | 0.788820  | 794.9743,  | 820.0352,  | 823.0863,  |
|                                                                                              | C | -1.028976 | -1.454546 | -0.047010 | 882.4065,  | 905.5087,  | 942.2554,  |
|                                                                                              | H | 0.163120  | 2.299770  | 0.109425  | 973.4889,  | 1023.7378, | 1050.9377, |
|                                                                                              | H | -0.736656 | 0.795781  | -1.610803 | 1073.0431, | 1105.8662, | 1149.9643, |
|                                                                                              | H | -2.090370 | 1.728655  | -0.990687 | 1182.0434, | 1234.3694, | 1273.9775, |
|                                                                                              | H | -1.512928 | -2.285024 | 0.475119  | 1289.3391, | 1304.6589, | 1314.0395, |
|                                                                                              | H | -2.747469 | -0.663518 | -1.103906 | 1351.4731, | 1367.3048, | 1375.9284, |
|                                                                                              | H | 1.006301  | 0.686731  | 1.860712  | 1383.0955, | 1403.2628, | 1457.4574, |
|                                                                                              | H | 0.501442  | -1.645966 | 1.577581  | 1489.9302, | 1497.8645, | 1507.2520, |
|                                                                                              | H | 1.214661  | -1.076161 | 0.006667  | 1553.4937, | 1566.7111, | 2972.6090, |
|                                                                                              | H | -0.677866 | -1.863970 | -1.001257 | 3005.1649, | 3015.4029, | 3024.5037, |
|                                                                                              | H | -2.651547 | -0.164250 | 0.578744  | 3054.0612, | 3054.8421, | 3062.9143, |
|                                                                                              | H | -1.116988 | 1.880466  | 1.226368  | 3067.6992, | 3092.9273, | 3171.3649  |
|                                                                                              | O | 2.139166  | 0.605484  | -0.326442 |            |            |            |
|                                                                                              | O | 2.235425  | -0.612540 | -0.692143 |            |            |            |
| TS6Te<br> | C | 0.354247  | 0.391507  | 1.045819  | 962.4361i, | 87.8234,   | 123.7695,  |
|                                                                                              | C | -0.477814 | 1.472015  | 0.427572  | 198.8786,  | 214.9183,  | 309.7678,  |
|                                                                                              | C | -1.355842 | 0.964190  | -0.722260 | 375.0404,  | 444.1196,  | 469.7034,  |
|                                                                                              | C | -2.052140 | -0.342491 | -0.322730 | 537.6043,  | 659.1597,  | 713.9941,  |
|                                                                                              | C | -1.028966 | -1.454552 | -0.046798 | 794.9753,  | 820.0365,  | 823.0876,  |
|                                                                                              | H | -2.090482 | 1.728556  | -0.990645 | 882.4068,  | 905.5074,  | 942.2571,  |
|                                                                                              | H | -1.116876 | 1.880586  | 1.226293  | 973.4907,  | 1023.7351, | 1050.9373, |
|                                                                                              | H | 0.163124  | 2.299777  | 0.109184  | 1073.0440, | 1105.8667, | 1149.9650, |

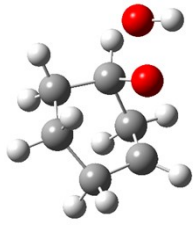
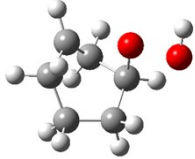
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|----------------------------------------------------------------------------------------------|---|-----------|-----------|-----------|------------|------------|------------|
|                                                                                              | H | 1.006459  | 0.686907  | 1.860559  | 1182.0428, | 1234.3687, | 1273.9769, |
|                                                                                              | H | -2.651487 | -0.164219 | 0.579010  | 1289.3369, | 1304.6571, | 1314.0370, |
|                                                                                              | H | -2.747574 | -0.663632 | -1.103588 | 1351.4726, | 1367.3056, | 1375.9318, |
|                                                                                              | H | -1.512861 | -2.285001 | 0.475432  | 1383.0949, | 1403.2631, | 1457.4633, |
|                                                                                              | H | -0.677932 | -1.864038 | -1.001046 | 1489.9292, | 1497.8612, | 1507.2490, |
|                                                                                              | H | -0.736824 | 0.795635  | -1.610814 | 1553.4921, | 1566.7109, | 2972.6115, |
|                                                                                              | C | 0.169207  | -0.969920 | 0.788893  | 3005.1652, | 3015.4020, | 3024.5041, |
|                                                                                              | H | 1.214675  | -1.076159 | 0.006670  | 3054.0611, | 3054.8418, | 3062.9133, |
|                                                                                              | H | 0.501580  | -1.645817 | 1.577693  | 3067.6994, | 3092.9277, | 3171.3650  |
|                                                                                              | O | 2.139133  | 0.605461  | -0.326690 |            |            |            |
|                                                                                              | O | 2.235373  | -0.612598 | -0.692275 |            |            |            |
| TS6Ti<br>   | C | -0.353895 | 0.391583  | 1.045886  | 963.1805i, | 87.8423,   | 123.6407,  |
|                                                                                              | C | 0.478071  | 1.471946  | 0.427296  | 198.8658,  | 214.7654,  | 309.6973,  |
|                                                                                              | C | 1.356524  | 0.964127  | -0.722213 | 374.7740,  | 444.1153,  | 469.7121,  |
|                                                                                              | C | 2.052232  | -0.342785 | -0.322567 | 537.5086,  | 658.9594,  | 713.8576,  |
|                                                                                              | C | 1.028704  | -1.454584 | -0.047026 | 794.8588,  | 820.0682,  | 823.0500,  |
|                                                                                              | H | 0.738005  | 0.795965  | -1.611185 | 882.3995,  | 905.5033,  | 942.1628,  |
|                                                                                              | H | -0.162846 | 2.299688  | 0.108773  | 973.4608,  | 1023.7311, | 1050.9762, |
|                                                                                              | H | 1.117044  | 1.880617  | 1.226071  | 1073.0792, | 1105.8579, | 1149.9838, |
|                                                                                              | H | -1.006394 | 0.687306  | 1.860252  | 1182.0904, | 1234.3193, | 1274.0427, |
|                                                                                              | H | 2.747836  | -0.664088 | -1.103222 | 1289.3413, | 1304.7500, | 1314.0452, |
|                                                                                              | H | 2.651308  | -0.164862 | 0.579431  | 1351.4917, | 1367.3484, | 1375.9672, |
|                                                                                              | H | 0.677566  | -1.863689 | -1.001426 | 1383.1495, | 1403.2203, | 1457.4507, |
|                                                                                              | H | 1.512409  | -2.285287 | 0.474977  | 1489.9332, | 1497.8721, | 1507.2709, |
|                                                                                              | H | 2.091471  | 1.728420  | -0.989988 | 1553.3759, | 1566.5921, | 2972.3689, |
|                                                                                              | C | -0.169288 | -0.969901 | 0.788950  | 3005.0851, | 3015.2445, | 3024.5144, |
|                                                                                              | H | -0.501323 | -1.645764 | 1.577899  | 3054.0028, | 3054.7812, | 3062.8168, |
|                                                                                              | H | -1.214870 | -1.075996 | 0.006633  | 3067.6586, | 3093.0869, | 3171.5881  |
|                                                                                              | O | -2.235813 | -0.612418 | -0.692204 |            |            |            |
|                                                                                              | O | -2.139724 | 0.605591  | -0.326566 |            |            |            |
| TS7Ca<br> | C | 2.111537  | 0.312393  | -0.266894 | 640.4762i, | 76.0532,   | 140.1410,  |
|                                                                                              | C | 1.559210  | -1.123293 | -0.336193 | 155.3924,  | 167.7752,  | 258.3774,  |
|                                                                                              | C | 0.346884  | -1.327454 | 0.505059  | 291.0112,  | 368.4445,  | 401.0467,  |
|                                                                                              | C | -0.602430 | -0.221585 | 0.796547  | 468.5317,  | 517.2981,  | 659.9788,  |
|                                                                                              | C | -0.036487 | 1.192342  | 0.732352  | 688.8589,  | 788.2713,  | 806.1037,  |
|                                                                                              | C | 0.993124  | 1.355076  | -0.392467 | 856.4611,  | 870.9907,  | 900.3582,  |
|                                                                                              | H | 1.302030  | -1.368560 | -1.378010 | 939.9183,  | 991.9965,  | 1009.0961, |
|                                                                                              | H | 2.322508  | -1.855960 | -0.048142 | 1051.3124, | 1057.9757, | 1080.1978, |
|                                                                                              | H | 2.629899  | 0.452684  | 0.689614  | 1140.8987, | 1161.1236, | 1199.5814, |
|                                                                                              | H | 2.860565  | 0.449728  | -1.052016 | 1256.6071, | 1285.0857, | 1302.8056, |
|                                                                                              | H | -1.206348 | -0.381601 | 1.696577  | 1352.6523, | 1360.6913, | 1370.9432, |
|                                                                                              | H | -0.873215 | 1.883212  | 0.604332  | 1385.1943, | 1400.0445, | 1413.3987, |
|                                                                                              | H | 0.427621  | 1.417346  | 1.701314  | 1450.6947, | 1474.8193, | 1493.1611, |
|                                                                                              | H | 0.491440  | 1.247022  | -1.359353 | 1501.0062, | 2973.7746, | 3009.0858, |
|                                                                                              | H | 1.416101  | 2.363468  | -0.363591 | 3010.0043, | 3027.5755, | 3030.9961, |
|                                                                                              | H | 0.064836  | -2.328143 | 0.809928  | 3033.5261, | 3062.2456, | 3072.5883, |

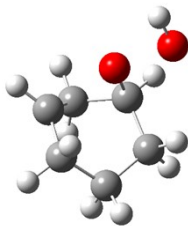
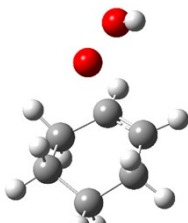
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| O | -1.286072 | -0.630443 | -0.362710 | 3085.5108, 3190.0235, 3801.5415 |
| O | -2.761755 | 0.310023  | -0.479207 |                                 |
| H | -3.283850 | -0.440709 | -0.795735 |                                 |

