Table S#. Cartesian coordinates for triBIP-cyclohexylimine: neutral. (-2086.47631873 Hartrees)

|  |  |  |  |
| --- | --- | --- | --- |
| atom | x | y | z |
| C | 1.683327 | 0.325129 | 0.811766 |
| C | 0.582343 | 1.159606 | 0.50527 |
| C | 0.775533 | 2.535448 | 0.339355 |
| C | 2.069272 | 3.032118 | 0.49009 |
| C | 3.15229 | 2.195237 | 0.803194 |
| C | 2.988532 | 0.813856 | 0.974442 |
| C | -0.186535 | -0.855556 | 0.686338 |
| H | -0.057017 | 3.1867 | 0.101869 |
| H | 2.249693 | 4.093237 | 0.364727 |
| H | 4.139127 | 2.630505 | 0.907216 |
| C | -2.468807 | -1.778997 | 0.506168 |
| C | -3.415223 | -2.828563 | 0.522128 |
| C | -2.997956 | -4.141362 | 0.760497 |
| C | -1.637214 | -4.359268 | 0.976751 |
| C | -0.704964 | -3.31057 | 0.95802 |
| C | -1.098137 | -1.985947 | 0.720947 |
| C | -4.502132 | -0.987399 | 0.098589 |
| H | -3.710108 | -4.957675 | 0.775135 |
| H | -1.283837 | -5.365841 | 1.165591 |
| H | 0.34102 | -3.533209 | 1.130754 |
| N | -0.570215 | 0.394583 | 0.434976 |
| C | -6.89273 | -0.564799 | -0.389805 |
| C | -5.57892 | -0.064602 | -0.216938 |
| C | -5.324332 | 1.311817 | -0.358184 |
| C | -6.337128 | 2.200654 | -0.680255 |
| C | -7.629164 | 1.670528 | -0.860189 |
| C | -7.94679 | 0.32182 | -0.723827 |
| H | -4.314192 | 1.670665 | -0.210703 |
| H | -8.422811 | 2.358155 | -1.118603 |
| C | -6.11022 | 3.706959 | -0.84461 |
| C | -9.382229 | -0.189613 | -0.918761 |
| O | -7.156857 | -1.881604 | -0.245165 |
| H | -6.298874 | -2.34666 | -0.016857 |
| N | -3.183561 | -0.634955 | 0.24093 |
| N | -4.671173 | -2.301499 | 0.267302 |
| H | -2.736459 | 0.271427 | 0.158559 |
| N | 1.165506 | -0.942572 | 0.916756 |
| H | 1.7407 | -1.753124 | 1.114379 |
| C | 4.068004 | -0.093754 | 1.325495 |
| N | 3.944015 | -1.418926 | 1.386735 |
| N | 5.33759 | 0.320413 | 1.650251 |
| C | 7.406371 | -0.94268 | 2.356888 |
| C | 7.838848 | -2.257037 | 2.569694 |
| C | 6.983715 | -3.357336 | 2.380812 |
| C | 5.656641 | -3.194035 | 1.985114 |
| C | 5.192199 | -1.890195 | 1.768611 |
| C | 6.072809 | -0.798761 | 1.945649 |
| H | 8.861684 | -2.424663 | 2.889967 |
| H | 7.366898 | -4.355767 | 2.556059 |
| H | 4.999059 | -4.044933 | 1.853804 |
| H | 5.732696 | 1.251679 | 1.718959 |
| C | 8.275016 | 0.214643 | 2.563479 |
| H | 9.289521 | -0.008571 | 2.903732 |
| N | 7.853451 | 1.406853 | 2.356821 |
| C | 8.742029 | 2.551722 | 2.54843 |
| C | 10.125151 | 2.279307 | 3.149871 |
| C | 8.875616 | 3.289196 | 1.204503 |
| H | 8.207078 | 3.226666 | 3.231751 |
| C | 10.906889 | 3.587153 | 3.322531 |
| H | 10.686314 | 1.609068 | 2.486752 |
| H | 10.023442 | 1.767269 | 4.112232 |
| C | 9.672602 | 4.58849 | 1.357902 |
| H | 9.381658 | 2.621469 | 0.496552 |
| H | 7.8784 | 3.488955 | 0.801332 |
| C | 11.044309 | 4.335861 | 1.992897 |
| H | 11.89338 | 3.376782 | 3.7472 |
| H | 10.383939 | 4.227028 | 4.044251 |
| H | 9.787381 | 5.072783 | 0.383281 |
| H | 9.105232 | 5.28117 | 1.991949 |
| H | 11.571351 | 5.283091 | 2.144517 |
| H | 11.655217 | 3.736936 | 1.305825 |
