Table S#. Cartesian coordinates for monoBIP-cyclohexylimine: neutral. (-1328.99836749 Hartrees)

|  |  |  |  |
| --- | --- | --- | --- |
| atom | x | y | z |
| C | -0.483053 | 2.715584 | 0.416145 |
| C | -1.881052 | 2.898359 | 0.327601 |
| C | -2.412894 | 4.190122 | 0.243421 |
| C | -1.520456 | 5.261988 | 0.256277 |
| C | -0.133595 | 5.064531 | 0.350314 |
| C | 0.427051 | 3.782688 | 0.429804 |
| C | -1.518543 | 0.752015 | 0.424651 |
| H | -3.482079 | 4.346339 | 0.169021 |
| H | -1.905266 | 6.273153 | 0.194132 |
| H | 0.529539 | 5.922761 | 0.360617 |
| N | -2.496427 | 1.656282 | 0.336302 |
| C | -3.063668 | -1.189037 | 0.352314 |
| C | -1.739219 | -0.685003 | 0.447265 |
| C | -0.658724 | -1.573623 | 0.540497 |
| C | -0.848757 | -2.950289 | 0.541355 |
| C | -2.167874 | -3.417641 | 0.446447 |
| C | -3.286126 | -2.585001 | 0.353326 |
| H | 0.347044 | -1.175374 | 0.612680 |
| H | -2.332312 | -4.483825 | 0.445491 |
| C | 0.361420 | -3.887798 | 0.614442 |
| C | -4.705200 | -3.167413 | 0.253385 |
| O | -4.117255 | -0.346876 | 0.257497 |
| H | -3.767809 | 0.591511 | 0.268641 |
| N | -0.287014 | 1.356600 | 0.476439 |
| H | 0.638260 | 0.947632 | 0.528152 |
| C | 1.869640 | 3.577070 | 0.516071 |
| H | 2.471751 | 4.490981 | 0.533986 |
| N | 2.383342 | 2.403646 | 0.562666 |
| C | 3.846217 | 2.273148 | 0.605015 |
| C | 4.417796 | 2.330347 | -0.823282 |
| C | 4.574369 | 3.275291 | 1.514632 |
| H | 4.045818 | 1.268606 | 0.997125 |
| C | 5.930590 | 2.085737 | -0.826620 |
| H | 4.198843 | 3.321293 | -1.239881 |
| H | 3.906197 | 1.596844 | -1.453374 |
| C | 6.083737 | 3.008000 | 1.520530 |
| H | 4.402404 | 4.296059 | 1.156042 |
| H | 4.163006 | 3.214757 | 2.526856 |
| C | 6.660178 | 3.063293 | 0.101127 |
| H | 6.316771 | 2.164127 | -1.847368 |
| H | 6.127826 | 1.059566 | -0.492795 |
| H | 6.585310 | 3.735122 | 2.166713 |
| H | 6.276761 | 2.017185 | 1.950502 |
| H | 7.732058 | 2.843665 | 0.116826 |
| H | 6.551014 | 4.082402 | -0.290657 |
| C | 1.245777 | -3.654521 | -0.627285 |
| H | 1.575562 | -2.614306 | -0.683508 |
| H | 2.133816 | -4.292376 | -0.588643 |
| H | 0.697384 | -3.887082 | -1.544179 |
| C | 1.182786 | -3.575549 | 1.880731 |
| H | 0.588653 | -3.743887 | 2.782861 |
| H | 2.064321 | -4.221634 | 1.926387 |
| H | 1.524899 | -2.537627 | 1.887374 |
| C | -0.049460 | -5.366088 | 0.652100 |
| H | -0.664682 | -5.591665 | 1.527396 |
| H | -0.608161 | -5.652070 | -0.243331 |
| H | 0.845240 | -5.991639 | 0.701283 |
| C | -5.359002 | -2.732161 | -1.075251 |
| H | -6.372934 | -3.138229 | -1.139958 |
| H | -5.413698 | -1.647265 | -1.155355 |
| H | -4.786354 | -3.113816 | -1.925275 |
| C | -5.557474 | -2.682549 | 1.445687 |
| H | -5.658132 | -1.598206 | 1.446625 |
| H | -6.556546 | -3.125767 | 1.394151 |
| H | -5.097957 | -2.986879 | 2.390277 |
| C | -4.694231 | -4.704659 | 0.283816 |
| H | -4.126052 | -5.123400 | -0.551056 |
| H | -4.268835 | -5.089758 | 1.214382 |
| H | -5.721459 | -5.069139 | 0.207540 |