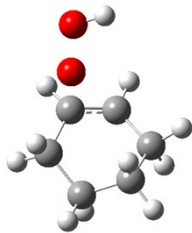
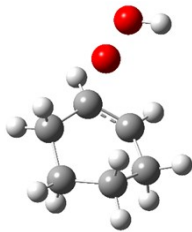
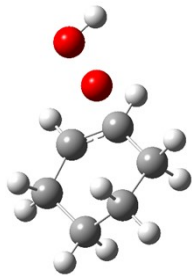
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|--------------------------------------------------------------------------------------------|---|-----------|-----------|-----------|---------------------------------|------------|------------|
| TS7Ce<br> | C | 1.559235  | -1.123291 | -0.336176 | 640.4740i,                      | 76.0536,   | 140.1410,  |
|                                                                                            | C | 0.346884  | -1.327450 | 0.505042  | 155.3948,                       | 167.7791,  | 258.3768,  |
|                                                                                            | C | -0.602433 | -0.221583 | 0.796537  | 291.0134,                       | 368.4445,  | 401.0499,  |
|                                                                                            | C | -0.036492 | 1.192344  | 0.732342  | 468.5318,                       | 517.3004,  | 659.9803,  |
|                                                                                            | C | 0.993123  | 1.355066  | -0.392477 | 688.8613,                       | 788.2724,  | 806.1045,  |
|                                                                                            | C | 2.111545  | 0.312401  | -0.266879 | 856.4610,                       | 870.9924,  | 900.3582,  |
|                                                                                            | H | 0.064825  | -2.328141 | 0.809892  | 939.9178,                       | 991.9953,  | 1009.0966, |
|                                                                                            | H | 2.322529  | -1.855947 | -0.048085 | 1051.3119,                      | 1057.9778, | 1080.1972, |
|                                                                                            | H | 1.302096  | -1.368580 | -1.377998 | 1140.8990,                      | 1161.1240, | 1199.5820, |
|                                                                                            | H | -0.873221 | 1.883212  | 0.604313  | 1256.6064,                      | 1285.0844, | 1302.8048, |
|                                                                                            | H | 0.427613  | 1.417355  | 1.701304  | 1352.6526,                      | 1360.6921, | 1370.9431, |
|                                                                                            | H | 0.491440  | 1.246986  | -1.359361 | 1385.1952,                      | 1400.0448, | 1413.3970, |
|                                                                                            | H | 1.416086  | 2.363464  | -0.363621 | 1450.6936,                      | 1474.8204, | 1493.1619, |
|                                                                                            | H | 2.860582  | 0.449740  | -1.051992 | 1501.0061,                      | 2973.7714, | 3009.0854, |
|                                                                                            | H | 2.629891  | 0.452707  | 0.689636  | 3010.0045,                      | 3027.5753, | 3030.9927, |
|                                                                                            | H | -1.206348 | -0.381606 | 1.696568  | 3033.5251,                      | 3062.2455, | 3072.5875, |
|                                                                                            | O | -1.286076 | -0.630435 | -0.362722 | 3085.5108, 3190.0224, 3801.5401 |            |            |
|                                                                                            | O | -2.761773 | 0.310012  | -0.479190 |                                 |            |            |
|                                                                                            | H | -3.283870 | -0.440728 | -0.795696 |                                 |            |            |

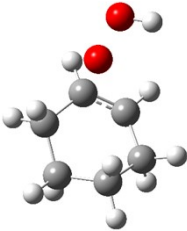
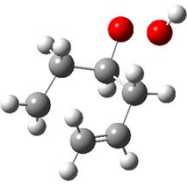
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|----------------------------------------------------------------------------------------------|---|-----------|-----------|-----------|---------------------------------|------------|------------|
| TS7Ta<br> | C | 2.111537  | 0.312394  | -0.266893 | 640.4904i,                      | 76.0534,   | 140.1446,  |
|                                                                                              | C | 1.559212  | -1.123293 | -0.336192 | 155.3898,                       | 167.7822,  | 258.3770,  |
|                                                                                              | C | 0.346885  | -1.327454 | 0.505058  | 291.0125,                       | 368.4431,  | 401.0488,  |
|                                                                                              | C | -0.602430 | -0.221585 | 0.796547  | 468.5334,                       | 517.2984,  | 659.9821,  |
|                                                                                              | C | -0.036487 | 1.192342  | 0.732352  | 688.8594,                       | 788.2724,  | 806.1001,  |
|                                                                                              | C | 0.993123  | 1.355076  | -0.392468 | 856.4610,                       | 870.9905,  | 900.3585,  |
|                                                                                              | H | 0.064837  | -2.328143 | 0.809925  | 939.9187,                       | 991.9968,  | 1009.0951, |
|                                                                                              | H | 1.302034  | -1.368560 | -1.378010 | 1051.3122,                      | 1057.9744, | 1080.1964, |
|                                                                                              | H | 2.322510  | -1.855958 | -0.048139 | 1140.8987,                      | 1161.1225, | 1199.5810, |
|                                                                                              | H | 1.416098  | 2.363468  | -0.363593 | 1256.6059,                      | 1285.0860, | 1302.8058, |
|                                                                                              | H | 2.860565  | 0.449730  | -1.052015 | 1352.6523,                      | 1360.6914, | 1370.9433, |
|                                                                                              | H | -1.206348 | -0.381602 | 1.696577  | 1385.1942,                      | 1400.0441, | 1413.3976, |
|                                                                                              | H | 0.427621  | 1.417346  | 1.701314  | 1450.6972,                      | 1474.8196, | 1493.1620, |
|                                                                                              | H | -0.873216 | 1.883211  | 0.604332  | 1501.0052,                      | 2973.7913, | 3009.0925, |
|                                                                                              | H | 0.491439  | 1.247020  | -1.359352 | 3010.0024,                      | 3027.5766, | 3031.0053, |
|                                                                                              | H | 2.629898  | 0.452686  | 0.689615  | 3033.5369,                      | 3062.2472, | 3072.5781, |
|                                                                                              | O | -1.286072 | -0.630443 | -0.362711 | 3085.5141, 3190.0222, 3801.5451 |            |            |
|                                                                                              | O | -2.761755 | 0.310023  | -0.479207 |                                 |            |            |
|                                                                                              | H | -3.283851 | -0.440710 | -0.795732 |                                 |            |            |

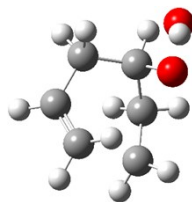
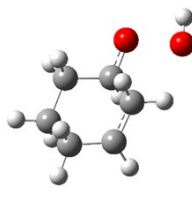
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|----------------------------------------------------------------------------------------------|---|-----------|-----------|-----------|-------------|------------|------------|
| TS7Te<br>   | C | 0.602432  | -0.221584 | 0.796542  | 640.4751i,  | 76.0534,   | 140.1407,  |
|                                                                                              | C | 0.036490  | 1.192343  | 0.732346  | 155.3931,   | 167.7767,  | 258.3769,  |
|                                                                                              | C | -0.993124 | 1.355071  | -0.392473 | 291.0122,   | 368.4445,  | 401.0487,  |
|                                                                                              | C | -2.111542 | 0.312397  | -0.266885 | 468.5316,   | 517.2993,  | 659.9795,  |
|                                                                                              | C | -1.559225 | -1.123292 | -0.336184 | 688.8601,   | 788.2718,  | 806.1040,  |
|                                                                                              | H | -1.416093 | 2.363466  | -0.363608 | 856.4608,   | 870.9915,  | 900.3582,  |
|                                                                                              | H | -0.427615 | 1.417352  | 1.701308  | 939.9183,   | 991.9961,  | 1009.0962, |
|                                                                                              | H | 0.873219  | 1.883212  | 0.604320  | 1051.3119,  | 1057.9768, | 1080.1974, |
|                                                                                              | H | 1.206348  | -0.381604 | 1.696573  | 1140.8988,  | 1161.1238, | 1199.5817, |
|                                                                                              | H | -2.629894 | 0.452696  | 0.689627  | 1256.6067,  | 1285.0850, | 1302.8051, |
|                                                                                              | H | -2.860575 | 0.449735  | -1.052002 | 1352.6525,  | 1360.6917, | 1370.9429, |
|                                                                                              | H | -2.322520 | -1.855953 | -0.048110 | 1385.1948,  | 1400.0447, | 1413.3976, |
|                                                                                              | H | -1.302068 | -1.368571 | -1.378003 | 1450.6942,  | 1474.8200, | 1493.1616, |
|                                                                                              | H | -0.491441 | 1.247002  | -1.359357 | 1501.0061,  | 2973.7723, | 3009.0851, |
|                                                                                              | C | -0.346884 | -1.327451 | 0.505049  | 3010.0045,  | 3027.5757, | 3030.9945, |
|                                                                                              | H | -0.064830 | -2.328141 | 0.809908  | 3033.5255,  | 3062.2456, | 3072.5878, |
|                                                                                              | O | 1.286075  | -0.630439 | -0.362716 | 3085.5107,  | 3190.0229, | 3801.5412  |
|                                                                                              | O | 2.761765  | 0.310017  | -0.479198 |             |            |            |
|                                                                                              | H | 3.283861  | -0.440720 | -0.795711 |             |            |            |
| TS7Ti<br> | C | -0.609267 | -0.079246 | 0.816370  | 636.4722i,  | 64.6377,   | 118.8165,  |
|                                                                                              | C | -0.028662 | 1.318719  | 0.561197  | 135.3079,   | 148.5230,  | 259.7318,  |
|                                                                                              | C | 1.417039  | 1.309384  | 0.026489  | 281.9979,   | 370.6918,  | 407.9658,  |
|                                                                                              | C | 1.682776  | 0.120671  | -0.904550 | 452.9478,   | 517.0088,  | 658.1442,  |
|                                                                                              | C | 1.531988  | -1.200199 | -0.134983 | 697.7634,   | 795.5724,  | 812.0587,  |
|                                                                                              | H | 1.622873  | 2.251827  | -0.488536 | 848.5475,   | 870.4064,  | 886.3699,  |
|                                                                                              | H | -0.701037 | 1.801741  | -0.152081 | 952.7453,   | 996.4267,  | 1010.0376, |
|                                                                                              | H | -0.079146 | 1.901826  | 1.485486  | 1048.9684,  | 1056.0198, | 1080.8431, |
|                                                                                              | H | -1.245078 | -0.104514 | 1.706921  | 1143.0305,  | 1167.3477, | 1197.7663, |
|                                                                                              | H | 0.976268  | 0.136630  | -1.739655 | 1256.5424,  | 1288.0645, | 1303.2540, |
|                                                                                              | H | 2.688979  | 0.181988  | -1.328614 | 1352.2569,  | 1359.3462, | 1362.9357, |
|                                                                                              | H | 1.547232  | -2.065406 | -0.809564 | 1384.6873,  | 1402.2799, | 1409.5285, |
|                                                                                              | H | 2.402716  | -1.341285 | 0.528897  | 1450.3656,  | 1482.3378, | 1491.4767, |
|                                                                                              | H | 2.121391  | 1.258320  | 0.866819  | 1500.8487,  | 2941.0710, | 3001.2912, |
|                                                                                              | C | 0.314969  | -1.236831 | 0.717865  | 3014.8471,  | 3028.5133, | 3037.6142, |
|                                                                                              | H | 0.032843  | -2.158712 | 1.212978  | 3046.4022,  | 3060.7570, | 3075.8931, |
|                                                                                              | O | -1.284065 | -0.640099 | -0.292780 | 3088.8774,  | 3186.1865, | 3801.4761  |
|                                                                                              | O | -2.711873 | 0.292934  | -0.579975 |             |            |            |
|                                                                                              | H | -3.252595 | -0.480089 | -0.794943 |             |            |            |
| TS8Ce<br> | C | -1.416854 | 1.269051  | 0.314922  | 1756.6902i, | 112.8434,  | 116.8055,  |
|                                                                                              | C | -0.039317 | 1.292301  | -0.367303 | 228.1276,   | 282.5858,  | 355.2538,  |
|                                                                                              | C | 0.713369  | -0.000003 | -0.148084 | 359.7599,   | 437.2042,  | 449.6643,  |
|                                                                                              | C | -0.039323 | -1.292306 | -0.367298 | 552.3714,   | 645.7478,  | 781.5509,  |
|                                                                                              | C | -1.416858 | -1.269047 | 0.314926  | 801.1031,   | 818.3050,  | 846.0341,  |
|                                                                                              | C | -2.204852 | 0.000003  | -0.039842 | 896.4697,   | 899.5395,  | 917.0069,  |
|                                                                                              | H | -0.162391 | 1.412679  | -1.454429 | 976.9034,   | 992.5103,  | 1029.6793, |
|                                                                                              | H | 0.569776  | 2.133946  | -0.028567 | 1079.1837,  | 1101.4875, | 1111.4909, |

