**Table S#.** Cartesian coordinates for unsub-monoBIP-cyclohexylimine: neutral. (-1000.81868882 Hartrees)

|  |  |  |  |
| --- | --- | --- | --- |
| atom | x | y | z |
| C | -0.471802 | 2.722723 | 0.443310 |
| C | -1.871767 | 2.899459 | 0.317472 |
| C | -2.408152 | 4.186799 | 0.204121 |
| C | -1.522447 | 5.260833 | 0.218935 |
| C | -0.132853 | 5.068795 | 0.345862 |
| C | 0.419239 | 3.794568 | 0.462094 |
| C | -1.517936 | 0.754492 | 0.440144 |
| H | -3.476711 | 4.333862 | 0.104043 |
| H | -1.909695 | 6.269666 | 0.132042 |
| H | 0.522568 | 5.932132 | 0.353976 |
| N | -2.490260 | 1.658528 | 0.321200 |
| C | -3.063165 | -1.187424 | 0.361181 |
| C | -1.738927 | -0.683865 | 0.458471 |
| C | -0.659758 | -1.574795 | 0.544670 |
| C | -0.849361 | -2.951304 | 0.540640 |
| C | -2.168657 | -3.417812 | 0.448074 |
| C | -3.286212 | -2.583583 | 0.359384 |
| H | 0.348704 | -1.182283 | 0.609838 |
| H | -2.333657 | -4.483886 | 0.443163 |
| C | 0.362442 | -3.887409 | 0.606004 |
| C | -4.705491 | -3.165536 | 0.259631 |
| O | -4.116051 | -0.344182 | 0.266260 |
| H | -3.764876 | 0.593734 | 0.265146 |
| N | -0.287388 | 1.354581 | 0.522300 |
| H | 0.597063 | 0.878639 | 0.609942 |
| C | 1.245627 | -3.645420 | -0.635110 |
| H | 1.574078 | -2.604514 | -0.686049 |
| H | 2.134937 | -4.281753 | -0.600644 |
| H | 0.697174 | -3.873580 | -1.553070 |
| C | 1.184672 | -3.582215 | 1.873652 |
| H | 0.592147 | -3.758562 | 2.775299 |
| H | 2.068169 | -4.226022 | 1.913691 |
| H | 1.524114 | -2.543558 | 1.887937 |
| C | -0.046683 | -5.366238 | 0.635030 |
| H | -0.660111 | -5.597953 | 1.509992 |
| H | -0.606655 | -5.647117 | -0.261186 |
| H | 0.848751 | -5.991159 | 0.678804 |
| C | -5.360351 | -2.728215 | -1.067792 |
| H | -6.374132 | -3.134647 | -1.132489 |
| H | -5.415470 | -1.643224 | -1.146011 |
| H | -4.788099 | -3.108300 | -1.918807 |
| C | -5.556228 | -2.682320 | 1.453634 |
| H | -5.656814 | -1.597940 | 1.456262 |
| H | -6.555381 | -3.125408 | 1.402799 |
| H | -5.095490 | -2.988033 | 2.397197 |
| C | -4.694862 | -4.702893 | 0.287551 |
| H | -4.128631 | -5.120375 | -0.549276 |
| H | -4.267527 | -5.089882 | 1.216460 |
| H | -5.722320 | -5.066982 | 0.212788 |
| H | 1.487330 | 3.644658 | 0.561168 |

