

The effect of cluster size on the intra-cluster ionic polymerization process

Estefania Rossich Molina¹ and Tamar Stein¹

¹Fritz Haber Research Center for Molecular Dynamics, The Hebrew University of Jerusalem, Jerusalem,
Israel, 9190401

*Corresponding author: tamar.stein@mail.huji.ac.il, Tel: +972-2-658-6108

Section 1 reports the cartesian coordinates of all optimized neutral structures for the decamers and eicosamers, used as starting structures in molecular dynamics simulations. “DEC” is used to report the decamers, while “EICO” is used to report the eicosamers.

In Section 2, the corresponding optimized cationic structures for each isomer are reported.

Indexes 1 to 20 were used to identify the correspondence between neutral and ionic structures at each cluster size.

Section 1: Optimized neutral structures

DEC 1

0 1

| | | | |
|---|-----------|-----------|-----------|
| C | 4.835087 | 3.147014 | -0.256465 |
| H | 5.303762 | 4.092289 | -0.408081 |
| C | 4.846693 | -1.875739 | -0.612386 |
| H | 4.035231 | -2.485598 | -0.946677 |
| C | 5.746639 | -1.184900 | -0.229840 |
| H | 6.546564 | -0.562915 | 0.101253 |
| C | 4.313060 | 2.083314 | -0.083370 |
| H | 3.841693 | 1.137080 | 0.074559 |
| C | 0.948010 | 3.319471 | -0.636404 |
| H | 1.994525 | 3.311021 | -0.418532 |
| C | -0.224103 | 3.328092 | -0.884626 |
| H | -1.268863 | 3.332220 | -1.109551 |
| C | -0.736431 | 0.023267 | -1.863018 |
| H | -0.120168 | 0.768406 | -2.315171 |
| C | -1.427369 | -0.797845 | -1.329640 |
| H | -2.037093 | -1.524555 | -0.838001 |
| C | 1.374503 | -3.161393 | -1.066281 |
| H | 0.902563 | -2.228014 | -1.289926 |
| C | 1.887753 | -4.211454 | -0.804214 |
| H | 2.335098 | -5.151418 | -0.574043 |
| C | -2.236007 | -3.021814 | 1.783366 |
| H | -3.278070 | -3.214912 | 1.901358 |
| C | 1.308713 | 0.060318 | 1.156867 |
| H | 0.492776 | 0.715846 | 0.938199 |
| C | 2.219161 | -0.679316 | 1.402928 |
| H | 3.040584 | -1.328734 | 1.607775 |
| C | -1.068205 | -2.799638 | 1.636418 |
| H | -0.030251 | -2.590388 | 1.494823 |
| C | -4.602659 | -0.823780 | 0.372177 |
| H | -4.044960 | -0.203094 | 1.041723 |
| C | -5.214039 | -1.517301 | -0.389120 |
| H | -5.765295 | -2.127985 | -1.067075 |
| C | -3.707449 | 2.305613 | -1.330393 |
| H | -3.389738 | 1.291437 | -1.446532 |
| C | -4.053500 | 3.444896 | -1.200364 |
| H | -4.374368 | 4.456048 | -1.093507 |
| C | -2.259511 | 1.672577 | 1.914295 |
| H | -2.543351 | 2.572144 | 1.416011 |
| C | -1.944679 | 0.656562 | 2.464944 |
| H | -1.658448 | -0.257606 | 2.935852 |

DEC 2

0 1

| | | | |
|---|-----------|-----------|----------|
| C | -0.579571 | -1.417488 | 1.283163 |
|---|-----------|-----------|----------|

| | | | |
|---|-----------|-----------|-----------|
| C | -0.959046 | -1.884740 | 2.319095 |
| H | -0.238436 | -1.001427 | 0.358204 |
| H | -1.298816 | -2.305601 | 3.237865 |
| C | -1.495412 | 3.125846 | -2.941352 |
| C | -0.558013 | 3.708979 | -2.477116 |
| H | -2.327427 | 2.596532 | -3.347557 |
| H | 0.280115 | 4.214999 | -2.048792 |
| C | -3.436905 | -3.549808 | 0.050490 |
| C | -3.825352 | -4.654909 | -0.197889 |
| H | -3.079161 | -2.566636 | 0.267153 |
| H | -4.181805 | -5.635501 | -0.415275 |
| C | -1.470958 | 3.079495 | 0.944985 |
| C | -1.117322 | 2.147683 | 1.609314 |
| H | -1.773642 | 3.906452 | 0.343702 |
| H | -0.784518 | 1.319073 | 2.194961 |
| C | 1.109593 | 0.661814 | -1.440739 |
| C | 2.001416 | 0.177357 | -0.802956 |
| H | 0.312913 | 1.107025 | -1.997401 |
| H | 2.783717 | -0.264972 | -0.226039 |
| C | 0.590321 | -2.969675 | -2.059853 |
| C | -0.244785 | -3.633204 | -1.514802 |
| H | 1.329088 | -2.363927 | -2.534407 |
| H | -1.005897 | -4.203487 | -1.028253 |
| C | 2.215619 | 1.665337 | 2.935008 |
| C | 2.076942 | 0.481273 | 2.820647 |
| H | 2.330811 | 2.721967 | 3.024637 |
| H | 1.949386 | -0.573131 | 2.708056 |
| C | 1.960680 | 3.893740 | 0.117328 |
| C | 2.213379 | 5.063974 | 0.079368 |
| H | 1.732475 | 2.849182 | 0.145654 |
| H | 2.444449 | 6.104037 | 0.051858 |
| C | 2.733436 | -2.871748 | 0.957769 |
| C | 3.727664 | -2.512234 | 1.520607 |
| H | 1.848829 | -3.186414 | 0.446389 |
| H | 4.612166 | -2.196929 | 2.025609 |
| C | -2.474966 | -0.701995 | -1.992736 |
| C | -2.483449 | 0.202047 | -1.206627 |
| H | -2.459191 | -1.518171 | -2.679132 |
| H | -2.460970 | 1.002512 | -0.497753 |

DEC 3

0 1

| | | | |
|---|-----------|-----------|-----------|
| C | 4.509700 | 0.740629 | -0.287207 |
| C | 5.192664 | 1.442630 | -0.976218 |
| H | 3.898770 | 0.115131 | 0.327297 |
| H | 5.805772 | 2.063399 | -1.588552 |
| C | 0.925645 | 3.986242 | -0.706973 |
| C | 1.979148 | 3.435361 | -0.562218 |
| H | -0.023353 | 4.456712 | -0.833486 |
| H | 2.908138 | 2.924026 | -0.428624 |
| C | -0.117249 | -2.291643 | 3.331652 |
| C | 0.172916 | -3.394669 | 3.698242 |
| H | -0.370745 | -1.308861 | 2.994491 |
| H | 0.422866 | -4.374065 | 4.037492 |
| C | 2.746610 | -2.389817 | -0.495864 |
| C | 2.366990 | -2.489334 | 0.635453 |
| H | 3.089926 | -2.286473 | -1.500542 |
| H | 2.022389 | -2.566827 | 1.643379 |
| C | -2.557758 | 3.659047 | -2.211223 |
| C | -2.474499 | 2.872801 | -1.311815 |
| H | -2.639460 | 4.356242 | -3.013286 |

| | | | |
|---|-----------|-----------|-----------|
| H | -2.405472 | 2.162136 | -0.516071 |
| C | -4.661936 | -0.776284 | -2.065189 |
| C | -3.547127 | -0.399248 | -2.289236 |
| H | -5.658777 | -1.098904 | -1.869382 |
| H | -2.550302 | -0.062617 | -2.479849 |
| C | -2.199903 | -3.358102 | -0.797415 |
| C | -1.493771 | -3.499400 | 0.159639 |
| H | -2.831008 | -3.206778 | -1.644365 |
| H | -0.871348 | -3.617617 | 1.018746 |
| C | 0.210193 | 0.601147 | -1.979172 |
| C | 0.016306 | -0.536257 | -1.652940 |
| H | 0.386835 | 1.621838 | -2.238351 |
| H | -0.154723 | -1.547092 | -1.351402 |
| C | -1.966290 | 0.883013 | 1.892786 |
| C | -2.376280 | -0.034293 | 1.239729 |
| H | -1.587533 | 1.691985 | 2.474963 |
| H | -2.731958 | -0.857382 | 0.657712 |
| C | 1.895368 | 0.804887 | 2.721929 |
| C | 1.392894 | 0.738260 | 1.636403 |
| H | 2.347078 | 0.877103 | 3.684758 |
| H | 0.942722 | 0.673957 | 0.666420 |

DEC4

0 1

| | | | |
|---|-----------|-----------|-----------|
| C | 5.158334 | 0.587004 | -0.729032 |
| C | 4.893038 | 1.438422 | -1.528614 |
| H | 5.376300 | -0.175512 | -0.012091 |
| H | 4.651205 | 2.196090 | -2.239093 |
| C | 2.047539 | 0.955619 | 1.161399 |
| C | 1.152658 | 0.513803 | 1.823318 |
| H | 2.847147 | 1.340463 | 0.566695 |
| H | 0.350268 | 0.121047 | 2.405906 |
| C | -3.845548 | 0.673222 | 4.149946 |
| C | -4.217383 | 0.170786 | 3.128905 |
| H | -3.516407 | 1.113336 | 5.063148 |
| H | -4.544040 | -0.268058 | 2.210867 |
| C | -2.185318 | -0.818677 | -2.499262 |
| C | -1.452967 | -0.037474 | -3.035210 |
| H | -2.841333 | -1.505696 | -2.013569 |
| H | -0.794961 | 0.657020 | -3.507754 |
| C | 4.164124 | -2.051314 | 1.477391 |
| C | 5.266962 | -2.442069 | 1.731736 |
| H | 3.184963 | -1.692499 | 1.243245 |
| H | 6.243827 | -2.796701 | 1.966897 |
| C | -5.638305 | -0.766349 | -0.338886 |
| H | -6.334237 | -1.555571 | -0.167586 |
| C | -1.545511 | 2.180090 | 0.088686 |
| H | -0.788639 | 2.084132 | -0.660162 |
| C | -2.375852 | 2.290411 | 0.945668 |
| H | -3.104078 | 2.373376 | 1.721772 |
| C | -4.862517 | 0.123253 | -0.540547 |
| H | -4.161161 | 0.909555 | -0.720063 |
| C | -1.710707 | -1.419937 | 0.894655 |
| H | -1.902922 | -0.377033 | 0.752402 |
| C | -1.479617 | -2.584032 | 1.056767 |
| H | -1.273964 | -3.619679 | 1.203904 |
| C | 1.417284 | -1.747090 | -1.319997 |
| H | 0.414299 | -1.707001 | -0.952624 |
| C | 2.542684 | -1.787367 | -1.728762 |
| H | 3.547996 | -1.819793 | -2.082908 |
| C | 1.483611 | 1.791661 | -2.266330 |
| H | 1.749018 | 0.782328 | -2.024862 |

| | | | |
|---|----------|----------|-----------|
| C | 1.176908 | 2.919360 | -2.531180 |
| H | 0.907957 | 3.924978 | -2.762189 |

DEC 5

0 1

| | | | |
|---|-----------|-----------|-----------|
| C | -3.916705 | -1.040678 | 0.360137 |
| C | -4.795146 | -1.833321 | 0.171442 |
| H | -3.131154 | -0.333046 | 0.525023 |
| H | -5.577843 | -2.538860 | 0.009057 |
| C | -0.485603 | -3.170957 | -2.067772 |
| C | -1.577779 | -2.722595 | -1.865720 |
| H | 0.493630 | -3.557542 | -2.238879 |
| H | -2.550046 | -2.326403 | -1.670049 |
| C | -6.831795 | 2.778136 | -0.012059 |
| C | -6.373831 | 1.679039 | 0.113543 |
| H | -7.246111 | 3.753686 | -0.125901 |
| H | -5.954224 | 0.701483 | 0.220112 |
| C | -1.765670 | 2.087649 | -0.361299 |
| C | -2.895579 | 2.441790 | -0.174179 |
| H | -0.758520 | 1.769007 | -0.532006 |
| H | -3.909171 | 2.742908 | -0.020769 |
| C | -0.294890 | -0.422591 | 1.846455 |
| C | -0.559373 | -1.499028 | 1.392489 |
| H | -0.057348 | 0.544335 | 2.234380 |
| H | -0.809270 | -2.444086 | 0.965883 |
| C | 1.897602 | 1.096518 | -1.323342 |
| C | 1.146783 | 0.169893 | -1.438307 |
| H | 2.576004 | 1.913294 | -1.220410 |
| H | 0.475407 | -0.656856 | -1.531777 |
| C | 3.080463 | -2.650605 | -0.957303 |
| C | 2.572014 | -3.362881 | -0.139663 |
| H | 3.540204 | -1.995226 | -1.665250 |
| H | 2.124607 | -3.992649 | 0.595754 |
| C | 5.518343 | 0.260906 | -2.501622 |
| C | 5.400070 | 0.125026 | -1.318006 |
| H | 5.626805 | 0.387754 | -3.554115 |
| H | 5.279130 | 0.003249 | -0.263252 |
| C | 3.496915 | -0.227737 | 1.782779 |
| C | 4.409175 | 0.202837 | 2.429418 |
| H | 2.686223 | -0.611925 | 1.199872 |
| H | 5.221614 | 0.574111 | 3.011601 |
| C | 0.479943 | 3.337216 | 1.914839 |
| C | 1.498817 | 2.756035 | 2.155500 |
| H | -0.432368 | 3.842037 | 1.690074 |
| H | 2.398676 | 2.220074 | 2.363322 |

DEC 6

0 1

| | | | |
|---|----------|-----------|-----------|
| C | 3.160054 | -3.947271 | 0.522252 |
| C | 2.771329 | -5.079608 | 0.502263 |
| H | 3.512705 | -2.938078 | 0.541302 |
| H | 2.431883 | -6.090018 | 0.485962 |
| C | 3.051426 | 3.888497 | -1.110632 |
| C | 3.491931 | 2.799168 | -1.340241 |
| H | 2.661691 | 4.860585 | -0.911139 |
| H | 3.884401 | 1.824442 | -1.528327 |
| C | 4.657560 | -0.313853 | 0.667925 |
| C | 3.472659 | -0.257486 | 0.499294 |
| H | 5.711783 | -0.338107 | 0.829017 |

| | | | |
|---|-----------|-----------|-----------|
| H | 2.415320 | -0.189614 | 0.349794 |
| C | 0.326923 | 1.079938 | -0.566423 |
| C | -0.224028 | 0.067041 | -0.239718 |
| H | 0.826607 | 1.980166 | -0.851445 |
| H | -0.716006 | -0.836478 | 0.053191 |
| C | -4.643133 | 2.918497 | 1.824507 |
| C | -5.279271 | 2.400072 | 2.696266 |
| H | -4.072302 | 3.365564 | 1.038527 |
| H | -5.845342 | 1.945507 | 3.476645 |
| C | -1.826817 | -3.272069 | 0.688564 |
| C | -0.657814 | -3.526377 | 0.622864 |
| H | -2.867721 | -3.040843 | 0.735322 |
| H | 0.385356 | -3.755585 | 0.570834 |
| C | 7.678955 | 2.326588 | 0.950035 |
| C | 6.534559 | 2.638074 | 0.789694 |
| H | 8.700682 | 2.059060 | 1.092416 |
| H | 5.514066 | 2.915713 | 0.642806 |
| C | -3.665315 | -0.727406 | -1.024084 |
| C | -4.060370 | -0.025192 | -0.137643 |
| H | -3.316926 | -1.369893 | -1.801110 |
| H | -4.408789 | 0.609512 | 0.649044 |
| C | -4.320547 | -4.584559 | -1.509481 |
| C | -5.212273 | -3.791097 | -1.422425 |
| H | -3.522925 | -5.288397 | -1.578819 |
| H | -5.999391 | -3.076657 | -1.341307 |
| C | -2.507345 | 3.115588 | -1.173529 |
| C | -2.752464 | 4.285628 | -1.245673 |
| H | -2.288035 | 2.071672 | -1.103850 |
| H | -2.970703 | 5.326118 | -1.321658 |

DEC 7

0 1

| | | | |
|---|-----------|-----------|-----------|
| C | 1.155365 | -3.917894 | 1.847158 |
| C | 0.488662 | -2.925470 | 1.916491 |
| H | 1.749730 | -4.800930 | 1.780288 |
| H | -0.094588 | -2.030208 | 1.964725 |
| C | 3.918928 | -3.451580 | -0.935581 |
| C | 3.394197 | -4.402230 | -1.439738 |
| H | 4.372270 | -2.596588 | -0.485215 |
| H | 2.932370 | -5.248948 | -1.893922 |
| C | 3.688027 | 0.226640 | 0.705654 |
| C | 3.191971 | -0.742988 | 1.204358 |
| H | 4.113354 | 1.096904 | 0.258707 |
| H | 2.730812 | -1.605306 | 1.637307 |
| C | 1.508338 | 3.162321 | -0.954072 |
| C | 1.352933 | 1.985412 | -1.117884 |
| H | 1.625812 | 4.214956 | -0.815879 |
| H | 1.207696 | 0.935333 | -1.256415 |
| C | -1.277465 | 0.554908 | 1.952417 |
| C | -0.097476 | 0.736218 | 1.851434 |
| H | -2.329723 | 0.394871 | 2.025168 |
| H | 0.954451 | 0.891663 | 1.748137 |
| C | -0.446979 | -1.174556 | -1.377602 |
| C | 0.590346 | -1.774348 | -1.413979 |
| H | -1.375523 | -0.647389 | -1.329274 |
| H | 1.511868 | -2.315937 | -1.434733 |
| C | -3.361711 | -4.680792 | -0.072791 |
| C | -2.299158 | -4.141113 | -0.188858 |
| H | -4.300214 | -5.174781 | 0.032246 |
| H | -1.353251 | -3.654379 | -0.293139 |
| C | -3.951087 | 0.326579 | -0.498496 |
| C | -3.919795 | -0.865465 | -0.382079 |

| | | | |
|---|-----------|-----------|-----------|
| H | -3.963582 | 1.389862 | -0.597921 |
| H | -3.876402 | -1.929270 | -0.283466 |
| C | -2.094499 | 3.450250 | -0.123015 |
| C | -3.061305 | 4.145119 | -0.258630 |
| H | -1.228536 | 2.833603 | -0.000777 |
| H | -3.923693 | 4.761674 | -0.376492 |
| C | 1.114722 | 7.073543 | -0.396760 |
| C | 0.120345 | 6.414372 | -0.299584 |
| H | 1.996740 | 7.665311 | -0.481549 |
| H | -0.763953 | 5.820638 | -0.216235 |

DEC 8

0 1

| | | | |
|---|-----------|-----------|-----------|
| C | 0.023693 | 3.466510 | -1.484733 |
| C | -0.172924 | 2.808976 | -0.491464 |
| H | 0.201197 | 4.049527 | -2.360998 |
| H | -0.365238 | 2.223434 | 0.385764 |
| C | 4.488807 | 3.925441 | 0.826664 |
| C | 3.424537 | 3.659216 | 0.324779 |
| H | 5.426005 | 4.167761 | 1.275590 |
| H | 2.471950 | 3.437466 | -0.109733 |
| C | 6.840754 | 0.519932 | -1.754992 |
| C | 6.044166 | 1.244001 | -1.210211 |
| H | 7.546986 | -0.112687 | -2.244399 |
| H | 5.345424 | 1.896770 | -0.728304 |
| C | 4.735954 | -2.106874 | -0.013346 |
| C | 4.093650 | -3.043546 | 0.395508 |
| H | 5.309264 | -1.278109 | -0.374363 |
| H | 3.501346 | -3.860533 | 0.750077 |
| C | -3.880479 | 0.060494 | -1.633030 |
| C | -3.037263 | 0.924272 | -1.669934 |
| H | -4.630248 | -0.703176 | -1.600512 |
| H | -2.281431 | 1.681467 | -1.697129 |
| C | 1.062775 | -1.483806 | -0.795372 |
| C | -0.116755 | -1.250117 | -0.907861 |
| H | 2.106425 | -1.700277 | -0.688383 |
| H | -1.153584 | -1.013567 | -1.022852 |
| C | -6.518915 | -2.679390 | -1.877178 |
| C | -6.528241 | -2.438892 | -0.695619 |
| H | -6.516176 | -2.901373 | -2.921009 |
| H | -6.539923 | -2.232330 | 0.351515 |
| C | 0.846908 | -4.678216 | 0.909073 |
| C | 1.265270 | -5.639841 | 1.505389 |
| H | 0.490643 | -3.818401 | 0.380340 |
| H | 1.617574 | -6.497461 | 2.033179 |
| C | -4.853212 | 2.267799 | 1.375347 |
| C | -5.157909 | 2.822885 | 2.402197 |
| H | -4.574238 | 1.774258 | 0.467282 |
| H | -5.441421 | 3.318977 | 3.303223 |
| C | -0.693538 | 0.313273 | 2.200535 |
| C | -1.656985 | 1.001142 | 2.435308 |
| H | 0.142118 | -0.307748 | 1.964374 |
| H | -2.526348 | 1.595151 | 2.623089 |

DEC 9

0 1

| | | | |
|---|-----------|----------|-----------|
| C | -0.070735 | 3.650745 | -1.780403 |
| C | -0.224718 | 2.914596 | -0.836220 |
| H | 0.069863 | 4.303739 | -2.612781 |
| H | -0.365716 | 2.260860 | 0.000584 |

| | | | |
|---|-----------|-----------|-----------|
| C | 4.346357 | 4.227992 | 0.610817 |
| C | 3.312213 | 3.900557 | 0.082831 |
| H | 5.257264 | 4.523276 | 1.081650 |
| H | 2.385039 | 3.628022 | -0.376990 |
| C | 6.951875 | 0.497870 | -1.099566 |
| C | 6.083600 | 1.273927 | -0.784240 |
| H | 7.722648 | -0.181745 | -1.387072 |
| H | 5.323222 | 1.974128 | -0.505052 |
| C | 4.539898 | -2.016528 | 0.370339 |
| C | 3.811283 | -2.933111 | 0.663846 |
| H | 5.185815 | -1.203740 | 0.109891 |
| H | 3.144294 | -3.732727 | 0.909393 |
| C | -3.669906 | 0.033541 | -1.354657 |
| C | -3.123001 | 1.044048 | -1.725295 |
| H | -4.118317 | -0.873548 | -1.011313 |
| H | -2.610203 | 1.929178 | -2.034579 |
| C | 1.125182 | -1.486795 | -1.190180 |
| C | -0.016963 | -1.146595 | -1.384885 |
| H | 2.135719 | -1.784440 | -1.000524 |
| H | -1.023291 | -0.827652 | -1.556011 |
| C | -3.305980 | -3.416984 | 0.465640 |
| C | -2.798875 | -2.452966 | 0.984850 |
| H | -3.746770 | -4.282115 | 0.023106 |
| H | -2.341463 | -1.596934 | 1.436010 |
| C | 0.510570 | -4.653227 | 0.631373 |
| C | 1.012512 | -5.603262 | 1.180109 |
| H | 0.073311 | -3.807020 | 0.144445 |
| H | 1.435389 | -6.453752 | 1.666030 |
| C | -4.512045 | 2.347986 | 1.609356 |
| C | -4.671263 | 2.875519 | 2.682513 |
| H | -4.360034 | 1.877407 | 0.660317 |
| H | -4.829917 | 3.349820 | 3.625057 |
| C | -0.362447 | 0.274337 | 1.855393 |
| C | -1.300690 | 0.925124 | 2.248308 |
| H | 0.451092 | -0.304773 | 1.475715 |
| H | -2.140590 | 1.499689 | 2.578630 |