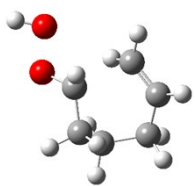
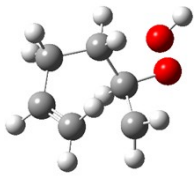
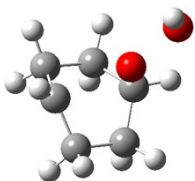
|                                                                                     |   |           |           |           |            |            |            |
|-------------------------------------------------------------------------------------|---|-----------|-----------|-----------|------------|------------|------------|
|                                                                                     | H | -1.281535 | 1.318626  | 1.402256  | 1150.9721, | 1157.9612, | 1243.2766, |
|                                                                                     | H | -1.980869 | 2.162137  | 0.030845  | 1266.8916, | 1284.3870, | 1298.5954, |
|                                                                                     | H | -0.162396 | -1.412685 | -1.454425 | 1342.0902, | 1366.4643, | 1368.7792, |
|                                                                                     | H | 0.569768  | -2.133951 | -0.028560 | 1377.5738, | 1387.5807, | 1464.3080, |
|                                                                                     | H | -1.980877 | -2.162132 | 0.030851  | 1473.7711, | 1488.6658, | 1492.0250, |
|                                                                                     | H | -1.281538 | -1.318619 | 1.402260  | 1504.1493, | 1933.5815, | 2977.5854, |
|                                                                                     | H | -2.431499 | 0.000002  | -1.113881 | 2983.0981, | 3003.7441, | 3014.8103, |
|                                                                                     | H | -3.167125 | 0.000004  | 0.481027  | 3018.0628, | 3059.6397, | 3062.0683, |
|                                                                                     | H | 1.260873  | 0.000002  | 1.061334  | 3065.5659, | 3077.1327, | 3078.3399  |
|                                                                                     | O | 2.525944  | 0.000005  | 0.795966  |            |            |            |
|                                                                                     | O | 2.032909  | -0.000006 | -0.617545 |            |            |            |
| TS9Ca                                                                               | C | 1.751947  | 0.294878  | -0.734740 | 690.3855i, | 103.1157,  | 161.5266,  |
|    | C | 1.052470  | -1.020903 | -0.628295 | 184.7796,  | 222.9412,  | 288.9383,  |
|                                                                                     | C | 0.582022  | -1.415226 | 0.742382  | 328.3265,  | 387.3811,  | 410.9970,  |
|                                                                                     | C | -0.528829 | -0.366652 | 0.835928  | 513.8310,  | 552.8240,  | 650.0580,  |
|                                                                                     | C | 0.054315  | 1.033372  | 1.059952  | 729.8047,  | 815.4032,  | 849.3532,  |
|                                                                                     | C | 0.894928  | 1.454061  | -0.160121 | 855.8001,  | 877.1779,  | 917.2301,  |
|                                                                                     | H | 0.175865  | -2.426706 | 0.764336  | 942.1289,  | 1007.6147, | 1014.3014, |
|                                                                                     | H | 1.127951  | -1.748038 | -1.427599 | 1039.0621, | 1054.3213, | 1096.7456, |
|                                                                                     | H | 2.692052  | 0.218314  | -0.161891 | 1107.1486, | 1133.0606, | 1186.1413, |
|                                                                                     | H | 2.033770  | 0.511595  | -1.767844 | 1209.9176, | 1256.8872, | 1288.6503, |
|                                                                                     | H | -1.350026 | -0.597318 | 1.516280  | 1303.0918, | 1336.6058, | 1341.3382, |
|                                                                                     | H | -0.756601 | 1.750548  | 1.205634  | 1358.9986, | 1383.9162, | 1393.5510, |
|                                                                                     | H | 0.651446  | 1.024772  | 1.979973  | 1471.0356, | 1479.3204, | 1485.7833, |
|                                                                                     | H | 0.208377  | 1.776628  | -0.944344 | 1496.2521, | 2940.6319, | 2990.5589, |
|                                                                                     | H | 1.534089  | 2.306450  | 0.085460  | 3017.6724, | 3048.4250, | 3069.5894, |
|                                                                                     | H | 1.351118  | -1.314715 | 1.520201  | 3076.8600, | 3084.3973, | 3098.7601, |
|                                                                                     | O | -0.973854 | -0.496011 | -0.537978 | 3103.5107, | 3186.5622, | 3812.8913  |
|                                                                                     | O | -2.485000 | 0.337947  | -0.486563 |            |            |            |
|                                                                                     | H | -2.838327 | -0.114206 | -1.264511 |            |            |            |
| TS9Ta                                                                               | C | -1.499854 | 1.147669  | -0.131526 | 704.0830i, | 105.2294,  | 149.1428,  |
|  | C | -1.534669 | -0.110380 | -1.024551 | 192.1673,  | 209.2041,  | 291.7091,  |
|                                                                                     | C | -0.858676 | -1.266998 | -0.361073 | 339.3739,  | 380.7552,  | 411.1262,  |
|                                                                                     | C | -0.472024 | -1.127064 | 1.086523  | 531.9332,  | 537.0437,  | 666.8221,  |
|                                                                                     | C | 0.541345  | 0.000062  | 0.867695  | 717.6870,  | 813.8793,  | 844.8805,  |
|                                                                                     | C | -0.140324 | 1.341022  | 0.580262  | 854.3633,  | 873.1678,  | 910.6055,  |
|                                                                                     | H | -0.830321 | -2.227911 | -0.861087 | 944.9679,  | 1002.3434, | 1010.5341, |
|                                                                                     | H | -2.578152 | -0.370086 | -1.260860 | 1049.8519, | 1065.0198, | 1098.0339, |
|                                                                                     | H | -1.049687 | 0.073933  | -1.990776 | 1101.9884, | 1121.8263, | 1176.8987, |
|                                                                                     | H | 0.550962  | 1.925577  | -0.030756 | 1206.8108, | 1256.4723, | 1282.8808, |
|                                                                                     | H | -2.286668 | 1.052550  | 0.624181  | 1306.6569, | 1340.1866, | 1357.2272, |
|                                                                                     | H | -1.301319 | -0.860054 | 1.755201  | 1365.8086, | 1384.3594, | 1389.0077, |
|                                                                                     | H | 0.012922  | -2.026755 | 1.464617  | 1457.0178, | 1481.2721, | 1483.1038, |
|                                                                                     | H | 1.333580  | 0.084625  | 1.613403  | 1509.6027, | 2968.2608, | 2991.5069, |
|                                                                                     | H | -0.288323 | 1.890461  | 1.516247  | 3016.9570, | 3027.6095, | 3036.7363, |
|                                                                                     | H | -1.754626 | 2.031961  | -0.720556 | 3069.3791, | 3078.9268, | 3091.3668, |