**Table S#.** Cartesian coordinates for unsub-monoBIP-cyclohexylimine: E0PT. (-1000.61974403 Hartrees)

|  |  |  |  |
| --- | --- | --- | --- |
| atom | x | y | z |
| C | -0.476280 | 2.748976 | 0.453646 |
| C | -1.889081 | 2.864294 | 0.303522 |
| C | -2.491128 | 4.128114 | 0.187570 |
| C | -1.657085 | 5.231819 | 0.226438 |
| C | -0.253106 | 5.101642 | 0.377442 |
| C | 0.362790 | 3.863798 | 0.495843 |
| C | -1.419161 | 0.741992 | 0.429069 |
| H | -3.563092 | 4.224299 | 0.071725 |
| H | -2.081216 | 6.224891 | 0.139839 |
| H | 0.355168 | 5.997667 | 0.401104 |
| N | -2.434039 | 1.606165 | 0.295295 |
| C | -2.992800 | -1.177100 | 0.341194 |
| C | -1.622599 | -0.683611 | 0.445112 |
| C | -0.581827 | -1.592793 | 0.533476 |
| C | -0.825432 | -2.973480 | 0.532616 |
| C | -2.169266 | -3.428525 | 0.445948 |
| C | -3.261320 | -2.593943 | 0.354705 |
| H | 0.439125 | -1.240279 | 0.596788 |
| H | -2.337787 | -4.492651 | 0.451894 |
| C | 0.348979 | -3.937522 | 0.597883 |
| C | -4.691387 | -3.129229 | 0.265311 |
| O | -3.981241 | -0.338149 | 0.227430 |
| H | -3.600275 | 0.641859 | 0.225932 |
| N | -0.224128 | 1.398929 | 0.530467 |
| H | 0.684995 | 0.975108 | 0.643368 |
| C | 1.231491 | -3.702213 | -0.650575 |
| H | 1.596208 | -2.673912 | -0.693565 |
| H | 2.095444 | -4.370335 | -0.611345 |
| H | 0.675050 | -3.910992 | -1.567145 |
| C | 1.179883 | -3.641011 | 1.866815 |
| H | 0.584410 | -3.796770 | 2.769170 |
| H | 2.036583 | -4.318601 | 1.898112 |
| H | 1.559133 | -2.616989 | 1.874488 |
| C | -0.091521 | -5.406937 | 0.627239 |
| H | -0.705299 | -5.628007 | 1.504145 |
| H | -0.652774 | -5.679742 | -0.270059 |
| H | 0.794959 | -6.042455 | 0.671604 |
| C | -5.329757 | -2.704140 | -1.076357 |
| H | -6.336963 | -3.123657 | -1.138503 |
| H | -5.403743 | -1.621515 | -1.169908 |
| H | -4.748464 | -3.088958 | -1.917817 |
| C | -5.528432 | -2.590090 | 1.447755 |
| H | -5.619299 | -1.505321 | 1.419250 |
| H | -6.531172 | -3.021927 | 1.400923 |
| H | -5.076413 | -2.877862 | 2.400101 |
| C | -4.710093 | -4.664895 | 0.332952 |
| H | -4.157587 | -5.114516 | -0.496146 |
| H | -4.286910 | -5.032486 | 1.271240 |
| H | -5.744695 | -5.007601 | 0.272311 |
| H | 1.434251 | 3.763740 | 0.611435 |

**Table S#.** Cartesian coordinates for unsub-monoBIP-cyclohexylimine: E1PT. (-1000.63576249 Hartrees)

|  |  |  |  |
| --- | --- | --- | --- |
| atom | x | y | z |
| C | -0.466074 | 2.739723 | 0.447772 |
| C | -1.854058 | 2.951118 | 0.319903 |
| C | -2.391934 | 4.233376 | 0.207908 |
| C | -1.486274 | 5.287507 | 0.227501 |
| C | -0.097537 | 5.074589 | 0.356415 |
| C | 0.441142 | 3.798102 | 0.470540 |
| C | -1.489418 | 0.745897 | 0.439084 |
| H | -3.457367 | 4.390739 | 0.106028 |
| H | -1.856717 | 6.301763 | 0.142565 |
| H | 0.566486 | 5.930269 | 0.367596 |
| N | -2.434650 | 1.695174 | 0.321927 |
| C | -3.103708 | -1.179348 | 0.349603 |
| C | -1.723529 | -0.680580 | 0.453203 |
| C | -0.666042 | -1.561581 | 0.538014 |
| C | -0.868526 | -2.958206 | 0.534195 |
| C | -2.188675 | -3.446638 | 0.445185 |
| C | -3.302983 | -2.633758 | 0.356297 |
| H | 0.349360 | -1.191372 | 0.603130 |
| H | -2.330652 | -4.515531 | 0.445347 |
| C | 0.343791 | -3.876337 | 0.600690 |
| C | -4.713453 | -3.208995 | 0.264086 |
| O | -4.064571 | -0.375411 | 0.253487 |
| N | -0.291768 | 1.366395 | 0.521904 |
| H | 0.595822 | 0.891890 | 0.609864 |
| C | 1.226697 | -3.601069 | -0.638167 |
| H | 1.551270 | -2.558835 | -0.674797 |
| H | 2.117380 | -4.233133 | -0.597240 |
| H | 0.685984 | -3.827008 | -1.560316 |
| C | 1.152204 | -3.560219 | 1.878360 |
| H | 0.556678 | -3.747504 | 2.774723 |
| H | 2.035294 | -4.202976 | 1.912131 |
| H | 1.491157 | -2.522096 | 1.899602 |
| C | -0.042479 | -5.360738 | 0.615579 |
| H | -0.649384 | -5.611748 | 1.489266 |
| H | -0.593772 | -5.643320 | -0.284788 |
| H | 0.865794 | -5.965453 | 0.654552 |
| C | -5.364450 | -2.780987 | -1.071188 |
| H | -6.367107 | -3.212023 | -1.134012 |
| H | -5.445635 | -1.697917 | -1.147513 |
| H | -4.782326 | -3.150539 | -1.919403 |
| C | -5.560336 | -2.696954 | 1.452165 |
| H | -5.663498 | -1.613622 | 1.424783 |
| H | -6.555431 | -3.147082 | 1.405798 |
| H | -5.100567 | -2.981869 | 2.402035 |
| C | -4.702021 | -4.745308 | 0.314682 |
| H | -4.140924 | -5.175143 | -0.519130 |
| H | -4.271843 | -5.116172 | 1.248558 |
| H | -5.729839 | -5.107860 | 0.249878 |
| H | 1.505306 | 3.630573 | 0.571254 |
| H | -3.413478 | 1.421064 | 0.249207 |