DEC 10

0 1

| | | | |
|---|-----------|-----------|-----------|
| C | -2.271891 | -1.172738 | -2.080760 |
| C | -1.214298 | -0.706014 | -1.764564 |
| H | -3.219321 | -1.578332 | -2.364322 |
| H | -0.274119 | -0.291891 | -1.470576 |
| C | 1.884670 | 0.979676 | 0.039766 |
| C | 1.098629 | 0.406925 | 0.737837 |
| H | 2.588991 | 1.492953 | -0.573971 |
| H | 0.389903 | -0.105769 | 1.352214 |
| C | -1.730021 | -1.145742 | 2.847517 |
| C | -1.890934 | -1.563199 | 1.736240 |
| H | -1.591086 | -0.787390 | 3.842051 |
| H | -2.040459 | -1.925921 | 0.741393 |
| C | -5.403674 | 0.715317 | -0.217727 |
| C | -4.514299 | 0.612832 | 0.578976 |
| H | -6.193120 | 0.809955 | -0.932585 |
| H | -3.716522 | 0.500682 | 1.279913 |
| C | -4.308231 | -4.107912 | -0.357374 |
| C | -4.709091 | -2.996713 | -0.160580 |
| H | -3.950960 | -5.098098 | -0.524702 |
| H | -5.050516 | -1.997605 | 0.010487 |
| C | -8.191516 | 2.145113 | -2.078533 |
| C | -8.391098 | 1.150828 | -2.716354 |
| H | -7.986254 | 3.029592 | -1.514062 |

| | | | |
|---|-----------|-----------|-----------|
| H | -8.554893 | 0.257502 | -3.275644 |
| C | -7.516537 | 4.543708 | -4.645266 |
| C | -6.922964 | 5.513914 | -5.018748 |
| H | -8.034755 | 3.673730 | -4.305290 |
| H | -6.397429 | 6.377898 | -5.355741 |
| C | -4.416043 | 2.895612 | -3.440161 |
| C | -3.638123 | 2.101630 | -2.992244 |
| H | -5.107513 | 3.612759 | -3.826986 |
| H | -2.953281 | 1.386851 | -2.588451 |
| C | -6.504377 | 5.324754 | -0.993570 |
| C | -5.809776 | 4.410581 | -0.653246 |
| H | -7.114587 | 6.141482 | -1.304925 |
| H | -5.190629 | 3.587556 | -0.368955 |
| C | -5.943103 | -1.906214 | -3.243061 |
| C | -5.647604 | -0.785490 | -3.546500 |
| H | -6.193011 | -2.903664 | -2.960457 |
| H | -5.372353 | 0.217514 | -3.796450 |

DEC 11

0 1

| | | | |
|---|-----------|-----------|-----------|
| C | 0.038294 | 1.664626 | -0.063768 |
| C | 1.055945 | 1.267917 | -0.555205 |
| H | -0.883129 | 2.005146 | 0.357801 |
| H | 1.954395 | 0.914510 | -1.008571 |
| C | 1.200264 | -0.582225 | -3.491721 |
| C | 2.079747 | -0.027815 | -4.085387 |
| H | 0.406021 | -1.064608 | -2.963471 |
| H | 2.861569 | 0.461436 | -4.619576 |
| C | -2.159768 | -0.918318 | 2.253928 |
| C | -1.043156 | -0.526311 | 2.440382 |
| H | -3.155959 | -1.260163 | 2.065653 |
| H | -0.047857 | -0.176657 | 2.595981 |
| C | -3.466627 | 2.304936 | -0.386800 |
| C | -3.653271 | 1.920386 | 0.732948 |
| H | -3.283262 | 2.643104 | -1.383284 |
| H | -3.832585 | 1.575698 | 1.728975 |
| C | -5.714986 | -1.750099 | 1.242896 |
| C | -5.115720 | -1.519177 | 0.231756 |
| H | -6.249435 | -1.944856 | 2.144520 |
| H | -4.583199 | -1.302068 | -0.669053 |
| C | -2.320031 | 2.695803 | -4.134471 |
| C | -1.499665 | 2.141848 | -3.459621 |
| H | -3.044070 | 3.189001 | -4.742468 |
| H | -0.761372 | 1.659649 | -2.854639 |
| C | -8.395259 | 1.656761 | 0.745970 |
| C | -7.285996 | 1.562058 | 0.304256 |
| H | -9.385484 | 1.743752 | 1.130448 |
| H | -6.294709 | 1.478583 | -0.087960 |
| C | -6.136758 | 0.141715 | -2.796417 |
| C | -5.013912 | 0.461837 | -3.062673 |
| H | -7.134334 | -0.139318 | -2.544761 |
| H | -4.010905 | 0.750555 | -3.291965 |
| C | -5.689184 | 0.896298 | 3.525733 |
| C | -4.760403 | 0.600889 | 4.221810 |
| H | -6.506480 | 1.160050 | 2.888626 |
| H | -3.928538 | 0.336535 | 4.834475 |
| C | -1.838617 | -1.204291 | -1.373206 |
| C | -2.238087 | -1.596946 | -2.432512 |
| H | -1.489029 | -0.858980 | -0.423035 |
| H | -2.601614 | -1.945953 | -3.372549 |

DEC 12

0 1

| | | | |
|---|-----------|-----------|-----------|
| C | 2.416750 | 3.022301 | 2.584205 |
| C | 2.507686 | 2.673992 | 3.726509 |
| H | 2.324253 | 3.320294 | 1.561345 |
| H | 2.587081 | 2.376581 | 4.747219 |
| C | -1.050267 | -0.155437 | 1.209615 |
| C | -0.217476 | 0.514845 | 1.751081 |
| H | -1.787547 | -0.754112 | 0.717717 |
| H | 0.516046 | 1.122386 | 2.235124 |
| C | -2.917954 | -2.883549 | -0.657910 |
| C | -2.766822 | -1.994862 | -1.447105 |
| H | -3.053095 | -3.672781 | 0.050003 |
| H | -2.622917 | -1.190896 | -2.135432 |
| C | -1.883122 | 1.581355 | -1.841520 |
| C | -2.917532 | 1.738688 | -2.425466 |
| H | -0.960438 | 1.440641 | -1.318693 |
| H | -3.840719 | 1.874792 | -2.941022 |
| C | -3.474065 | -5.369723 | 2.316928 |
| C | -2.353665 | -4.948448 | 2.293543 |
| H | -4.470838 | -5.746022 | 2.347476 |
| H | -1.354945 | -4.570390 | 2.257317 |
| C | 3.372426 | -0.958394 | 0.373837 |
| C | 3.581235 | -0.183070 | 1.262330 |
| H | 3.174306 | -1.646480 | -0.417123 |
| H | 3.757508 | 0.518151 | 2.047671 |
| C | -1.461169 | 5.269717 | -2.097437 |
| C | -0.969792 | 6.361476 | -2.106499 |
| H | -1.890432 | 4.290433 | -2.087061 |
| H | -0.544016 | 7.338471 | -2.116556 |
| C | 0.803062 | -3.178795 | 1.107270 |
| C | 0.872657 | -4.286730 | 0.656657 |
| H | 0.736788 | -2.181269 | 1.488377 |
| H | 0.937245 | -5.274043 | 0.259274 |
| C | 1.343260 | 3.290919 | -1.154556 |
| C | 1.794553 | 2.227684 | -0.833806 |
| H | 0.921936 | 4.228918 | -1.445891 |
| H | 2.193223 | 1.279075 | -0.540360 |
| C | 0.601826 | -1.432561 | -2.063300 |
| C | 1.001793 | -0.540501 | -2.755226 |
| H | 0.238258 | -2.225705 | -1.447000 |
| H | 1.350060 | 0.262489 | -3.364503 |

DEC 13

0 1

| | | | |
|---|-----------|-----------|-----------|
| C | -3.929926 | -0.628092 | -1.730362 |
| C | -3.114600 | -1.505128 | -1.726938 |
| H | -4.651165 | 0.157159 | -1.738237 |
| H | -2.374692 | -2.276467 | -1.716921 |
| C | 1.021953 | 0.216966 | -1.327659 |
| C | -0.161646 | 0.392676 | -1.257599 |
| H | 2.075184 | 0.048844 | -1.385950 |
| H | -1.218371 | 0.538760 | -1.201021 |
| C | 4.401290 | 1.147229 | 0.282380 |
| C | 3.622947 | 2.046345 | 0.426339 |
| H | 5.081192 | 0.335801 | 0.151593 |
| H | 2.922333 | 2.842809 | 0.553502 |
| C | 0.805244 | 3.907576 | -1.059511 |
| C | 0.930503 | 5.039111 | -0.687279 |
| H | 0.696163 | 2.889751 | -1.372147 |
| H | 1.046252 | 6.047080 | -0.360453 |
| C | 4.333008 | -1.959934 | -1.853546 |
| C | 3.546976 | -2.333073 | -1.030790 |
| H | 5.029360 | -1.636748 | -2.593078 |

| | | | |
|---|-----------|-----------|-----------|
| H | 2.838046 | -2.658999 | -0.300709 |
| C | -0.173746 | -3.155953 | -0.320594 |
| C | -0.129662 | -4.199559 | -0.907062 |
| H | -0.211152 | -2.222451 | 0.198944 |
| H | -0.084377 | -5.127763 | -1.428980 |
| C | -2.621677 | 3.188328 | -0.329381 |
| C | -2.877351 | 2.228409 | 0.340056 |
| H | -2.381669 | 4.042858 | -0.920764 |
| H | -3.075637 | 1.362811 | 0.935129 |
| C | -2.526074 | -1.251706 | 1.773562 |
| C | -1.610431 | -0.602185 | 2.192403 |
| H | -3.334893 | -1.829016 | 1.386492 |
| H | -0.788470 | -0.021018 | 2.552518 |
| C | 1.050877 | 2.119536 | 3.097218 |
| C | 0.295397 | 2.492067 | 2.245506 |
| H | 1.727292 | 1.786448 | 3.851226 |
| H | -0.382672 | 2.820704 | 1.487262 |
| C | 1.657960 | -2.072428 | 2.520655 |
| C | 2.113824 | -1.071795 | 2.045281 |
| H | 1.243091 | -2.961647 | 2.937899 |
| H | 2.520726 | -0.178762 | 1.619592 |

DEC 14

0 1

| | | | |
|---|-----------|-----------|-----------|
| C | 0.133098 | 1.341688 | 0.351361 |
| C | 1.308420 | 1.132469 | 0.454927 |
| H | -0.910010 | 1.541738 | 0.256279 |
| H | 2.361302 | 0.958040 | 0.534866 |
| C | 1.944800 | 0.636456 | -3.107754 |
| C | 2.554695 | 0.362329 | -4.101388 |
| H | 1.413008 | 0.889456 | -2.215721 |
| H | 3.095210 | 0.129745 | -4.990367 |
| C | 1.563587 | 4.391610 | 2.073718 |
| C | 1.885291 | 5.543284 | 2.141058 |
| H | 1.287796 | 3.361337 | 1.999979 |
| H | 2.185440 | 6.564381 | 2.200900 |
| C | 4.674962 | 0.407001 | -0.784699 |
| C | 5.100152 | 0.723779 | 0.290001 |
| H | 4.284991 | 0.145773 | -1.745185 |
| H | 5.462271 | 1.014797 | 1.250638 |
| C | 5.284728 | 4.274282 | 1.177707 |
| C | 6.208133 | 4.363556 | 1.935430 |
| H | 4.460784 | 4.194502 | 0.499367 |
| H | 7.033755 | 4.448811 | 2.604242 |
| C | 2.840652 | 3.580297 | -5.536978 |
| C | 3.178237 | 3.713317 | -6.678310 |
| H | 2.547615 | 3.457357 | -4.516266 |
| H | 3.467525 | 3.839405 | -7.696356 |
| C | 6.524309 | 1.786455 | -3.333087 |
| C | 5.919500 | 2.236927 | -4.263484 |
| H | 7.050112 | 1.384217 | -2.496747 |
| H | 5.367889 | 2.648038 | -5.081164 |
| C | -1.079483 | 4.803894 | -0.287821 |
| C | -1.399174 | 4.456316 | -1.387970 |
| H | -0.774172 | 5.110965 | 0.687994 |
| H | -1.685949 | 4.152692 | -2.369183 |
| C | 2.433480 | 4.034167 | -1.505379 |
| C | 3.479009 | 3.601468 | -1.901376 |
| H | 1.495264 | 4.405345 | -1.153844 |
| H | 4.405927 | 3.204184 | -2.257456 |
| C | 3.199713 | 0.891350 | 3.594007 |
| C | 3.648089 | 1.993433 | 3.458314 |
| H | 2.797757 | -0.088477 | 3.715411 |

| | | | |
|---|----------|----------|----------|
| H | 4.045851 | 2.974856 | 3.317279 |
|---|----------|----------|----------|

DEC 15

0 1

| | | | |
|---|-----------|-----------|-----------|
| C | -0.383005 | 4.727688 | 1.844644 |
| C | -0.382027 | 3.767114 | 1.129426 |
| H | -0.396910 | 5.582206 | 2.481486 |
| H | -0.376285 | 2.911716 | 0.487745 |
| C | -5.592004 | 0.137326 | -0.223086 |
| C | -6.134285 | 0.297529 | 0.832139 |
| H | -5.097391 | -0.005023 | -1.159536 |
| H | -6.624717 | 0.438683 | 1.767937 |
| C | 3.208457 | 3.529783 | 1.057908 |
| C | 4.222255 | 3.010198 | 0.686678 |
| H | 2.293711 | 3.984125 | 1.374339 |
| H | 5.114019 | 2.535224 | 0.343523 |
| C | -2.271723 | 0.325598 | 1.204007 |
| C | -1.106088 | 0.061743 | 1.296164 |
| H | -3.312391 | 0.554011 | 1.117463 |
| H | -0.062128 | -0.161030 | 1.370855 |
| C | 2.601733 | -0.193820 | 1.542418 |
| C | 2.357607 | -1.362285 | 1.435358 |
| H | 2.827166 | 0.848389 | 1.622161 |
| H | 2.139024 | -2.404852 | 1.339663 |
| C | -2.495251 | -3.200815 | 0.304434 |
| C | -2.681926 | -4.179034 | -0.361537 |
| H | -2.328068 | -2.315603 | 0.882738 |
| H | -2.854507 | -5.054470 | -0.945660 |
| C | 0.921103 | -4.763507 | 0.749358 |
| C | 2.049274 | -5.102301 | 0.963622 |
| H | -0.087229 | -4.465693 | 0.556112 |
| H | 3.051853 | -5.411631 | 1.152096 |
| C | 5.408837 | 0.684676 | -2.168582 |
| C | 4.565163 | 0.160216 | -1.500178 |
| H | 6.157351 | 1.144137 | -2.772261 |
| H | 3.809548 | -0.302757 | -0.902331 |
| C | -3.032236 | 0.111655 | -3.125574 |
| C | -2.891117 | -0.895823 | -2.493391 |
| H | -3.148623 | 1.007796 | -3.691900 |
| H | -2.766428 | -1.793966 | -1.926667 |
| C | 0.297974 | 1.146360 | -1.669506 |
| C | 1.323615 | 1.746014 | -1.514911 |
| H | -0.617031 | 0.612737 | -1.808561 |
| H | 2.240557 | 2.273621 | -1.370066 |

DEC16

0 1

| | | | |
|---|-----------|----------|-----------|
| C | -0.938110 | 2.179200 | 0.797943 |
| C | 0.139332 | 1.851158 | 0.388076 |
| H | -1.903646 | 2.472428 | 1.151596 |
| H | 1.103651 | 1.566729 | 0.028159 |
| C | 1.164724 | 3.060758 | -2.724310 |
| C | 1.233340 | 2.075190 | -3.401769 |
| H | 1.092252 | 3.936984 | -2.115423 |
| H | 1.281252 | 1.199952 | -4.008373 |
| C | 1.701725 | 3.246531 | 3.282604 |
| C | 2.608434 | 3.878340 | 3.745062 |
| H | 0.891661 | 2.692172 | 2.856465 |
| H | 3.412308 | 4.440372 | 4.162656 |
| C | 3.792990 | 1.910065 | -0.468124 |
| C | 3.868221 | 1.757255 | 0.717418 |
| H | 3.703927 | 2.053397 | -1.522407 |

| | | | |
|---|-----------|----------|-----------|
| H | 3.925990 | 1.631730 | 1.775363 |
| C | -3.714576 | 1.717026 | -2.916402 |
| C | -2.617498 | 1.900702 | -2.472938 |
| H | -4.690500 | 1.546155 | -3.308507 |
| H | -1.641220 | 2.068354 | -2.071625 |
| C | -2.271483 | 1.813996 | 4.463212 |
| C | -1.922658 | 2.938948 | 4.247643 |
| H | -2.573861 | 0.810308 | 4.656632 |
| H | -1.611191 | 3.939128 | 4.036223 |
| C | 2.273707 | 5.188699 | 0.104189 |
| C | 1.767028 | 6.169697 | -0.360022 |
| H | 2.725756 | 4.310904 | 0.512669 |
| H | 1.306838 | 7.037733 | -0.774409 |
| C | -1.787835 | 6.075481 | 2.341815 |
| C | -0.602444 | 5.918317 | 2.418238 |
| H | -2.843846 | 6.201086 | 2.255635 |
| H | 0.453901 | 5.767705 | 2.472131 |
| C | -1.738164 | 5.225612 | -2.370492 |
| C | -1.481074 | 5.320916 | -1.204432 |
| H | -1.966971 | 5.120788 | -3.406250 |
| H | -1.251803 | 5.396997 | -0.162862 |
| C | -4.195864 | 3.687710 | 0.483830 |
| C | -4.397928 | 3.523328 | 1.653149 |
| H | -3.995108 | 3.816612 | -0.557909 |
| H | -4.563570 | 3.362296 | 2.694460 |

DEC 17

0 1

| | | | |
|---|-----------|-----------|-----------|
| C | 0.597204 | 0.893690 | 0.123884 |
| C | 1.743302 | 0.583182 | 0.285844 |
| H | -0.425159 | 1.169677 | -0.025508 |
| H | 2.768167 | 0.318284 | 0.416024 |
| C | 0.944188 | 2.660975 | -3.006151 |
| C | 0.119854 | 3.220817 | -3.670631 |
| H | 1.678802 | 2.160565 | -2.412848 |
| H | -0.613343 | 3.720272 | -4.261942 |
| C | 0.621531 | 2.337947 | 3.441744 |
| C | 1.147688 | 3.342110 | 3.829386 |
| H | 0.149211 | 1.448109 | 3.085410 |
| H | 1.607266 | 4.245625 | 4.161588 |
| C | 4.343463 | 2.235841 | -1.426873 |
| C | 4.727252 | 1.294088 | -2.058950 |
| H | 3.985956 | 3.074182 | -0.867877 |
| H | 5.073324 | 0.460029 | -2.625164 |
| C | -2.898941 | 0.942107 | -1.294739 |
| C | -2.185949 | 0.715509 | -2.229423 |
| H | -3.516126 | 1.148892 | -0.449787 |
| H | -1.540520 | 0.532203 | -3.058327 |
| C | -3.711657 | 4.040776 | 4.483964 |
| C | -2.517860 | 3.949299 | 4.447178 |
| H | -4.773183 | 4.130466 | 4.525667 |
| H | -1.452768 | 3.861149 | 4.395001 |
| C | 2.535110 | 5.303010 | -0.085294 |
| C | 2.055471 | 4.360722 | 0.478497 |
| H | 2.956386 | 6.143307 | -0.588947 |
| H | 1.619304 | 3.523966 | 0.982374 |
| C | -1.335681 | 3.943563 | -0.188230 |
| C | -1.863827 | 4.181191 | 0.860681 |
| H | -0.859360 | 3.728182 | -1.120736 |
| H | -2.329338 | 4.406064 | 1.794996 |
| C | -2.583048 | 0.766642 | 2.624132 |
| C | -2.170390 | -0.182204 | 2.020826 |

| | | | |
|---|-----------|-----------|----------|
| H | -2.942031 | 1.614102 | 3.167794 |
| H | -1.803787 | -1.022046 | 1.474694 |
| C | -0.467136 | 6.874141 | 3.774454 |
| C | -0.012038 | 6.465114 | 2.745134 |
| H | -0.880487 | 7.239388 | 4.686567 |
| H | 0.386370 | 6.091999 | 1.826160 |

DEC 18

0 1

| | | | |
|---|-----------|-----------|-----------|
| C | 0.844917 | -1.335036 | 0.047246 |
| C | -0.144087 | -1.472864 | 0.710259 |
| H | 1.730395 | -1.203287 | -0.539072 |
| H | -1.023420 | -1.600011 | 1.305063 |
| C | -1.432645 | -0.952341 | -2.805596 |
| C | -1.930960 | -0.587843 | -3.832125 |
| H | -0.979276 | -1.268064 | -1.888867 |
| H | -2.370312 | -0.271747 | -4.750881 |
| C | 2.317240 | 1.483528 | 1.590806 |
| C | 3.373561 | 1.983985 | 1.851711 |
| H | 1.380269 | 1.034346 | 1.343179 |
| H | 4.312502 | 2.440031 | 2.068804 |
| C | -3.601787 | -1.655814 | 2.016941 |
| C | -3.168145 | -2.005862 | 3.077265 |
| H | -3.996704 | -1.338873 | 1.073425 |
| H | -2.780510 | -2.319581 | 4.019798 |
| C | 4.937230 | -2.719864 | 1.733488 |
| C | 4.345608 | -1.683643 | 1.834595 |
| H | 5.458568 | -3.646219 | 1.656090 |
| H | 3.818124 | -0.757243 | 1.923858 |
| C | 5.068620 | 2.869402 | -1.054533 |
| C | 5.203723 | 4.053027 | -0.934961 |
| H | 4.936674 | 1.814388 | -1.165281 |
| H | 5.330036 | 5.106400 | -0.833153 |
| C | 3.501184 | -0.204700 | -2.296213 |
| C | 4.188510 | -0.893891 | -1.597659 |
| H | 2.879603 | 0.421370 | -2.897817 |
| H | 4.784033 | -1.505488 | -0.956450 |
| C | -7.003681 | -0.620982 | 2.882154 |
| C | -8.092921 | -0.197091 | 2.624114 |
| H | -6.028848 | -0.995114 | 3.107783 |
| H | -9.067033 | 0.176526 | 2.405753 |
| C | -4.826909 | -0.405242 | -1.311694 |
| C | -5.739288 | -0.288850 | -0.544358 |
| H | -4.012474 | -0.507063 | -1.996303 |
| H | -6.542984 | -0.188868 | 0.152389 |
| C | 0.488758 | 2.046274 | -2.077521 |
| C | 1.431781 | 2.604017 | -1.593223 |
| H | -0.350378 | 1.543818 | -2.505741 |
| H | 2.276909 | 3.089452 | -1.155866 |