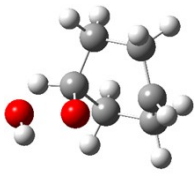
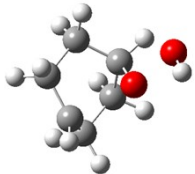
|                                                                                                                  |   |           |           |           |                                 |            |            |
|------------------------------------------------------------------------------------------------------------------|---|-----------|-----------|-----------|---------------------------------|------------|------------|
|                                                                                                                  | O | 1.093211  | -0.530532 | -0.366744 | 3107.6506, 3183.0935, 3812.3655 |            |            |
|                                                                                                                  | O | 2.533076  | 0.379228  | -0.523241 |                                 |            |            |
|                                                                                                                  | H | 2.966547  | -0.269729 | -1.093720 |                                 |            |            |
| <hr/>                                                                                                            |   |           |           |           |                                 |            |            |
| <div>TS9Ti</div> <div></div>    | C | -0.858917 | -1.266461 | -0.361831 | 704.3814i,                      | 105.2293,  | 149.6252,  |
|                                                                                                                  | C | -1.534447 | -0.109281 | -1.024716 | 192.3089,                       | 209.0904,  | 291.6789,  |
|                                                                                                                  | C | -1.498814 | 1.148593  | -0.131313 | 339.4454,                       | 380.6599,  | 411.0582,  |
|                                                                                                                  | C | -0.139474 | 1.340509  | 0.581464  | 531.9391,                       | 537.1719,  | 667.1885,  |
|                                                                                                                  | C | 0.541310  | -0.001039 | 0.867929  | 717.7646,                       | 813.8123,  | 844.8648,  |
|                                                                                                                  | H | -1.752247 | 2.033261  | -0.720348 | 854.3305,                       | 873.1240,  | 910.5227,  |
|                                                                                                                  | H | -1.049574 | 0.075146  | -1.990964 | 944.8796,                       | 1002.3129, | 1010.4886, |
|                                                                                                                  | H | -2.578103 | -0.368383 | -1.260869 | 1049.7125,                      | 1064.8237, | 1097.9835, |
|                                                                                                                  | H | -0.831229 | -2.227244 | -0.862142 | 1102.0633,                      | 1121.8190, | 1176.9388, |
|                                                                                                                  | H | 0.552508  | 1.925375  | -0.028448 | 1206.7506,                      | 1256.4176, | 1282.8275, |
|                                                                                                                  | H | -0.287749 | 1.888919  | 1.518006  | 1306.6296,                      | 1340.1667, | 1357.2485, |
|                                                                                                                  | H | 1.333652  | 0.082262  | 1.613642  | 1365.7857,                      | 1384.3186, | 1389.0308, |
|                                                                                                                  | H | -2.286193 | 1.054127  | 0.623874  | 1457.0024,                      | 1481.2793, | 1483.0952, |
|                                                                                                                  | C | -0.472905 | -1.127704 | 1.085970  | 1509.6715,                      | 2968.3899, | 2991.5263, |
|                                                                                                                  | H | -1.302319 | -0.860562 | 1.754449  | 3017.0624,                      | 3027.6662, | 3036.8109, |
|                                                                                                                  | H | 0.011279  | -2.027934 | 1.463764  | 3069.4278,                      | 3079.0717, | 3091.4948, |
|                                                                                                                  | O | 1.092954  | -0.531132 | -0.366973 | 3107.6278, 3183.0335, 3812.4146 |            |            |
|                                                                                                                  | O | 2.532401  | 0.379514  | -0.523403 |                                 |            |            |
|                                                                                                                  | H | 2.966619  | -0.269739 | -1.092969 |                                 |            |            |
| <hr/>                                                                                                            |   |           |           |           |                                 |            |            |
| <div>TS10Ca</div> <div></div> | C | -2.213629 | 0.217102  | -0.266653 | 466.2518i,                      | 51.8162,   | 85.7083,   |
|                                                                                                                  | C | -1.255655 | 1.417851  | -0.197391 | 141.7039,                       | 214.3522,  | 259.0222,  |
|                                                                                                                  | C | -0.038062 | 1.141427  | 0.632130  | 326.8186,                       | 364.5865,  | 408.6677,  |
|                                                                                                                  | C | 0.448369  | -0.140224 | 0.855349  | 456.9822,                       | 502.9135,  | 667.9766,  |
|                                                                                                                  | C | -0.418958 | -1.346016 | 0.586805  | 727.9826,                       | 809.2297,  | 820.6835,  |
|                                                                                                                  | C | -1.448822 | -1.087545 | -0.521488 | 877.1035,                       | 891.1253,  | 911.0602,  |
|                                                                                                                  | H | -0.935253 | 1.690272  | -1.215792 | 936.3297,                       | 1017.1884, | 1035.8282, |
|                                                                                                                  | H | -1.772432 | 2.303705  | 0.189184  | 1046.9669,                      | 1065.5225, | 1083.4673, |
|                                                                                                                  | H | -2.759060 | 0.136502  | 0.681547  | 1149.5744,                      | 1158.6007, | 1226.0930, |
|                                                                                                                  | H | -2.962882 | 0.383470  | -1.046392 | 1262.2144,                      | 1295.6123, | 1353.6810, |
|                                                                                                                  | H | 1.229114  | -0.262429 | 1.598028  | 1360.1597,                      | 1362.9386, | 1374.0323, |
|                                                                                                                  | H | 0.220422  | -2.196175 | 0.337616  | 1385.3163,                      | 1419.2938, | 1458.2707, |
|                                                                                                                  | H | -0.935114 | -1.604264 | 1.521743  | 1469.5885,                      | 1492.7629, | 1500.1841, |
|                                                                                                                  | H | -0.931994 | -1.027434 | -1.485423 | 1507.0062,                      | 2959.2659, | 2998.7983, |
|                                                                                                                  | H | -2.143270 | -1.930568 | -0.586039 | 3009.9479,                      | 3025.8961, | 3031.9364, |
|                                                                                                                  | H | 0.550669  | 1.988813  | 0.971595  | 3058.1808,                      | 3065.8983, | 3076.1525, |
|                                                                                                                  | O | 1.685695  | -0.362934 | -0.600417 | 3145.8911, 3167.6348, 3733.8621 |            |            |
|                                                                                                                  | O | 2.937583  | 0.157027  | -0.238247 |                                 |            |            |
|                                                                                                                  | H | 3.014123  | 0.949802  | -0.789271 |                                 |            |            |

|                                                                                               |   |           |           |           |            |            |            |
|-----------------------------------------------------------------------------------------------|---|-----------|-----------|-----------|------------|------------|------------|
| TS10Ce<br>   | C | -1.150126 | 1.490727  | 0.076176  | 467.3989i, | 54.8460,   | 86.0509,   |
|                                                                                               | C | 0.025343  | 0.970659  | 0.844700  | 142.1367,  | 198.9606,  | 282.8545,  |
|                                                                                               | C | 0.437675  | -0.358487 | 0.800412  | 334.5107,  | 358.0545,  | 401.9092,  |
|                                                                                               | C | -0.498845 | -1.440069 | 0.297713  | 462.1655,  | 497.4811,  | 674.3785,  |
|                                                                                               | C | -1.894451 | -0.910067 | -0.069397 | 722.5142,  | 805.0851,  | 819.4540,  |
|                                                                                               | C | -1.790783 | 0.421803  | -0.820703 | 881.3354,  | 884.7385,  | 907.2188,  |
|                                                                                               | H | 0.629491  | 1.686495  | 1.394713  | 936.1112,  | 1008.4909, | 1051.2569, |
|                                                                                               | H | -1.894940 | 1.875429  | 0.790763  | 1060.4523, | 1066.4520, | 1082.0286, |
|                                                                                               | H | -0.849251 | 2.365179  | -0.515862 | 1152.6107, | 1164.7570, | 1220.5538, |
|                                                                                               | H | -0.033642 | -1.913320 | -0.574058 | 1261.3516, | 1293.6521, | 1351.4309, |
|                                                                                               | H | -0.575889 | -2.221696 | 1.060265  | 1357.9500, | 1366.9890, | 1367.1938, |
|                                                                                               | H | -2.424139 | -1.653941 | -0.671262 | 1383.1430, | 1417.6924, | 1453.8987, |
|                                                                                               | H | -2.487989 | -0.762822 | 0.841346  | 1474.6675, | 1494.5514, | 1502.4839, |
|                                                                                               | H | -1.176480 | 0.282878  | -1.716982 | 1504.1660, | 2962.9606, | 3002.9941, |
|                                                                                               | H | -2.776088 | 0.757762  | -1.156353 | 3009.2395, | 3025.0355, | 3028.5194, |
|                                                                                               | H | 1.192117  | -0.667155 | 1.514842  | 3054.1938, | 3064.2740, | 3068.2172, |
|                                                                                               | O | 1.672401  | -0.375758 | -0.640042 | 3147.1146, | 3170.5261, | 3736.6932  |
|                                                                                               | O | 2.912713  | 0.150361  | -0.241109 |            |            |            |
|                                                                                               | H | 2.943027  | 1.006976  | -0.691612 |            |            |            |
| TS10Ta<br> | C | -1.894451 | -0.910067 | -0.069397 | 467.3989i, | 54.8460,   | 86.0508,   |
|                                                                                               | C | -0.498845 | -1.440069 | 0.297713  | 142.1367,  | 198.9606,  | 282.8545,  |
|                                                                                               | C | 0.437675  | -0.358487 | 0.800412  | 334.5107,  | 358.0544,  | 401.9091,  |
|                                                                                               | C | 0.025343  | 0.970659  | 0.844700  | 462.1655,  | 497.4811,  | 674.3785,  |
|                                                                                               | C | -1.150126 | 1.490727  | 0.076176  | 722.5142,  | 805.0851,  | 819.4540,  |
|                                                                                               | C | -1.790783 | 0.421803  | -0.820703 | 881.3354,  | 884.7385,  | 907.2188,  |
|                                                                                               | H | 1.192117  | -0.667155 | 1.514842  | 936.1112,  | 1008.4909, | 1051.2569, |
|                                                                                               | H | -0.575889 | -2.221696 | 1.060265  | 1060.4523, | 1066.4521, | 1082.0286, |
|                                                                                               | H | -0.033642 | -1.913320 | -0.574058 | 1152.6107, | 1164.7570, | 1220.5538, |
|                                                                                               | H | -1.176479 | 0.282878  | -1.716982 | 1261.3516, | 1293.6521, | 1351.4309, |
|                                                                                               | H | -2.487989 | -0.762822 | 0.841345  | 1357.9500, | 1366.9890, | 1367.1938, |
|                                                                                               | H | 0.629491  | 1.686495  | 1.394713  | 1383.1430, | 1417.6923, | 1453.8987, |
|                                                                                               | H | -0.849251 | 2.365179  | -0.515862 | 1474.6674, | 1494.5514, | 1502.4839, |
|                                                                                               | H | -1.894940 | 1.875429  | 0.790763  | 1504.1659, | 2962.9606, | 3002.9941, |
|                                                                                               | H | -2.776088 | 0.757762  | -1.156353 | 3009.2395, | 3025.0355, | 3028.5194, |
|                                                                                               | H | -2.424139 | -1.653941 | -0.671262 | 3054.1938, | 3064.2740, | 3068.2172, |
|                                                                                               | O | 1.672401  | -0.375758 | -0.640042 | 3147.1146, | 3170.5261, | 3736.6932  |
|                                                                                               | O | 2.912713  | 0.150361  | -0.241109 |            |            |            |
|                                                                                               | H | 2.943026  | 1.006976  | -0.691612 |            |            |            |
| TS10Te<br> | C | -0.431630 | -0.186271 | 0.896575  | 465.7039i, | 52.8185,   | 97.5013,   |
|                                                                                               | C | 0.459346  | -1.363364 | 0.578103  | 131.9006,  | 204.5670,  | 260.5385,  |
|                                                                                               | C | 1.451361  | -1.053953 | -0.552239 | 333.3817,  | 369.5564,  | 408.8808,  |
|                                                                                               | C | 2.181318  | 0.270361  | -0.297470 | 457.5375,  | 501.6296,  | 661.7256,  |
|                                                                                               | C | 1.186648  | 1.436968  | -0.181881 | 730.9561,  | 810.2829,  | 820.6739,  |
|                                                                                               | H | 2.169508  | -1.873937 | -0.648123 | 876.4934,  | 890.7966,  | 910.9983,  |
|                                                                                               | H | 1.005725  | -1.632589 | 1.492349  | 931.4260,  | 1012.7620, | 1023.8395, |
|                                                                                               | H | -0.162764 | -2.225769 | 0.323519  | 1045.9773, | 1065.0910, | 1083.1637, |

