**Table S#.** Cartesian coordinates for diBIP-cyclohexylimine: neutral. (-1707.73604777 Hartrees)

|  |  |  |  |
| --- | --- | --- | --- |
| atom | x | y | z |
| C | 1.579646 | 1.136284 | -0.019745 |
| C | 0.355893 | 1.840489 | -0.092226 |
| C | 0.362978 | 3.230381 | -0.262889 |
| C | 1.597756 | 3.869434 | -0.363470 |
| C | 2.804621 | 3.153702 | -0.289169 |
| C | 2.830903 | 1.763921 | -0.117108 |
| C | -0.137715 | -0.252300 | 0.152837 |
| H | -0.566227 | 3.784842 | -0.318110 |
| H | 1.632829 | 4.944331 | -0.496917 |
| H | 3.746349 | 3.685758 | -0.369261 |
| C | -2.294973 | -1.447086 | 0.243218 |
| C | -3.099072 | -2.606364 | 0.320701 |
| C | -2.500455 | -3.862028 | 0.462987 |
| C | -1.107351 | -3.913422 | 0.519312 |
| C | -0.317965 | -2.756965 | 0.426261 |
| C | -0.893110 | -1.486640 | 0.282551 |
| C | -4.442588 | -0.903056 | 0.118962 |
| H | -3.101625 | -4.760623 | 0.526456 |
| H | -0.615908 | -4.872186 | 0.634263 |
| H | 0.760516 | -2.852417 | 0.470382 |
| N | -0.698828 | 0.948693 | 0.021320 |
| C | -6.907407 | -0.758504 | -0.129589 |
| C | -5.652859 | -0.106102 | -0.004073 |
| C | -5.591059 | 1.295062 | 0.000445 |
| C | -6.737564 | 2.072803 | -0.112340 |
| C | -7.960695 | 1.398395 | -0.249255 |
| C | -8.087971 | 0.006995 | -0.264163 |
| H | -4.626123 | 1.777567 | 0.105101 |
| H | -8.860185 | 1.987260 | -0.342553 |
| C | -6.632765 | 3.602781 | -0.094821 |
| C | -9.460204 | -0.665236 | -0.425656 |
| O | -6.985743 | -2.108799 | -0.127919 |
| H | -6.064722 | -2.472012 | 0.014244 |
| N | -3.168783 | -0.393205 | 0.121262 |
| N | -4.431224 | -2.233015 | 0.236694 |
| H | -2.847068 | 0.564431 | 0.031955 |
| N | 1.235487 | -0.182725 | 0.137535 |
| H | 1.928737 | -0.918827 | 0.199437 |
| C | 4.081740 | 1.017629 | -0.038901 |
| H | 4.994280 | 1.618192 | -0.124222 |
| N | 4.104334 | -0.255385 | 0.116217 |
| C | 5.424452 | -0.904756 | 0.179755 |
| C | 6.223189 | -0.728433 | -1.122776 |
| C | 6.249245 | -0.433770 | 1.389520 |
| H | 5.232464 | -1.976407 | 0.307943 |
| C | 7.572009 | -1.451524 | -1.048620 |
| H | 6.391038 | 0.342368 | -1.290540 |
| H | 5.631004 | -1.096572 | -1.965785 |
| C | 7.597186 | -1.159373 | 1.459603 |
| H | 6.421442 | 0.645534 | 1.301154 |
| H | 5.674858 | -0.593491 | 2.306775 |
| C | 8.390516 | -0.984866 | 0.160142 |
| H | 8.129706 | -1.289658 | -1.976028 |
| H | 7.398311 | -2.532068 | -0.968534 |
| H | 8.172723 | -0.790951 | 2.314312 |
| H | 7.422579 | -2.228855 | 1.633580 |
| H | 9.334991 | -1.535121 | 0.214542 |
| H | 8.645678 | 0.075026 | 0.033517 |
| C | -5.823565 | 4.067776 | -1.322262 |
| H | -5.708832 | 5.155979 | -1.312118 |
| H | -4.825860 | 3.621147 | -1.327972 |
| H | -6.328601 | 3.784734 | -2.249842 |
| C | -5.907264 | 4.056108 | 1.187732 |
| H | -4.898761 | 3.639775 | 1.244164 |
| H | -5.821367 | 5.146489 | 1.207647 |
| H | -6.455869 | 3.738729 | 2.078624 |
| C | -8.012688 | 4.273603 | -0.131216 |
| H | -8.559145 | 4.020360 | -1.043486 |