DEC 19

0 1

| | | | |
|---|-----------|-----------|-----------|
| C | 1.111187 | -0.497885 | -0.890557 |
| C | 0.257322 | 0.306747 | -1.137636 |
| H | 1.866721 | -1.221464 | -0.666369 |
| H | -0.512667 | 1.021173 | -1.338742 |
| C | 3.777117 | 1.898671 | -1.337462 |
| C | 4.896254 | 2.262928 | -1.116075 |
| H | 2.776787 | 1.566280 | -1.516440 |
| H | 5.894362 | 2.586219 | -0.927707 |
| C | -2.469424 | -1.508190 | 0.144044 |

| | | | |
|---|-----------|-----------|-----------|
| C | -3.198937 | -2.163174 | -0.544394 |
| H | -1.816672 | -0.918686 | 0.753044 |
| H | -3.832244 | -2.755533 | -1.164757 |
| C | 1.372857 | 4.178994 | -0.343348 |
| C | 0.602520 | 3.558712 | 0.331857 |
| H | 2.073254 | 4.719923 | -0.937617 |
| H | -0.078655 | 2.994376 | 0.932225 |
| C | -0.234445 | -4.560911 | -2.957708 |
| C | -0.389647 | -3.488297 | -2.448338 |
| H | -0.102461 | -5.513367 | -3.417302 |
| H | -0.529585 | -2.531169 | -1.993136 |
| C | 3.041418 | -0.602563 | 2.665259 |
| C | 3.306257 | 0.273781 | 1.892812 |
| H | 2.804038 | -1.383047 | 3.352042 |
| H | 3.545146 | 1.049103 | 1.196202 |
| C | 2.761861 | -3.687744 | -0.567126 |
| C | 3.611433 | -3.126312 | 0.062899 |
| H | 1.994499 | -4.168000 | -1.134654 |
| H | 4.360424 | -2.616104 | 0.624874 |
| C | -3.048437 | 1.983399 | -0.972944 |
| C | -2.429747 | 2.984943 | -1.193856 |
| H | -3.597898 | 1.090905 | -0.767937 |
| H | -1.866265 | 3.871079 | -1.381064 |
| C | -0.438530 | 0.817073 | 2.398345 |
| C | -1.592127 | 1.139092 | 2.443006 |
| H | 0.593305 | 0.539305 | 2.347586 |
| H | -2.625974 | 1.407181 | 2.470102 |
| C | -5.415398 | 1.440483 | 1.756894 |
| C | -5.116837 | 0.281176 | 1.767083 |
| H | -5.684741 | 2.472159 | 1.744638 |
| H | -4.840285 | -0.749532 | 1.757893 |

DEC 20

0 1

| | | | |
|---|-----------|----------|-----------|
| C | -0.274663 | 1.945110 | 1.344550 |
| C | 0.674526 | 1.327346 | 1.734308 |
| H | -1.114344 | 2.507155 | 0.996175 |
| H | 1.527087 | 0.783917 | 2.074257 |
| C | 0.926345 | 4.394264 | -6.043908 |
| C | 1.512634 | 3.650816 | -6.776415 |
| H | 0.407064 | 5.053127 | -5.382121 |
| H | 2.034818 | 2.996190 | -7.436160 |
| C | 1.566049 | 4.082993 | 3.926995 |
| C | 1.740211 | 3.700748 | 5.048854 |
| H | 1.417711 | 4.416907 | 2.920956 |
| H | 1.889255 | 3.369222 | 6.051114 |
| C | 4.597201 | 2.000122 | 1.044952 |
| C | 4.114753 | 2.380249 | 2.073730 |
| H | 5.032261 | 1.667822 | 0.126624 |
| H | 3.680886 | 2.724574 | 2.987482 |
| C | -3.197236 | 3.124900 | 4.575416 |
| C | -2.013360 | 3.061868 | 4.406555 |
| H | -4.250539 | 3.173074 | 4.731694 |
| H | -0.956121 | 3.006018 | 4.258833 |
| C | 4.984104 | 1.500033 | -2.524413 |
| C | 6.174758 | 1.391683 | -2.459892 |
| H | 3.921300 | 1.607010 | -2.577988 |
| H | 7.235228 | 1.296877 | -2.411272 |
| C | -2.656439 | 4.725089 | 1.178831 |
| C | -2.501023 | 4.901538 | 0.003979 |
| H | -2.789065 | 4.548992 | 2.224993 |
| H | -2.351421 | 5.067002 | -1.040598 |

| | | | |
|---|-----------|----------|-----------|
| C | 1.418263 | 2.406341 | -3.067346 |
| C | 1.346457 | 2.221863 | -1.884984 |
| H | 1.471658 | 2.585432 | -4.120110 |
| H | 1.260990 | 2.056938 | -0.830991 |
| C | -0.955046 | 6.465562 | -3.235930 |
| C | -0.242626 | 5.612629 | -2.788297 |
| H | -1.583548 | 7.231628 | -3.629744 |
| H | 0.392559 | 4.850231 | -2.387779 |
| C | 1.057349 | 5.521952 | 0.471398 |
| C | 2.095776 | 4.929377 | 0.395690 |
| H | 0.124344 | 6.036799 | 0.532097 |
| H | 3.016485 | 4.390034 | 0.343220 |

EICO 1

0 1

| | | | |
|---|----------|-----------|-----------|
| C | 4.003288 | 4.769306 | 10.739661 |
| C | 4.991851 | 5.385470 | 11.021343 |
| H | 3.124578 | 4.222654 | 10.475621 |
| H | 5.882196 | 5.929618 | 11.251014 |
| C | 2.371399 | 8.966396 | 10.801754 |
| C | 2.420419 | 8.048350 | 11.569676 |
| H | 2.342909 | 9.783730 | 10.112753 |
| H | 2.476723 | 7.226375 | 12.246655 |
| C | 8.412986 | 7.227034 | 10.734827 |
| C | 8.188338 | 6.383343 | 9.914545 |
| H | 8.617328 | 7.987210 | 11.454209 |
| H | 7.977660 | 5.629824 | 9.184929 |
| C | 7.203601 | 3.581505 | 7.496350 |
| C | 6.736850 | 3.222372 | 8.540187 |
| H | 7.590767 | 3.915061 | 6.557731 |
| H | 6.294417 | 2.917324 | 9.462778 |
| C | 0.749266 | 4.568399 | 8.602834 |
| C | 0.955124 | 5.648050 | 9.078402 |
| H | 0.565219 | 3.609434 | 8.175025 |
| H | 1.147901 | 6.608827 | 9.504211 |
| C | 6.685641 | 9.815259 | 8.856993 |
| C | 6.446888 | 10.980325 | 8.716408 |
| H | 6.917311 | 8.778822 | 8.973285 |
| H | 6.225392 | 12.014921 | 8.586317 |
| C | 2.752732 | 3.525025 | 1.368561 |
| C | 3.644952 | 3.491153 | 2.166947 |
| H | 1.961677 | 3.555665 | 0.653996 |
| H | 4.451173 | 3.475233 | 2.868316 |
| C | 5.874494 | 0.235196 | 4.566777 |
| C | 6.285253 | 0.613994 | 5.626017 |
| H | 5.506850 | -0.112450 | 3.628093 |
| H | 6.637886 | 0.969391 | 6.570063 |
| C | 6.713278 | 6.620252 | -0.182531 |
| C | 5.861717 | 5.936391 | 0.307494 |
| H | 7.471065 | 7.234169 | -0.612772 |
| H | 5.095518 | 5.335520 | 0.745991 |
| C | 3.447820 | 1.812880 | 8.886043 |
| C | 3.297684 | 1.069374 | 9.813209 |
| H | 3.586107 | 2.480599 | 8.060561 |
| H | 3.159613 | 0.405477 | 10.635804 |
| C | 3.491838 | 7.921647 | 6.910721 |
| C | 3.692502 | 7.493053 | 8.012636 |
| H | 3.330876 | 8.309561 | 5.927016 |
| H | 3.870459 | 7.103947 | 8.992586 |
| C | 8.184431 | 9.097920 | 2.959276 |
| C | 8.262658 | 7.931247 | 2.700712 |

| | | | |
|---|----------|-----------|----------|
| H | 8.102308 | 10.134646 | 3.195841 |
| H | 8.316078 | 6.890928 | 2.465929 |
| C | 3.004661 | 11.302819 | 7.991537 |
| C | 2.165712 | 12.064946 | 8.380715 |
| H | 3.755479 | 10.620581 | 7.650872 |
| H | 1.427296 | 12.750607 | 8.729411 |
| C | 7.970439 | 7.208368 | 6.250109 |
| C | 6.851416 | 6.840304 | 6.470689 |
| H | 8.963277 | 7.538103 | 6.042883 |
| H | 5.848032 | 6.525282 | 6.666345 |
| C | 4.654833 | 7.524864 | 3.187067 |
| C | 3.769518 | 6.773728 | 3.486711 |
| H | 5.454732 | 8.181831 | 2.921957 |
| H | 2.969861 | 6.116594 | 3.754855 |
| C | 1.491609 | 9.491822 | 4.035643 |
| C | 1.267929 | 10.040869 | 5.076575 |
| H | 1.706744 | 8.993657 | 3.116722 |
| H | 1.097883 | 10.530293 | 6.010606 |
| C | 4.131162 | 3.508878 | 5.771312 |
| C | 3.429389 | 4.375711 | 6.211820 |
| H | 4.762241 | 2.731217 | 5.396916 |
| H | 2.809007 | 5.149105 | 6.612241 |
| C | 6.774090 | 4.565065 | 3.749363 |
| C | 7.373164 | 3.536395 | 3.611605 |
| H | 6.223619 | 5.474445 | 3.867465 |
| H | 7.896991 | 2.615210 | 3.495931 |
| C | 0.395419 | 6.089767 | 4.794456 |
| C | 0.641676 | 5.006121 | 4.347730 |
| H | 0.190919 | 7.060794 | 5.188466 |
| H | 0.885056 | 4.044007 | 3.955375 |
| C | 4.881732 | 10.927928 | 4.784271 |
| C | 5.669704 | 10.194703 | 5.310478 |
| H | 4.164177 | 11.568328 | 4.324101 |
| H | 6.355399 | 9.524992 | 5.783537 |

EICO 2

0 1

| | | | |
|---|----------|-----------|-----------|
| C | 3.865470 | 4.523555 | 11.118779 |
| C | 4.921625 | 5.040873 | 11.349163 |
| H | 2.923807 | 4.074175 | 10.890331 |
| H | 5.865110 | 5.508408 | 11.527342 |
| C | 2.909731 | 8.809619 | 11.008267 |
| C | 2.837147 | 7.970926 | 11.860358 |
| H | 2.978845 | 9.552349 | 10.243233 |
| H | 2.785227 | 7.214786 | 12.609786 |
| C | 7.998284 | 7.176682 | 10.517253 |
| C | 7.718248 | 6.459970 | 9.598957 |
| H | 8.251318 | 7.825291 | 11.324947 |
| H | 7.463509 | 5.821996 | 8.778731 |
| C | 6.128036 | 4.196057 | 6.900359 |
| C | 5.720696 | 3.870808 | 7.980051 |
| H | 6.491331 | 4.473857 | 5.933392 |
| H | 5.345345 | 3.598153 | 8.942438 |
| C | 0.426757 | 4.671684 | 9.345786 |
| C | 0.884500 | 5.738359 | 9.642554 |
| H | 0.022277 | 3.721889 | 9.077850 |
| H | 1.303007 | 6.684433 | 9.914402 |
| C | 6.117612 | 9.960893 | 9.195349 |
| C | 5.825796 | 11.115920 | 9.318555 |
| H | 6.386553 | 8.931498 | 9.094497 |
| H | 5.557342 | 12.141785 | 9.428421 |
| C | 2.936119 | 3.517482 | 1.461841 |

| | | | |
|---|-----------|-----------|-----------|
| C | 4.031881 | 3.638195 | 1.930802 |
| H | 1.961675 | 3.411713 | 1.042919 |
| H | 5.010480 | 3.756717 | 2.348212 |
| C | 4.552372 | 0.869409 | 4.115307 |
| C | 4.791968 | 1.299046 | 5.207490 |
| H | 4.334074 | 0.495843 | 3.140796 |
| H | 5.005888 | 1.698779 | 6.175566 |
| C | 7.023918 | 6.387400 | 0.117870 |
| C | 5.860083 | 6.263726 | 0.372024 |
| H | 8.064961 | 6.491724 | -0.089052 |
| H | 4.829077 | 6.134535 | 0.617459 |
| C | 2.824253 | 2.022382 | 8.548566 |
| C | 3.059218 | 1.302779 | 9.476902 |
| H | 2.621846 | 2.666957 | 7.718229 |
| H | 3.270235 | 0.659463 | 10.300477 |
| C | 3.483526 | 7.729389 | 7.247486 |
| C | 3.853767 | 7.099571 | 8.198420 |
| H | 3.153227 | 8.282497 | 6.393854 |
| H | 4.168361 | 6.539121 | 9.053346 |
| C | 9.212181 | 7.957212 | 2.489695 |
| C | 9.999676 | 7.063812 | 2.616475 |
| H | 8.501273 | 8.747394 | 2.373027 |
| H | 10.694419 | 6.263364 | 2.733264 |
| C | 2.548297 | 11.211617 | 8.080087 |
| C | 1.581167 | 11.552901 | 8.699286 |
| H | 3.415643 | 10.908697 | 7.532105 |
| H | 0.724567 | 11.857131 | 9.256184 |
| C | 8.129277 | 7.697444 | 5.919141 |
| C | 6.971759 | 7.527805 | 6.178864 |
| H | 9.156181 | 7.842574 | 5.672134 |
| H | 5.938755 | 7.375683 | 6.412793 |
| C | 4.750515 | 7.521907 | 3.502481 |
| C | 4.158756 | 6.558930 | 3.902771 |
| H | 5.282779 | 8.381026 | 3.154179 |
| H | 3.627969 | 5.708909 | 4.277319 |
| C | 1.491960 | 9.020438 | 4.322001 |
| C | 1.049318 | 9.717922 | 5.189429 |
| H | 1.906797 | 8.390034 | 3.566818 |
| H | 0.671319 | 10.334067 | 5.974677 |
| C | 6.436338 | 10.641171 | 2.059001 |
| C | 6.352915 | 9.849075 | 1.164086 |
| H | 6.489395 | 11.337825 | 2.865637 |
| H | 6.277992 | 9.121412 | 0.385664 |
| C | 7.392979 | 4.629956 | 3.395456 |
| C | 7.314278 | 3.452400 | 3.604524 |
| H | 7.466849 | 5.679571 | 3.209366 |
| H | 7.221833 | 2.407217 | 3.799524 |
| C | 1.907490 | 4.607981 | 6.053081 |
| C | 2.151884 | 3.729831 | 5.274269 |
| H | 1.702355 | 5.385845 | 6.757223 |
| H | 2.394961 | 2.953386 | 4.582366 |
| C | 4.520868 | 10.923974 | 5.026510 |
| C | 5.499396 | 10.678624 | 5.673212 |
| H | 3.639150 | 11.119803 | 4.458034 |
| H | 6.361957 | 10.443852 | 6.257233 |

EICO 3

0 1

| | | | |
|---|----------|----------|-----------|
| C | 4.162118 | 5.932192 | 10.627904 |
| C | 5.266015 | 6.231743 | 11.013961 |
| H | 3.191992 | 5.669434 | 10.262347 |
| H | 6.254660 | 6.504739 | 11.312728 |

| | | | |
|---|-----------|-----------|-----------|
| C | 1.022392 | 8.440920 | 9.767693 |
| C | 2.026691 | 8.612982 | 10.414405 |
| H | 0.150105 | 8.285268 | 9.170075 |
| H | 2.929588 | 8.741636 | 10.968699 |
| C | 8.858111 | 7.772875 | 10.432590 |
| C | 8.598854 | 6.848114 | 9.700937 |
| H | 9.103328 | 8.588151 | 11.075827 |
| H | 8.375297 | 6.021053 | 9.056352 |
| C | 8.793227 | 3.899355 | 7.471418 |
| C | 7.877598 | 3.424917 | 8.098418 |
| H | 9.597696 | 4.316226 | 6.903732 |
| H | 7.060341 | 2.997830 | 8.641051 |
| C | 1.848870 | 3.653041 | 8.867980 |
| C | 1.270509 | 4.513622 | 8.249061 |
| H | 2.388391 | 2.900031 | 9.401574 |
| H | 0.761173 | 5.269309 | 7.690350 |
| C | 5.877886 | 9.496968 | 8.802755 |
| C | 4.926524 | 10.212509 | 8.599889 |
| H | 6.719232 | 8.862996 | 8.989580 |
| H | 4.069807 | 10.821562 | 8.401775 |
| C | -0.116852 | 4.762045 | 4.376430 |
| C | 0.797056 | 3.974645 | 4.347761 |
| H | -0.917504 | 5.465364 | 4.435876 |
| H | 1.625584 | 3.300361 | 4.340014 |
| C | 4.711273 | -1.252746 | 6.879594 |
| C | 4.677899 | -0.118548 | 6.469588 |
| H | 4.741951 | -2.262047 | 7.224342 |
| H | 4.645048 | 0.890336 | 6.110500 |
| C | 6.907496 | 8.551570 | 2.228278 |
| C | 7.324877 | 7.786863 | 1.392997 |
| H | 6.529344 | 9.227462 | 2.967309 |
| H | 7.707552 | 7.105123 | 0.666986 |
| C | 4.921951 | 1.459499 | 9.684634 |
| C | 4.980236 | 2.454576 | 10.366487 |
| H | 4.875874 | 0.592790 | 9.058552 |
| H | 5.022329 | 3.356263 | 10.940557 |
| C | 3.112667 | 7.017774 | 5.704277 |
| C | 3.087178 | 7.523694 | 6.801008 |
| H | 3.146743 | 6.573970 | 4.732397 |
| H | 3.052617 | 7.967852 | 7.772886 |
| C | 11.665298 | 5.825008 | 5.476631 |
| C | 10.860952 | 5.372470 | 4.698942 |
| H | 12.388882 | 6.220660 | 6.153772 |
| H | 10.138151 | 4.972669 | 4.017744 |
| C | 1.961954 | 11.165436 | 6.668292 |
| C | 1.349245 | 11.336352 | 7.693971 |
| H | 2.512261 | 10.995217 | 5.767069 |
| H | 0.811266 | 11.472627 | 8.605062 |
| C | 7.960619 | 7.382641 | 5.794748 |
| C | 6.780136 | 7.243164 | 6.008546 |
| H | 9.008937 | 7.469889 | 5.609660 |
| H | 5.732342 | 7.129892 | 6.200307 |
| C | 3.766410 | 6.588444 | 1.905654 |
| C | 2.721709 | 6.018754 | 2.112927 |
| H | 4.700705 | 7.081067 | 1.726993 |
| H | 1.807194 | 5.507673 | 2.329800 |
| C | 0.585570 | 10.218123 | 3.574224 |
| C | 1.320096 | 9.355106 | 3.159540 |
| H | -0.057989 | 10.982548 | 3.947707 |
| H | 1.959697 | 8.581510 | 2.788583 |
| C | 4.754750 | 3.359571 | 4.920059 |
| C | 4.017223 | 3.535492 | 5.860476 |
| H | 5.438438 | 3.250063 | 4.105848 |

| | | | |
|---|-----------|-----------|----------|
| H | 3.361131 | 3.709997 | 6.689072 |
| C | 7.621746 | 4.755770 | 3.162274 |
| C | 7.944643 | 3.806235 | 2.489888 |
| H | 7.348079 | 5.597127 | 3.766727 |
| H | 8.223199 | 2.966175 | 1.893758 |
| C | -1.555837 | 7.256694 | 7.024783 |
| C | -0.607249 | 7.776515 | 6.487821 |
| H | -2.401929 | 6.802844 | 7.490587 |
| H | 0.236259 | 8.234744 | 6.014596 |
| C | 4.740102 | 11.025255 | 3.946914 |
| C | 5.202953 | 10.562558 | 4.961311 |
| H | 4.320677 | 11.431916 | 3.054032 |
| H | 5.595237 | 10.157824 | 5.871014 |