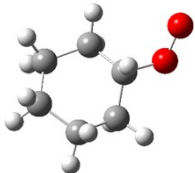
|                                                                                     |   |           |           |           |            |            |            |
|-------------------------------------------------------------------------------------|---|-----------|-----------|-----------|------------|------------|------------|
|                                                                                     | H | -1.173376 | -0.342031 | 1.674045  | 1150.0908, | 1156.0178, | 1225.1135, |
|                                                                                     | H | 2.757716  | 0.194014  | 0.632742  | 1262.0243, | 1295.5406, | 1354.0044, |
|                                                                                     | H | 2.900636  | 0.472561  | -1.096550 | 1364.5768, | 1367.8932, | 1374.7721, |
|                                                                                     | H | 1.684895  | 2.338020  | 0.193369  | 1385.4529, | 1419.3542, | 1456.7362, |
|                                                                                     | H | 0.814200  | 1.705378  | -1.183364 | 1469.9632, | 1492.4252, | 1500.2051, |
|                                                                                     | H | 0.905602  | -0.993678 | -1.499313 | 1508.5080, | 2963.6047, | 2999.5441, |
|                                                                                     | C | 0.009258  | 1.112479  | 0.683688  | 3009.5042, | 3028.8338, | 3033.8404, |
|                                                                                     | H | -0.603658 | 1.934914  | 1.038622  | 3058.6546, | 3063.7148, | 3071.2798, |
|                                                                                     | O | -1.689192 | -0.460942 | -0.543059 | 3140.7461, | 3164.5217, | 3712.7276  |
|                                                                                     | O | -2.813287 | 0.369433  | -0.433803 |            |            |            |
|                                                                                     | H | -3.416470 | -0.142133 | 0.126943  |            |            |            |
| TS10Ti                                                                              | C | 0.437671  | -0.358494 | 0.800425  | 467.4015i, | 54.8461,   | 86.0524,   |
|    | C | -0.498852 | -1.440072 | 0.297723  | 142.1366,  | 198.9612,  | 282.8536,  |
|                                                                                     | C | -1.894447 | -0.910060 | -0.069418 | 334.5138,  | 358.0546,  | 401.9089,  |
|                                                                                     | C | -1.790759 | 0.421814  | -0.820713 | 462.1653,  | 497.4821,  | 674.3778,  |
|                                                                                     | C | -1.150115 | 1.490730  | 0.076184  | 722.5137,  | 805.0842,  | 819.4539,  |
|                                                                                     | H | -2.424123 | -1.653928 | -0.671301 | 881.3352,  | 884.7380,  | 907.2189,  |
|                                                                                     | H | -0.033637 | -1.913334 | -0.574034 | 936.1111,  | 1008.4906, | 1051.2571, |
|                                                                                     | H | -0.575918 | -2.221690 | 1.060283  | 1060.4507, | 1066.4527, | 1082.0284, |
|                                                                                     | H | 1.192110  | -0.667167 | 1.514857  | 1152.6113, | 1164.7568, | 1220.5538, |
|                                                                                     | H | -1.176439 | 0.282895  | -1.716982 | 1261.3519, | 1293.6527, | 1351.4312, |
|                                                                                     | H | -2.776057 | 0.757778  | -1.156378 | 1357.9509, | 1366.9894, | 1367.1943, |
|                                                                                     | H | -0.849236 | 2.365189  | -0.515841 | 1383.1434, | 1417.6923, | 1453.8984, |
|                                                                                     | H | -1.894936 | 1.875423  | 0.790769  | 1474.6667, | 1494.5514, | 1502.4844, |
|                                                                                     | H | -2.488008 | -0.762818 | 0.841310  | 1504.1652, | 2962.9590, | 3002.9943, |
|                                                                                     | C | 0.025348  | 0.970655  | 0.844713  | 3009.2399, | 3025.0382, | 3028.5181, |
|                                                                                     | H | 0.629498  | 1.686487  | 1.394731  | 3054.1961, | 3064.2743, | 3068.2167, |
|                                                                                     | O | 1.672391  | -0.375782 | -0.640032 | 3147.1152, | 3170.5260, | 3736.6932  |
|                                                                                     | O | 2.912695  | 0.150375  | -0.241126 |            |            |            |
|                                                                                     | H | 2.942981  | 1.006982  | -0.691646 |            |            |            |
| TS11Ce                                                                              | C | -1.317576 | -1.410195 | -0.244618 | 439.9491i, | 102.1431,  | 127.4632,  |
|  | C | 0.054553  | -1.151179 | 0.303956  | 175.3639,  | 190.7090,  | 233.2875,  |
|                                                                                     | C | 0.561906  | 0.214880  | -0.209489 | 296.4950,  | 353.4123,  | 399.4504,  |
|                                                                                     | C | -0.313878 | 1.397829  | 0.237452  | 442.5414,  | 458.0638,  | 514.0452,  |
|                                                                                     | C | -1.695278 | 1.400483  | -0.353156 | 539.6662,  | 675.3107,  | 745.9717,  |
|                                                                                     | C | -2.394607 | -0.736339 | 0.239601  | 828.3312,  | 860.6194,  | 913.0234,  |
|                                                                                     | H | 0.039472  | -1.113014 | 1.399522  | 922.5074,  | 932.9965,  | 958.4816,  |
|                                                                                     | H | 0.763494  | -1.924262 | 0.000460  | 965.4558,  | 1011.4141, | 1020.5979, |
|                                                                                     | H | -1.393752 | -1.924026 | -1.199008 | 1062.2542, | 1096.8996, | 1164.8301, |
|                                                                                     | H | -0.367790 | 1.403823  | 1.332549  | 1209.8868, | 1260.5038, | 1277.2696, |
|                                                                                     | H | 0.221780  | 2.317140  | -0.043281 | 1290.8862, | 1311.7839, | 1359.2171, |
|                                                                                     | H | -2.446231 | 2.013206  | 0.135788  | 1375.5947, | 1387.9915, | 1432.1562, |
|                                                                                     | H | -1.788582 | 1.334376  | -1.432350 | 1460.5177, | 1476.3436, | 1496.3964, |
|                                                                                     | H | -2.393813 | -0.343745 | 1.250942  | 1577.6738, | 2970.2717, | 3012.4481, |
|                                                                                     | H | -3.368150 | -0.823407 | -0.229913 | 3021.3931, | 3035.9770, | 3088.4540, |
|                                                                                     | H | 0.629085  | 0.199686  | -1.304210 | 3112.3173, | 3125.3956, | 3144.3493, |

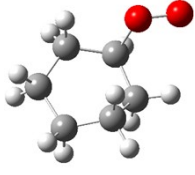
|                                                                                                       |   |           |           |           |                                 |            |            |
|-------------------------------------------------------------------------------------------------------|---|-----------|-----------|-----------|---------------------------------|------------|------------|
|                                                                                                       | O | 1.862771  | 0.528857  | 0.306442  | 3204.2034, 3209.6500, 3785.2830 |            |            |
|                                                                                                       | O | 2.819065  | -0.368922 | -0.331421 |                                 |            |            |
|                                                                                                       | H | 3.279080  | -0.712133 | 0.446857  |                                 |            |            |
| <hr/>                                                                                                 |   |           |           |           |                                 |            |            |
| <div>TS11Te</div>    | C | 0.586542  | 0.262079  | 0.722127  | 439.3999i,                      | 79.5695,   | 120.5851,  |
|                                                                                                       | C | -0.513221 | 1.343881  | 0.774171  | 130.4537,                       | 166.9192,  | 256.3627,  |
|                                                                                                       | C | -1.422857 | 1.408750  | -0.423972 | 289.9084,                       | 326.0235,  | 357.0717,  |
|                                                                                                       | C | -1.579769 | -0.824876 | -1.014695 | 425.7948,                       | 502.6192,  | 522.7976,  |
|                                                                                                       | C | -1.287400 | -1.382529 | 0.191312  | 613.0678,                       | 717.5353,  | 762.6300,  |
|                                                                                                       | H | -2.464281 | 1.657168  | -0.253666 | 792.7068,                       | 850.3969,  | 875.3194,  |
|                                                                                                       | H | -1.095319 | 1.154159  | 1.681720  | 916.0450,                       | 939.6116,  | 942.2649,  |
|                                                                                                       | H | -0.015006 | 2.312127  | 0.918260  | 958.3911,                       | 968.5048,  | 1016.7196, |
|                                                                                                       | H | 1.307758  | 0.447749  | 1.525327  | 1068.7362,                      | 1112.1907, | 1147.7749, |
|                                                                                                       | H | -2.577666 | -0.903690 | -1.431480 | 1191.0442,                      | 1261.9385, | 1294.3703, |
|                                                                                                       | H | -0.794730 | -0.562006 | -1.712276 | 1304.3180,                      | 1335.4679, | 1361.5724, |
|                                                                                                       | H | -2.091686 | -1.796846 | 0.792322  | 1382.3394,                      | 1390.2290, | 1436.7740, |
|                                                                                                       | H | -1.003913 | 1.780595  | -1.352389 | 1457.5601,                      | 1468.1447, | 1475.8743, |
|                                                                                                       | C | 0.048699  | -1.181687 | 0.854311  | 1576.4212,                      | 2991.1402, | 3012.2455, |
|                                                                                                       | H | 0.818801  | -1.857071 | 0.461671  | 3031.0991,                      | 3053.2406, | 3057.0329, |
|                                                                                                       | H | -0.030890 | -1.413107 | 1.921247  | 3123.0544,                      | 3136.4400, | 3146.6048, |
|                                                                                                       | O | 1.269180  | 0.493417  | -0.519236 | 3215.0671, 3223.1194, 3789.1065 |            |            |
|                                                                                                       | O | 2.530781  | -0.238812 | -0.458188 |                                 |            |            |
|                                                                                                       | H | 2.555289  | -0.609623 | -1.350868 |                                 |            |            |
| <hr/>                                                                                                 |   |           |           |           |                                 |            |            |
| <div>TS12Ce</div>  | C | -1.099498 | -1.442271 | -0.185341 | 861.4708i,                      | 76.3378,   | 149.1093,  |
|                                                                                                       | C | 0.187228  | -1.098666 | 0.329795  | 171.2880,                       | 197.6631,  | 245.7897,  |
|                                                                                                       | C | 0.577577  | 0.441402  | -0.292294 | 312.1592,                       | 341.6901,  | 382.9042,  |
|                                                                                                       | C | -0.577003 | 1.359353  | 0.176217  | 440.9647,                       | 472.6393,  | 518.2582,  |
|                                                                                                       | C | -1.949609 | 0.855785  | -0.279463 | 543.8440,                       | 720.7315,  | 807.1065,  |
|                                                                                                       | C | -2.255085 | -0.594897 | 0.208684  | 847.7623,                       | 877.2473,  | 882.3247,  |
|                                                                                                       | H | 0.211496  | -0.897175 | 1.402812  | 920.9340,                       | 946.4006,  | 969.8289,  |
|                                                                                                       | H | 1.017153  | -1.729735 | 0.027498  | 1028.1223,                      | 1053.2763, | 1089.3100, |
|                                                                                                       | H | -1.176847 | -2.057829 | -1.077503 | 1122.0577,                      | 1165.0352, | 1185.5181, |
|                                                                                                       | H | -0.530879 | 1.446145  | 1.266174  | 1204.7471,                      | 1242.5063, | 1273.6158, |
|                                                                                                       | H | -0.394538 | 2.355669  | -0.235743 | 1299.2862,                      | 1316.5944, | 1334.4053, |
|                                                                                                       | H | -2.724365 | 1.525405  | 0.104322  | 1357.9219,                      | 1366.6444, | 1422.8926, |
|                                                                                                       | H | -2.014720 | 0.888483  | -1.372106 | 1480.0424,                      | 1482.8252, | 1493.6121, |
|                                                                                                       | H | -2.362549 | -0.574275 | 1.300348  | 1512.7893,                      | 2946.6915, | 3008.7254, |
|                                                                                                       | H | -3.196955 | -0.945909 | -0.217344 | 3028.9356,                      | 3037.9820, | 3062.3274, |
|                                                                                                       | H | 0.580733  | 0.331432  | -1.388902 | 3070.5317,                      | 3082.6690, | 3087.2424, |
|                                                                                                       | O | 1.740032  | 0.832016  | 0.205015  | 3150.1230, 3177.3676, 3807.8408 |            |            |
|                                                                                                       | O | 2.960965  | -0.529091 | -0.142440 |                                 |            |            |
|                                                                                                       | H | 3.681835  | 0.110156  | -0.055755 |                                 |            |            |