| H | -8.621763 | 3.975402 | 0.726470 |
| H | -7.892483 | 5.359255 | -0.100500 |
| C | -9.472073 | -1.512027 | -1.715444 |
| H | -8.697785 | -2.278585 | -1.692806 |
| H | -10.443817 | -2.001634 | -1.830641 |
| H | -9.306983 | -0.876791 | -2.590095 |
| C | -9.764863 | -1.560093 | 0.795199 |
| H | -10.744141 | -2.031779 | 0.669086 |
| H | -9.015180 | -2.340198 | 0.915013 |
| H | -9.793595 | -0.960055 | 1.708980 |
| C | -10.594370 | 0.366618 | -0.531112 |
| H | -10.658891 | 0.990042 | 0.364579 |
| H | -10.472351 | 1.023477 | -1.396497 |
| H | -11.544965 | -0.160808 | -0.644661 |

**Table S#.** Cartesian coordinates for diBIP-cyclohexylimine: E0PT. (-1707.53809208 Hartrees)

|  |  |  |  |
| --- | --- | --- | --- |
| atom | x | y | z |
| C | 1.610101 | 1.119883 | -0.016592 |
| C | 0.387656 | 1.823096 | -0.110287 |
| C | 0.394710 | 3.214202 | -0.279632 |
| C | 1.629510 | 3.853350 | -0.353541 |
| C | 2.836706 | 3.137914 | -0.255890 |
| C | 2.862618 | 1.749108 | -0.088019 |
| C | -0.103131 | -0.271397 | 0.119371 |
| H | -0.533868 | 3.767138 | -0.354503 |
| H | 1.667300 | 4.928378 | -0.484298 |
| H | 3.778460 | 3.672297 | -0.314961 |
| C | -2.275850 | -1.433338 | 0.174278 |
| C | -3.111216 | -2.583342 | 0.225820 |
| C | -2.541321 | -3.860289 | 0.354030 |
| C | -1.158460 | -3.930605 | 0.424495 |
| C | -0.336480 | -2.780903 | 0.359909 |
| C | -0.871185 | -1.500346 | 0.226931 |
| C | -4.394122 | -0.832702 | 0.047233 |
| H | -3.161207 | -4.746075 | 0.396066 |
| H | -0.681793 | -4.897402 | 0.528314 |
| H | 0.737996 | -2.907235 | 0.417622 |
| N | -0.665704 | 0.928925 | -0.017998 |
| C | -6.863890 | -0.743781 | -0.156652 |
| C | -5.588834 | -0.044256 | -0.056591 |
| C | -5.562568 | 1.346985 | -0.066492 |
| C | -6.744588 | 2.077089 | -0.172470 |
| C | -7.980363 | 1.366129 | -0.289263 |
| C | -8.091217 | -0.003048 | -0.292257 |
| H | -4.611982 | 1.855483 | 0.014406 |
| H | -8.880074 | 1.956966 | -0.374776 |
| C | -6.779707 | 3.595639 | -0.158115 |
| C | -9.435184 | -0.719512 | -0.436069 |
| O | -6.895862 | -2.046517 | -0.124920 |
| H | -5.923588 | -2.409292 | -0.004699 |
| N | -3.111042 | -0.358834 | 0.066848 |
| N | -4.416139 | -2.172553 | 0.138836 |
| H | -2.744952 | 0.589115 | -0.006368 |
| N | 1.266954 | -0.201072 | 0.128893 |
| H | 1.964434 | -0.933313 | 0.203255 |
| C | 4.111998 | 1.001782 | 0.009376 |
| H | 5.026329 | 1.601080 | -0.059890 |
| N | 4.127943 | -0.271481 | 0.160363 |
| C | 5.445441 | -0.925356 | 0.238983 |
| C | 6.255362 | -0.751213 | -1.057132 |
| C | 6.260564 | -0.455195 | 1.455688 |
| H | 5.248440 | -1.996106 | 0.365956 |
| C | 7.602365 | -1.475987 | -0.971520 |
| H | 6.426131 | 0.319317 | -1.223561 |
| H | 5.669185 | -1.118262 | -1.904836 |
| C | 7.607012 | -1.182458 | 1.536398 |
| H | 6.435451 | 0.623749 | 1.368878 |
| H | 5.678669 | -0.613913 | 2.368429 |
| C | 8.411143 | -1.008744 | 0.243479 |
| H | 8.167328 | -1.315508 | -1.894690 |