| C | -9.425032 | -1.215329 | -2.071101 |
| H | -8.759357 | -2.055827 | -1.879648 |
| H | -10.444406 | -1.59518 | -2.189532 |
| H | -9.13042 | -0.742532 | -3.012408 |
| C | -6.464197 | 4.117945 | -2.288548 |
| H | -7.500838 | 3.869218 | -2.529012 |
| H | -6.335354 | 5.196677 | -2.418323 |
| H | -5.8165 | 3.607916 | -3.006693 |
| C | -9.887829 | -0.841923 | 0.385551 |
| H | -10.909069 | -1.208007 | 0.243896 |
| H | -9.257404 | -1.678752 | 0.683053 |
| H | -9.899134 | -0.109627 | 1.197958 |
| C | -10.348894 | 0.950764 | -1.275031 |
| H | -10.392201 | 1.707305 | -0.486569 |
| H | -10.067065 | 1.445575 | -2.208291 |
| H | -11.35406 | 0.54161 | -1.402317 |
| C | -7.018723 | 4.475176 | 0.136833 |
| H | -6.875627 | 5.552971 | 0.015981 |
| H | -8.075104 | 4.25631 | -0.036501 |
| H | -6.782726 | 4.211949 | 1.171294 |
| C | -4.654137 | 4.102836 | -0.562847 |
| H | -4.361292 | 3.848584 | 0.459706 |
| H | -3.961195 | 3.608968 | -1.249138 |
| H | -4.537081 | 5.182212 | -0.687496 |

Table S#. Cartesian coordinates for triBIP-cyclohexylimine: E0PT. (-2086.27776155 Hartrees)

|  |  |  |  |
| --- | --- | --- | --- |
| atom | x | y | z |
| C | 1.686007 | 0.361764 | 0.917055 |
| C | 0.587259 | 1.199034 | 0.612043 |
| C | 0.781258 | 2.577313 | 0.459913 |
| C | 2.073885 | 3.070049 | 0.620924 |
| C | 3.156511 | 2.22836 | 0.928872 |
| C | 2.992176 | 0.846886 | 1.086213 |
| C | -0.175816 | -0.819539 | 0.760356 |
| H | -0.048969 | 3.231254 | 0.222734 |
| H | 2.256553 | 4.131793 | 0.505466 |
| H | 4.144159 | 2.661027 | 1.036227 |
| C | -2.457463 | -1.726367 | 0.511476 |
| C | -3.422329 | -2.771591 | 0.513707 |
| C | -3.031633 | -4.093691 | 0.780862 |
| C | -1.686896 | -4.314528 | 1.034131 |
| C | -0.734355 | -3.268717 | 1.029245 |
| C | -1.092581 | -1.946301 | 0.771582 |
| C | -4.454516 | -0.910681 | 0.048987 |
| H | -3.755302 | -4.898672 | 0.786894 |
| H | -1.343566 | -5.319447 | 1.245453 |
| H | 0.301583 | -3.509219 | 1.234449 |
| N | -0.56263 | 0.432344 | 0.522127 |
| C | -6.865163 | -0.574484 | -0.430357 |
| C | -5.526322 | -0.015226 | -0.283247 |
| C | -5.326245 | 1.348937 | -0.466756 |
| C | -6.392165 | 2.185937 | -0.79247 |
| C | -7.695144 | 1.612193 | -0.928495 |
| C | -7.976947 | 0.278642 | -0.760882 |
| H | -4.329455 | 1.752444 | -0.360179 |
| H | -8.504791 | 2.280429 | -1.180295 |
| C | -6.230046 | 3.680577 | -1.012574 |
| C | -9.389126 | -0.290113 | -0.910883 |
| O | -7.061045 | -1.851551 | -0.263356 |
| H | -6.149231 | -2.309657 | -0.030923 |
| N | -3.137661 | -0.578505 | 0.217569 |
| N | -4.646336 | -2.227914 | 0.225349 |
| H | -2.66262 | 0.320861 | 0.161308 |
| N | 1.170722 | -0.908587 | 1.001906 |
| H | 1.748706 | -1.719982 | 1.192281 |
| C | 4.070961 | -0.070391 | 1.412813 |
| N | 3.935711 | -1.395031 | 1.455332 |
| N | 5.351149 | 0.327495 | 1.712416 |
| C | 7.428833 | -0.969099 | 2.330569 |
| C | 7.853077 | -2.290988 | 2.508251 |
| C | 6.979725 | -3.379393 | 2.33432 |
| C | 5.644065 | -3.196506 | 1.979771 |