EICO 4

0 1

| | | | |
|---|-----------|-----------|-----------|
| C | 1.594720 | 2.176830 | 2.917653 |
| C | 2.528469 | 1.776487 | 2.265569 |
| H | 0.754154 | 2.505331 | 3.490289 |
| H | 3.359708 | 1.424132 | 1.692317 |
| C | 5.710317 | 2.493602 | 0.583227 |
| C | 5.560589 | 1.698308 | -0.313081 |
| H | 5.833559 | 3.187609 | 1.389132 |
| H | 5.443851 | 0.997838 | -1.113488 |
| C | -0.695231 | 2.970987 | 0.305799 |
| C | -1.847066 | 2.725186 | 0.575475 |
| H | 0.317986 | 3.202459 | 0.048450 |
| H | -2.854193 | 2.478287 | 0.838470 |
| C | 7.446772 | -3.316367 | 0.335300 |
| C | 7.022888 | -2.695149 | -0.607903 |
| H | 7.834663 | -3.865700 | 1.163700 |
| H | 6.640059 | -2.145692 | -1.442629 |
| C | -5.037936 | 0.866058 | 1.811564 |
| C | -4.419904 | 1.273101 | 2.765944 |
| H | -5.578415 | 0.494708 | 0.965645 |
| H | -3.858519 | 1.634716 | 3.601831 |
| C | -1.469011 | 1.563879 | 4.880843 |
| C | -1.708737 | 2.586569 | 5.475120 |
| H | -1.257911 | 0.667271 | 4.335450 |
| H | -1.912083 | 3.486364 | 6.011830 |
| C | 4.771516 | 4.354135 | 3.531897 |
| C | 5.789673 | 4.984800 | 3.677205 |
| H | 3.875252 | 3.785579 | 3.388964 |
| H | 6.684217 | 5.548613 | 3.819740 |
| C | 2.834515 | -1.697773 | 1.674429 |
| C | 3.955884 | -2.013319 | 1.355415 |
| H | 1.846445 | -1.403130 | 1.961013 |
| H | 4.948807 | -2.295545 | 1.071783 |
| C | -4.308524 | 3.224340 | -2.948788 |
| C | -5.044549 | 2.292446 | -2.733364 |
| H | -3.664940 | 4.059461 | -3.127078 |
| H | -5.684131 | 1.459736 | -2.530892 |
| C | -1.745028 | 5.562450 | -2.006464 |
| C | -1.733661 | 6.327133 | -2.940247 |
| H | -1.742484 | 4.873595 | -1.185916 |
| H | -1.729832 | 7.011348 | -3.759223 |
| C | -0.830675 | -1.539137 | 2.738330 |
| C | -0.852228 | -0.598707 | 1.980705 |
| H | -0.819786 | -2.378226 | 3.398032 |
| H | -0.877110 | 0.236510 | 1.310980 |
| C | 2.746094 | 4.088959 | -1.250819 |
| C | 1.810527 | 4.679247 | -1.733311 |

| | | | |
|---|-----------|-----------|-----------|
| H | 3.584686 | 3.568352 | -0.837540 |
| H | 0.974226 | 5.198550 | -2.150309 |
| C | -0.500890 | -2.311812 | -6.246207 |
| C | -1.001868 | -1.804531 | -5.272871 |
| H | -0.076441 | -2.748349 | -7.122384 |
| H | -1.436439 | -1.363109 | -4.399530 |
| C | -2.313848 | -0.030158 | -2.054716 |
| C | -1.850912 | -1.085223 | -1.690580 |
| H | -2.742061 | 0.903746 | -2.355597 |
| H | -1.424766 | -2.006821 | -1.350999 |
| C | 2.060000 | -2.571827 | -1.826778 |
| C | 1.598281 | -2.588399 | -2.942881 |
| H | 2.459250 | -2.538080 | -0.832997 |
| H | 1.152082 | -2.586306 | -3.915780 |
| C | 6.052515 | -0.334169 | -3.456979 |
| C | 4.977688 | -0.837695 | -3.235056 |
| H | 6.998090 | 0.112500 | -3.671072 |
| H | 4.023875 | -1.288228 | -3.044317 |
| C | -1.455488 | -4.158201 | 0.249383 |
| C | -0.646945 | -4.555744 | -0.554462 |
| H | -2.178303 | -3.808439 | 0.958771 |
| H | 0.089940 | -4.858999 | -1.265024 |
| C | -4.283659 | -7.801805 | 1.406515 |
| C | -3.450737 | -7.144010 | 0.833190 |
| H | -5.014388 | -8.398459 | 1.904853 |
| H | -2.707773 | -6.548913 | 0.344806 |
| C | -5.741415 | -1.003024 | -1.314533 |
| C | -6.922308 | -0.791265 | -1.181348 |
| H | -4.690811 | -1.168459 | -1.441956 |
| H | -7.971524 | -0.631600 | -1.068093 |
| C | -4.240627 | -2.774415 | 2.513523 |
| C | -4.342418 | -3.973647 | 2.423656 |
| H | -4.169802 | -1.709136 | 2.579131 |
| H | -4.424456 | -5.035155 | 2.320824 |

EICO 5

0 1

| | | | |
|---|----------|-----------|-----------|
| C | 4.622980 | 4.178759 | 11.942645 |
| C | 5.647477 | 4.816179 | 11.907884 |
| H | 3.718570 | 3.611497 | 11.948028 |
| H | 6.550999 | 5.385512 | 11.838592 |
| C | 3.007125 | 8.872901 | 11.330570 |
| C | 3.509208 | 7.888502 | 11.815787 |
| H | 2.560392 | 9.733738 | 10.880261 |
| H | 3.954525 | 7.008200 | 12.227617 |
| C | 8.507301 | 7.247699 | 10.688745 |
| C | 8.050933 | 6.544920 | 9.819867 |
| H | 8.918951 | 7.879674 | 11.443532 |
| H | 7.636489 | 5.925387 | 9.051104 |
| C | 6.478723 | 3.951971 | 7.343853 |
| C | 6.144332 | 3.747220 | 8.486072 |
| H | 6.748823 | 4.115123 | 6.322217 |
| H | 5.834939 | 3.606330 | 9.499654 |
| C | 2.595365 | 1.582372 | 4.005710 |
| C | 2.603499 | 1.623007 | 5.212021 |
| H | 2.611411 | 1.576136 | 2.937327 |
| H | 2.617749 | 1.667674 | 6.280636 |
| C | 7.827996 | 10.373553 | 8.747473 |
| C | 7.985866 | 11.555623 | 8.931943 |
| H | 7.683999 | 9.326056 | 8.583084 |
| H | 8.134523 | 12.597575 | 9.106674 |
| C | 3.032797 | 3.223169 | 0.435099 |

| | | | |
|---|-----------|-----------|-----------|
| C | 3.956655 | 3.282603 | 1.209560 |
| H | 2.228981 | 3.172991 | -0.264774 |
| H | 4.773748 | 3.326422 | 1.901039 |
| C | 5.461763 | -0.624553 | 6.319087 |
| C | 5.675988 | 0.401678 | 6.916220 |
| H | 5.269205 | -1.536347 | 5.799660 |
| H | 5.863270 | 1.324446 | 7.425875 |
| C | 7.633152 | 5.975974 | 0.227180 |
| C | 6.452181 | 6.078518 | 0.453770 |
| H | 8.677802 | 5.876226 | 0.034592 |
| H | 5.406239 | 6.172245 | 0.659650 |
| C | 2.621093 | 3.087352 | 8.792480 |
| C | 2.629879 | 1.924483 | 9.117005 |
| H | 2.614169 | 4.119717 | 8.505374 |
| H | 2.638016 | 0.895385 | 9.399342 |
| C | 2.433729 | 6.560750 | 7.158465 |
| C | 2.770480 | 6.907744 | 8.265579 |
| H | 2.111210 | 6.255577 | 6.184382 |
| H | 3.048742 | 7.234121 | 9.247054 |
| C | 9.199946 | 6.993749 | 3.285124 |
| C | 10.041754 | 6.212443 | 3.656348 |
| H | 8.446245 | 7.686504 | 2.971750 |
| H | 10.791418 | 5.523968 | 3.976778 |
| C | 1.816686 | 11.029585 | 8.450246 |
| C | 0.758020 | 11.092005 | 9.026779 |
| H | 2.748865 | 10.978624 | 7.925158 |
| H | -0.176374 | 11.149327 | 9.539116 |
| C | 7.326991 | 7.511474 | 6.230165 |
| C | 6.176043 | 7.504534 | 6.595143 |
| H | 8.333264 | 7.495935 | 5.872705 |
| H | 5.153763 | 7.483853 | 6.910799 |
| C | 3.498369 | 7.860494 | 1.621207 |
| C | 2.789392 | 6.891826 | 1.751308 |
| H | 4.160286 | 8.695967 | 1.538058 |
| H | 2.169769 | 6.033370 | 1.896100 |
| C | 1.137665 | 9.314341 | 4.070496 |
| C | 0.746864 | 9.669932 | 5.156150 |
| H | 1.501279 | 8.964239 | 3.126925 |
| H | 0.436924 | 9.993718 | 6.126882 |
| C | 6.465567 | 9.769873 | 2.887250 |
| C | 6.825202 | 9.458965 | 1.777203 |
| H | 6.134981 | 10.046923 | 3.867609 |
| H | 7.138688 | 9.150102 | 0.804439 |
| C | 7.022218 | 3.655453 | 3.434581 |
| C | 6.513882 | 2.681098 | 3.935956 |
| H | 7.475318 | 4.514525 | 2.986799 |
| H | 6.069766 | 1.823489 | 4.397217 |
| C | 0.249902 | 5.846573 | 4.250407 |
| C | 0.731318 | 4.739324 | 4.263447 |
| H | -0.150579 | 6.837047 | 4.256438 |
| H | 1.160700 | 3.758584 | 4.293922 |
| C | 4.180345 | 10.837980 | 5.700605 |
| C | 5.167035 | 11.016400 | 6.374284 |
| H | 3.295679 | 10.656667 | 5.126304 |
| H | 6.039397 | 11.157469 | 6.979507 |

EICO 6

0 1

| | | | |
|---|----------|----------|-----------|
| C | 3.388059 | 4.853993 | -1.244800 |
| C | 4.002528 | 4.811267 | -0.206784 |
| H | 2.818642 | 4.875055 | -2.148491 |

| | | | |
|---|-----------|-----------|-----------|
| H | 4.523805 | 4.743590 | 0.723324 |
| C | 5.427757 | 0.199750 | -0.829340 |
| C | 5.094517 | 1.350271 | -0.979221 |
| H | 5.730177 | -0.817664 | -0.693960 |
| H | 4.798955 | 2.371267 | -1.097323 |
| C | 4.740722 | 3.126238 | 3.353405 |
| C | 3.614012 | 2.995871 | 2.940167 |
| H | 5.734486 | 3.235777 | 3.726245 |
| H | 2.613715 | 2.889108 | 2.574250 |
| C | -0.131380 | 3.417347 | 1.642429 |
| C | 0.664488 | 4.226264 | 1.229400 |
| H | -0.852325 | 2.702521 | 1.978860 |
| H | 1.393048 | 4.909013 | 0.848121 |
| C | -4.679585 | 2.127407 | -2.780683 |
| C | -3.600379 | 2.654109 | -2.904235 |
| H | -5.620822 | 1.643182 | -2.636735 |
| H | -2.641977 | 3.119438 | -2.999527 |
| C | 5.258231 | -0.607788 | 2.876057 |
| C | 5.852236 | -1.650045 | 2.745781 |
| H | 4.744736 | 0.324192 | 2.984786 |
| H | 6.377253 | -2.566921 | 2.595902 |
| C | -6.864605 | -0.811347 | -1.174718 |
| C | -6.011881 | -0.250895 | -0.529852 |
| H | -7.622198 | -1.311949 | -1.735057 |
| H | -5.255282 | 0.249252 | 0.040684 |
| C | -3.637177 | 5.603039 | -0.932935 |
| C | -2.595321 | 5.351279 | -0.378836 |
| H | -4.555292 | 5.827473 | -1.427558 |
| H | -1.679220 | 5.103898 | 0.115638 |
| C | -7.044237 | -2.674635 | 3.754103 |
| C | -6.506809 | -2.557969 | 2.680350 |
| H | -7.538674 | -2.778133 | 4.693922 |
| H | -6.026491 | -2.456829 | 1.729988 |
| C | 0.289052 | 3.326865 | -2.705162 |
| C | -0.072381 | 4.420242 | -3.067519 |
| H | 0.603633 | 2.354838 | -2.382951 |
| H | -0.401621 | 5.386732 | -3.378220 |
| C | 0.601167 | -0.367516 | -1.778729 |
| C | 1.733912 | -0.076490 | -1.472995 |
| H | -0.396417 | -0.636773 | -2.061832 |
| H | 2.743007 | 0.171808 | -1.208405 |
| C | -2.076216 | -1.647348 | 4.062014 |
| C | -3.249183 | -1.896009 | 4.205396 |
| H | -1.042277 | -1.409074 | 3.923598 |
| H | -4.292117 | -2.117018 | 4.297677 |
| C | 5.732748 | -3.583855 | -0.395035 |
| C | 6.912139 | -3.487762 | -0.632187 |
| H | 4.687224 | -3.658315 | -0.175348 |
| H | 7.953494 | -3.413006 | -0.851977 |
| C | 1.142273 | 0.275041 | 3.616052 |
| C | 1.038386 | -0.062119 | 2.461346 |
| H | 1.241709 | 0.579226 | 4.634203 |
| H | 0.962313 | -0.364532 | 1.437822 |
| C | -3.295473 | -3.239847 | 0.891725 |
| C | -3.648122 | -2.905109 | -0.213432 |
| H | -2.983383 | -3.485017 | 1.883317 |
| H | -3.933582 | -2.587802 | -1.193058 |
| C | -0.865714 | -4.825676 | -1.598808 |
| C | 0.073227 | -4.873224 | -2.356799 |
| H | -1.701784 | -4.750042 | -0.935570 |
| H | 0.917276 | -4.879078 | -3.014076 |
| C | -3.331181 | 1.064866 | 1.778906 |
| C | -3.475779 | 2.018024 | 1.051133 |

| | | | |
|---|-----------|-----------|-----------|
| H | -3.201950 | 0.219491 | 2.423316 |
| H | -3.594158 | 2.863417 | 0.405638 |
| C | -2.247333 | -2.045445 | -3.466020 |
| C | -2.786401 | -0.964919 | -3.459503 |
| H | -1.761842 | -2.998141 | -3.443714 |
| H | -3.254793 | -0.002033 | -3.451801 |
| C | 1.944543 | -3.477735 | 0.591580 |
| C | 2.674824 | -2.958193 | 1.400678 |
| H | 1.283624 | -3.932653 | -0.116421 |
| H | 3.330088 | -2.479644 | 2.098132 |
| C | 3.203458 | -3.887623 | -4.400838 |
| C | 2.717273 | -2.975252 | -3.778898 |
| H | 3.650191 | -4.680674 | -4.957464 |
| H | 2.285466 | -2.167980 | -3.224035 |

EICO 7

0 1

| | | | |
|---|-----------|-----------|-----------|
| C | -1.762153 | -3.090171 | 1.020188 |
| C | -2.524349 | -2.348032 | 0.448523 |
| H | -1.069713 | -3.715539 | 1.541565 |
| H | -3.205918 | -1.698408 | -0.059219 |
| C | -5.201826 | -1.767261 | -1.963717 |
| C | -4.890135 | -0.638342 | -2.258547 |
| H | -5.469480 | -2.766424 | -1.686524 |
| H | -4.633418 | 0.363967 | -2.531732 |
| C | 1.031976 | -2.485248 | -1.315931 |
| C | 2.083665 | -2.371015 | -0.732452 |
| H | 0.110146 | -2.582435 | -1.851742 |
| H | 2.997023 | -2.257235 | -0.186692 |
| C | -7.323192 | 3.091347 | 0.635522 |
| C | -6.670572 | 3.179741 | -0.375240 |
| H | -7.910309 | 3.021726 | 1.523989 |
| H | -6.087859 | 3.251428 | -1.269827 |
| C | 5.015130 | -1.600338 | 1.840428 |
| C | 4.169144 | -2.301459 | 2.341474 |
| H | 5.766573 | -0.978819 | 1.399772 |
| H | 3.415535 | -2.921919 | 2.779966 |
| C | 0.866547 | -3.377770 | 3.556134 |
| C | 1.116854 | -4.557589 | 3.603540 |
| H | 0.650413 | -2.331176 | 3.488823 |
| H | 1.333070 | -5.601042 | 3.661358 |
| C | -4.971199 | -4.947392 | -0.218677 |
| C | -5.970935 | -5.413276 | -0.707599 |
| H | -4.088186 | -4.515234 | 0.205178 |
| H | -6.851494 | -5.844134 | -1.128708 |
| C | -2.926810 | 0.963268 | 1.767638 |
| C | -4.004739 | 1.404314 | 1.446425 |
| H | -1.967148 | 0.572199 | 2.037857 |
| H | -4.957538 | 1.795642 | 1.152704 |
| C | 5.467729 | -1.426303 | -3.549462 |
| C | 6.204838 | -0.834941 | -2.798874 |
| H | 4.818651 | -1.966190 | -4.206000 |
| H | 6.845088 | -0.313873 | -2.119765 |
| C | 2.677270 | -3.573252 | -4.341176 |
| C | 2.877119 | -3.755141 | -5.517561 |
| H | 2.493170 | -3.398710 | -3.300265 |
| H | 3.054349 | -3.927563 | -6.555722 |
| C | 0.680233 | 0.409301 | 2.813940 |
| C | 0.619262 | -0.256930 | 1.808156 |
| H | 0.774019 | 1.015884 | 3.687148 |
| H | 0.581895 | -0.845332 | 0.914762 |
| C | -1.954172 | -2.470644 | -3.867843 |

| | | | |
|---|-----------|-----------|-----------|
| C | -0.916533 | -2.813968 | -4.379641 |
| H | -2.877868 | -2.160579 | -3.425543 |
| H | 0.008842 | -3.113849 | -4.823043 |
| C | 1.885714 | 5.281845 | -3.731991 |
| C | 2.274750 | 4.329611 | -3.101409 |
| H | 1.559962 | 6.123298 | -4.301387 |
| H | 2.613561 | 3.484690 | -2.537299 |
| C | 3.490873 | 1.126694 | -1.352216 |
| C | 3.035760 | 1.773543 | -0.438585 |
| H | 3.910240 | 0.533598 | -2.138418 |
| H | 2.618913 | 2.334335 | 0.373845 |
| C | -1.507761 | 3.581041 | -0.375399 |
| C | -0.775388 | 4.089338 | -1.190411 |
| H | -2.149431 | 3.104551 | 0.337280 |
| H | -0.100521 | 4.512974 | -1.905849 |
| C | -4.923894 | 2.833818 | -3.757053 |
| C | -3.956604 | 3.071307 | -3.074604 |
| H | -5.771408 | 2.626909 | -4.372301 |
| H | -3.094626 | 3.292364 | -2.477173 |
| C | 2.214341 | 3.701314 | 2.723277 |
| C | 1.364313 | 4.094893 | 1.962106 |
| H | 2.949949 | 3.323811 | 3.401028 |
| H | 0.606553 | 4.418543 | 1.280405 |
| C | 6.760253 | 1.224651 | 0.191769 |
| C | 7.856163 | 0.801885 | 0.470049 |
| H | 5.782320 | 1.580773 | -0.061994 |
| H | 8.829685 | 0.445096 | 0.723184 |
| C | 3.788018 | 0.819514 | 4.617591 |
| C | 3.603137 | 1.583662 | 5.533322 |
| H | 3.951997 | 0.129642 | 3.815318 |
| H | 3.444709 | 2.247379 | 6.353759 |
| C | -4.705949 | 0.940214 | 5.165473 |
| C | -5.106578 | 0.926863 | 6.302493 |
| H | -4.350131 | 0.953750 | 4.156689 |
| H | -5.460525 | 0.913236 | 7.308566 |

EICO 8

0 1

| | | | |
|---|-----------|-----------|-----------|
| C | -6.267227 | 5.552069 | 3.069243 |
| C | -5.964783 | 5.541983 | 1.900708 |
| H | -6.549310 | 5.570600 | 4.098351 |
| H | -5.683696 | 5.527693 | 0.866971 |
| C | -4.698520 | 5.099545 | -1.790657 |
| C | -3.828870 | 5.308523 | -0.980018 |
| H | -5.431663 | 4.872398 | -2.532701 |
| H | -3.064215 | 5.468773 | -0.248586 |
| C | -5.637079 | 2.335055 | -4.548447 |
| C | -4.747513 | 2.245232 | -3.738816 |
| H | -6.420303 | 2.402920 | -5.269356 |
| H | -3.960287 | 2.167382 | -3.018100 |
| C | 1.220871 | -0.388065 | -2.725513 |
| C | 1.768057 | 0.673049 | -2.906223 |
| H | 0.766576 | -1.337709 | -2.540155 |
| H | 2.273436 | 1.603907 | -3.050155 |
| C | 1.737593 | 3.037612 | -0.087166 |
| C | 1.604735 | 4.104798 | -0.635044 |
| H | 1.861127 | 2.088182 | 0.392040 |
| H | 1.483820 | 5.049391 | -1.116170 |
| C | 2.884188 | -0.254302 | 1.447640 |
| C | 1.716781 | -0.500639 | 1.635745 |
| H | 3.914733 | -0.026638 | 1.278842 |
| H | 0.683190 | -0.732449 | 1.786227 |

| | | | |
|---|-----------|-----------|-----------|
| C | -1.613178 | 1.725510 | -1.372994 |
| C | -2.529018 | 2.020441 | -0.642535 |
| H | -0.788397 | 1.462572 | -2.001689 |
| H | -3.326523 | 2.271181 | 0.024423 |
| C | -2.278157 | 5.101078 | 2.289066 |
| C | -1.286640 | 4.698673 | 1.730710 |
| H | -3.172605 | 5.439201 | 2.765704 |
| H | -0.408510 | 4.334616 | 1.238994 |
| C | -4.532047 | 0.852032 | 2.322911 |
| C | -5.058461 | 1.936375 | 2.376139 |
| H | -4.049900 | -0.100011 | 2.271527 |
| H | -5.523395 | 2.897697 | 2.434235 |
| C | -5.287298 | -6.563023 | 3.188450 |
| C | -5.175631 | -6.042402 | 2.105976 |
| H | -5.402858 | -7.022126 | 4.144663 |
| H | -5.062314 | -5.580805 | 1.147280 |
| C | -3.867979 | -4.067775 | -0.916406 |
| C | -4.556124 | -4.830221 | -1.550872 |
| H | -3.262764 | -3.383625 | -0.357413 |
| H | -5.164357 | -5.498223 | -2.119354 |
| C | -1.759351 | -2.204470 | 1.555119 |
| C | -1.873133 | -1.196233 | 0.898639 |
| H | -1.646994 | -3.124766 | 2.089611 |
| H | -1.959600 | -0.296633 | 0.321736 |
| C | 4.840871 | -1.069207 | -1.701938 |
| C | 5.949050 | -1.007911 | -1.226714 |
| H | 3.856912 | -1.102916 | -2.119854 |
| H | 6.924357 | -0.952517 | -0.791736 |
| C | 5.553222 | 2.359553 | 1.813004 |
| C | 5.354936 | 2.737084 | 0.683382 |
| H | 5.716486 | 1.991572 | 2.802584 |
| H | 5.160950 | 3.069543 | -0.314704 |
| C | 6.501148 | -0.688841 | 3.505857 |
| C | 5.443527 | -0.714927 | 4.085690 |
| H | 7.427494 | -0.659854 | 2.972924 |
| H | 4.505094 | -0.750181 | 4.592525 |
| C | 9.380446 | -0.306365 | 0.726888 |
| C | 8.552851 | 0.571879 | 0.756611 |
| H | 10.126882 | -1.068566 | 0.694474 |
| H | 7.805019 | 1.338235 | 0.790320 |
| C | 4.791444 | 3.457868 | -3.231182 |
| C | 5.097266 | 2.326482 | -2.942901 |
| H | 4.534734 | 4.457564 | -3.501536 |
| H | 5.357997 | 1.323702 | -2.670857 |
| C | -1.617289 | -5.927605 | 1.927441 |
| C | -0.636958 | -5.532072 | 1.344584 |
| H | -2.501531 | -6.277444 | 2.416648 |
| H | 0.218376 | -5.171898 | 0.812291 |
| C | 1.249338 | -4.071866 | -1.509860 |
| C | 1.748082 | -3.303753 | -0.722332 |
| H | 0.793269 | -4.755319 | -2.196466 |
| H | 2.178097 | -2.607194 | -0.032643 |
| C | -1.344416 | -6.036748 | -3.144280 |
| C | -0.528974 | -6.525014 | -3.887455 |
| H | -2.071299 | -5.603336 | -2.488630 |
| H | 0.180902 | -6.966763 | -4.550530 |