| H | 7.426916 | -2.556250 | -0.891905 |
| H | 8.175962 | -0.814608 | 2.395630 |
| H | 7.430042 | -2.251724 | 1.709004 |
| H | 9.354823 | -1.559294 | 0.306033 |
| H | 8.667791 | 0.050935 | 0.118290 |
| C | -7.470514 | 4.095689 | -1.447673 |
| H | -8.490284 | 3.717250 | -1.539750 |
| H | -7.517707 | 5.186948 | -1.425971 |
| H | -6.909152 | 3.789816 | -2.333539 |
| C | -7.599160 | 4.051843 | 1.072452 |
| H | -7.684396 | 5.141438 | 1.062828 |
| H | -8.607614 | 3.632469 | 1.067684 |
| H | -7.104036 | 3.752218 | 1.999033 |
| C | -5.377687 | 4.212210 | -0.079000 |
| H | -4.858618 | 3.917732 | 0.836575 |
| H | -4.765204 | 3.920627 | -0.935755 |
| H | -5.464905 | 5.300479 | -0.079885 |
| C | -9.423869 | -1.582651 | -1.716963 |
| H | -8.645552 | -2.344805 | -1.685668 |
| H | -10.390793 | -2.081529 | -1.821153 |
| H | -9.266635 | -0.958115 | -2.599853 |
| C | -10.588784 | 0.287923 | -0.549637 |
| H | -10.660965 | 0.921666 | 0.337767 |
| H | -10.482898 | 0.931564 | -1.426532 |
| H | -11.526753 | -0.261773 | -0.649550 |
| C | -9.702914 | -1.606796 | 0.800333 |
| H | -10.679377 | -2.085145 | 0.688893 |
| H | -8.949350 | -2.384195 | 0.913878 |
| H | -9.722634 | -1.001766 | 1.710050 |

**Table S#.** Cartesian coordinates for diBIP-cyclohexylimine: E1PT. (-1707.55346068 Hartrees)

|  |  |  |  |
| --- | --- | --- | --- |
| atom | x | y | z |
| C | 1.544444 | 1.095848 | -0.051665 |
| C | 0.306818 | 1.773909 | -0.129153 |
| C | 0.283341 | 3.163491 | -0.309520 |
| C | 1.504058 | 3.825007 | -0.414714 |
| C | 2.727063 | 3.133936 | -0.335477 |
| C | 2.783196 | 1.748067 | -0.153649 |
| C | -0.136172 | -0.327905 | 0.129720 |
| H | -0.656922 | 3.698350 | -0.369246 |
| H | 1.517485 | 4.899365 | -0.555490 |
| H | 3.657122 | 3.685289 | -0.419961 |
| C | -2.278139 | -1.534629 | 0.220001 |
| C | -3.070012 | -2.691845 | 0.296456 |
| C | -2.494973 | -3.955313 | 0.440265 |
| C | -1.104240 | -3.998364 | 0.498552 |
| C | -0.309799 | -2.840712 | 0.406288 |
| C | -0.876061 | -1.571531 | 0.261253 |
| C | -4.412252 | -0.909159 | 0.085186 |
| H | -3.098734 | -4.850629 | 0.503063 |
| H | -0.612829 | -4.956133 | 0.615141 |
| H | 0.767604 | -2.940784 | 0.451601 |
| N | -0.726106 | 0.859064 | -0.008890 |
| C | -6.909029 | -0.772199 | -0.154003 |
| C | -5.606002 | -0.103524 | -0.025275 |
| C | -5.520727 | 1.272420 | -0.000232 |
| C | -6.673547 | 2.081028 | -0.101259 |
| C | -7.927450 | 1.449850 | -0.244850 |
| C | -8.098564 | 0.078571 | -0.273781 |
| H | -4.556271 | 1.751700 | 0.112747 |
| H | -8.799574 | 2.078725 | -0.328449 |
| C | -6.524791 | 3.594508 | -0.016874 |
| C | -9.475988 | -0.559735 | -0.419910 |
| O | -6.981423 | -2.027034 | -0.159084 |
| N | -3.138042 | -0.464939 | 0.095951 |
| N | -4.379568 | -2.251662 | 0.204315 |
| H | -2.770430 | 0.483759 | 0.010548 |
| N | 1.231225 | -0.230038 | 0.114239 |
| H | 1.944620 | -0.947666 | 0.182051 |
| C | 4.047556 | 1.024336 | -0.068581 |
| H | 4.949837 | 1.638520 | -0.158411 |