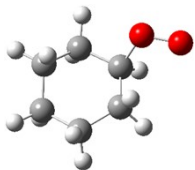
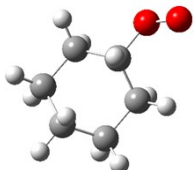
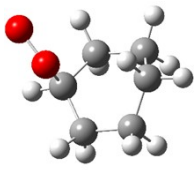
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|-----------------------------------------------------------------------------------------------|---|-----------|-----------|-----------|------------|------------|------------|
| TS12Te<br>   | C | -0.791383 | -0.323356 | 0.685942  | 496.2175i, | 60.9878,   | 88.7190,   |
|                                                                                               | C | 0.335354  | -1.321006 | 0.590501  | 165.7376,  | 189.0352,  | 222.8914,  |
|                                                                                               | C | 1.312035  | -1.081211 | -0.582684 | 285.7660,  | 290.6123,  | 378.8069,  |
|                                                                                               | C | 2.264646  | 0.108095  | -0.324590 | 400.1011,  | 519.2139,  | 537.1338,  |
|                                                                                               | C | 1.542416  | 1.287392  | 0.276009  | 647.7493,  | 689.0278,  | 795.3523,  |
|                                                                                               | H | 1.904490  | -1.985375 | -0.751616 | 814.6312,  | 834.2092,  | 885.4527,  |
|                                                                                               | H | 0.883702  | -1.283553 | 1.537920  | 928.2755,  | 946.7231,  | 962.4210,  |
|                                                                                               | H | -0.082286 | -2.334098 | 0.516069  | 974.1822,  | 1014.3412, | 1071.7179, |
|                                                                                               | H | -1.165493 | -0.022065 | 1.664266  | 1096.7301, | 1135.0496, | 1187.1057, |
|                                                                                               | H | 3.059894  | -0.210527 | 0.358807  | 1220.4402, | 1268.3159, | 1282.4954, |
|                                                                                               | H | 2.770675  | 0.378585  | -1.262719 | 1333.8871, | 1343.8183, | 1364.3004, |
|                                                                                               | H | 2.009554  | 1.800680  | 1.111311  | 1368.0127, | 1374.1038, | 1427.3106, |
|                                                                                               | H | 0.733167  | -0.920691 | -1.496776 | 1468.6132, | 1479.3587, | 1501.2730, |
|                                                                                               | C | 0.237633  | 1.548203  | -0.029250 | 1567.5926, | 2975.3775, | 2993.1572, |
|                                                                                               | H | -0.190315 | 1.237858  | -0.976121 | 3026.5900, | 3036.6806, | 3050.0025, |
|                                                                                               | H | -0.294012 | 2.352412  | 0.466872  | 3073.2817, | 3093.7149, | 3127.0418, |
|                                                                                               | O | -1.769640 | -0.617213 | -0.221524 | 3145.8513, | 3209.5527, | 3780.9363  |
|                                                                                               | O | -2.672128 | 0.564329  | -0.321769 |            |            |            |
|                                                                                               | H | -3.499435 | 0.101147  | -0.517238 |            |            |            |
| TS13Te<br> | C | -0.584063 | 0.295710  | -0.231281 | 438.5844i, | 54.7265,   | 137.5570,  |
|                                                                                               | C | 0.164916  | 1.579876  | -0.029134 | 145.6776,  | 172.4035,  | 257.0656,  |
|                                                                                               | C | 2.316687  | 0.789606  | 0.223257  | 275.0557,  | 336.4388,  | 376.9199,  |
|                                                                                               | C | 2.212986  | -0.387227 | -0.453521 | 445.1704,  | 486.7564,  | 541.9190,  |
|                                                                                               | C | 1.250808  | -1.464855 | -0.023442 | 553.6906,  | 662.0555,  | 772.6666,  |
|                                                                                               | H | 2.947609  | 1.588610  | -0.149717 | 815.7980,  | 839.8435,  | 847.7899,  |
|                                                                                               | H | 0.242625  | 2.262474  | -0.867049 | 907.5931,  | 937.3959,  | 946.1480,  |
|                                                                                               | H | 0.070242  | 2.043716  | 0.948006  | 951.3506,  | 977.5221,  | 1005.4582, |
|                                                                                               | H | -0.587326 | 0.024337  | -1.294142 | 1070.9976, | 1109.4822, | 1149.6805, |
|                                                                                               | H | 2.677221  | -0.479603 | -1.431030 | 1211.4662, | 1232.4459, | 1285.6710, |
|                                                                                               | H | 0.989576  | -2.076550 | -0.893214 | 1306.3472, | 1331.7304, | 1362.6397, |
|                                                                                               | H | 1.716998  | -2.152935 | 0.694502  | 1372.1995, | 1386.3018, | 1427.9528, |
|                                                                                               | H | 2.059377  | 0.853220  | 1.273446  | 1458.9569, | 1478.0524, | 1501.5407, |
|                                                                                               | C | -0.041513 | -0.882243 | 0.594566  | 1574.1615, | 2994.8078, | 3013.2889, |
|                                                                                               | H | 0.131167  | -0.545849 | 1.622412  | 3032.0811, | 3045.7976, | 3092.0387, |
|                                                                                               | H | -0.803124 | -1.663483 | 0.634428  | 3118.7560, | 3134.5176, | 3147.9795, |
|                                                                                               | O | -1.943288 | 0.625912  | 0.130953  | 3213.4074, | 3221.4947, | 3793.0345  |
|                                                                                               | O | -2.804938 | -0.484947 | -0.315833 |            |            |            |
|                                                                                               | H | -3.377488 | -0.566860 | 0.458729  |            |            |            |
| TS14Ca<br> | C | -0.466941 | -0.224156 | 0.777024  | 629.2784i, | 48.1608,   | 88.7181,   |
|                                                                                               | C | 0.138688  | 1.161450  | 1.017086  | 110.5052,  | 193.4125,  | 278.7034,  |
|                                                                                               | C | 1.044318  | 1.466186  | -0.219359 | 305.6402,  | 375.2592,  | 390.7528,  |
|                                                                                               | C | 1.126495  | 0.239802  | -1.068601 | 542.9241,  | 545.5346,  | 656.9089,  |
|                                                                                               | C | 1.562989  | -1.030394 | -0.417302 | 780.2289,  | 804.6112,  | 821.4062,  |
|                                                                                               | C | 0.611393  | -1.311669 | 0.789007  | 852.9526,  | 881.3647,  | 896.6204,  |
|                                                                                               | H | 0.646817  | 2.301706  | -0.797153 | 925.0477,  | 964.9099,  | 1025.1343, |
|                                                                                               | H | -0.657908 | 1.903530  | 1.093301  | 1042.7681, | 1092.7816, | 1099.5336, |

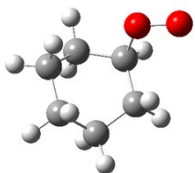
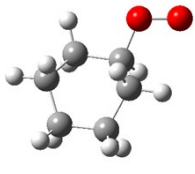
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|-----------------------------------------------------------------------------------------------|---|-----------|-----------|-----------|------------|------------|------------|
|                                                                                               | H | 0.701461  | 1.179974  | 1.955289  | 1107.2449, | 1153.8922, | 1198.5908, |
|                                                                                               | H | -1.272211 | -0.454466 | 1.474242  | 1207.7838, | 1245.2626, | 1267.2771, |
|                                                                                               | H | 1.114299  | 0.323491  | -2.148495 | 1314.5398, | 1324.6190, | 1331.8609, |
|                                                                                               | H | 1.546507  | -1.855788 | -1.130406 | 1333.4154, | 1364.5319, | 1387.0896, |
|                                                                                               | H | 2.602314  | -0.936884 | -0.065426 | 1466.3325, | 1475.2796, | 1487.4473, |
|                                                                                               | H | 0.143983  | -2.292085 | 0.680046  | 1501.9273, | 2958.3775, | 2964.9680, |
|                                                                                               | H | 1.144448  | -1.300214 | 1.744516  | 3038.6173, | 3045.2007, | 3079.2564, |
|                                                                                               | H | 2.051694  | 1.761870  | 0.112444  | 3080.3281, | 3096.6753, | 3098.3732, |
|                                                                                               | O | -1.001313 | -0.221332 | -0.555182 | 3103.7077, | 3187.8855, | 3803.6020  |
|                                                                                               | O | -2.653093 | -0.064225 | -0.312218 |            |            |            |
|                                                                                               | H | -2.887811 | -0.153994 | -1.246290 |            |            |            |
| TS14Ce<br>   | C | -1.044344 | 1.466172  | -0.219369 | 629.2807i, | 48.1578,   | 88.7164,   |
|                                                                                               | C | -0.138666 | 1.161480  | 1.017055  | 110.5057,  | 193.4136,  | 278.7018,  |
|                                                                                               | C | 0.466942  | -0.224143 | 0.777034  | 305.6391,  | 375.2572,  | 390.7576,  |
|                                                                                               | C | -0.611410 | -1.311641 | 0.789040  | 542.9234,  | 545.5336,  | 656.9088,  |
|                                                                                               | C | -1.562973 | -1.030409 | -0.417303 | 780.2357,  | 804.6125,  | 821.4065,  |
|                                                                                               | C | -1.126487 | 0.239785  | -1.068605 | 852.9506,  | 881.3634,  | 896.6227,  |
|                                                                                               | H | 0.657942  | 1.903553  | 1.093200  | 925.0491,  | 964.9080,  | 1025.1348, |
|                                                                                               | H | -0.701402 | 1.180057  | 1.955279  | 1042.7659, | 1092.7823, | 1099.5369, |
|                                                                                               | H | -2.051726 | 1.761801  | 0.112464  | 1107.2494, | 1153.8909, | 1198.5937, |
|                                                                                               | H | -0.646908 | 2.301716  | -0.797173 | 1207.7840, | 1245.2621, | 1267.2765, |
|                                                                                               | H | -0.144015 | -2.292072 | 0.680145  | 1314.5391, | 1324.6172, | 1331.8609, |
|                                                                                               | H | -1.144487 | -1.300124 | 1.744537  | 1333.4143, | 1364.5320, | 1387.0913, |
|                                                                                               | H | -1.546446 | -1.855815 | -1.130393 | 1466.3339, | 1475.2814, | 1487.4500, |
|                                                                                               | H | -2.602312 | -0.936926 | -0.065462 | 1501.9299, | 2958.3732, | 2964.9631, |
|                                                                                               | H | -1.114286 | 0.323465  | -2.148500 | 3038.6167, | 3045.2004, | 3079.2534, |
|                                                                                               | H | 1.272212  | -0.454440 | 1.474257  | 3080.3275, | 3096.6738, | 3098.3745, |
|                                                                                               | O | 1.001315  | -0.221353 | -0.555174 | 3103.7086, | 3187.8860, | 3803.5988  |
|                                                                                               | O | 2.653092  | -0.064243 | -0.312221 |            |            |            |
|                                                                                               | H | 2.887797  | -0.153913 | -1.246307 |            |            |            |
| TS14Ti<br> | C | 1.126482  | 0.239771  | -1.068609 | 629.2823i, | 48.1551,   | 88.7148,   |
|                                                                                               | C | 1.562960  | -1.030422 | -0.417303 | 110.5063,  | 193.4144,  | 278.7009,  |
|                                                                                               | C | 0.611420  | -1.311622 | 0.789064  | 305.6384,  | 375.2560,  | 390.7606,  |
|                                                                                               | C | -0.466943 | -0.224131 | 0.777041  | 542.9231,  | 545.5329,  | 656.9088,  |
|                                                                                               | C | 0.138654  | 1.161502  | 1.017034  | 780.2404,  | 804.6134,  | 821.4066,  |
|                                                                                               | H | 0.144035  | -2.292062 | 0.680215  | 852.9493,  | 881.3623,  | 896.6243,  |
|                                                                                               | H | 1.546401  | -1.855836 | -1.130383 | 925.0500,  | 964.9067,  | 1025.1352, |
|                                                                                               | H | 2.602309  | -0.936958 | -0.065487 | 1042.7643, | 1092.7829, | 1099.5392, |
|                                                                                               | H | 1.114277  | 0.323443  | -2.148504 | 1107.2525, | 1153.8900, | 1198.5956, |
|                                                                                               | H | -1.272213 | -0.454418 | 1.474268  | 1207.7842, | 1245.2618, | 1267.2760, |
|                                                                                               | H | -0.657962 | 1.903573  | 1.093130  | 1314.5386, | 1324.6160, | 1331.8609, |
|                                                                                               | H | 0.701366  | 1.180113  | 1.955271  | 1333.4135, | 1364.5321, | 1387.0924, |
|                                                                                               | H | 1.144512  | -1.300061 | 1.744552  | 1466.3349, | 1475.2826, | 1487.4519, |
|                                                                                               | C | 1.044363  | 1.466160  | -0.219378 | 1501.9317, | 2958.3698, | 2964.9595, |
|                                                                                               | H | 2.051751  | 1.761751  | 0.112475  | 3038.6162, | 3045.2001, | 3079.2512, |
|                                                                                               | H | 0.646974  | 2.301722  | -0.797189 | 3080.3270, | 3096.6727, | 3098.3755, |