EICO 9

0 1

| | | | |
|---|-----------|-----------|----------|
| C | -1.685197 | -1.171494 | 1.436978 |
| C | -2.299329 | -0.808927 | 2.411639 |
| H | -1.151367 | -1.499412 | 0.569396 |

| | | | |
|---|-----------|-----------|-----------|
| H | -2.860764 | -0.450701 | 3.247184 |
| C | -1.022982 | 3.827324 | -3.834058 |
| C | -0.328245 | 4.221342 | -2.928962 |
| H | -1.655187 | 3.483731 | -4.624985 |
| H | 0.294902 | 4.561378 | -2.128898 |
| C | -3.341346 | -4.463765 | 0.970934 |
| C | -3.353816 | -5.563900 | 0.473641 |
| H | -3.324735 | -3.484942 | 1.405297 |
| H | -3.376469 | -6.535810 | 0.032964 |
| C | -2.771750 | 4.065434 | 0.172893 |
| C | -1.820275 | 3.541809 | 0.700176 |
| H | -3.605362 | 4.539394 | -0.296198 |
| H | -0.973568 | 3.082368 | 1.168659 |
| C | 1.371170 | 1.078013 | -2.248633 |
| C | 2.219407 | 0.437117 | -1.674572 |
| H | 0.620942 | 1.662507 | -2.739479 |
| H | 2.961124 | -0.135898 | -1.159922 |
| C | 0.030422 | -2.523958 | -1.769163 |
| C | -0.602257 | -3.447726 | -1.316005 |
| H | 0.587530 | -1.694062 | -2.152539 |
| H | -1.191520 | -4.236558 | -0.899134 |
| C | 1.267374 | 2.498812 | 2.580824 |
| C | 0.646252 | 1.465086 | 2.639789 |
| H | 1.814169 | 3.411647 | 2.491588 |
| H | 0.072509 | 0.562382 | 2.678169 |
| C | 2.384435 | 4.137297 | -0.322427 |
| C | 2.183616 | 5.284805 | -0.006327 |
| H | 2.551369 | 3.119142 | -0.606962 |
| H | 2.020768 | 6.302127 | 0.271531 |
| C | 3.110672 | -3.015167 | 0.007024 |
| C | 4.027762 | -2.400706 | 0.495559 |
| H | 2.279326 | -3.531226 | -0.422843 |
| H | 4.813246 | -1.820470 | 0.927800 |
| C | -2.515925 | -0.268856 | -2.357106 |
| C | -2.454861 | 0.833262 | -1.868311 |
| H | -2.548233 | -1.259161 | -2.753346 |
| H | -2.393722 | 1.804723 | -1.423609 |
| C | 4.421996 | -0.573150 | -4.182785 |
| C | 4.963894 | -1.643792 | -4.054782 |
| H | 3.919219 | 0.363408 | -4.277126 |
| H | 5.425213 | -2.600259 | -3.923205 |
| C | 5.375905 | 1.080013 | 0.552197 |
| C | 4.422290 | 1.093405 | 1.292773 |
| H | 6.215635 | 1.064946 | -0.112016 |
| H | 3.567269 | 1.118110 | 1.934509 |
| C | -4.825955 | 1.702443 | 4.204222 |
| C | -4.255692 | 2.120334 | 3.225244 |
| H | -5.341941 | 1.332893 | 5.066254 |
| H | -3.746187 | 2.508756 | 2.368044 |
| C | -3.816623 | 2.338971 | -6.317238 |
| C | -3.581185 | 1.732002 | -5.300743 |
| H | -4.027965 | 2.863155 | -7.222564 |
| H | -3.360069 | 1.207245 | -4.392703 |
| C | 6.312384 | -5.172148 | -3.069551 |
| C | 5.707334 | -4.627351 | -2.179247 |
| H | 6.852486 | -5.666315 | -3.845568 |
| H | 5.164638 | -4.138033 | -1.396645 |
| C | 7.589551 | 0.410918 | -2.336805 |
| C | 8.496223 | 0.896201 | -1.705587 |
| H | 6.785367 | -0.019605 | -2.898404 |
| H | 9.308851 | 1.320240 | -1.159328 |
| C | -6.919986 | 0.256588 | 7.195300 |
| C | -6.863235 | -0.496127 | 6.254184 |

| | | | |
|---|-----------|-----------|-----------|
| H | -6.981298 | 0.910464 | 8.036116 |
| H | -6.799417 | -1.147369 | 5.406850 |
| C | -6.569883 | -6.461166 | 4.171327 |
| C | -5.693014 | -6.227153 | 3.376738 |
| H | -7.340124 | -6.681880 | 4.875870 |
| H | -4.920967 | -6.006649 | 2.669485 |
| C | -6.172312 | -2.657427 | 3.134273 |
| C | -5.928812 | -1.503969 | 2.873263 |
| H | -6.377041 | -3.685289 | 3.350982 |
| H | -5.708131 | -0.478498 | 2.665347 |
| C | -8.204458 | 2.660091 | -3.735732 |
| C | -7.139367 | 2.520961 | -4.283044 |
| H | -9.146822 | 2.780481 | -3.250851 |
| H | -6.193463 | 2.396324 | -4.766058 |

EICO 10

0 1

| | | | |
|---|------------|-----------|-----------|
| C | -2.688822 | 3.442184 | -0.069161 |
| C | -2.117912 | 3.494294 | -1.122096 |
| H | -3.215808 | 3.385817 | 0.860213 |
| H | -1.621555 | 3.513626 | -2.068926 |
| C | 1.760903 | 0.062423 | -1.278301 |
| C | 1.715385 | 1.118801 | -0.715526 |
| H | 1.802469 | -0.883313 | -1.769403 |
| H | 1.675118 | 2.052452 | -0.195894 |
| C | -2.201944 | -1.170482 | -2.105693 |
| C | -1.917583 | -0.231977 | -1.415748 |
| H | -2.474346 | -2.017521 | -2.697763 |
| H | -1.683871 | 0.601011 | -0.786963 |
| C | -5.198769 | 1.207517 | 0.035746 |
| C | -4.666101 | 0.213909 | 0.441881 |
| H | -5.673576 | 2.094834 | -0.322934 |
| H | -4.193315 | -0.681232 | 0.787850 |
| C | -7.027060 | -6.217098 | -0.301279 |
| C | -5.859961 | -6.059905 | -0.082791 |
| H | -8.068898 | -6.339039 | -0.499064 |
| H | -4.819838 | -5.903180 | 0.099659 |
| C | -6.684062 | 4.784082 | -0.301665 |
| C | -5.809043 | 4.572770 | -1.091923 |
| H | -7.455171 | 4.977379 | 0.409129 |
| H | -5.019926 | 4.360290 | -1.779962 |
| C | -8.274626 | 4.413341 | -3.814060 |
| C | -8.729699 | 4.139411 | -4.886855 |
| H | -7.860861 | 4.650046 | -2.857312 |
| H | -9.142734 | 3.901334 | -5.840243 |
| C | -5.514362 | 2.078112 | -3.800953 |
| C | -4.538718 | 1.567969 | -3.326196 |
| H | -6.386425 | 2.536537 | -4.215343 |
| H | -3.675135 | 1.101262 | -2.900462 |
| C | 1.766482 | 4.094635 | 1.744120 |
| C | 0.700180 | 4.035796 | 1.201093 |
| H | 2.714264 | 4.153706 | 2.229375 |
| H | -0.250484 | 3.974230 | 0.712381 |
| C | -7.332551 | -2.410194 | -1.286178 |
| C | -6.660509 | -1.520179 | -1.726020 |
| H | -7.937745 | -3.204879 | -0.906886 |
| H | -6.064613 | -0.719403 | -2.108082 |
| C | -8.195966 | -2.935096 | 2.587310 |
| C | -7.859470 | -4.076338 | 2.447016 |
| H | -8.481175 | -1.912296 | 2.708992 |
| H | -7.540959 | -5.085363 | 2.304019 |
| C | -10.435995 | -4.823342 | -1.314683 |

| | | | |
|---|------------|-----------|-----------|
| C | -10.305447 | -4.529875 | -0.161179 |
| H | -10.559076 | -5.077288 | -2.342995 |
| H | -10.170154 | -4.258221 | 0.862945 |
| C | 0.120514 | -2.778190 | 0.180548 |
| C | 0.799355 | -3.407529 | 0.940638 |
| H | -0.497556 | -2.208061 | -0.482579 |
| H | 1.404447 | -3.968328 | 1.615873 |
| C | -4.045788 | -4.188518 | -2.398789 |
| C | -3.109806 | -4.774550 | -2.862653 |
| H | -4.882188 | -3.665151 | -1.985012 |
| H | -2.281743 | -5.304145 | -3.274989 |
| C | -8.613105 | 1.009551 | 2.402042 |
| C | -8.158618 | 0.447022 | 1.446695 |
| H | -9.021917 | 1.511834 | 3.249032 |
| H | -7.743533 | -0.057504 | 0.599487 |
| C | -5.008831 | 2.694524 | 3.087839 |
| C | -4.131872 | 3.332287 | 3.598485 |
| H | -5.778880 | 2.111628 | 2.629944 |
| H | -3.340416 | 3.877414 | 4.065428 |
| C | -4.462290 | -3.167858 | 1.381691 |
| C | -3.264569 | -3.200811 | 1.361049 |
| H | -5.530180 | -3.129906 | 1.403784 |
| H | -2.196478 | -3.228349 | 1.346808 |
| C | -1.677741 | 0.815627 | 2.333437 |
| C | -0.661192 | 0.330387 | 1.924504 |
| H | -2.584659 | 1.244409 | 2.703466 |
| H | 0.237795 | -0.110632 | 1.553731 |
| C | -0.380321 | 1.915673 | -3.891111 |
| C | -1.254064 | 2.350361 | -4.585394 |
| H | 0.389240 | 1.521141 | -3.263066 |
| H | -2.042740 | 2.722672 | -5.199274 |
| C | -1.109228 | 3.582968 | 5.786547 |
| C | -0.592384 | 3.533051 | 4.707611 |
| H | -1.563542 | 3.616992 | 6.750073 |
| H | -0.124576 | 3.485024 | 3.747728 |

EICO 11

0 1

| | | | |
|---|-----------|-----------|-----------|
| C | -2.482010 | 3.105471 | -3.085835 |
| C | -1.951460 | 4.061924 | -2.595204 |
| H | -2.951891 | 2.242176 | -3.507943 |
| H | -1.480119 | 4.906641 | -2.145318 |
| C | 0.992884 | 4.013179 | -0.196971 |
| C | 0.141702 | 4.394227 | 0.554996 |
| H | 1.749548 | 3.668882 | -0.865162 |
| H | -0.625511 | 4.729481 | 1.219715 |
| C | -1.977108 | -2.755262 | -2.185874 |
| C | -1.338992 | -2.076154 | -1.432575 |
| H | -2.554903 | -3.350812 | -2.856700 |
| H | -0.792311 | -1.449197 | -0.761526 |
| C | -4.891892 | 1.380413 | -1.376041 |
| C | -4.243088 | 0.372396 | -1.378706 |
| H | -5.445145 | 2.295160 | -1.375439 |
| H | -3.653333 | -0.519258 | -1.401685 |
| C | -7.131455 | -1.783999 | 0.083384 |
| C | -7.595325 | -0.679250 | 0.094848 |
| H | -6.700216 | -2.760869 | 0.062443 |
| H | -7.984560 | 0.316004 | 0.100657 |
| C | -8.492306 | 2.542221 | -2.089373 |
| C | -8.980382 | 1.507217 | -2.444477 |
| H | -8.041533 | 3.460044 | -1.777164 |
| H | -9.403459 | 0.579513 | -2.757772 |

| | | | |
|---|-----------|-----------|-----------|
| C | -6.108051 | 2.488726 | -4.891521 |
| C | -5.158111 | 2.890897 | -5.500435 |
| H | -6.953182 | 2.132036 | -4.342275 |
| H | -4.306803 | 3.239178 | -6.040336 |
| C | -3.376309 | -0.171688 | -4.837058 |
| C | -2.211076 | -0.268833 | -4.576065 |
| H | -4.417925 | -0.075858 | -5.051921 |
| H | -1.178378 | -0.356850 | -4.320369 |
| C | -3.524875 | 3.992494 | 1.849960 |
| C | -3.222592 | 3.478401 | 0.809814 |
| H | -3.806356 | 4.435528 | 2.780440 |
| H | -2.958080 | 3.016982 | -0.117302 |
| C | -7.183823 | -1.321791 | -4.658283 |
| C | -6.803698 | -0.886036 | -3.608347 |
| H | -7.522930 | -1.704052 | -5.594269 |
| H | -6.456551 | -0.493361 | -2.674032 |
| C | -1.535511 | 2.157632 | 4.370634 |
| C | -1.613259 | 2.397946 | 5.542019 |
| H | -1.483446 | 1.930382 | 3.325507 |
| H | -1.679187 | 2.604360 | 6.585898 |
| C | 0.463335 | 1.184658 | -2.375145 |
| C | 1.322556 | 0.349795 | -2.381201 |
| H | -0.307034 | 1.928324 | -2.376340 |
| H | 2.084143 | -0.396126 | -2.389525 |
| C | -5.532189 | -4.021886 | -2.311837 |
| C | -5.047862 | -4.813252 | -1.554436 |
| H | -5.970483 | -3.313161 | -2.981920 |
| H | -4.619302 | -5.514616 | -0.874882 |
| C | -3.643735 | -3.039301 | 1.173109 |
| C | -4.154188 | -2.969061 | 2.254365 |
| H | -3.178233 | -3.089185 | 0.211968 |
| H | -4.605358 | -2.889558 | 3.217066 |
| C | -0.851101 | 0.800463 | 0.941896 |
| C | -1.778810 | 0.155745 | 1.343334 |
| H | -0.039076 | 1.393880 | 0.582569 |
| H | -2.612083 | -0.409320 | 1.705205 |
| C | -5.681471 | 4.899496 | -2.217168 |
| C | -5.869593 | 5.109708 | -1.052778 |
| H | -5.504506 | 4.692212 | -3.250225 |
| H | -6.023637 | 5.285237 | -0.011903 |
| C | -1.629964 | 6.882570 | 3.589842 |
| C | -1.403293 | 5.781810 | 4.003125 |
| H | -1.826378 | 7.862812 | 3.220072 |
| H | -1.213857 | 4.792648 | 4.362652 |
| C | -8.060634 | 3.038658 | 1.417971 |
| C | -6.886238 | 2.799536 | 1.411968 |
| H | -9.106221 | 3.247604 | 1.418133 |
| H | -5.835677 | 2.593576 | 1.414305 |
| C | -5.657335 | 4.003070 | 4.740110 |
| C | -4.879393 | 4.771783 | 5.227905 |
| H | -6.342706 | 3.317342 | 4.291936 |
| H | -4.184364 | 5.462232 | 5.649437 |
| C | -5.315862 | 0.145520 | 2.847955 |
| C | -4.665386 | 0.696425 | 3.690541 |
| H | -5.889342 | -0.339093 | 2.085333 |
| H | -4.076630 | 1.198017 | 4.427298 |

EICO 12

0 1

| | | | |
|---|----------|----------|----------|
| C | 1.299849 | 1.292583 | 2.022093 |
| C | 1.837207 | 0.527938 | 2.773252 |
| H | 0.815646 | 1.973042 | 1.352924 |

| | | | |
|---|-----------|-----------|-----------|
| H | 2.326806 | -0.150717 | 3.437732 |
| C | -2.239190 | 0.046250 | 0.114861 |
| C | -1.552836 | -0.162131 | 1.074485 |
| H | -2.867830 | 0.213506 | -0.730758 |
| H | -0.930528 | -0.349938 | 1.922959 |
| C | -5.424034 | -1.723784 | -0.821078 |
| C | -5.741578 | -0.680837 | -0.325145 |
| H | -5.132342 | -2.655604 | -1.251180 |
| H | -6.008583 | 0.250224 | 0.124294 |
| C | -4.682715 | 1.785350 | 2.091164 |
| C | -5.031465 | 2.783154 | 1.527852 |
| H | -4.373152 | 0.890236 | 2.586796 |
| H | -5.336889 | 3.677156 | 1.033558 |
| C | -3.082842 | -4.300897 | 0.286871 |
| C | -2.208006 | -3.567515 | -0.079715 |
| H | -3.880331 | -4.931666 | 0.614958 |
| H | -1.417905 | -2.915481 | -0.389491 |
| C | 4.590119 | -1.083508 | -0.311933 |
| C | 4.871669 | 0.037339 | 0.006315 |
| H | 4.327136 | -2.084434 | -0.577177 |
| H | 5.105267 | 1.043323 | 0.282779 |
| C | -1.381512 | 3.636310 | 0.858659 |
| C | -0.508189 | 4.384060 | 0.520398 |
| H | -2.158518 | 2.967580 | 1.161518 |
| H | 0.274083 | 5.043643 | 0.211630 |
| C | 1.216972 | -1.934110 | -0.383764 |
| C | 1.177481 | -2.797510 | -1.214662 |
| H | 1.258415 | -1.154481 | 0.346721 |
| H | 1.127359 | -3.562328 | -1.960720 |
| C | 0.805221 | 1.900640 | -1.703301 |
| C | 1.832201 | 1.287799 | -1.632624 |
| H | -0.109716 | 2.447828 | -1.743893 |
| H | 2.736045 | 0.722913 | -1.554013 |
| C | 3.566417 | -4.484907 | 0.895417 |
| C | 4.746957 | -4.653303 | 0.773998 |
| H | 2.511215 | -4.344995 | 0.988663 |
| H | 5.795596 | -4.820307 | 0.655764 |
| C | 0.239955 | -6.226543 | 0.516004 |
| C | 1.094215 | -7.048265 | 0.341836 |
| H | -0.524406 | -5.494762 | 0.669248 |
| H | 1.860394 | -7.773982 | 0.186325 |
| C | 0.307469 | -5.747289 | -3.171631 |
| C | 0.283067 | -5.054676 | -4.148078 |
| H | 0.335578 | -6.351588 | -2.290565 |
| H | 0.261313 | -4.442885 | -5.020691 |
| C | 3.705764 | -6.770160 | -1.983057 |
| C | 3.763888 | -7.648779 | -2.794930 |
| H | 3.660626 | -5.990304 | -1.251747 |
| H | 3.805581 | -8.423873 | -3.525692 |
| C | -0.463803 | -3.055506 | 3.029803 |
| C | 0.728406 | -2.987667 | 3.128849 |
| H | -1.526878 | -3.114391 | 2.942060 |
| H | 1.791394 | -2.928232 | 3.227067 |
| C | -4.359610 | -1.837849 | 3.878245 |
| C | -4.092094 | -1.835524 | 2.710140 |
| H | -4.596341 | -1.843121 | 4.917715 |
| H | -3.847963 | -1.829019 | 1.668957 |
| C | 4.172861 | 3.242196 | 1.490282 |
| C | 4.763347 | 3.919341 | 0.698455 |
| H | 3.627571 | 2.635546 | 2.180370 |
| H | 5.272021 | 4.537861 | -0.005663 |
| C | -6.660889 | -5.538990 | 1.096413 |
| C | -6.449820 | -4.438514 | 1.518030 |

| | | | |
|---|-----------|-----------|-----------|
| H | -6.859735 | -6.517885 | 0.724458 |
| H | -6.255773 | -3.457876 | 1.894045 |
| C | 2.385738 | 5.166660 | -1.535514 |
| C | 2.387935 | 6.360029 | -1.435338 |
| H | 2.372538 | 4.100152 | -1.615874 |
| H | 2.394171 | 7.422487 | -1.349705 |
| C | 7.240623 | -6.359571 | -1.211089 |
| C | 8.200899 | -5.895103 | -0.667582 |
| H | 6.380635 | -6.770815 | -1.694586 |
| H | 9.062612 | -5.486910 | -0.191093 |
| C | 4.401643 | -1.837961 | 3.330117 |
| C | 4.158620 | -2.174258 | 4.453907 |
| H | 4.614960 | -1.533543 | 2.326680 |
| H | 3.953401 | -2.482434 | 5.453753 |