| N | 4.087581 | -0.246382 | 0.097765 |
| C | 5.415473 | -0.878413 | 0.168648 |
| C | 6.217129 | -0.698209 | -1.131580 |
| C | 6.229553 | -0.391763 | 1.379498 |
| H | 5.235956 | -1.951702 | 0.300747 |
| C | 7.570612 | -1.411486 | -1.049254 |
| H | 6.378877 | 0.373159 | -1.301227 |
| H | 5.630530 | -1.072105 | -1.975971 |
| C | 7.582746 | -1.106709 | 1.458285 |
| H | 6.392408 | 0.688626 | 1.285396 |
| H | 5.652759 | -0.551300 | 2.295287 |
| C | 8.380126 | -0.933134 | 0.161113 |
| H | 8.130810 | -1.249016 | -1.974941 |
| H | 7.404253 | -2.492910 | -0.965717 |
| H | 8.152511 | -0.730039 | 2.313102 |
| H | 7.414700 | -2.176397 | 1.637091 |
| H | 9.328228 | -1.476161 | 0.222484 |
| H | 8.628185 | 0.127906 | 0.030297 |
| H | -5.252851 | -2.776503 | 0.177687 |
| C | -7.858748 | 4.325319 | -0.216881 |
| H | -7.692620 | 5.402336 | -0.147339 |
| H | -8.290298 | 4.112548 | -1.198198 |
| H | -8.589063 | 4.050968 | 0.548364 |
| C | -5.529280 | 4.073943 | -1.094980 |
| H | -4.542725 | 3.622441 | -0.968839 |
| H | -5.894081 | 3.835512 | -2.096744 |
| H | -5.412991 | 5.157927 | -1.018992 |
| C | -5.967030 | 3.945125 | 1.381647 |
| H | -6.652995 | 3.619136 | 2.166971 |
| H | -4.997045 | 3.474413 | 1.557188 |
| H | -5.839563 | 5.027547 | 1.462989 |
| C | -9.515274 | -1.398385 | -1.717217 |
| H | -8.772271 | -2.194523 | -1.693536 |
| H | -10.506821 | -1.845005 | -1.828421 |
| H | -9.325704 | -0.767566 | -2.589450 |
| C | -10.588152 | 0.496896 | -0.495892 |
| H | -10.613857 | 1.121144 | 0.400776 |
| H | -10.478054 | 1.148368 | -1.366656 |
| H | -11.550965 | -0.011790 | -0.580254 |
| C | -9.768528 | -1.463580 | 0.800807 |
| H | -10.765138 | -1.899004 | 0.690154 |
| H | -9.039638 | -2.267402 | 0.883948 |
| H | -9.755842 | -0.877188 | 1.723194 |

**Table S#.** Cartesian coordinates for diBIP-cyclohexylimine: E2PT. (-1707.55886850 Hartrees)

|  |  |  |  |
| --- | --- | --- | --- |
| atom | x | y | z |
| C | 1.534153 | 1.142325 | -0.140101 |
| C | 0.315025 | 1.827814 | -0.253790 |
| C | 0.273384 | 3.207213 | -0.458280 |
| C | 1.500366 | 3.861097 | -0.548959 |
| C | 2.720728 | 3.171848 | -0.431608 |
| C | 2.773444 | 1.789941 | -0.226388 |
| C | -0.108695 | -0.350362 | 0.055363 |
| H | -0.665880 | 3.737222 | -0.545725 |
| H | 1.516647 | 4.932365 | -0.707580 |
| H | 3.651427 | 3.722650 | -0.502527 |
| C | -2.278102 | -1.507903 | 0.168358 |
| C | -3.037888 | -2.700357 | 0.275050 |
| C | -2.441462 | -3.949887 | 0.433622 |
| C | -1.046816 | -3.985527 | 0.481724 |
| C | -0.270702 | -2.823557 | 0.364502 |
| C | -0.865947 | -1.566600 | 0.204374 |
| C | -4.348952 | -0.922040 | 0.052803 |
| H | -3.031374 | -4.853871 | 0.517318 |
| H | -0.546391 | -4.937090 | 0.610165 |
| H | 0.808607 | -2.905738 | 0.401647 |
| N | -0.671792 | 0.862816 | -0.120683 |
| C | -6.873592 | -0.783310 | -0.132787 |
| C | -5.561363 | -0.128729 | -0.042350 |
| C | -5.467298 | 1.248997 | -0.035209 |
| C | -6.611719 | 2.065600 | -0.106061 |