| C | 5.188533 | -1.88433 | 1.795467 |
| C | 6.084172 | -0.804011 | 1.96594 |
| H | 8.884109 | -2.473742 | 2.791689 |
| H | 7.35705 | -4.38397 | 2.484442 |
| H | 4.973665 | -4.038513 | 1.856276 |
| H | 5.750776 | 1.255507 | 1.797534 |
| C | 8.320415 | 0.171532 | 2.531401 |
| H | 9.352001 | -0.078248 | 2.792875 |
| N | 7.901059 | 1.37642 | 2.414537 |
| C | 8.814559 | 2.500511 | 2.623062 |
| C | 10.267968 | 2.166125 | 2.976745 |
| C | 8.752164 | 3.410805 | 1.385044 |
| H | 8.388489 | 3.072323 | 3.460435 |
| C | 11.090846 | 3.442544 | 3.185458 |
| H | 10.708468 | 1.577679 | 2.162488 |
| H | 10.304669 | 1.543792 | 3.876337 |
| C | 9.578409 | 4.685121 | 1.586077 |
| H | 9.138058 | 2.849257 | 0.525241 |
| H | 7.706634 | 3.65187 | 1.169926 |
| C | 11.028828 | 4.359772 | 1.959519 |
| H | 12.12859 | 3.18036 | 3.413937 |
| H | 10.703031 | 3.982537 | 4.058361 |
| H | 9.546556 | 5.298528 | 0.680359 |
| H | 9.12697 | 5.281368 | 2.388822 |
| H | 11.586158 | 5.282382 | 2.149875 |
| H | 11.515951 | 3.860104 | 1.112788 |
| C | -6.685369 | 4.022195 | -2.450814 |
| H | -7.72299 | 3.735241 | -2.632275 |
| H | -6.600659 | 5.101277 | -2.601974 |
| H | -6.053716 | 3.51953 | -3.186585 |
| C | -7.124903 | 4.433955 | -0.000992 |
| H | -7.019185 | 5.509076 | -0.16515 |
| H | -8.179858 | 4.176727 | -0.115206 |
| H | -6.823093 | 4.211327 | 1.024918 |
| C | -4.780006 | 4.146408 | -0.831349 |
| H | -4.418788 | 3.956864 | 0.182534 |
| H | -4.106444 | 3.65436 | -1.537307 |
| H | -4.723383 | 5.221842 | -1.010553 |
| C | -9.415464 | -1.329564 | -2.052973 |
| H | -8.729265 | -2.154076 | -1.866168 |
| H | -10.427027 | -1.733096 | -2.145576 |
| H | -9.148057 | -0.860107 | -3.003169 |
| C | -10.395511 | 0.817707 | -1.255115 |
| H | -10.440315 | 1.579446 | -0.472201 |
| H | -10.149592 | 1.308101 | -2.200405 |
| H | -11.389654 | 0.376978 | -1.352606 |
| C | -9.834112 | -0.943758 | 0.416199 |
| H | -9.189509 | -1.775767 | 0.697028 |
| H | -9.828947 | -0.20831 | 1.225054 |
| H | -10.853691 | -1.32036 | 0.303823 |

Table S#. Cartesian coordinates for triBIP-cyclohexylimine: E1PT. (-2086.29343325 Hartrees)

|  |  |  |  |
| --- | --- | --- | --- |
| atom | x | y | z |
| C | 1.614824 | 0.282626 | 1.100875 |
| C | 0.50204 | 1.104017 | 0.804249 |
| C | 0.671437 | 2.487186 | 0.666569 |
| C | 1.955459 | 3.000159 | 0.831828 |
| C | 3.053265 | 2.173613 | 1.128226 |
| C | 2.912826 | 0.788286 | 1.271886 |
| C | -0.22326 | -0.93065 | 0.924476 |
| H | -0.170602 | 3.128585 | 0.436249 |
| H | 2.119829 | 4.065994 | 0.727692 |
| H | 4.033667 | 2.622098 | 1.239201 |
| C | -2.479831 | -1.86757 | 0.625047 |
| C | -3.412588 | -2.917874 | 0.594331 |
| C | -3.031368 | -4.236384 | 0.846418 |
| C | -1.684848 | -4.445862 | 1.130147 |
| C | -0.747994 | -3.395768 | 1.159293 |
| C | -1.12097 | -2.072625 | 0.910249 |
| C | -4.469599 | -0.999371 | 0.122409 |
| H | -3.746461 | -5.047836 | 0.824551 |
| H | -1.340592 | -5.451811 | 1.334329 |
| H | 0.286389 | -3.623296 | 1.384751 |
| N | -0.63266 | 0.317216 | 0.701599 |