Table S#. Cartesian coordinates for monoBIP-cyclohexylimine: E0PT. (-1328.80078256 Hartrees)

|  |  |  |  |
| --- | --- | --- | --- |
| atom | x | y | z |
| C | -0.439440 | 2.706702 | 0.233437 |
| C | -1.853311 | 2.850428 | 0.181340 |
| C | -2.429226 | 4.130552 | 0.090664 |
| C | -1.563901 | 5.212027 | 0.063520 |
| C | -0.157618 | 5.052289 | 0.121858 |
| C | 0.445060 | 3.799185 | 0.207637 |
| C | -1.402749 | 0.722167 | 0.305223 |
| H | -3.503059 | 4.256798 | 0.044728 |
| H | -1.968018 | 6.214719 | -0.002494 |
| H | 0.472399 | 5.934041 | 0.100720 |
| N | -2.415280 | 1.603316 | 0.228748 |
| C | -2.999650 | -1.174786 | 0.386006 |
| C | -1.621065 | -0.695104 | 0.370601 |
| C | -0.574464 | -1.613381 | 0.410639 |
| C | -0.831237 | -2.980675 | 0.474553 |
| C | -2.191578 | -3.420842 | 0.513391 |
| C | -3.278998 | -2.583328 | 0.479802 |
| H | 0.445112 | -1.255711 | 0.389146 |
| H | -2.365061 | -4.484469 | 0.574653 |
| C | 0.269738 | -4.027582 | 0.492357 |
| C | -4.717358 | -3.103367 | 0.531321 |
| O | -3.988374 | -0.329443 | 0.309942 |
| H | -3.605028 | 0.640678 | 0.257613 |
| N | -0.193794 | 1.365944 | 0.309553 |
| H | 0.759381 | 1.012910 | 0.363181 |
| C | 1.893310 | 3.609600 | 0.268696 |
| H | 2.499635 | 4.519893 | 0.229757 |
| N | 2.395102 | 2.434920 | 0.362530 |
| C | 3.858521 | 2.306049 | 0.420645 |
| C | 4.523200 | 2.728347 | -0.900440 |
| C | 4.480820 | 3.069454 | 1.601497 |
| H | 4.060451 | 1.239359 | 0.569807 |
| C | 6.037375 | 2.498321 | -0.842440 |
| H | 4.315097 | 3.791488 | -1.070852 |
| H | 4.076671 | 2.173459 | -1.730843 |
| C | 5.994034 | 2.833810 | 1.663334 |
| H | 4.288400 | 4.141430 | 1.475245 |
| H | 3.996318 | 2.762428 | 2.532841 |
| C | 6.669576 | 3.231840 | 0.345642 |
| H | 6.501609 | 2.815720 | -1.780936 |
| H | 6.229190 | 1.422408 | -0.744130 |
| H | 6.422655 | 3.395072 | 2.499215 |
| H | 6.185828 | 1.772057 | 1.862442 |
| H | 7.743456 | 3.026819 | 0.391654 |
| H | 6.557747 | 4.313665 | 0.199753 |
| C | -5.445873 | -2.513320 | 1.759564 |
| H | -5.512598 | -1.427384 | 1.707410 |
| H | -6.459874 | -2.919027 | 1.801482 |
| H | -4.930297 | -2.789100 | 2.682986 |
| C | -4.745119 | -4.634511 | 0.658226 |
| H | -5.784161 | -4.965060 | 0.709220 |
| H | -4.278356 | -5.125191 | -0.199970 |
| H | -4.238938 | -4.972103 | 1.566425 |
| C | -5.460758 | -2.714377 | -0.765995 |
| H | -5.548313 | -1.633984 | -0.873552 |
| H | -4.938023 | -3.110790 | -1.640021 |
| H | -6.466519 | -3.141702 | -0.745004 |
| C | 0.115348 | -4.901007 | 1.758254 |
| H | -0.853380 | -5.403221 | 1.792669 |
| H | 0.893241 | -5.668761 | 1.758513 |
| H | 0.224080 | -4.298236 | 2.662557 |
| C | 1.671192 | -3.405321 | 0.488863 |
| H | 1.842969 | -2.805151 | -0.407908 |
| H | 1.833030 | -2.775727 | 1.367253 |
| H | 2.417216 | -4.202656 | 0.504637 |
| C | 0.113216 | -4.917393 | -0.763085 |
| H | 0.882649 | -5.693537 | -0.748728 |
| H | -0.862473 | -5.406452 | -0.794656 |
| H | 0.233535 | -4.328006 | -1.674794 |