|   |           |           |           |                                 |
|---|-----------|-----------|-----------|---------------------------------|
| O | -1.001316 | -0.221366 | -0.555168 | 3103.7093, 3187.8863, 3803.5966 |
| O | -2.653093 | -0.064253 | -0.312223 |                                 |
| H | -2.887788 | -0.153867 | -1.246317 |                                 |

|                                                                                           |   |           |           |           |            |            |            |
|-------------------------------------------------------------------------------------------|---|-----------|-----------|-----------|------------|------------|------------|
| TSH1<br> | C | 1.603190  | -1.235640 | -0.225197 | 224.6893i, | 38.9981,   | 75.5401,   |
|                                                                                           | C | 0.225905  | -1.268843 | 0.450802  | 174.0117,  | 261.5223,  | 361.4493,  |
|                                                                                           | C | 1.387431  | 1.398045  | 0.135920  | 431.9844,  | 466.0317,  | 526.9043,  |
|                                                                                           | H | -0.238674 | -2.248791 | 0.312666  | 653.2584,  | 732.5976,  | 779.8317,  |
|                                                                                           | H | 0.308396  | -1.093946 | 1.529593  | 803.2838,  | 894.6068,  | 904.9369,  |
|                                                                                           | H | 2.268820  | -1.944236 | 0.273937  | 925.6822,  | 948.6742,  | 993.3739,  |
|                                                                                           | H | 1.479659  | -1.608196 | -1.247688 | 1056.0833, | 1110.5328, | 1115.9355, |
|                                                                                           | H | 1.594070  | 2.209061  | -0.565657 | 1143.8507, | 1157.8980, | 1181.3336, |
|                                                                                           | H | 1.734330  | 1.759985  | 1.106070  | 1248.2942, | 1285.9436, | 1290.6984, |
|                                                                                           | C | -0.155304 | 1.203332  | 0.234869  | 1302.1452, | 1313.5939, | 1334.9708, |
|                                                                                           | H | -0.682348 | 1.953622  | -0.357613 | 1354.6348, | 1374.7928, | 1376.7596, |
|                                                                                           | H | -0.471606 | 1.346073  | 1.272999  | 1387.7144, | 1397.2635, | 1489.8927, |
|                                                                                           | C | 2.262983  | 0.171582  | -0.272330 | 1494.6549, | 1505.1563, | 1512.3176, |
|                                                                                           | H | 2.638423  | 0.333514  | -1.285661 | 1528.3087, | 3019.4153, | 3025.7397, |
|                                                                                           | H | 3.149042  | 0.169585  | 0.367034  | 3032.4038, | 3039.3479, | 3051.6614, |
|                                                                                           | C | -0.632361 | -0.184972 | -0.172668 | 3053.4834, | 3056.2394, | 3067.8332, |
|                                                                                           | H | -0.684788 | -0.302538 | -1.258923 | 3078.4509, | 3082.5058, | 3098.0921  |
|                                                                                           | O | -2.010358 | -0.380132 | 0.308699  |            |            |            |
|                                                                                           | O | -2.895440 | 0.245737  | -0.440591 |            |            |            |

|                                                                                             |   |           |           |           |            |            |            |
|---------------------------------------------------------------------------------------------|---|-----------|-----------|-----------|------------|------------|------------|
| TSH2<br> | C | -0.156558 | -1.087047 | 0.615102  | 182.1472i, | 41.1840,   | 107.7146,  |
|                                                                                             | C | 0.934853  | -1.363045 | -0.418871 | 247.9244,  | 300.6675,  | 348.6057,  |
|                                                                                             | C | 0.332543  | 1.423504  | 0.095763  | 432.1012,  | 519.4498,  | 537.2167,  |
|                                                                                             | C | -0.676449 | 0.345257  | 0.535800  | 643.6561,  | 726.5537,  | 773.8215,  |
|                                                                                             | H | 1.214062  | -2.420383 | -0.397058 | 792.1760,  | 864.0915,  | 883.3429,  |
|                                                                                             | H | 0.559534  | -1.157501 | -1.428346 | 910.1706,  | 946.3721,  | 998.4258,  |
|                                                                                             | H | -1.011236 | -1.761229 | 0.518533  | 1048.3377, | 1081.8274, | 1124.1957, |
|                                                                                             | H | 0.252688  | -1.246510 | 1.620175  | 1127.5076, | 1167.7918, | 1188.9701, |
|                                                                                             | H | 0.264480  | 2.266980  | 0.785732  | 1196.5779, | 1281.5138, | 1291.9184, |
|                                                                                             | H | -0.041573 | 1.801416  | -0.859463 | 1304.9400, | 1327.6543, | 1349.2372, |
|                                                                                             | H | -1.191590 | 0.615846  | 1.458326  | 1357.8532, | 1365.2750, | 1383.1931, |
|                                                                                             | C | 1.828895  | 1.023392  | -0.082800 | 1392.8249, | 1400.4774, | 1484.1406, |
|                                                                                             | H | 2.421796  | 1.499023  | 0.702389  | 1487.2567, | 1497.0138, | 1501.9200, |
|                                                                                             | H | 2.172834  | 1.469203  | -1.019509 | 1520.4934, | 3011.0116, | 3015.3317, |
|                                                                                             | C | 2.152451  | -0.491190 | -0.099906 | 3023.8948, | 3035.3560, | 3050.3564, |
|                                                                                             | H | 2.962276  | -0.682435 | -0.809412 | 3052.4974, | 3064.2518, | 3067.8253, |
|                                                                                             | H | 2.530395  | -0.795838 | 0.882932  | 3079.0352, | 3080.5027, | 3094.3843  |
|                                                                                             | O | -1.747117 | 0.408018  | -0.507113 |            |            |            |
|                                                                                             | O | -2.831392 | -0.244743 | -0.158489 |            |            |            |