EICO 13

0 1

| | | | |
|---|-----------|-----------|-----------|
| C | 5.984653 | 0.842480 | -0.860939 |
| C | 6.324670 | 1.549598 | 0.044664 |
| H | 5.683565 | 0.222051 | -1.678376 |
| H | 6.633122 | 2.180302 | 0.847283 |
| C | 2.600829 | 4.204047 | 0.873791 |
| C | 3.175023 | 3.338357 | 1.470686 |
| H | 2.079002 | 4.958908 | 0.325746 |
| H | 3.657960 | 2.553412 | 2.008274 |
| C | 0.098198 | 5.312589 | -1.602875 |
| C | 1.117651 | 5.666385 | -2.123466 |
| H | -0.815133 | 4.979781 | -1.157880 |
| H | 2.017853 | 5.966165 | -2.614341 |
| C | 3.369687 | 2.570025 | -2.362872 |
| C | 3.549164 | 2.204483 | -3.490645 |
| H | 3.204066 | 2.875305 | -1.351395 |
| H | 3.698813 | 1.861912 | -4.492351 |
| C | -3.189394 | 3.328160 | -1.185132 |
| C | -2.570054 | 3.059735 | -0.194542 |
| H | -3.735070 | 3.550193 | -2.075614 |
| H | -2.013783 | 2.805742 | 0.684194 |
| C | -0.177305 | 2.080532 | 2.408844 |
| C | -1.131964 | 1.762517 | 3.060342 |
| H | 0.672148 | 2.368302 | 1.826251 |
| H | -1.985439 | 1.493875 | 3.644347 |
| C | 3.044915 | -1.169118 | -1.955479 |
| C | 3.431707 | -2.218975 | -1.525648 |
| H | 2.697527 | -0.225980 | -2.321801 |
| H | 3.755983 | -3.152510 | -1.122940 |
| C | 3.248704 | -3.893765 | 1.623531 |
| C | 3.080567 | -5.021596 | 1.257815 |
| H | 3.380583 | -2.881217 | 1.940970 |
| H | 2.932717 | -6.028857 | 0.941635 |
| C | 0.314766 | 1.606088 | -1.550500 |
| C | 0.467647 | 0.744275 | -0.730731 |
| H | 0.187480 | 2.368060 | -2.289501 |
| H | 0.597700 | -0.031583 | -0.006526 |
| C | -1.112125 | -1.808426 | 1.295911 |
| C | -0.139568 | -2.489046 | 1.132945 |
| H | -1.984480 | -1.205726 | 1.431754 |
| H | 0.725355 | -3.097771 | 0.983960 |
| C | 2.399739 | -0.301178 | 2.380954 |
| C | 3.315365 | -0.205980 | 1.613369 |
| H | 1.562334 | -0.378468 | 3.038841 |
| H | 4.122747 | -0.110381 | 0.918828 |
| C | 5.637934 | -0.786188 | -4.335607 |

| | | | |
|---|-----------|-----------|-----------|
| C | 6.412213 | 0.108474 | -4.522205 |
| H | 4.936065 | -1.569006 | -4.151024 |
| H | 7.089964 | 0.918554 | -4.677176 |
| C | -3.801251 | -1.064352 | -1.929634 |
| C | -2.747381 | -0.500264 | -1.847190 |
| H | -4.734331 | -1.576342 | -1.992154 |
| H | -1.803971 | -0.000782 | -1.757813 |
| C | 3.826362 | 5.460717 | -4.798069 |
| C | 2.946827 | 6.098913 | -5.302254 |
| H | 4.612192 | 4.887963 | -4.353059 |
| H | 2.162794 | 6.663375 | -5.753701 |
| C | -4.271657 | 1.830864 | -4.254520 |
| C | -4.546084 | 2.773772 | -4.940502 |
| H | -4.022365 | 0.993496 | -3.635698 |
| H | -4.795203 | 3.608177 | -5.555735 |
| C | 3.299325 | 0.386872 | -6.797732 |
| C | 2.231394 | 0.865953 | -6.544436 |
| H | 4.252934 | -0.040651 | -7.009310 |
| H | 1.285813 | 1.302764 | -6.305822 |
| C | -4.295512 | 0.328604 | 1.389514 |
| C | -4.467337 | -0.278352 | 2.407858 |
| H | -4.133538 | 0.859063 | 0.475956 |
| H | -4.621203 | -0.811154 | 3.318692 |
| C | 6.862597 | 3.481318 | -3.377769 |
| C | 7.296416 | 4.049223 | -4.339201 |
| H | 6.471193 | 2.967945 | -2.525234 |
| H | 7.683268 | 4.561377 | -5.190548 |
| C | -4.378016 | 1.975747 | 4.948610 |
| C | -3.772853 | 1.699205 | 5.943560 |
| H | -4.909779 | 2.213387 | 4.054870 |
| H | -3.237506 | 1.461489 | 6.834162 |
| C | -0.755182 | 2.949693 | -4.977567 |
| C | 0.339708 | 3.419141 | -4.847027 |
| H | -1.739981 | 2.548586 | -5.082031 |
| H | 1.315475 | 3.836968 | -4.719778 |

EICO 14

0 1

| | | | |
|---|----------|-----------|-----------|
| C | 1.405885 | 2.545698 | 0.461805 |
| C | 1.996962 | 2.197394 | 1.444538 |
| H | 0.900581 | 2.855187 | -0.427631 |
| H | 2.531795 | 1.889353 | 2.316813 |
| C | 2.710971 | 1.244359 | -2.603565 |
| C | 2.152775 | 0.191384 | -2.730619 |
| H | 3.211501 | 2.182854 | -2.473329 |
| H | 1.657120 | -0.747009 | -2.832189 |
| C | 0.935278 | 5.133816 | 3.176774 |
| C | 1.010671 | 6.006191 | 3.994021 |
| H | 0.881593 | 4.353886 | 2.446086 |
| H | 1.072216 | 6.790867 | 4.713073 |
| C | 5.164275 | 1.153544 | 0.340199 |
| C | 5.664868 | 1.805624 | 1.212167 |
| H | 4.712306 | 0.601522 | -0.454596 |
| H | 6.106970 | 2.393924 | 1.987257 |
| C | 2.901248 | 2.621228 | 5.000135 |
| C | 3.955731 | 2.082627 | 4.817145 |
| H | 1.964555 | 3.108860 | 5.155162 |
| H | 4.894218 | 1.594742 | 4.662488 |
| C | 3.808733 | 0.763324 | -6.093077 |
| C | 4.678172 | 0.715048 | -6.915514 |
| H | 3.052575 | 0.805154 | -5.339224 |
| H | 5.464326 | 0.684286 | -7.635673 |

| | | | |
|---|-----------|-----------|-----------|
| C | 6.688489 | 1.983679 | -2.709492 |
| C | 6.252578 | 1.216436 | -3.520551 |
| H | 7.058501 | 2.663667 | -1.972182 |
| H | 5.852094 | 0.548222 | -4.250163 |
| C | 2.463855 | 7.283521 | 0.292973 |
| C | 2.115537 | 7.988016 | -0.612022 |
| H | 2.782257 | 6.669418 | 1.108127 |
| H | 1.816338 | 8.609644 | -1.426941 |
| C | 4.167764 | 4.237653 | -1.075365 |
| C | 4.339448 | 4.534494 | -2.224118 |
| H | 4.017287 | 3.950800 | -0.057473 |
| H | 4.494576 | 4.787257 | -3.251642 |
| C | 5.285949 | 5.588299 | 1.967336 |
| C | 4.534406 | 5.182964 | 2.808577 |
| H | 5.965072 | 5.918586 | 1.211998 |
| H | 3.866082 | 4.811978 | 3.554345 |
| C | 7.821253 | 2.463471 | -6.535185 |
| C | 7.815696 | 2.713450 | -7.706314 |
| H | 7.821055 | 2.256204 | -5.486119 |
| H | 7.820511 | 2.946328 | -8.746369 |
| C | 7.770455 | 4.958380 | -0.618017 |
| C | 8.226387 | 4.318370 | 0.286874 |
| H | 7.355183 | 5.521824 | -1.426332 |
| H | 8.619071 | 3.751707 | 1.102042 |
| C | 0.304186 | 4.036703 | -2.965376 |
| C | 0.791808 | 4.859789 | -2.244153 |
| H | -0.123370 | 3.296867 | -3.603016 |
| H | 1.240979 | 5.589849 | -1.603388 |
| C | 5.439391 | 7.645449 | -2.188766 |
| C | 6.444921 | 7.876058 | -2.799369 |
| H | 4.541965 | 7.432127 | -1.645783 |
| H | 7.344801 | 8.054810 | -3.343769 |
| C | 2.447574 | 8.582394 | -4.279706 |
| C | 1.940882 | 7.496998 | -4.302287 |
| H | 2.894336 | 9.551146 | -4.236274 |
| H | 1.494640 | 6.526383 | -4.315183 |
| C | 6.485493 | -0.960624 | 4.747929 |
| C | 6.254082 | -0.704315 | 3.601235 |
| H | 6.685367 | -1.197912 | 5.767851 |
| H | 6.041077 | -0.460345 | 2.582260 |
| C | 4.082701 | 10.979045 | -2.158060 |
| C | 3.191097 | 11.768776 | -2.280274 |
| H | 4.871912 | 10.265943 | -2.054532 |
| H | 2.401374 | 12.477631 | -2.380814 |
| C | 8.066584 | 5.210783 | -4.436683 |
| C | 9.070349 | 5.199829 | -3.783288 |
| H | 7.169146 | 5.209697 | -5.018267 |
| H | 9.958714 | 5.179915 | -3.194278 |
| C | 7.579957 | 3.544004 | 3.949071 |
| C | 8.022183 | 2.430973 | 3.974213 |
| H | 7.167522 | 4.528189 | 3.916095 |
| H | 8.396735 | 1.432370 | 4.003016 |
| C | 4.540487 | 5.621727 | -5.703394 |
| C | 4.727380 | 4.461433 | -5.939688 |
| H | 4.352184 | 6.648810 | -5.477553 |
| H | 4.890138 | 3.425913 | -6.151425 |

EICO 15

0 1

| | | | |
|---|-----------|-----------|----------|
| C | -0.428681 | -0.946221 | 2.362900 |
| C | 0.528777 | -0.437924 | 1.852612 |
| H | -1.275528 | -1.403476 | 2.821780 |

| | | | |
|---|-----------|-----------|------------|
| H | 1.380359 | 0.010373 | 1.385283 |
| C | 3.078901 | 1.040716 | -4.408574 |
| C | 3.533288 | 0.479555 | -3.452440 |
| H | 2.684752 | 1.554478 | -5.256278 |
| H | 3.926086 | 0.001917 | -2.580205 |
| C | -0.060569 | 2.956706 | 3.210887 |
| C | 0.242771 | 4.101131 | 3.396290 |
| H | -0.321994 | 1.937832 | 3.023717 |
| H | 0.523735 | 5.119612 | 3.559691 |
| C | 1.198041 | 1.857582 | -0.954979 |
| C | 1.256479 | 2.711192 | -0.114925 |
| H | 1.153578 | 1.082986 | -1.690195 |
| H | 1.315647 | 3.458305 | 0.646960 |
| C | 3.695546 | 2.880922 | 2.993318 |
| C | 4.284286 | 3.314894 | 2.043201 |
| H | 3.167046 | 2.519655 | 3.847757 |
| H | 4.798954 | 3.706939 | 1.191827 |
| C | 4.944281 | 7.369280 | -2.808346 |
| C | 5.764984 | 6.592689 | -3.206157 |
| H | 4.213329 | 8.056989 | -2.447600 |
| H | 6.502515 | 5.900195 | -3.549879 |
| C | 6.540514 | 5.987514 | 0.404538 |
| C | 7.182144 | 5.800420 | 1.399222 |
| H | 5.960268 | 6.155686 | -0.478216 |
| H | 7.733729 | 5.644846 | 2.298838 |
| C | 1.656790 | 7.579234 | 3.785935 |
| C | 2.461371 | 6.961446 | 4.423825 |
| H | 0.932767 | 8.113542 | 3.211482 |
| H | 3.175801 | 6.409842 | 4.995620 |
| C | 1.595003 | 4.299465 | -3.575791 |
| C | 2.571137 | 4.777401 | -4.080027 |
| H | 0.736881 | 3.868215 | -3.110257 |
| H | 3.448241 | 5.200853 | -4.518014 |
| C | 2.806855 | 5.885873 | -0.489787 |
| C | 2.999205 | 6.196553 | 0.652315 |
| H | 2.645729 | 5.596197 | -1.507479 |
| H | 3.164869 | 6.466969 | 1.673467 |
| C | 6.326099 | 6.190300 | 5.368860 |
| C | 5.833065 | 5.364760 | 4.654391 |
| H | 6.764541 | 6.930085 | 5.998851 |
| H | 5.383364 | 4.633948 | 4.013690 |
| C | 0.259794 | -1.585308 | -1.575664 |
| C | 0.764813 | -1.576833 | -2.661595 |
| H | -0.179707 | -1.577696 | -0.602109 |
| H | 1.221157 | -1.553714 | -3.625490 |
| C | 4.685350 | 2.938870 | -1.448828 |
| C | 5.876819 | 3.031218 | -1.351757 |
| H | 3.621675 | 2.849668 | -1.522762 |
| H | 6.937355 | 3.131368 | -1.280992 |
| C | 4.988327 | 0.486051 | -7.425056 |
| C | 4.625457 | -0.119689 | -8.392211 |
| H | 5.309956 | 1.033553 | -6.565255 |
| H | 4.300049 | -0.667508 | -9.246782 |
| C | 6.151904 | 3.240680 | -9.591363 |
| C | 6.565469 | 4.313809 | -9.924304 |
| H | 5.781300 | 2.285441 | -9.285503 |
| H | 6.930780 | 5.266539 | -10.232531 |
| C | 6.116741 | 3.724751 | -6.045575 |
| C | 5.812945 | 3.336099 | -4.952566 |
| H | 6.373258 | 4.055273 | -7.029191 |
| H | 5.533558 | 2.998977 | -3.975648 |
| C | 2.245370 | 3.747866 | 6.313222 |
| C | 3.385056 | 3.856305 | 6.664220 |

| | | | |
|---|-----------|-----------|-----------|
| H | 1.234927 | 3.649426 | 5.983313 |
| H | 4.401537 | 3.962546 | 6.968662 |
| C | -1.542146 | 7.224207 | 1.596162 |
| C | -0.527135 | 6.943702 | 1.026402 |
| H | -2.451887 | 7.464856 | 2.096651 |
| H | 0.384179 | 6.690033 | 0.527959 |
| C | 8.860725 | 4.295449 | -3.198489 |
| C | 8.872050 | 4.953728 | -2.197949 |
| H | 8.838787 | 3.714023 | -4.092789 |
| H | 8.863627 | 5.537040 | -1.303316 |
| C | 3.568499 | -1.164557 | -0.119292 |
| C | 4.047115 | -0.147843 | 0.295895 |
| H | 3.125126 | -2.060323 | -0.492073 |
| H | 4.461660 | 0.763051 | 0.669419 |

EICO 16

0 1

| | | | |
|---|-----------|-----------|-----------|
| C | 0.367803 | 2.535481 | -0.458241 |
| C | 1.466129 | 2.358094 | -0.011607 |
| H | -0.615611 | 2.692358 | -0.845104 |
| H | 2.444853 | 2.197920 | 0.387490 |
| C | 1.429784 | 1.221463 | -3.508862 |
| C | 1.281749 | 0.040105 | -3.641423 |
| H | 1.575296 | 2.270976 | -3.367356 |
| H | 1.155004 | -1.013878 | -3.742028 |
| C | 0.277541 | 3.396462 | 3.161908 |
| C | 0.809189 | 4.111324 | 3.963766 |
| H | -0.183634 | 2.756726 | 2.439822 |
| H | 1.281080 | 4.768001 | 4.660690 |
| C | 4.364994 | 0.963115 | -1.372130 |
| C | 5.202747 | 1.563902 | -0.761129 |
| H | 3.594859 | 0.437663 | -1.896169 |
| H | 5.929717 | 2.109638 | -0.202870 |
| C | -3.186518 | 1.514204 | -1.869883 |
| C | -2.217790 | 1.165187 | -2.482734 |
| H | -4.047488 | 1.822205 | -1.317911 |
| H | -1.342312 | 0.870284 | -3.021158 |
| C | -3.585886 | 2.363650 | 4.475217 |
| C | -2.927416 | 3.363352 | 4.424070 |
| H | -4.181575 | 1.479587 | 4.501323 |
| H | -2.338093 | 4.252151 | 4.353094 |
| C | 0.846054 | 7.189348 | 0.341240 |
| C | 0.879449 | 5.999652 | 0.483249 |
| H | 0.821727 | 8.249879 | 0.232982 |
| H | 0.911856 | 4.936653 | 0.608337 |
| C | -2.363859 | 4.703447 | 0.594879 |
| C | -2.665066 | 3.620064 | 1.009372 |
| H | -2.075663 | 5.668616 | 0.242505 |
| H | -2.932818 | 2.660767 | 1.398592 |
| C | -1.259710 | 0.009702 | 2.247816 |
| C | -1.571596 | 0.108085 | 1.094700 |
| H | -0.966424 | -0.071364 | 3.273320 |
| H | -1.844990 | 0.206316 | 0.065819 |
| C | 2.115855 | 7.645620 | 4.514309 |
| C | 2.584887 | 7.041293 | 3.591929 |
| H | 1.689883 | 8.177766 | 5.336834 |
| H | 2.998397 | 6.490735 | 2.774394 |
| C | -6.621529 | 5.510686 | 2.930357 |
| C | -5.525107 | 5.258902 | 2.519182 |
| H | -7.596155 | 5.736376 | 3.298060 |
| H | -4.547668 | 5.027733 | 2.149873 |
| C | 4.105216 | 4.559174 | 0.921997 |

| | | | |
|---|-----------|-----------|-----------|
| C | 4.211449 | 4.007973 | 1.980410 |
| H | 3.991130 | 5.025059 | -0.032728 |
| H | 4.296940 | 3.498660 | 2.914003 |
| C | 2.687747 | 0.815773 | 3.117979 |
| C | 3.362059 | 0.025381 | 2.520303 |
| H | 2.073920 | 1.515286 | 3.643647 |
| H | 3.950228 | -0.687810 | 1.984434 |
| C | 2.396937 | -2.214378 | -0.638980 |
| C | 1.693345 | -1.311089 | -0.286718 |
| H | 3.034168 | -3.017744 | -0.930434 |
| H | 1.076106 | -0.502536 | 0.042445 |
| C | 2.611534 | 4.999159 | -2.523293 |
| C | 3.515712 | 4.259291 | -2.786879 |
| H | 1.811250 | 5.656343 | -2.264082 |
| H | 4.314805 | 3.586332 | -3.003909 |
| C | 5.781918 | -1.947477 | 0.402031 |
| C | 5.867405 | -2.889562 | 1.136043 |
| H | 5.691867 | -1.097823 | -0.240465 |
| H | 5.948485 | -3.727593 | 1.789632 |
| C | -2.636653 | 7.017728 | 3.696874 |
| C | -1.490631 | 6.876856 | 3.374853 |
| H | -3.663458 | 7.127801 | 3.967200 |
| H | -0.469627 | 6.750365 | 3.081472 |
| C | -0.392026 | 0.840126 | 5.679283 |
| C | 0.425895 | -0.034588 | 5.656226 |
| H | -1.124426 | 1.618635 | 5.678110 |
| H | 1.164624 | -0.803117 | 5.626916 |
| C | -0.655046 | 8.274245 | 6.703897 |
| C | -0.037797 | 8.669394 | 7.650644 |
| H | -1.198455 | 7.920268 | 5.853635 |
| H | 0.503618 | 9.019501 | 8.499365 |
| C | -5.637094 | 1.715000 | 1.562554 |
| C | -5.100011 | 0.660432 | 1.377217 |
| H | -6.103678 | 2.659345 | 1.742980 |
| H | -4.612070 | -0.276001 | 1.225677 |

EICO 17

0 1

| | | | |
|---|-----------|-----------|-----------|
| C | 1.132982 | -2.989334 | -1.535512 |
| C | 0.700581 | -1.871817 | -1.488460 |
| H | 1.529021 | -3.983098 | -1.568267 |
| H | 0.329960 | -0.869496 | -1.438097 |
| C | -2.414684 | -3.810391 | -1.615345 |
| C | -3.519930 | -4.225029 | -1.406263 |
| H | -1.427592 | -3.432309 | -1.785002 |
| H | -4.512425 | -4.574169 | -1.216682 |
| C | 1.076232 | -2.823645 | 2.190416 |
| C | 1.998891 | -3.136096 | 2.888271 |
| H | 0.251545 | -2.535969 | 1.573593 |
| H | 2.823953 | -3.405603 | 3.508464 |
| C | -2.193828 | -1.120700 | 0.771364 |
| C | -1.439669 | -0.309610 | 1.231028 |
| H | -2.863705 | -1.836085 | 0.346041 |
| H | -0.757705 | 0.409777 | 1.633649 |
| C | 5.273515 | -2.431723 | -0.471360 |
| C | 4.234181 | -2.611504 | 0.098906 |
| H | 6.187873 | -2.253118 | -0.995428 |
| H | 3.308193 | -2.764094 | 0.613873 |
| C | 4.298894 | 1.681058 | 1.197479 |
| C | 4.698113 | 1.576607 | 0.072350 |
| H | 3.935638 | 1.751562 | 2.199486 |
| H | 5.042125 | 1.469695 | -0.932545 |

| | | | |
|---|-----------|-----------|-----------|
| C | 3.539281 | 0.757703 | -3.523274 |
| C | 3.533805 | -0.231417 | -2.846440 |
| H | 3.506129 | 1.642658 | -4.119975 |
| H | 3.516654 | -1.108768 | -2.235539 |
| C | -4.648837 | 1.258364 | 2.190440 |
| C | -5.615511 | 1.928461 | 2.417567 |
| H | -3.787301 | 0.658942 | 1.977834 |
| H | -6.478284 | 2.518326 | 2.628006 |
| C | -4.826251 | -0.868425 | -1.895323 |
| C | -5.240080 | -0.121075 | -1.055820 |
| H | -4.446194 | -1.539785 | -2.632428 |
| H | -5.589784 | 0.548885 | -0.300999 |
| C | 1.679047 | 5.553380 | -0.637631 |
| C | 2.497734 | 4.821226 | -0.159789 |
| H | 0.939822 | 6.187663 | -1.074018 |
| H | 3.230295 | 4.160200 | 0.250323 |
| C | 7.082406 | -0.824490 | -3.158671 |
| C | 8.162925 | -1.198220 | -2.802890 |
| H | 6.114817 | -0.491972 | -3.469528 |
| H | 9.130207 | -1.525458 | -2.496879 |
| C | -2.067901 | 3.762740 | 1.925535 |
| C | -1.035536 | 3.999657 | 1.364770 |
| H | -2.990292 | 3.535818 | 2.412926 |
| H | -0.115805 | 4.198254 | 0.855185 |
| C | -0.939723 | -8.456710 | -2.259695 |
| C | -1.428449 | -7.390000 | -2.021404 |
| H | -0.512201 | -9.409071 | -2.475070 |
| H | -1.873238 | -6.440231 | -1.813115 |
| C | -0.059444 | 1.863617 | -1.147323 |
| C | 1.042272 | 1.607653 | -0.750950 |
| H | -1.040613 | 2.109725 | -1.488326 |
| H | 2.024700 | 1.382328 | -0.393043 |
| C | 1.961344 | 4.094494 | -4.974574 |
| C | 1.762445 | 3.781107 | -3.835480 |
| H | 2.139866 | 4.374790 | -5.987511 |
| H | 1.578949 | 3.499951 | -2.819323 |
| C | -1.926127 | 5.115497 | -1.812785 |
| C | -1.330594 | 5.081515 | -2.851287 |
| H | -2.444561 | 5.133416 | -0.880213 |
| H | -0.787699 | 5.040559 | -3.769287 |
| C | 4.922956 | -0.997188 | 3.266335 |
| C | 4.645439 | -0.773783 | 4.409701 |
| H | 5.161009 | -1.188972 | 2.242152 |
| H | 4.400826 | -0.568305 | 5.426773 |
| C | -6.956535 | -3.603403 | -0.662469 |
| C | -7.280135 | -4.748986 | -0.534349 |
| H | -6.657586 | -2.584042 | -0.782272 |
| H | -7.578289 | -5.765582 | -0.416236 |
| C | 2.188924 | -6.512955 | -1.261620 |
| C | 3.208212 | -5.919611 | -1.052457 |
| H | 1.275452 | -7.036117 | -1.448914 |
| H | 4.108755 | -5.378229 | -0.864392 |
| C | 1.004681 | 1.775244 | 3.240473 |
| C | 1.485894 | 0.678498 | 3.196539 |
| H | 0.552162 | 2.741431 | 3.272057 |
| H | 1.908319 | -0.302840 | 3.154641 |