Table S#. Cartesian coordinates for monoBIP-cyclohexylimine: E1PT. (-1328.81564424 Hartrees)

|  |  |  |  |
| --- | --- | --- | --- |
| atom | x | y | z |
| C | -0.500700 | 2.795099 | 0.366564 |
| C | -1.888756 | 2.988755 | 0.285152 |
| C | -2.439117 | 4.269532 | 0.195180 |
| C | -1.539354 | 5.331386 | 0.197421 |
| C | -0.147530 | 5.133655 | 0.282622 |
| C | 0.414372 | 3.857939 | 0.366325 |
| C | -1.472879 | 0.789421 | 0.397006 |
| H | -3.507434 | 4.423448 | 0.125656 |
| H | -1.920620 | 6.342852 | 0.132039 |
| H | 0.511075 | 5.994513 | 0.282171 |
| N | -2.443276 | 1.720964 | 0.307419 |
| C | -3.051167 | -1.165079 | 0.324995 |
| C | -1.681522 | -0.639533 | 0.436730 |
| C | -0.608879 | -1.496606 | 0.563803 |
| C | -0.787015 | -2.897044 | 0.585282 |
| C | -2.095986 | -3.411943 | 0.477239 |
| C | -3.223380 | -2.622391 | 0.349004 |
| H | 0.395795 | -1.102185 | 0.650899 |
| H | -2.218517 | -4.483276 | 0.495940 |
| C | 0.439552 | -3.791576 | 0.699391 |
| C | -4.620524 | -3.224009 | 0.230773 |
| O | -4.026144 | -0.380290 | 0.211266 |
| N | -0.287163 | 1.435613 | 0.433712 |
| H | 0.662886 | 1.069181 | 0.482507 |
| C | 1.855667 | 3.620564 | 0.438970 |
| H | 2.487593 | 4.512926 | 0.429056 |
| N | 2.319926 | 2.428818 | 0.504615 |
| C | 3.776936 | 2.240335 | 0.536736 |
| C | 4.373273 | 2.434557 | -0.868008 |
| C | 4.511964 | 3.116880 | 1.562939 |
| H | 3.936810 | 1.194257 | 0.820326 |
| C | 5.875025 | 2.129741 | -0.872772 |
| H | 4.202597 | 3.474257 | -1.173386 |
| H | 3.843548 | 1.797243 | -1.582001 |
| C | 6.011139 | 2.797698 | 1.565411 |
| H | 4.372407 | 4.175044 | 1.314526 |
| H | 4.078484 | 2.957532 | 2.554789 |
| C | 6.620745 | 2.970221 | 0.169900 |
| H | 6.285843 | 2.309867 | -1.870635 |
| H | 6.025716 | 1.064803 | -0.656505 |
| H | 6.525113 | 3.438601 | 2.287819 |
| H | 6.157286 | 1.763038 | 1.900122 |
| H | 7.681306 | 2.701871 | 0.183810 |
| H | 6.564094 | 4.027534 | -0.117509 |
| H | -3.417409 | 1.425694 | 0.257575 |
| C | -5.508812 | -2.709140 | 1.386591 |
| H | -5.627835 | -1.628402 | 1.339394 |
| H | -6.494993 | -3.175805 | 1.317385 |
| H | -5.072553 | -2.972996 | 2.353618 |
| C | -4.585105 | -4.758692 | 0.305618 |
| H | -3.994593 | -5.192688 | -0.505392 |
| H | -4.175341 | -5.106811 | 1.257247 |
| H | -5.604931 | -5.138941 | 0.219065 |
| C | 0.080920 | -5.282855 | 0.729016 |
| H | -0.539622 | -5.533050 | 1.593350 |
| H | -0.446737 | -5.587369 | -0.178160 |
| H | 0.999174 | -5.869919 | 0.794722 |
| C | 1.347725 | -3.520089 | -0.521647 |
| H | 0.833683 | -3.773873 | -1.451824 |
| H | 1.649485 | -2.471465 | -0.569562 |
| H | 2.250453 | -4.131637 | -0.448319 |
| C | 1.207268 | -3.438260 | 1.991994 |
| H | 0.587763 | -3.612041 | 2.874598 |
| H | 2.095175 | -4.070806 | 2.065117 |
| H | 1.534375 | -2.396151 | 1.998954 |
| C | -5.243062 | -2.825314 | -1.126819 |
| H | -6.240036 | -3.266669 | -1.206510 |
| H | -5.332081 | -1.744307 | -1.222704 |
| H | -4.637640 | -3.202658 | -1.954963 |