| C | -6.872154 | -0.579852 | -0.46554 |
| C | -5.515645 | -0.068543 | -0.222763 |
| C | -5.236839 | 1.283151 | -0.323863 |
| C | -6.236085 | 2.204174 | -0.679801 |
| C | -7.543716 | 1.716751 | -0.939377 |
| C | -7.902614 | 0.391281 | -0.853928 |
| H | -4.234609 | 1.638648 | -0.127991 |
| H | -8.295692 | 2.439271 | -1.221849 |
| C | -5.964079 | 3.69779 | -0.796748 |
| C | -9.317264 | -0.08954 | -1.16101 |
| O | -7.121439 | -1.8054 | -0.345642 |
| N | -3.166989 | -0.710003 | 0.331273 |
| N | -4.624596 | -2.329458 | 0.280457 |
| H | -2.679924 | 0.186611 | 0.297035 |
| N | 1.123098 | -0.998071 | 1.169297 |
| H | 1.715934 | -1.800816 | 1.352701 |
| C | 4.00993 | -0.113375 | 1.578565 |
| N | 3.892142 | -1.439001 | 1.642855 |
| N | 5.294176 | 0.303183 | 1.828158 |
| C | 7.412624 | -0.958359 | 2.371441 |
| C | 7.861457 | -2.27218 | 2.547474 |
| C | 6.994121 | -3.373106 | 2.428972 |
| C | 5.64245 | -3.212382 | 2.127878 |
| C | 5.162495 | -1.908755 | 1.944164 |
| C | 6.051022 | -0.815836 | 2.0642 |
| H | 8.907546 | -2.438243 | 2.781249 |
| H | 7.390758 | -4.370747 | 2.576425 |
| H | 4.979526 | -4.064931 | 2.041335 |
| H | 5.690205 | 1.23571 | 1.873959 |
| C | 8.297251 | 0.198499 | 2.500169 |
| H | 9.343495 | -0.02687 | 2.723249 |
| N | 7.852997 | 1.3916 | 2.358774 |
| C | 8.749457 | 2.540515 | 2.477267 |
| C | 10.228508 | 2.256384 | 2.763596 |
| C | 8.599157 | 3.399014 | 1.210101 |
| H | 8.353241 | 3.134374 | 3.313587 |
| C | 11.021118 | 3.564099 | 2.883605 |
| H | 10.643516 | 1.651737 | 1.947132 |
| H | 10.331616 | 1.669555 | 3.682192 |
| C | 9.393751 | 4.70346 | 1.321609 |
| H | 8.961541 | 2.815726 | 0.354697 |
| H | 7.537433 | 3.600011 | 1.036856 |
| C | 10.870119 | 4.43028 | 1.628518 |
| H | 12.076736 | 3.342681 | 3.068782 |
| H | 10.658528 | 4.124411 | 3.7543 |
| H | 9.295558 | 5.279792 | 0.396362 |
| H | 8.965865 | 5.316158 | 2.125052 |
| H | 11.414524 | 5.372151 | 1.749678 |
| H | 11.322372 | 3.90695 | 0.776701 |
| H | -5.548068 | -2.741782 | 0.151909 |
| C | -9.269712 | -1.091594 | -2.338215 |
| H | -8.694496 | -1.977828 | -2.074189 |
| H | -10.287939 | -1.396381 | -2.594923 |
| H | -8.819302 | -0.627062 | -3.219384 |
| C | -10.238215 | 1.073084 | -1.559592 |
| H | -11.233422 | 0.676176 | -1.769253 |
| H | -10.333179 | 1.81099 | -0.758097 |
| H | -9.884751 | 1.585383 | -2.458162 |
| C | -9.922243 | -0.770651 | 0.087455 |
| H | -9.338156 | -1.639292 | 0.386842 |
| H | -9.964617 | -0.069444 | 0.924964 |
| H | -10.942679 | -1.092127 | -0.13764 |
| C | -6.268425 | 4.142905 | -2.245032 |
| H | -7.302724 | 3.931265 | -2.524577 |
| H | -6.107342 | 5.220123 | -2.334253 |
| H | -5.60922 | 3.636356 | -2.953794 |
| C | -6.896269 | 4.453622 | 0.176822 |
| H | -6.728926 | 5.528816 | 0.074773 |
| H | -7.949442 | 4.255241 | -0.032204 |
| H | -6.690564 | 4.168713 | 1.211187 |
| C | -4.510266 | 4.058138 | -0.461138 |
| H | -4.252688 | 3.777283 | 0.563397 |
| H | -3.805042 | 3.574602 | -1.142043 |
| H | -4.378624 | 5.13788 | -0.55671 |