EICO 18

0 1

| | | | |
|---|-----------|-----------|-----------|
| C | 0.195913 | -0.331904 | -1.173616 |
| C | -0.462030 | 0.565818 | -1.620287 |
| H | 0.774024 | -1.136553 | -0.768844 |

| | | | |
|---|-----------|-----------|-----------|
| H | -1.066835 | 1.355391 | -2.015876 |
| C | 2.641131 | 2.431214 | -0.824717 |
| C | 3.511612 | 3.149264 | -0.421754 |
| H | 1.856534 | 1.793067 | -1.176291 |
| H | 4.281418 | 3.793171 | -0.060310 |
| C | -3.612691 | -0.518979 | -0.138006 |
| C | -4.592714 | -1.060564 | -0.565308 |
| H | -2.739307 | -0.036184 | 0.248356 |
| H | -5.469717 | -1.539643 | -0.938695 |
| C | -0.276880 | 4.697581 | -0.698426 |
| C | -1.140607 | 4.054286 | -0.172266 |
| H | 0.494012 | 5.272445 | -1.164144 |
| H | -1.910775 | 3.480573 | 0.298147 |
| C | -1.050378 | -4.366581 | -1.987805 |
| C | -1.636541 | -3.404956 | -1.578947 |
| H | -0.520960 | -5.214883 | -2.358512 |
| H | -2.161689 | -2.547033 | -1.214533 |
| C | 5.317355 | -0.538822 | 2.229866 |
| C | 4.764841 | 0.202449 | 1.469162 |
| H | 5.811627 | -1.194625 | 2.909826 |
| H | 4.272575 | 0.868281 | 0.792911 |
| C | 1.351828 | -3.187486 | 0.759141 |
| C | 2.327839 | -2.538625 | 1.008422 |
| H | 0.470543 | -3.748967 | 0.539095 |
| H | 3.197994 | -1.960865 | 1.236246 |
| C | -3.534195 | 2.052191 | -2.640161 |
| C | -2.945075 | 3.059356 | -2.914412 |
| H | -4.048972 | 1.154523 | -2.377073 |
| H | -2.429025 | 3.963368 | -3.157746 |
| C | -0.735197 | 1.251222 | 1.971236 |
| C | -1.688434 | 1.097744 | 2.680584 |
| H | 0.106146 | 1.399669 | 1.331917 |
| H | -2.537490 | 0.956602 | 3.312977 |
| C | -5.354314 | 0.021521 | 3.998954 |
| C | -4.724326 | -0.770615 | 3.357825 |
| H | -5.922897 | 0.719090 | 4.571324 |
| H | -4.151280 | -1.474255 | 2.790834 |
| C | -7.389356 | 1.759556 | -2.918352 |
| C | -6.877709 | 1.951923 | -1.852322 |
| H | -7.842462 | 1.592269 | -3.868857 |
| H | -6.405585 | 2.134313 | -0.909152 |
| C | 2.220644 | 6.740778 | -3.167907 |
| C | 2.547020 | 5.612345 | -2.931554 |
| H | 1.926020 | 7.742876 | -3.397033 |
| H | 2.840718 | 4.611134 | -2.703176 |
| C | -5.738839 | 4.696808 | -4.445162 |
| C | -6.374067 | 5.568585 | -4.965981 |
| H | -5.175461 | 3.921092 | -3.970324 |
| H | -6.948178 | 6.340720 | -5.424681 |
| C | -4.990155 | -5.979406 | 0.638496 |
| C | -4.194216 | -5.594267 | -0.168880 |
| H | -5.701565 | -6.329451 | 1.351140 |
| H | -3.474181 | -5.244213 | -0.877489 |
| C | -2.365564 | -3.409494 | 2.016312 |
| C | -1.613241 | -2.519565 | 2.295263 |
| H | -3.033969 | -4.202034 | 1.756362 |
| H | -0.943183 | -1.722565 | 2.532792 |
| C | -2.289168 | 6.227967 | -4.441052 |
| C | -1.113378 | 6.009416 | -4.363549 |
| H | -3.343737 | 6.393669 | -4.494209 |
| H | -0.063878 | 5.822220 | -4.289132 |
| C | -4.839916 | 2.449410 | 1.251799 |
| C | -4.745558 | 3.487509 | 0.659698 |

| | | | |
|---|-----------|-----------|-----------|
| H | -4.930814 | 1.522144 | 1.775822 |
| H | -4.661133 | 4.410633 | 0.124305 |
| C | -3.701823 | 6.424018 | -1.292817 |
| C | -4.877533 | 6.509475 | -1.508552 |
| H | -2.654943 | 6.327867 | -1.103607 |
| H | -5.927093 | 6.571866 | -1.701255 |
| C | -8.802563 | 6.426072 | -1.408013 |
| C | -8.392592 | 5.392464 | -1.852426 |
| H | -9.176159 | 7.341117 | -1.009152 |
| H | -8.025081 | 4.469294 | -2.246612 |
| C | 1.142305 | 10.055230 | -4.789631 |
| C | 0.201890 | 9.314909 | -4.768325 |
| H | 1.974197 | 10.720776 | -4.816318 |
| H | -0.631168 | 8.646172 | -4.750207 |

EICO 19

0 1

| | | | |
|---|-----------|-----------|-----------|
| C | 1.057626 | 2.428330 | 1.247224 |
| C | 0.470027 | 1.433163 | 1.567563 |
| H | 1.593460 | 3.310563 | 0.961634 |
| H | -0.059265 | 0.548554 | 1.854335 |
| C | -2.663462 | 2.944178 | 2.221715 |
| C | -3.801328 | 2.860429 | 1.855179 |
| H | -1.644238 | 3.013381 | 2.534043 |
| H | -4.813226 | 2.805503 | 1.517069 |
| C | 3.381319 | -0.409062 | 0.333317 |
| C | 4.163812 | -1.179901 | -0.145977 |
| H | 2.681884 | 0.281937 | 0.754474 |
| H | 4.850730 | -1.872581 | -0.579118 |
| C | -0.896179 | 6.875166 | 0.728128 |
| C | -0.503560 | 7.502808 | 1.669105 |
| H | -1.251713 | 6.313028 | -0.108464 |
| H | -0.160796 | 8.062734 | 2.509086 |
| C | 3.592454 | 4.979795 | 0.437686 |
| C | 2.659773 | 5.721403 | 0.561443 |
| H | 4.419228 | 4.312153 | 0.323692 |
| H | 1.819503 | 6.372515 | 0.670782 |
| C | -2.357273 | 4.756281 | -2.281166 |
| C | -2.372363 | 4.140935 | -1.253393 |
| H | -2.335135 | 5.294728 | -3.201345 |
| H | -2.395026 | 3.600457 | -0.330194 |
| C | 0.877813 | -3.345997 | 0.529927 |
| C | 1.010153 | -4.438358 | 1.006022 |
| H | 0.755059 | -2.375182 | 0.096295 |
| H | 1.159052 | -5.411856 | 1.421396 |
| C | -1.640175 | -1.699937 | 2.361773 |
| C | -2.312075 | -0.713969 | 2.253409 |
| H | -1.045919 | -2.581774 | 2.453787 |
| H | -2.905440 | 0.169131 | 2.153286 |
| C | 6.808897 | 2.958763 | -0.191000 |
| C | 5.968424 | 2.114450 | -0.319583 |
| H | 7.561375 | 3.705584 | -0.076083 |
| H | 5.220825 | 1.355835 | -0.427362 |
| C | 5.045715 | -5.070756 | -1.508110 |
| C | 4.008523 | -4.635535 | -1.096206 |
| H | 5.970171 | -5.454793 | -1.875036 |
| H | 3.086234 | -4.250585 | -0.713971 |
| C | -2.731955 | -4.260796 | -0.111372 |
| C | -3.925993 | -4.358780 | -0.105896 |
| H | -1.666340 | -4.182366 | -0.110110 |
| H | -4.991199 | -4.451009 | -0.102348 |

| | | | |
|---|-----------|-----------|-----------|
| C | 3.188932 | -7.284822 | 1.332561 |
| C | 2.514076 | -7.863706 | 2.134133 |
| H | 3.788426 | -6.765193 | 0.616832 |
| H | 1.921969 | -8.387076 | 2.849432 |
| C | -5.981670 | 3.787645 | -0.906399 |
| C | -6.794691 | 2.952271 | -0.630338 |
| H | -5.249410 | 4.523842 | -1.154940 |
| H | -7.515149 | 2.202174 | -0.386847 |
| C | -4.158492 | 0.415362 | -1.080884 |
| C | -3.888582 | -0.712813 | -0.777378 |
| H | -4.417241 | 1.415100 | -1.354721 |
| H | -3.639470 | -1.719706 | -0.510219 |
| C | -8.538107 | -0.431296 | 0.755697 |
| C | -7.399209 | -0.455815 | 0.385168 |
| H | -9.550636 | -0.413301 | 1.089581 |
| H | -6.382666 | -0.470133 | 0.049428 |
| C | 3.368955 | 2.837581 | -2.480506 |
| C | 2.416693 | 2.192679 | -2.145464 |
| H | 4.216236 | 3.419163 | -2.764591 |
| H | 1.566399 | 1.616141 | -1.848558 |
| C | -7.745428 | -4.139110 | -0.154868 |
| C | -7.583768 | -5.297697 | -0.409264 |
| H | -7.893969 | -3.105021 | 0.070251 |
| H | -7.445086 | -6.329788 | -0.637101 |
| C | 8.099166 | 0.174799 | 2.153073 |
| C | 8.740554 | -0.528761 | 2.878018 |
| H | 7.528774 | 0.805364 | 1.506782 |
| H | 9.309729 | -1.155326 | 3.524970 |
| C | 3.828762 | -0.899910 | -3.631028 |
| C | 3.858058 | -2.089112 | -3.771042 |
| H | 3.788550 | 0.159158 | -3.490343 |
| H | 3.892115 | -3.149309 | -3.882569 |
| C | 0.609202 | -0.843832 | -1.971158 |
| C | -0.388699 | -0.422100 | -1.457742 |
| H | 1.505132 | -1.208020 | -2.429090 |
| H | -1.291010 | -0.056122 | -1.016745 |

EICO 20

0 1

| | | | |
|---|-----------|----------|-----------|
| C | 1.098640 | 2.511734 | 2.550715 |
| C | 2.179571 | 2.006783 | 2.435438 |
| H | 0.135108 | 2.964200 | 2.648552 |
| H | 3.147694 | 1.572162 | 2.324151 |
| C | 2.548318 | 5.244999 | -5.304312 |
| C | 2.894043 | 4.097294 | -5.345083 |
| H | 2.245072 | 6.270057 | -5.260332 |
| H | 3.180194 | 3.067938 | -5.369135 |
| C | 0.913457 | 5.462562 | 4.359546 |
| C | 0.421148 | 5.081170 | 5.383728 |
| H | 1.344825 | 5.791259 | 3.437404 |
| H | -0.024710 | 4.739695 | 6.292260 |
| C | 5.468184 | 3.135217 | 0.660509 |
| C | 5.415177 | 3.291812 | 1.847602 |
| H | 5.516236 | 3.002280 | -0.399008 |
| H | 5.349963 | 3.427778 | 2.906218 |
| C | -2.929805 | 2.702936 | 3.473051 |
| C | -2.074986 | 2.342996 | 4.232345 |
| H | -3.682670 | 3.013349 | 2.779931 |
| H | -1.309265 | 2.018411 | 4.905837 |
| C | 4.408497 | 1.978836 | -2.706553 |
| C | 5.514331 | 1.758594 | -3.111946 |
| H | 3.421654 | 2.190740 | -2.347515 |

| | | | |
|---|-----------|-----------|-----------|
| H | 6.499215 | 1.564685 | -3.471614 |
| C | -1.287206 | 5.461950 | 1.780305 |
| C | -0.791741 | 5.495876 | 0.689439 |
| H | -1.705731 | 5.421265 | 2.761574 |
| H | -0.335722 | 5.530121 | -0.277182 |
| C | 1.219886 | 3.533123 | -2.150821 |
| C | 1.307407 | 3.131915 | -1.024555 |
| H | 1.153965 | 3.900655 | -3.151682 |
| H | 1.375086 | 2.781439 | -0.015977 |
| C | 0.382057 | 7.268175 | -2.698129 |
| C | 1.369465 | 6.896960 | -2.129118 |
| H | -0.488406 | 7.595588 | -3.221329 |
| H | 2.241278 | 6.549310 | -1.616731 |
| C | 2.395597 | 6.967673 | 1.271070 |
| C | 2.948191 | 5.904999 | 1.240020 |
| H | 1.886198 | 7.904650 | 1.289662 |
| H | 3.447797 | 4.959775 | 1.203845 |
| C | -1.227559 | 3.336768 | -7.635046 |
| C | -0.110884 | 3.667494 | -7.355762 |
| H | -2.220362 | 3.042833 | -7.889179 |
| H | 0.880671 | 3.967252 | -7.089819 |
| C | 1.220833 | 0.913713 | -5.383875 |
| C | 2.152548 | 0.386787 | -4.847282 |
| H | 0.391703 | 1.384374 | -5.864925 |
| H | 2.982496 | -0.076544 | -4.363735 |
| C | -5.515176 | 3.770490 | 0.724352 |
| C | -4.439587 | 4.267660 | 0.552294 |
| H | -6.475723 | 3.330790 | 0.865938 |
| H | -3.474541 | 4.706926 | 0.414117 |
| C | 3.879525 | 3.422441 | 5.285843 |
| C | 4.842882 | 2.745471 | 5.506554 |
| H | 3.008657 | 4.017519 | 5.103137 |
| H | 5.699026 | 2.144784 | 5.713044 |
| C | -2.589852 | 4.075032 | 7.303515 |
| C | -2.185283 | 4.447868 | 8.367033 |
| H | -2.941699 | 3.745071 | 6.349637 |
| H | -1.833947 | 4.786345 | 9.314942 |
| C | 0.124641 | 1.611484 | 7.115988 |
| C | 0.934628 | 1.563732 | 6.234925 |
| H | -0.601307 | 1.666846 | 7.895426 |
| H | 1.653847 | 1.530196 | 5.446037 |
| C | 5.137533 | 6.070811 | -1.389323 |
| C | 4.793757 | 5.509893 | -2.390891 |
| H | 5.435477 | 6.555353 | -0.486821 |
| H | 4.477849 | 5.014711 | -3.284110 |
| C | 0.873825 | 10.690329 | -3.617625 |
| C | 0.067787 | 11.485555 | -4.007455 |
| H | 1.589414 | 9.969973 | -3.285467 |
| H | -0.648166 | 12.199717 | -4.344878 |
| C | -0.203645 | 8.241991 | -6.063412 |
| C | -0.508238 | 7.170323 | -6.503427 |
| H | 0.055484 | 9.194782 | -5.654930 |
| H | -0.780477 | 6.214893 | -6.895500 |
| C | 3.949992 | 8.426002 | -4.374475 |
| C | 3.494945 | 9.034470 | -5.299907 |
| H | 4.357176 | 7.873301 | -3.555308 |
| H | 3.091808 | 9.578506 | -6.123517 |

Section 2: Optimized cationic structures

DEC1

1 2

| | | | |
|---|-----------|-----------|-----------|
| C | 3.469658 | 2.231326 | 0.067951 |
| H | 3.175997 | 2.785834 | 0.931997 |
| C | 4.829678 | -2.073870 | -1.172262 |
| H | 4.391825 | -2.783644 | -1.838168 |
| C | 5.353504 | -1.302055 | -0.420684 |
| H | 5.844468 | -0.619982 | 0.237292 |
| C | 3.833014 | 1.649085 | -0.915764 |
| H | 4.188037 | 1.131607 | -1.780325 |
| C | 0.593868 | 3.492377 | -1.998175 |
| H | 1.654621 | 3.512307 | -2.115629 |
| C | -0.597736 | 3.499920 | -1.869441 |
| H | -1.660614 | 3.536394 | -1.751023 |
| C | -0.038805 | 0.314207 | -0.681928 |
| H | -0.029980 | 1.154084 | -1.364791 |
| C | -0.329115 | -0.719510 | -0.044971 |
| H | -0.822134 | -1.616951 | 0.305687 |
| C | 1.402850 | -3.766132 | -0.145456 |
| H | 0.570068 | -3.982080 | -0.777195 |
| C | 2.341677 | -3.574303 | 0.573744 |
| H | 3.197636 | -3.437074 | 1.196868 |
| C | -2.376430 | -3.289947 | 1.285614 |
| H | -3.291087 | -3.059775 | 0.784224 |
| C | 0.771762 | 0.181347 | 0.731414 |
| H | 0.420412 | 0.773106 | 1.569889 |
| C | 2.042707 | -0.209569 | 0.577305 |
| H | 2.642330 | -0.800422 | -0.108721 |
| C | -1.358329 | -3.567978 | 1.853350 |
| H | -0.460675 | -3.851549 | 2.356358 |
| C | -3.720386 | -0.557176 | -0.482009 |
| H | -3.696108 | -0.182428 | 0.519042 |
| C | -3.750345 | -0.980342 | -1.602522 |
| H | -3.802733 | -1.359515 | -2.598894 |
| C | -4.102862 | 3.024456 | -0.634695 |
| H | -4.395527 | 2.113722 | -1.109675 |
| C | -3.797787 | 4.054587 | -0.104906 |
| H | -3.552699 | 4.984660 | 0.357943 |
| C | -2.327582 | 1.316276 | 2.237148 |
| H | -2.549066 | 2.203008 | 1.681305 |
| C | -2.119075 | 0.315696 | 2.863019 |
| H | -1.957179 | -0.570480 | 3.436418 |

DEC 2

1 2

| | | | |
|---|-----------|-----------|-----------|
| C | -0.029403 | -1.263902 | 2.689157 |
| C | -1.030638 | -1.920709 | 2.634019 |
| H | 0.871082 | -0.689656 | 2.761344 |
| H | -1.927463 | -2.500195 | 2.599375 |
| C | -0.753949 | 1.784953 | -3.017195 |
| C | -0.558594 | 3.064041 | -2.724907 |
| H | -1.039119 | 1.466657 | -4.017569 |
| H | -0.276911 | 3.651450 | -1.856819 |
| C | -4.354501 | -2.014591 | 0.894508 |
| C | -4.071221 | -3.124851 | 0.544895 |
| H | -4.624967 | -1.030949 | 1.209170 |
| H | -3.849575 | -4.123680 | 0.240499 |
| C | -3.177351 | 1.657369 | 0.264163 |
| C | -2.469780 | 1.055000 | 1.021544 |
| H | -3.826773 | 2.199690 | -0.387118 |
| H | -1.853373 | 0.505242 | 1.703567 |
| C | 2.772462 | 0.714454 | -2.253685 |
| C | 2.723114 | 0.591720 | -1.062265 |

| | | | |
|---|-----------|-----------|-----------|
| H | 2.847720 | 0.825818 | -3.312565 |
| H | 2.710373 | 0.489175 | 0.003933 |
| C | -0.020989 | -1.522703 | -1.193759 |
| C | -1.241923 | -1.403644 | -0.922702 |
| H | 0.997472 | -1.872459 | -1.122950 |
| H | -2.197066 | -1.576730 | -0.449231 |
| C | 2.858532 | 1.123301 | 2.664397 |
| C | 3.424284 | 0.076977 | 2.520687 |
| H | 2.370085 | 2.061894 | 2.805996 |
| H | 3.934189 | -0.853614 | 2.401376 |
| C | 1.274748 | 3.405827 | 0.331876 |
| C | 0.199205 | 3.443090 | 0.859600 |
| H | 2.238815 | 3.381195 | -0.127358 |
| H | -0.754992 | 3.489820 | 1.336911 |
| C | 2.473924 | -3.025845 | 0.731556 |
| C | 3.308409 | -2.743766 | -0.080637 |
| H | 1.737249 | -3.283742 | 1.460955 |
| H | 4.064608 | -2.505607 | -0.795477 |
| C | -0.788439 | -0.557747 | -2.177131 |
| C | -0.594810 | 0.806376 | -1.984652 |
| H | -1.053183 | -0.920056 | -3.166109 |
| H | -0.313895 | 1.157725 | -0.994212 |

DEC 3

1 2

| | | | |
|---|-----------|-----------|-----------|
| C | 4.237570 | 1.174320 | -0.420402 |
| C | 4.425134 | 1.094083 | -1.601125 |
| H | 4.082911 | 1.245467 | 0.634444 |
| H | 4.627463 | 1.026306 | -2.647094 |
| C | 0.989522 | 4.677113 | -0.425756 |
| C | 1.950796 | 4.043793 | -0.757531 |
| H | 0.155325 | 5.278431 | -0.139708 |
| H | 2.823868 | 3.500297 | -1.048628 |
| C | -0.334463 | -2.380621 | 3.164954 |
| C | 0.556023 | -3.147814 | 3.396548 |
| H | -1.134464 | -1.697261 | 2.979972 |
| H | 1.335169 | -3.840930 | 3.625299 |
| C | 1.517297 | -1.298726 | -0.398574 |
| C | 1.342650 | -2.500671 | 0.143067 |
| H | 2.506675 | -0.892934 | -0.600208 |
| H | 0.520834 | -3.141654 | 0.441062 |
| C | -0.818931 | 1.090438 | -2.253997 |
| C | -0.792397 | 1.687842 | -1.147526 |
| H | -1.149709 | 0.822186 | -3.241242 |
| H | -1.082433 | 2.374947 | -0.374226 |
| C | -3.983451 | -0.913623 | -2.075106 |
| C | -4.367535 | 0.208095 | -2.244033 |
| H | -3.666100 | -1.921198 | -1.919164 |
| H | -4.735245 | 1.197075 | -2.404089 |
| C | -1.751509 | -3.800910 | -1.040380 |
| C | -2.192300 | -3.505798 | 0.034031 |
| H | -1.375108 | -4.093883 | -1.995710 |
| H | -2.599635 | -3.277986 | 0.994575 |
| C | 0.419188 | 0.722478 | -1.349048 |
| C | 0.365906 | -0.527420 | -0.724293 |
| H | 1.390856 | 1.151609 | -1.575783 |
| H | -0.614069 | -0.942139 | -0.491709 |
| C | -1.893802 | 0.643371 | 1.955474 |
| C | -2.739397 | 0.247806 | 1.203049 |
| H | -1.143921 | 1.004195 | 2.625962 |
| H | -3.501622 | -0.074888 | 0.525502 |
| C | 1.684667 | 0.654188 | 2.551415 |
| C | 1.634290 | 1.729566 | 2.024314 |

| | | | |
|---|----------|-----------|----------|
| H | 1.720495 | -0.297722 | 3.035930 |
| H | 1.602891 | 2.693459 | 1.561442 |