Table S#. Cartesian coordinates for monoBIP-cyclohexylimine: E2PT. (-1328.82800246 Hartrees)

|  |  |  |  |
| --- | --- | --- | --- |
| atom | x | y | z |
| C | -0.528073 | 2.742572 | 0.404197 |
| C | -1.921436 | 2.980419 | 0.301064 |
| C | -2.451704 | 4.265809 | 0.212852 |
| C | -1.550554 | 5.334546 | 0.236214 |
| C | -0.170901 | 5.128033 | 0.341490 |
| C | 0.373135 | 3.833989 | 0.422135 |
| C | -1.476384 | 0.809681 | 0.407582 |
| H | -3.518023 | 4.431858 | 0.127295 |
| H | -1.930374 | 6.346308 | 0.172118 |
| H | 0.499623 | 5.979267 | 0.359395 |
| N | -2.483178 | 1.726588 | 0.306580 |
| C | -3.060964 | -1.168598 | 0.322868 |
| C | -1.700320 | -0.624250 | 0.437828 |
| C | -0.618761 | -1.472146 | 0.564038 |
| C | -0.778274 | -2.871255 | 0.591400 |
| C | -2.082512 | -3.404573 | 0.481720 |
| C | -3.216356 | -2.628047 | 0.346212 |
| H | 0.371068 | -1.041120 | 0.641954 |
| H | -2.192376 | -4.477493 | 0.503258 |
| C | 0.459199 | -3.752098 | 0.713784 |
| C | -4.606812 | -3.245875 | 0.216236 |
| O | -4.050358 | -0.398428 | 0.206418 |
| N | -0.270650 | 1.400503 | 0.468577 |
| C | 1.787972 | 3.650514 | 0.503480 |
| H | 2.430179 | 4.524088 | 0.516824 |
| N | 2.355102 | 2.483039 | 0.555389 |
| C | 3.811698 | 2.240422 | 0.578233 |
| C | 4.374110 | 2.283257 | -0.851756 |
| C | 4.545498 | 3.216531 | 1.502221 |
| H | 3.920675 | 1.227482 | 0.972873 |
| C | 5.881885 | 2.008778 | -0.845664 |
| H | 4.175034 | 3.277269 | -1.268103 |
| H | 3.849587 | 1.555510 | -1.476661 |
| C | 6.049534 | 2.919561 | 1.503417 |
| H | 4.393648 | 4.242088 | 1.149431 |
| H | 4.129611 | 3.150194 | 2.510928 |
| C | 6.626406 | 2.971977 | 0.084535 |
| H | 6.267702 | 2.081106 | -1.866169 |
| H | 6.056732 | 0.978853 | -0.512923 |
| H | 6.556979 | 3.637847 | 2.153217 |
| H | 6.224463 | 1.925172 | 1.931036 |
| H | 7.692933 | 2.730728 | 0.101749 |
| H | 6.537202 | 3.994116 | -0.303449 |
| H | -3.454655 | 1.434506 | 0.245286 |
| H | 1.725533 | 1.671887 | 0.519365 |
| C | -5.220585 | -2.855122 | -1.147165 |
| H | -6.215850 | -3.299278 | -1.235630 |
| H | -5.310687 | -1.774484 | -1.246725 |
| H | -4.606579 | -3.232660 | -1.969068 |
| C | -5.513324 | -2.742357 | 1.361939 |
| H | -5.640604 | -1.662598 | 1.314981 |
| H | -6.494929 | -3.217532 | 1.282137 |
| H | -5.085021 | -3.003350 | 2.333502 |
| C | -4.556574 | -4.779951 | 0.292061 |
| H | -3.953177 | -5.208439 | -0.512409 |
| H | -4.152113 | -5.123254 | 1.247789 |
| H | -5.571438 | -5.171520 | 0.195653 |
| C | 0.118948 | -5.247457 | 0.757546 |
| H | -0.501333 | -5.496081 | 1.622661 |
| H | -0.404050 | -5.567051 | -0.147173 |
| H | 1.043267 | -5.824453 | 0.831086 |
| C | 1.222104 | -3.377016 | 2.002363 |
| H | 2.122267 | -3.991682 | 2.082176 |
| H | 1.527087 | -2.328136 | 1.998990 |
| H | 0.606277 | -3.554211 | 2.887099 |
| C | 1.365468 | -3.482177 | -0.508343 |
| H | 0.854895 | -3.749925 | -1.436629 |
| H | 1.651813 | -2.429646 | -0.565562 |
| H | 2.276450 | -4.081239 | -0.430712 |