Table S#. Cartesian coordinates for triBIP-cyclohexylimine: E2PT. (-2086.29902013 Hartrees)

|  |  |  |  |
| --- | --- | --- | --- |
| atom | x | y | z |
| C | 1.590076 | 0.353309 | 1.105904 |
| C | 0.492351 | 1.177945 | 0.812503 |
| C | 0.633962 | 2.557454 | 0.67219 |
| C | 1.919519 | 3.068944 | 0.838583 |
| C | 3.019434 | 2.246619 | 1.133778 |
| C | 2.885387 | 0.86105 | 1.276796 |
| C | -0.213832 | -0.944387 | 0.938511 |
| H | -0.211686 | 3.191796 | 0.441712 |
| H | 2.079306 | 4.134964 | 0.735069 |
| H | 3.997295 | 2.698653 | 1.245443 |
| C | -2.484304 | -1.84141 | 0.6231 |
| C | -3.387661 | -2.934367 | 0.591313 |
| C | -2.979665 | -4.244318 | 0.835453 |
| C | -1.628403 | -4.443541 | 1.120011 |
| C | -0.711583 | -3.382115 | 1.155355 |
| C | -1.118147 | -2.06508 | 0.912626 |
| C | -4.417542 | -1.020855 | 0.136819 |
| H | -3.678857 | -5.070455 | 0.808031 |
| H | -1.271294 | -5.446508 | 1.316902 |
| H | 0.327271 | -3.590642 | 1.378654 |
| N | -0.600436 | 0.329673 | 0.722078 |
| C | -6.842799 | -0.60309 | -0.456427 |
| C | -5.483757 | -0.102899 | -0.211715 |
| C | -5.201471 | 1.250854 | -0.316407 |
| C | -6.192369 | 2.175159 | -0.667828 |
| C | -7.506448 | 1.696029 | -0.92632 |
| C | -7.869415 | 0.373394 | -0.842298 |
| H | -4.190074 | 1.578375 | -0.122265 |
| H | -8.254886 | 2.423672 | -1.206294 |
| C | -5.915115 | 3.669325 | -0.781606 |
| C | -9.288102 | -0.101067 | -1.14902 |
| O | -7.104696 | -1.829519 | -0.342165 |
| N | -3.139247 | -0.669561 | 0.341904 |
| N | -4.599892 | -2.368266 | 0.281083 |
| N | 1.11327 | -0.943128 | 1.173115 |
| C | 3.976165 | -0.048739 | 1.581876 |
| N | 3.831799 | -1.371101 | 1.657056 |
| N | 5.268419 | 0.344844 | 1.816342 |
| C | 7.365048 | -0.954931 | 2.352861 |
| C | 7.787992 | -2.275529 | 2.535078 |
| C | 6.89702 | -3.360529 | 2.434395 |
| C | 5.547415 | -3.176832 | 2.143046 |
| C | 5.093317 | -1.864573 | 1.951695 |
| C | 6.003737 | -0.788399 | 2.054525 |
| H | 8.831818 | -2.461089 | 2.763678 |
| H | 7.275921 | -4.364063 | 2.587369 |
| H | 4.866719 | -4.01637 | 2.069412 |
| C | 8.271161 | 0.186719 | 2.472751 |
| H | 9.31342 | -0.055712 | 2.696045 |
| N | 7.845137 | 1.386151 | 2.329888 |
| C | 8.756791 | 2.522264 | 2.456255 |
| C | 10.230957 | 2.21656 | 2.744199 |
| C | 8.620235 | 3.394279 | 1.197032 |
| H | 8.366469 | 3.114047 | 3.296901 |
| C | 11.037725 | 3.513639 | 2.881653 |
| H | 10.641782 | 1.615897 | 1.922677 |
| H | 10.323367 | 1.618808 | 3.656847 |
| C | 9.429924 | 4.688145 | 1.324462 |
| H | 8.978007 | 2.815412 | 0.336744 |
| H | 7.561478 | 3.610189 | 1.023471 |
| C | 10.901751 | 4.395594 | 1.635753 |
| H | 12.0899 | 3.278187 | 3.068716 |
| H | 10.677712 | 4.068161 | 3.757125 |
| H | 9.343141 | 5.274637 | 0.404349 |
| H | 9.005162 | 5.29788 | 2.131818 |
| H | 11.45489 | 5.330499 | 1.770534 |
| H | 11.352947 | 3.877322 | 0.780308 |
| H | -1.580292 | 0.545535 | 0.516636 |
| H | -5.515798 | -2.787873 | 0.147649 |
| H | 1.737346 | -1.726651 | 1.360575 |
| H | 5.689365 | 1.267912 | 1.850279 |