|                                                                                             |   |           |           |           |            |            |            |
|---------------------------------------------------------------------------------------------|---|-----------|-----------|-----------|------------|------------|------------|
| TSH3<br>   | C | -1.415548 | 1.382261  | -0.089223 | 181.0955i, | 36.0663,   | 81.5904,   |
|                                                                                             | C | 0.124209  | 1.236564  | 0.106604  | 256.4341,  | 304.6884,  | 366.4896,  |
|                                                                                             | C | -1.470130 | -1.118409 | -0.485251 | 425.0701,  | 473.9995,  | 521.4698,  |
|                                                                                             | H | 0.618785  | 1.494090  | -0.831899 | 646.5740,  | 745.8543,  | 761.3753,  |
|                                                                                             | H | 0.475981  | 1.975074  | 0.828228  | 800.7524,  | 868.4055,  | 890.5802,  |
|                                                                                             | H | -1.802083 | 2.135267  | 0.602323  | 915.4450,  | 935.5962,  | 998.5090,  |
|                                                                                             | H | -1.585856 | 1.783017  | -1.092745 | 1050.2125, | 1085.3014, | 1123.4690, |
|                                                                                             | H | -1.169458 | -0.944477 | -1.525581 | 1136.5148, | 1157.4122, | 1186.1799, |
|                                                                                             | H | -2.100829 | -2.012208 | -0.484834 | 1205.5519, | 1283.0219, | 1295.8262, |
|                                                                                             | C | -0.244400 | -1.359210 | 0.397364  | 1302.9826, | 1323.5194, | 1349.5372, |
|                                                                                             | H | 0.350020  | -2.205599 | 0.041590  | 1357.9573, | 1372.7690, | 1382.7311, |
|                                                                                             | H | -0.588801 | -1.624518 | 1.402854  | 1387.6596, | 1400.3597, | 1478.4683, |
|                                                                                             | C | 0.686641  | -0.146483 | 0.519354  | 1486.4055, | 1496.9709, | 1501.4820, |
|                                                                                             | H | 1.124538  | -0.100858 | 1.517174  | 1515.7801, | 3002.8977, | 3016.1847, |
|                                                                                             | C | -2.237724 | 0.089793  | 0.054533  | 3026.6358, | 3029.8610, | 3054.8823, |
|                                                                                             | H | -3.195512 | 0.211945  | -0.459311 | 3062.5641, | 3064.0988, | 3065.2651, |
|                                                                                             | H | -2.474644 | -0.094477 | 1.110071  | 3071.2981, | 3080.6749, | 3102.8094  |
|                                                                                             | O | 1.842384  | -0.468380 | -0.359935 |            |            |            |
|                                                                                             | O | 2.868812  | 0.327837  | -0.156084 |            |            |            |
| TSB4<br> | C | -2.054129 | 0.224625  | -0.583746 | 91.1508i,  | 77.1509,   | 129.9731,  |
|                                                                                             | C | -1.401645 | 1.368974  | 0.207439  | 231.9596,  | 271.8854,  | 362.5343,  |
|                                                                                             | C | 0.127719  | 1.161883  | 0.413209  | 414.3926,  | 468.4809,  | 502.6519,  |
|                                                                                             | C | -0.212948 | -1.352342 | 0.303112  | 595.5047,  | 785.4339,  | 792.3800,  |
|                                                                                             | C | -1.733075 | -1.147874 | 0.031341  | 836.1875,  | 892.1336,  | 899.4858,  |
|                                                                                             | H | 0.703376  | 1.974731  | -0.034144 | 914.7868,  | 951.4700,  | 998.5163,  |
|                                                                                             | H | -1.585745 | 2.319190  | -0.300194 | 1052.8097, | 1086.3962, | 1109.0041, |
|                                                                                             | H | -1.890783 | 1.443434  | 1.183879  | 1123.8049, | 1156.7916, | 1183.9196, |
|                                                                                             | H | -3.138138 | 0.367898  | -0.616801 | 1221.5734, | 1259.4616, | 1300.3793, |
|                                                                                             | H | -1.713535 | 0.253892  | -1.625295 | 1308.9291, | 1315.4379, | 1324.0917, |
|                                                                                             | H | 0.153202  | -2.262091 | -0.178049 | 1359.6039, | 1365.7451, | 1380.0735, |
|                                                                                             | H | -0.030945 | -1.470611 | 1.375661  | 1385.9429, | 1392.4021, | 1487.2831, |
|                                                                                             | H | -2.103738 | -1.938071 | -0.626501 | 1495.2688, | 1505.0337, | 1507.3197, |
|                                                                                             | H | -2.282904 | -1.250174 | 0.971987  | 1524.5871, | 3014.2114, | 3026.7074, |
|                                                                                             | H | 0.369681  | 1.153018  | 1.480521  | 3028.4371, | 3042.1389, | 3043.6884, |
|                                                                                             | C | 0.606213  | -0.162044 | -0.180392 | 3058.6645, | 3062.5542, | 3067.0882, |
|                                                                                             | H | 0.651240  | -0.115887 | -1.270276 | 3073.9025, | 3088.3893, | 3097.8949  |
|                                                                                             | O | 1.991349  | -0.414950 | 0.250899  |            |            |            |
|                                                                                             | O | 2.868086  | 0.285617  | -0.439220 |            |            |            |
| TSB5<br> | C | -1.466936 | 0.388040  | -0.936888 | 84.4779i,  | 80.7910,   | 144.1039,  |
|                                                                                             | C | -1.064353 | 1.468482  | 0.077324  | 250.1120,  | 285.0747,  | 325.3359,  |
|                                                                                             | C | 0.178973  | 1.075157  | 0.919865  | 432.5581,  | 465.5098,  | 549.9767,  |
|                                                                                             | C | 0.662963  | -0.355716 | 0.696029  | 703.9976,  | 754.8651,  | 775.0622,  |
|                                                                                             | C | -0.446794 | -1.398420 | 0.613967  | 795.8304,  | 862.2878,  | 870.1142,  |
|                                                                                             | C | -1.667182 | -0.969329 | -0.248093 | 906.7150,  | 923.1313,  | 994.8621,  |
|                                                                                             | H | 1.022718  | 1.741466  | 0.726485  | 1045.2463, | 1065.1372, | 1127.3915, |
|                                                                                             | H | -0.876621 | 2.412186  | -0.440957 | 1131.9860, | 1165.2019, | 1187.3214, |
|                                                                                             | H | -1.912734 | 1.650879  | 0.746143  | 1198.0126, | 1270.9691, | 1283.7686, |
|                                                                                             | H | -2.391739 | 0.682963  | -1.441816 | 1307.1488, | 1324.3664, | 1351.0469, |

|                                                                                             |   |           |           |           |            |            |            |
|---------------------------------------------------------------------------------------------|---|-----------|-----------|-----------|------------|------------|------------|
|                                                                                             | H | -0.700286 | 0.301087  | -1.712738 | 1355.6021, | 1366.7965, | 1381.4009, |
|                                                                                             | H | 1.403208  | -0.629178 | 1.450620  | 1386.6973, | 1391.6266, | 1475.0696, |
|                                                                                             | H | -0.011606 | -2.329560 | 0.241828  | 1484.1115, | 1500.7483, | 1501.6774, |
|                                                                                             | H | -0.763837 | -1.601504 | 1.641460  | 1515.0338, | 3017.6385, | 3020.3076, |
|                                                                                             | H | -1.879164 | -1.736788 | -0.996566 | 3032.4753, | 3040.5220, | 3041.9129, |
|                                                                                             | H | -2.555922 | -0.909208 | 0.389404  | 3060.0877, | 3060.9215, | 3071.3606, |
|                                                                                             | H | -0.041485 | 1.170803  | 1.987930  | 3077.6305, | 3083.5893, | 3087.9688  |
|                                                                                             | O | 1.400536  | -0.452315 | -0.594435 |            |            |            |
|                                                                                             | O | 2.540394  | 0.202012  | -0.571192 |            |            |            |
| TSB6<br>   | C | -1.279976 | -1.262491 | -0.359275 | 77.4044i,  | 68.4767,   | 136.4352,  |
|                                                                                             | C | -1.939025 | 0.103650  | -0.710364 | 242.3233,  | 307.6717,  | 367.8654,  |
|                                                                                             | C | -1.455936 | 1.244770  | 0.197672  | 446.1885,  | 495.4718,  | 508.5153,  |
|                                                                                             | C | 0.709347  | -0.039026 | 0.665548  | 617.6231,  | 769.3409,  | 779.9355,  |
|                                                                                             | C | -0.302564 | -1.167798 | 0.823981  | 808.9715,  | 863.4039,  | 880.1342,  |
|                                                                                             | H | -1.845903 | 2.200561  | -0.164388 | 890.0964,  | 961.0162,  | 1002.6385, |
|                                                                                             | H | -1.707049 | 0.363124  | -1.748405 | 1039.7759, | 1073.6238, | 1104.1065, |
|                                                                                             | H | -3.028246 | 0.027224  | -0.651671 | 1130.7720, | 1164.9443, | 1181.3845, |
|                                                                                             | H | -2.045316 | -2.006533 | -0.123205 | 1194.0200, | 1253.7311, | 1278.6605, |
|                                                                                             | H | -0.740219 | -1.647303 | -1.227981 | 1299.9689, | 1339.5185, | 1348.4123, |
|                                                                                             | H | 1.323211  | 0.064695  | 1.562147  | 1355.7153, | 1366.7741, | 1377.9465, |
|                                                                                             | H | 0.230788  | -2.112843 | 0.959117  | 1385.7376, | 1392.5924, | 1479.3115, |
|                                                                                             | H | -0.849350 | -0.986226 | 1.755233  | 1484.3632, | 1491.3958, | 1504.1718, |
|                                                                                             | H | -1.860080 | 1.117039  | 1.208461  | 1516.2932, | 3015.8851, | 3024.7775, |
|                                                                                             | C | 0.076578  | 1.309344  | 0.254144  | 3035.8201, | 3043.4530, | 3044.6825, |
|                                                                                             | H | 0.403125  | 2.094114  | 0.940106  | 3055.5378, | 3062.5955, | 3071.3415, |
|                                                                                             | H | 0.468796  | 1.582051  | -0.729962 | 3073.1263, | 3084.9930, | 3090.1246  |
|                                                                                             | O | 1.651664  | -0.508109 | -0.376778 |            |            |            |
|                                                                                             | O | 2.698298  | 0.279784  | -0.499432 |            |            |            |
| TSB7<br> | C | -1.565173 | -1.093765 | -0.426087 | 56.1530i,  | 90.0572,   | 156.1946,  |
|                                                                                             | C | -2.271152 | 0.151634  | 0.133042  | 257.3283,  | 284.3963,  | 371.0090,  |
|                                                                                             | C | -1.340919 | 1.400567  | 0.157193  | 420.1717,  | 486.5476,  | 533.5304,  |
|                                                                                             | C | 0.659845  | -0.108086 | 0.375151  | 596.0284,  | 765.6232,  | 784.8181,  |
|                                                                                             | C | -0.238141 | -1.357794 | 0.301199  | 824.0771,  | 874.6311,  | 881.0373,  |
|                                                                                             | H | -1.764728 | 2.205305  | -0.448654 | 913.3969,  | 963.9868,  | 1010.8518, |
|                                                                                             | H | -3.169774 | 0.358845  | -0.454156 | 1033.9168, | 1081.7758, | 1115.6347, |
|                                                                                             | H | -2.616113 | -0.068458 | 1.148972  | 1138.8574, | 1146.6290, | 1184.8933, |
|                                                                                             | H | -2.214727 | -1.968367 | -0.329420 | 1205.9898, | 1257.7397, | 1262.2973, |
|                                                                                             | H | -1.381672 | -0.968550 | -1.498253 | 1302.7005, | 1336.0586, | 1342.5865, |
|                                                                                             | H | 0.911476  | 0.153787  | 1.405081  | 1357.7034, | 1370.9846, | 1373.5179, |
|                                                                                             | H | 0.319436  | -2.153993 | -0.200460 | 1382.1586, | 1391.0139, | 1483.5809, |
|                                                                                             | H | -0.440379 | -1.712901 | 1.316197  | 1489.8764, | 1496.3194, | 1510.9510, |
|                                                                                             | H | -1.273833 | 1.793944  | 1.176685  | 1522.2155, | 3017.4432, | 3027.3182, |
|                                                                                             | C | 0.078472  | 1.097622  | -0.354304 | 3034.1243, | 3034.9882, | 3041.4043, |
|                                                                                             | H | 0.735153  | 1.958364  | -0.211462 | 3054.8015, | 3064.6002, | 3067.5309, |
|                                                                                             | H | 0.057799  | 0.883040  | -1.427672 | 3077.3097, | 3080.9874, | 3094.9544  |
|                                                                                             | O | 1.947850  | -0.485320 | -0.246803 |            |            |            |
|                                                                                             | O | 2.914620  | 0.357560  | 0.047551  |            |            |            |