| C | -7.877779 | 1.444123 | -0.211075 |
| C | -8.059004 | 0.075981 | -0.227844 |
| H | -4.485265 | 1.698439 | 0.040518 |
| H | -8.747942 | 2.078414 | -0.273797 |
| C | -6.449960 | 3.581379 | -0.067926 |
| C | -9.447241 | -0.551184 | -0.337219 |
| O | -6.962599 | -2.039847 | -0.127289 |
| N | -3.106236 | -0.421567 | 0.035106 |
| N | -4.344608 | -2.281821 | 0.191841 |
| N | 1.230480 | -0.192235 | 0.047300 |
| H | 1.969166 | -0.885637 | 0.148488 |
| C | 4.030018 | 1.054855 | -0.097681 |
| H | 4.940919 | 1.656206 | -0.174951 |
| N | 4.041872 | -0.212230 | 0.091524 |
| C | 5.353622 | -0.871238 | 0.208090 |
| C | 6.194503 | -0.717626 | -1.070957 |
| C | 6.137886 | -0.383612 | 1.438361 |
| H | 5.147609 | -1.938469 | 0.345929 |
| C | 7.534885 | -1.447354 | -0.941694 |
| H | 6.376808 | 0.348979 | -1.247371 |
| H | 5.625603 | -1.091894 | -1.927140 |
| C | 7.479028 | -1.114445 | 1.560975 |
| H | 6.316955 | 0.693713 | 1.338195 |
| H | 5.531666 | -0.526349 | 2.337963 |
| C | 8.315027 | -0.962841 | 0.285339 |
| H | 8.122485 | -1.304704 | -1.853693 |
| H | 7.352474 | -2.525321 | -0.848692 |
| H | 8.029561 | -0.737298 | 2.427894 |
| H | 7.293501 | -2.180318 | 1.743739 |
| H | 9.255061 | -1.514921 | 0.379881 |
| H | 8.578245 | 0.093929 | 0.149809 |
| H | -5.211756 | -2.810984 | 0.188414 |
| H | -1.691093 | 0.960487 | -0.139304 |
| C | -9.526998 | -1.400333 | -1.625307 |
| H | -8.793265 | -2.205122 | -1.608902 |
| H | -10.526368 | -1.835258 | -1.712967 |
| H | -9.346323 | -0.780989 | -2.507913 |
| C | -5.622697 | 4.022820 | -1.295365 |
| H | -5.484875 | 5.107199 | -1.271184 |
| H | -4.635681 | 3.554017 | -1.302590 |
| H | -6.134566 | 3.760829 | -2.224559 |
| C | -10.551804 | 0.514721 | -0.396939 |
| H | -10.553540 | 1.146172 | 0.495235 |
| H | -10.455307 | 1.159329 | -1.274649 |
| H | -11.521079 | 0.014454 | -0.455811 |
| C | -9.722305 | -1.442671 | 0.896001 |
| H | -8.999767 | -2.253510 | 0.967530 |
| H | -9.681222 | -0.850622 | 1.814109 |
| H | -10.726122 | -1.868667 | 0.814377 |
| C | -7.798508 | 4.312813 | -0.087578 |
| H | -8.356786 | 4.101101 | -1.002757 |
| H | -8.417169 | 4.031174 | 0.768416 |
| H | -7.625670 | 5.389851 | -0.039270 |
| C | -5.695433 | 3.974899 | 1.220613 |
| H | -6.248859 | 3.660539 | 2.108845 |
| H | -4.700883 | 3.525304 | 1.259073 |
| H | -5.577395 | 5.061103 | 1.256579 |

**Table S#.** Cartesian coordinates for diBIP-cyclohexylimine: E3PT. (-1707.56917917 Hartrees)

|  |  |  |  |
| --- | --- | --- | --- |
| atom | x | y | z |
| C | 1.515357 | 1.140998 | -0.113375 |
| C | 0.308673 | 1.872680 | -0.241594 |
| C | 0.292942 | 3.245087 | -0.467487 |
| C | 1.527908 | 3.897325 | -0.571223 |
| C | 2.732150 | 3.201040 | -0.446946 |
| C | 2.756622 | 1.811201 | -0.220445 |
| C | -0.081832 | -0.285406 | 0.094216 |
| H | -0.637967 | 3.789279 | -0.565962 |
| H | 1.549083 | 4.965497 | -0.747010 |
| H | 3.672401 | 3.733311 | -0.529121 |