| C | -9.248969 | -1.09888 | -2.32946 |
| H | -8.67235 | -1.985926 | -2.071166 |
| H | -10.268345 | -1.402843 | -2.583722 |
| H | -8.802008 | -0.631607 | -3.211162 |
| C | -10.205549 | 1.0662 | -1.54256 |
| H | -11.203314 | 0.674855 | -1.751737 |
| H | -10.295234 | 1.802486 | -0.73887 |
| H | -9.851195 | 1.580211 | -2.439877 |
| C | -9.895604 | -0.782897 | 0.097174 |
| H | -9.311168 | -1.651693 | 0.395491 |
| H | -9.936945 | -0.082734 | 0.935857 |
| H | -10.916738 | -1.103794 | -0.126782 |
| C | -6.222936 | 4.124135 | -2.225421 |
| H | -7.258799 | 3.916115 | -2.50229 |
| H | -6.059635 | 5.201475 | -2.312244 |
| H | -5.568269 | 3.618522 | -2.939327 |
| C | -6.837215 | 4.426649 | 0.199678 |
| H | -6.667023 | 5.502185 | 0.103232 |
| H | -7.892424 | 4.233066 | -0.004193 |
| H | -6.627858 | 4.135409 | 1.23172 |
| C | -4.457741 | 4.020198 | -0.451412 |
| H | -4.197621 | 3.730977 | 0.570119 |
| H | -3.759671 | 3.532939 | -1.137082 |
| H | -4.318358 | 5.099707 | -0.542347 |

Table S#. Cartesian coordinates for triBIP-cyclohexylimine: E3PT. (-2086.30288096 Hartrees)

|  |  |  |  |
| --- | --- | --- | --- |
| atom | x | y | z |
| C | 1.596536 | 0.409325 | 1.107915 |
| C | 0.512513 | 1.270575 | 0.806546 |
| C | 0.669602 | 2.646846 | 0.674798 |
| C | 1.956833 | 3.159702 | 0.854289 |
| C | 3.046402 | 2.333488 | 1.15454 |
| C | 2.891325 | 0.945378 | 1.286021 |
| C | -0.144983 | -0.846332 | 0.931189 |
| H | -0.168067 | 3.291836 | 0.440843 |
| H | 2.119135 | 4.226003 | 0.757651 |
| H | 4.023834 | 2.7817 | 1.282101 |
| C | -2.431903 | -1.780219 | 0.602381 |
| C | -3.311364 | -2.894303 | 0.562873 |
| C | -2.877321 | -4.198679 | 0.798545 |
| C | -1.523295 | -4.36641 | 1.082825 |
| C | -0.632158 | -3.280615 | 1.125626 |
| C | -1.060799 | -1.971543 | 0.892163 |
| C | -4.386471 | -1.002861 | 0.117645 |
| H | -3.558906 | -5.039178 | 0.764048 |
| H | -1.141423 | -5.362195 | 1.273167 |
| H | 0.414116 | -3.451793 | 1.344681 |
| N | -0.575294 | 0.432823 | 0.70544 |
| C | -6.821986 | -0.639363 | -0.472993 |
| C | -5.474724 | -0.109438 | -0.225118 |
| C | -5.225301 | 1.253087 | -0.322134 |
| C | -6.236108 | 2.154369 | -0.668622 |
| C | -7.539063 | 1.645395 | -0.932307 |
| C | -7.870342 | 0.314625 | -0.855918 |
| H | -4.222023 | 1.602144 | -0.123663 |
| H | -8.303788 | 2.357006 | -1.209823 |
| C | -5.99413 | 3.655679 | -0.774989 |
| C | -9.277937 | -0.191981 | -1.165245 |
| O | -7.056781 | -1.872289 | -0.363379 |
| N | -3.118646 | -0.622202 | 0.325139 |
| N | -4.536867 | -2.356437 | 0.255044 |
| N | 1.167087 | -0.89763 | 1.179074 |
| C | 3.981818 | 0.054196 | 1.591617 |
| N | 3.842619 | -1.28528 | 1.689921 |
| N | 5.276655 | 0.35408 | 1.819952 |
| C | 7.337154 | -0.998425 | 2.363971 |
| C | 7.731822 | -2.325548 | 2.55766 |
| C | 6.817846 | -3.391551 | 2.473737 |
| C | 5.469542 | -3.188983 | 2.186274 |
| C | 5.066008 | -1.868357 | 1.986021 |
| C | 5.980648 | -0.808118 | 2.068399 |
| H | 8.771348 | -2.531728 | 2.785534 |
| H | 7.174932 | -4.400847 | 2.636374 |
| H | 4.76868 | -4.011011 | 2.124231 |
| C | 8.25891 | 0.13452 | 2.472607 |
| H | 9.298519 | -0.115339 | 2.695666 |
| N | 7.836485 | 1.333446 | 2.323783 |
| C | 8.747704 | 2.470194 | 2.445384 |
| C | 10.221561 | 2.162277 | 2.729495 |
| C | 8.606114 | 3.341797 | 1.18659 |
| H | 8.357426 | 3.059954 | 3.28704 |
| C | 11.028445 | 3.459469 | 2.866185 |
| H | 10.629885 | 1.562489 | 1.906105 |
| H | 10.315756 | 1.564212 | 3.641694 |
| C | 9.416257 | 4.635447 | 1.314321 |
| H | 8.962252 | 2.764016 | 0.325111 |
| H | 7.546875 | 3.558148 | 1.016542 |
| C | 10.888883 | 4.342637 | 1.621552 |
| H | 12.080895 | 3.223375 | 3.050081 |
| H | 10.670743 | 4.012603 | 3.743387 |
| H | 9.326874 | 5.22259 | 0.395031 |
| H | 8.993102 | 5.243913 | 2.123369 |
| H | 11.441785 | 5.277572 | 1.756286 |
| H | 11.338204 | 3.825646 | 0.764406 |
| H | 2.923611 | -1.718731 | 1.555333 |
| H | -1.549383 | 0.648876 | 0.495146 |
| H | -5.441314 | -2.797775 | 0.118639 |
| H | 5.756071 | 1.253414 | 1.842896 |
| C | -9.215986 | -1.191455 | -2.34322 |
| H | -8.618047 | -2.063361 | -2.082391 |
| H | -10.227799 | -1.520817 | -2.59631 |
| H | -8.781105 | -0.715536 | -3.226401 |
| C | -10.220014 | 0.953842 | -1.563618 |
| H | -10.328394 | 1.689872 | -0.762048 |
| H | -9.873452 | 1.473421 | -2.460916 |
| H | -11.208743 | 0.541198 | -1.775387 |
| C | -9.871232 | -0.884159 | 0.081859 |
| H | -9.263672 | -1.735191 | 0.38583 |
| H | -9.933123 | -0.181336 | 0.917147 |
| H | -10.882559 | -1.234505 | -0.142751 |
| C | -6.306379 | 4.109621 | -2.217967 |
| H | -7.337216 | 3.882245 | -2.498543 |
| H | -6.163684 | 5.190228 | -2.301258 |
| H | -5.640253 | 3.619413 | -2.931969 |
| C | -6.93774 | 4.387973 | 0.204387 |
| H | -6.789072 | 5.467474 | 0.115965 |
| H | -7.987368 | 4.173826 | -0.007955 |
| H | -6.729379 | 4.094687 | 1.236027 |
| C | -4.546379 | 4.038264 | -0.437361 |
| H | -4.285162 | 3.754294 | 0.585361 |
| H | -3.834639 | 3.565731 | -1.119318 |
| H | -4.428915 | 5.120398 | -0.527469 |

Table S#. Cartesian coordinates for triBIP-cyclohexylimine: E4PT. (-2086.31247864 Hartrees)

|  |  |  |  |
| --- | --- | --- | --- |
| atom | x | y | z |
| C | 1.604844 | 0.342192 | 1.143316 |
| C | 0.532362 | 1.214834 | 0.830867 |
| C | 0.703427 | 2.590103 | 0.690696 |
| C | 1.995276 | 3.087488 | 0.871799 |
| C | 3.072571 | 2.246059 | 1.181922 |
| C | 2.90449 | 0.862822 | 1.323041 |
| C | -0.15302 | -0.893168 | 0.964898 |
| H | -0.127128 | 3.241678 | 0.4492 |
| H | 2.171002 | 4.151587 | 0.769096 |
| H | 4.063571 | 2.661969 | 1.313863 |
| C | -2.45256 | -1.800755 | 0.626472 |
| C | -3.346813 | -2.903666 | 0.591933 |
| C | -2.932565 | -4.21171 | 0.843294 |
| C | -1.582927 | -4.393911 | 1.137545 |
| C | -0.677271 | -3.319364 | 1.175072 |
| C | -1.085682 | -2.006655 | 0.927679 |
| C | -4.394612 | -1.002596 | 0.123099 |
| H | -3.625716 | -5.042896 | 0.812812 |
| H | -1.21525 | -5.392741 | 1.339843 |
| H | 0.36528 | -3.502932 | 1.401743 |
| N | -0.566337 | 0.391091 | 0.729067 |