| C | -2.272992 | -1.460771 | 0.234428 |
| C | -3.016043 | -2.665142 | 0.341462 |
| C | -2.404517 | -3.909929 | 0.489163 |
| C | -1.010435 | -3.925905 | 0.520427 |
| C | -0.252675 | -2.750184 | 0.397408 |
| C | -0.859411 | -1.499147 | 0.251958 |
| C | -4.356214 | -0.906714 | 0.132121 |
| H | -2.983627 | -4.820872 | 0.573741 |
| H | -0.495114 | -4.871656 | 0.636236 |
| H | 0.828555 | -2.803754 | 0.409898 |
| N | -0.681957 | 0.927611 | -0.097725 |
| C | -6.879499 | -0.810955 | -0.103068 |
| C | -5.582276 | -0.134692 | 0.031679 |
| C | -5.516293 | 1.245149 | 0.068201 |
| C | -6.671872 | 2.040615 | -0.031255 |
| C | -7.922482 | 1.398102 | -0.190796 |
| C | -8.076947 | 0.027657 | -0.230796 |
| H | -4.546112 | 1.709954 | 0.189757 |
| H | -8.799787 | 2.019769 | -0.277898 |
| C | -6.544524 | 3.556888 | 0.074777 |
| C | -9.447257 | -0.625856 | -0.397001 |
| O | -6.946999 | -2.069191 | -0.108687 |
| N | -3.123378 | -0.386420 | 0.111698 |
| N | -4.329869 | -2.267896 | 0.268065 |
| N | 1.255571 | -0.189484 | 0.093918 |
| C | 4.001304 | 1.121071 | -0.106654 |
| H | 4.924805 | 1.684958 | -0.189515 |
| N | 4.096070 | -0.160800 | 0.087095 |
| C | 5.375658 | -0.891611 | 0.197985 |
| C | 6.187284 | -0.761060 | -1.097890 |
| C | 6.174028 | -0.410074 | 1.417200 |
| H | 5.095126 | -1.936276 | 0.343303 |
| C | 7.522237 | -1.502980 | -0.979322 |
| H | 6.377508 | 0.302025 | -1.285565 |
| H | 5.599050 | -1.140875 | -1.937030 |
| C | 7.509154 | -1.155238 | 1.519466 |
| H | 6.362323 | 0.664684 | 1.309027 |
| H | 5.577949 | -0.547807 | 2.322882 |
| C | 8.326027 | -1.016644 | 0.231031 |
| H | 8.093280 | -1.369857 | -1.902371 |
| H | 7.330377 | -2.578034 | -0.877054 |
| H | 8.071669 | -0.776056 | 2.376925 |
| H | 7.315477 | -2.217573 | 1.711498 |
| H | 9.260827 | -1.578396 | 0.313730 |
| H | 8.597413 | 0.036372 | 0.085366 |
| H | -5.185939 | -2.813474 | 0.251305 |
| H | -1.696305 | 1.033360 | -0.116055 |
| H | 3.211821 | -0.677874 | 0.158998 |
| C | -5.535374 | 4.065575 | -0.975956 |
| H | -5.429324 | 5.149627 | -0.882881 |
| H | -4.548559 | 3.618252 | -0.837955 |
| H | -5.878587 | 3.839113 | -1.988264 |
| C | -7.882798 | 4.276424 | -0.139841 |
| H | -8.297517 | 4.068366 | -1.129436 |
| H | -8.622464 | 3.987476 | 0.610946 |
| H | -7.729313 | 5.354780 | -0.057932 |
| C | -6.020210 | 3.896363 | 1.488051 |
| H | -6.719918 | 3.553592 | 2.253992 |
| H | -5.051818 | 3.428352 | 1.677373 |
| H | -5.902500 | 4.978643 | 1.587970 |
| C | -9.461036 | -1.466752 | -1.692736 |
| H | -8.703895 | -2.249278 | -1.660534 |
| H | -10.443110 | -1.931823 | -1.814976 |
| H | -9.273961 | -0.833483 | -2.563984 |
| C | -10.570062 | 0.418313 | -0.492375 |
| H | -10.622793 | 1.037990 | 0.406449 |
| H | -10.446665 | 1.076250 | -1.356561 |
| H | -11.525737 | -0.099631 | -0.602165 |
| C | -9.750987 | -1.530077 | 0.819721 |
| H | -10.736804 | -1.985715 | 0.691573 |
| H | -9.008135 | -2.318874 | 0.921224 |
| H | -9.767487 | -0.939849 | 1.739808 |