| C | -6.822926 | -0.611006 | -0.478253 |
| C | -5.468898 | -0.097712 | -0.2322 |
| C | -5.199856 | 1.260589 | -0.341423 |
| C | -6.197082 | 2.172494 | -0.69728 |
| C | -7.507509 | 1.67969 | -0.955856 |
| C | -7.857801 | 0.35473 | -0.867917 |
| H | -4.191491 | 1.596592 | -0.145931 |
| H | -8.262195 | 2.399393 | -1.239901 |
| C | -5.934537 | 3.669095 | -0.819181 |
| C | -9.272198 | -0.134051 | -1.175052 |
| O | -7.074293 | -1.840216 | -0.361922 |
| N | -3.123466 | -0.636554 | 0.334467 |
| N | -4.56333 | -2.353152 | 0.271485 |
| N | 1.154485 | -0.96128 | 1.220378 |
| C | 4.016652 | -0.010783 | 1.640127 |
| N | 3.858344 | -1.364953 | 1.743326 |
| N | 5.28492 | 0.363604 | 1.858379 |
| C | 7.330595 | -0.998773 | 2.407874 |
| C | 7.769664 | -2.320286 | 2.614394 |
| C | 6.885358 | -3.399416 | 2.540184 |
| C | 5.527168 | -3.216551 | 2.251387 |
| C | 5.08627 | -1.913868 | 2.042226 |
| C | 5.962174 | -0.802679 | 2.109382 |
| H | 8.81544 | -2.495229 | 2.838255 |
| H | 7.259304 | -4.401487 | 2.708227 |
| H | 4.84818 | -4.058293 | 2.196119 |
| C | 8.244206 | 0.098278 | 2.507746 |
| H | 9.284985 | -0.098539 | 2.737241 |
| N | 7.877901 | 1.33346 | 2.346072 |
| C | 8.722076 | 2.534033 | 2.434866 |
| C | 10.191668 | 2.225119 | 2.705817 |
| C | 8.543776 | 3.364325 | 1.156961 |
| H | 8.320742 | 3.110005 | 3.276647 |
| C | 10.986705 | 3.533889 | 2.80917 |
| H | 10.590503 | 1.617522 | 1.884335 |
| H | 10.296919 | 1.647068 | 3.62865 |
| C | 9.339986 | 4.669398 | 1.260983 |
| H | 8.900378 | 2.773708 | 0.306185 |
| H | 7.480873 | 3.568555 | 0.99606 |
| C | 10.819358 | 4.394506 | 1.552111 |
| H | 12.041962 | 3.303938 | 2.978772 |
| H | 10.638626 | 4.094908 | 3.684367 |
| H | 9.22981 | 5.238573 | 0.333939 |
| H | 8.918458 | 5.283668 | 2.065724 |
| H | 11.363823 | 5.336438 | 1.665915 |
| H | 11.261917 | 3.869178 | 0.697063 |
| H | 6.882607 | 1.479253 | 2.125144 |
| H | 2.951443 | -1.814538 | 1.613233 |
| H | -1.535219 | 0.619805 | 0.512439 |
| H | -5.472586 | -2.784224 | 0.135154 |
| C | -9.222821 | -1.135623 | -2.351643 |
| H | -8.637116 | -2.01534 | -2.08896 |
| H | -10.238684 | -1.451451 | -2.60593 |
| H | -8.779722 | -0.667146 | -3.234709 |
| C | -6.243692 | 4.112844 | -2.266081 |
| H | -7.277642 | 3.895225 | -2.542983 |
| H | -6.088388 | 5.190868 | -2.360042 |
| H | -5.584515 | 3.6076 | -2.976145 |
| C | -10.199857 | 1.023152 | -1.574367 |
| H | -10.297025 | 1.762136 | -0.773983 |
| H | -9.848782 | 1.536759 | -2.473296 |
| H | -11.194084 | 0.622529 | -1.783322 |
| C | -9.87525 | -0.817127 | 0.07239 |
| H | -9.280519 | -1.67704 | 0.376339 |
| H | -9.926793 | -0.11351 | 0.907691 |
| H | -10.891942 | -1.151921 | -0.151907 |
| C | -6.865428 | 4.42408 | 0.155179 |
| H | -6.704131 | 5.50061 | 0.05379 |
| H | -7.918478 | 4.220657 | -0.050627 |
| H | -6.656813 | 4.140181 | 1.189476 |
| C | -4.481145 | 4.03559 | -0.488424 |
| H | -4.221109 | 3.757044 | 0.536099 |
| H | -3.777356 | 3.547957 | -1.167917 |
| H | -4.350227 | 5.115435 | -0.58823 |