DEC 4

1 2

| | | | |
|---|-----------|-----------|-----------|
| C | 2.442078 | 1.278628 | 1.444467 |
| C | 1.383937 | 1.703004 | 1.073519 |
| H | 3.392914 | 0.920783 | 1.774666 |
| H | 0.444918 | 2.107686 | 0.755522 |
| C | 0.911168 | -1.654101 | 0.374732 |
| C | -0.181906 | -1.445833 | 1.229242 |
| H | 1.908770 | -1.595454 | 0.807691 |
| H | 0.022383 | -1.238627 | 2.274178 |
| C | -1.248737 | 1.005907 | 3.640656 |
| C | -2.356047 | 0.662077 | 3.339171 |
| H | -0.270825 | 1.324659 | 3.926783 |
| H | -3.349880 | 0.366130 | 3.082554 |
| C | -2.059937 | 0.058013 | -2.703526 |
| C | -0.924481 | 0.345035 | -2.958033 |
| H | -3.077647 | -0.185200 | -2.485802 |
| H | 0.084611 | 0.602030 | -3.200906 |
| C | 4.903093 | -1.762785 | 0.753125 |
| C | 4.897394 | -0.883666 | -0.061201 |
| H | 4.952179 | -2.544920 | 1.478196 |
| H | 4.916408 | -0.104730 | -0.792481 |
| C | -5.039244 | -0.614357 | 0.064886 |
| H | -5.411831 | -1.613517 | 0.100892 |
| C | -1.870151 | 2.905542 | -0.484813 |
| H | -1.755086 | 2.780765 | -1.539263 |
| C | -2.015735 | 3.057027 | 0.695426 |
| H | -2.149573 | 3.201576 | 1.745116 |
| C | -4.661165 | 0.521370 | 0.022101 |
| H | -4.338271 | 1.538904 | -0.018027 |
| C | -1.485471 | -0.818613 | 0.610612 |
| H | -1.775843 | 0.180753 | 0.330372 |
| C | -1.568281 | -2.052172 | 0.846218 |
| H | -2.028481 | -3.019616 | 0.943856 |
| C | 0.839891 | -1.937105 | -1.016706 |
| H | -0.119471 | -1.975681 | -1.525364 |
| C | 1.983046 | -2.128149 | -1.670866 |
| H | 3.043441 | -2.139553 | -1.442016 |
| C | 2.757878 | 1.024378 | -2.339219 |
| H | 2.542998 | 1.479142 | -1.395555 |
| C | 3.012778 | 0.523636 | -3.397897 |
| H | 3.248835 | 0.101140 | -4.349719 |

DEC 5

1 2

| | | | |
|---|-----------|-----------|-----------|
| C | -4.021940 | -0.970195 | 1.152496 |
| C | -4.293097 | -1.816470 | 0.349642 |
| H | -3.811754 | -0.219116 | 1.881347 |
| H | -4.556352 | -2.576438 | -0.351603 |
| C | -0.816358 | -2.530899 | -1.401734 |
| C | -1.532637 | -1.497862 | -1.549794 |
| H | -0.421170 | -3.505385 | -1.631161 |
| H | -2.246604 | -0.837342 | -2.010008 |
| C | -5.654678 | 2.816844 | 0.059827 |
| C | -6.046440 | 1.686754 | 0.112964 |
| H | -5.325557 | 3.830440 | 0.008864 |
| H | -6.411790 | 0.685829 | 0.163108 |
| C | -1.394115 | 2.244106 | -1.542073 |

| | | | |
|---|-----------|-----------|-----------|
| C | -2.388606 | 1.901063 | -0.967868 |
| H | -0.528627 | 2.579903 | -2.067378 |
| H | -3.303277 | 1.631058 | -0.480098 |
| C | 0.462006 | -0.688658 | -0.173384 |
| C | -0.697549 | -1.507979 | -0.247793 |
| H | 0.767539 | -0.359633 | 0.818562 |
| H | -1.209898 | -1.719769 | 0.685493 |
| C | 2.341892 | 0.524641 | -0.957119 |
| C | 1.241180 | -0.241614 | -1.241656 |
| H | 2.555426 | 0.765662 | 0.082413 |
| H | 0.992280 | -0.506203 | -2.264308 |
| C | 2.881615 | -3.323196 | -0.165567 |
| C | 2.309034 | -3.480834 | 0.874447 |
| H | 3.407467 | -3.210974 | -1.087435 |
| H | 1.815179 | -3.649733 | 1.805591 |
| C | 3.259995 | 1.027057 | -1.948053 |
| C | 4.342457 | 1.688676 | -1.573607 |
| H | 3.058994 | 0.835784 | -3.000526 |
| H | 4.812249 | 2.005633 | -0.650767 |
| C | 4.364336 | -0.326689 | 1.852983 |
| C | 4.553086 | 0.796124 | 2.225612 |
| H | 4.208310 | -1.335158 | 1.535362 |
| H | 4.740191 | 1.785294 | 2.580773 |
| C | 0.249215 | 2.085519 | 1.875826 |
| C | 1.031082 | 1.655576 | 2.675478 |
| H | -0.455572 | 2.471862 | 1.171350 |
| H | 1.722483 | 1.286321 | 3.399795 |

DEC 6

1 2

| | | | |
|---|-----------|-----------|-----------|
| C | 2.709866 | -2.454792 | -0.875470 |
| C | 2.718327 | -2.710983 | -2.046013 |
| H | 2.710630 | -2.235010 | 0.170211 |
| H | 2.751372 | -2.954638 | -3.084974 |
| C | 3.073844 | 2.122032 | -2.249799 |
| C | 3.771909 | 1.219118 | -1.884866 |
| H | 2.465036 | 2.932402 | -2.587003 |
| H | 4.410259 | 0.418800 | -1.580758 |
| C | 1.320538 | -0.602913 | 2.169826 |
| C | 0.729021 | -1.640956 | 2.068490 |
| H | 1.844148 | 0.322827 | 2.281456 |
| H | 0.221990 | -2.578786 | 1.983303 |
| C | 0.385704 | 0.010593 | -1.606245 |
| C | -0.575614 | -0.935790 | -1.161428 |
| H | 1.387555 | -0.002085 | -2.005112 |
| H | -0.473712 | -1.996798 | -0.933189 |
| C | -2.430916 | 2.068613 | 2.087094 |
| C | -1.765246 | 1.226108 | 2.619086 |
| H | -3.034354 | 2.824817 | 1.634831 |
| H | -1.171068 | 0.480252 | 3.100965 |
| C | -1.442947 | -4.081307 | 0.337990 |
| C | -0.377512 | -4.442695 | -0.075854 |
| H | -2.398453 | -3.776021 | 0.708114 |
| H | 0.566066 | -4.785128 | -0.441084 |
| C | 1.302281 | 3.065077 | 2.015294 |
| C | 2.169851 | 2.886477 | 1.207345 |
| H | 0.539162 | 3.235598 | 2.743022 |
| H | 2.948853 | 2.740765 | 0.489436 |
| C | -1.524433 | 0.008878 | -0.686113 |
| C | -0.317395 | 0.764467 | -0.624420 |
| H | -2.461363 | -0.028717 | -0.151723 |

| | | | |
|---|-----------|-----------|-----------|
| H | 0.067623 | 1.394338 | 0.174904 |
| C | -4.499957 | -1.902529 | 0.252055 |
| C | -4.191304 | -1.421279 | 1.304832 |
| H | -4.807807 | -2.337028 | -0.673228 |
| H | -3.947002 | -0.984613 | 2.248041 |
| C | -0.950130 | 3.311808 | -2.198001 |
| C | -0.368287 | 3.751271 | -1.246553 |
| H | -1.476503 | 2.960153 | -3.057662 |
| H | 0.152331 | 4.156521 | -0.405776 |

DEC 7

1 2

| | | | |
|---|-----------|-----------|-----------|
| C | 1.596727 | -2.398815 | 1.827301 |
| C | 0.958491 | -2.210825 | 2.823652 |
| H | 2.158984 | -2.577258 | 0.933738 |
| H | 0.389989 | -2.052381 | 3.711541 |
| C | 3.133619 | -4.183433 | -1.167796 |
| C | 2.532351 | -3.274616 | -1.667221 |
| H | 3.671421 | -4.996742 | -0.737718 |
| H | 1.981818 | -2.449854 | -2.089733 |
| C | 3.362632 | 1.201332 | 0.631154 |
| C | 3.450413 | 0.656141 | 1.694002 |
| H | 3.265414 | 1.677976 | -0.320894 |
| H | 3.528374 | 0.152197 | 2.630330 |
| C | 1.755858 | 3.137308 | -2.187506 |
| C | 1.744067 | 2.032671 | -2.652790 |
| H | 1.757537 | 4.119737 | -1.772208 |
| H | 1.701431 | 1.028949 | -3.027415 |
| C | -1.953562 | 0.354666 | 1.046050 |
| C | -0.698435 | 0.075182 | 0.350736 |
| H | -1.845960 | 0.813414 | 2.026954 |
| H | 0.216468 | 0.295301 | 0.898876 |
| C | -0.555721 | -0.434158 | -0.913012 |
| C | 0.723566 | -0.623359 | -1.486590 |
| H | -1.450386 | -0.666679 | -1.489541 |
| H | 1.462649 | -0.346559 | -0.709100 |
| C | -2.969917 | -4.357271 | 1.106719 |
| C | -1.893723 | -3.833065 | 1.079904 |
| H | -3.921671 | -4.836861 | 1.125888 |
| H | -0.930265 | -3.370191 | 1.065098 |
| C | -3.215332 | 0.632356 | 0.244801 |
| C | -3.166080 | -0.527922 | 0.775219 |
| H | -3.656537 | 1.397508 | -0.370192 |
| H | -3.523044 | -1.525262 | 0.966388 |
| C | -1.946142 | 2.986632 | -2.163393 |
| C | -2.992626 | 3.563373 | -2.248456 |
| H | -1.004235 | 2.483825 | -2.094211 |
| H | -3.920538 | 4.079451 | -2.342937 |
| C | 0.569189 | 3.282263 | 1.364751 |
| C | -0.447297 | 3.716888 | 0.904342 |
| H | 1.478554 | 2.883127 | 1.757438 |
| H | -1.348084 | 4.094960 | 0.475836 |

DEC 8

1 2

| | | | |
|---|-----------|----------|-----------|
| C | 0.941329 | 4.203983 | -0.628538 |
| C | 0.312058 | 4.666165 | 0.280632 |
| H | 1.511845 | 3.804353 | -1.439484 |
| H | -0.234174 | 5.108841 | 1.084070 |
| C | 3.352246 | 0.934818 | 1.954082 |
| C | 2.686483 | 1.896924 | 1.695705 |
| H | 3.964978 | 0.098370 | 2.207760 |

| | | | |
|---|-----------|-----------|-----------|
| H | 2.118112 | 2.772351 | 1.462716 |
| C | 2.523937 | 1.268913 | -2.946662 |
| C | 3.075078 | 1.358026 | -1.886629 |
| H | 2.059407 | 1.199539 | -3.904881 |
| H | 3.569041 | 1.444803 | -0.942939 |
| C | 2.165928 | -2.034954 | -0.858051 |
| C | 1.822210 | -2.297660 | 0.331208 |
| H | 2.832084 | -1.783504 | -1.665145 |
| H | 1.945331 | -2.459189 | 1.389266 |
| C | -2.225651 | 1.003221 | -1.074830 |
| C | -2.928440 | 2.114978 | -1.217611 |
| H | -2.648851 | 0.045406 | -1.367482 |
| H | -2.802498 | 3.176035 | -1.037855 |
| C | 0.654163 | -2.333507 | -0.681703 |
| C | -0.262992 | -1.242675 | -0.739214 |
| H | 0.276127 | -3.298363 | -1.005799 |
| H | -1.253783 | -1.477790 | -1.123187 |
| C | -3.229325 | -2.530719 | -2.720247 |
| C | -3.379404 | -2.888231 | -1.586738 |
| H | -3.121371 | -2.239774 | -3.741436 |
| H | -3.526168 | -3.213322 | -0.580412 |
| C | 0.564638 | -2.301404 | 3.820360 |
| C | 0.865265 | -1.171185 | 3.559965 |
| H | 0.298085 | -3.301750 | 4.081870 |
| H | 1.147299 | -0.162197 | 3.349654 |
| C | -3.584259 | -1.006269 | 1.383044 |
| C | -2.546490 | -1.251684 | 1.928770 |
| H | -4.521817 | -0.790262 | 0.921163 |
| H | -1.635954 | -1.459847 | 2.449303 |
| C | 0.018309 | 0.069264 | -0.370426 |
| C | -0.891565 | 1.089237 | -0.535572 |
| H | 0.995066 | 0.314479 | 0.031384 |
| H | -0.565655 | 2.086987 | -0.248303 |

DEC 9

1 2

| | | | |
|---|-----------|-----------|-----------|
| C | 0.896725 | 2.407726 | -1.835629 |
| C | -0.049817 | 2.755310 | -1.186795 |
| H | 1.754530 | 2.131146 | -2.409847 |
| H | -0.886648 | 3.084069 | -0.605880 |
| C | 3.165550 | 2.035517 | 2.398091 |
| C | 2.453090 | 2.396049 | 1.504744 |
| H | 3.803412 | 1.739914 | 3.201279 |
| H | 1.828532 | 2.725109 | 0.701210 |
| C | 4.554313 | 1.061123 | -2.251012 |
| C | 4.517548 | 1.912954 | -1.409495 |
| H | 4.622249 | 0.317285 | -3.013273 |
| H | 4.505350 | 2.677471 | -0.664196 |
| C | 2.603139 | -0.804372 | 0.107811 |
| C | 2.067448 | -1.914639 | 0.364604 |
| H | 3.354401 | -0.032463 | 0.069775 |
| H | 1.933915 | -2.914379 | 0.752764 |
| C | -3.416271 | 0.025570 | -1.147530 |
| C | -2.933431 | 0.791530 | -1.932443 |
| H | -3.860164 | -0.666663 | -0.466731 |
| H | -2.520131 | 1.474140 | -2.642068 |
| C | 1.205317 | -0.984848 | -0.569348 |
| C | 0.072005 | -0.382423 | -0.009574 |
| H | 1.174024 | -1.214024 | -1.629229 |
| H | -0.782310 | -0.196201 | -0.657527 |
| C | -1.872497 | -3.070891 | -0.787707 |
| C | -1.690227 | -3.251704 | 0.382395 |
| H | -2.059212 | -2.922369 | -1.828303 |

| | | | |
|---|-----------|-----------|----------|
| H | -1.534914 | -3.448347 | 1.420044 |
| C | 0.980686 | -5.233765 | 1.296225 |
| C | 1.487881 | -4.928416 | 2.337393 |
| H | 0.523060 | -5.528429 | 0.377850 |
| H | 1.942254 | -4.693567 | 3.274064 |
| C | -2.943996 | 3.161398 | 1.040511 |
| C | -2.176558 | 3.796672 | 1.706275 |
| H | -3.635181 | 2.609163 | 0.442087 |
| H | -1.513182 | 4.384696 | 2.301033 |
| C | -0.081410 | 0.001089 | 1.355855 |
| C | -1.248655 | 0.490455 | 1.755463 |
| H | 0.751256 | -0.101722 | 2.052256 |
| H | -1.707857 | 0.865287 | 2.661290 |

DEC 10

1 2

| | | | |
|---|-----------|-----------|-----------|
| C | -2.294845 | -0.845082 | -3.108130 |
| C | -1.596234 | 0.039160 | -2.697814 |
| H | -2.916931 | -1.617159 | -3.508483 |
| H | -0.962781 | 0.825732 | -2.343435 |
| C | -1.023494 | 3.403290 | -0.738657 |
| C | -1.150207 | 2.423077 | -0.060398 |
| H | -0.866554 | 4.286604 | -1.316080 |
| H | -1.227876 | 1.543708 | 0.544440 |
| C | -1.841028 | -0.645870 | 2.081244 |
| C | -1.973015 | -1.054089 | 0.963126 |
| H | -1.691710 | -0.304649 | 3.079122 |
| H | -2.080356 | -1.435222 | -0.027817 |
| C | -5.991168 | 0.500920 | -0.134181 |
| C | -5.010517 | 0.460833 | 0.649601 |
| H | -6.992289 | 0.415093 | -0.522426 |
| H | -4.428607 | 0.265997 | 1.534683 |
| C | -4.107478 | -3.528361 | -0.919369 |
| C | -4.794191 | -3.150268 | -0.013893 |
| H | -3.493640 | -3.902265 | -1.707782 |
| H | -5.401762 | -2.854834 | 0.811738 |
| C | -8.349361 | 2.709416 | -1.816172 |
| C | -8.207647 | 1.737323 | -2.501720 |
| H | -8.517249 | 3.568002 | -1.205131 |
| H | -8.094647 | 0.866669 | -3.112060 |
| C | -5.228680 | 3.000313 | -4.308213 |
| C | -4.119332 | 2.792549 | -4.712882 |
| H | -6.220474 | 3.196737 | -3.954237 |
| H | -3.139558 | 2.599538 | -5.093251 |
| C | -4.387792 | 2.223747 | -1.106354 |
| C | -4.611790 | 0.877286 | -0.813683 |
| H | -3.742912 | 2.451815 | -1.951136 |
| H | -4.139437 | 0.137526 | -1.447667 |
| C | -4.720550 | 4.562512 | -0.886963 |
| C | -4.968213 | 3.343872 | -0.429305 |
| H | -4.154676 | 5.038410 | -1.679091 |
| H | -5.628027 | 3.182180 | 0.418594 |
| C | -6.167013 | -1.566130 | -3.179803 |
| C | -5.816908 | -0.573157 | -3.752692 |
| H | -6.452083 | -2.461815 | -2.668031 |
| H | -5.491162 | 0.303261 | -4.271104 |

DEC 11

1 2

| | | | |
|---|----------|----------|-----------|
| C | 0.473840 | 2.136983 | 0.585875 |
| C | 0.438268 | 1.586381 | -0.477741 |

| | | | |
|---|-----------|-----------|-----------|
| H | 0.547151 | 2.633004 | 1.527931 |
| H | 0.448078 | 1.103071 | -1.432765 |
| C | 0.762590 | -0.455629 | -3.691116 |
| C | 0.918859 | 0.669951 | -4.069589 |
| H | 0.632878 | -1.466121 | -3.373688 |
| H | 1.076360 | 1.665378 | -4.421062 |
| C | -1.843777 | -2.025487 | 1.854400 |
| C | -1.249059 | -1.057392 | 1.472968 |
| H | -2.340399 | -2.900186 | 2.211564 |
| H | -0.693388 | -0.205518 | 1.137393 |
| C | -3.240736 | 2.286064 | 0.281621 |
| C | -3.243136 | 2.877492 | 1.546870 |
| H | -2.545920 | 2.173363 | -0.539344 |
| H | -2.495347 | 3.419495 | 2.110447 |
| C | -4.409064 | 0.334094 | 0.603067 |
| C | -4.786506 | -0.677695 | -0.297540 |
| H | -3.780370 | 0.045570 | 1.444641 |
| H | -4.376432 | -1.668885 | -0.133739 |
| C | -3.382023 | 2.313618 | -3.410526 |
| C | -2.549447 | 1.451585 | -3.431731 |
| H | -4.105867 | 3.097840 | -3.421867 |
| H | -1.794416 | 0.694453 | -3.475071 |
| C | -4.548026 | 2.500205 | 1.810745 |
| C | -4.682774 | 1.754862 | 0.485998 |
| H | -5.231155 | 2.589530 | 2.644563 |
| H | -5.448878 | 2.047344 | -0.229306 |
| C | -6.167598 | -0.562811 | -1.017668 |
| C | -5.184558 | -0.279126 | -1.754441 |
| H | -7.187384 | -0.757275 | -0.735127 |
| H | -4.634563 | 0.008424 | -2.635349 |
| C | -7.807156 | 0.878749 | 1.825850 |
| C | -7.271169 | 0.022520 | 2.469161 |
| H | -8.315806 | 1.642340 | 1.280006 |
| H | -6.827014 | -0.743037 | 3.065918 |
| C | -2.075506 | -2.106995 | -1.980713 |
| C | -2.478271 | -2.229897 | -3.102441 |
| H | -1.709348 | -2.021947 | -0.979537 |
| H | -2.820092 | -2.359006 | -4.105613 |

DEC 12

1 2

| | | | |
|---|-----------|-----------|-----------|
| C | 1.251651 | 2.944845 | -0.148735 |
| C | 2.042526 | 2.249546 | 0.542080 |
| H | 0.641763 | 3.792724 | -0.432778 |
| H | 2.693337 | 1.945830 | 1.343633 |
| C | -1.783243 | 0.497313 | 1.983774 |
| C | -1.160213 | 1.379512 | 2.503535 |
| H | -2.348151 | -0.289980 | 1.528247 |
| H | -0.635296 | 2.167279 | 2.996440 |
| C | -2.973227 | -2.461138 | -0.047609 |
| C | -3.303786 | -1.482534 | -0.656613 |
| H | -2.693440 | -3.351480 | 0.477921 |
| H | -3.616370 | -0.618827 | -1.201483 |
| C | -2.148019 | 2.095449 | -1.143585 |
| C | -1.916829 | 1.906159 | -2.304268 |
| H | -2.364954 | 2.266279 | -0.110936 |
| H | -1.735776 | 1.748255 | -3.344619 |
| C | -1.922580 | -5.961247 | 0.270672 |
| C | -1.626221 | -5.712131 | 1.403663 |
| H | -2.197516 | -6.208164 | -0.730133 |
| H | -1.364369 | -5.510517 | 2.418046 |
| C | 3.691786 | -0.938548 | 0.840124 |

| | | | |
|---|-----------|-----------|-----------|
| C | 4.604243 | -0.296827 | 0.403665 |
| H | 2.894527 | -1.531995 | 1.234796 |
| H | 5.439797 | 0.249329 | 0.025958 |
| C | -0.984947 | 5.541622 | -1.233896 |
| C | -0.191815 | 6.201097 | -0.625209 |
| H | -1.703446 | 4.971710 | -1.779939 |
| H | 0.498113 | 6.817526 | -0.093160 |
| C | 0.365662 | -2.252981 | 1.973643 |
| C | 0.667991 | -3.165747 | 1.258385 |
| H | 0.087849 | -1.452182 | 2.623590 |
| H | 0.925886 | -4.002399 | 0.646682 |
| C | 1.735020 | 1.645390 | -0.877580 |
| C | 0.891650 | 0.533659 | -0.882331 |
| H | 2.493117 | 1.731566 | -1.650185 |
| H | 0.131732 | 0.466815 | -0.104852 |
| C | 0.108128 | -1.524517 | -1.750611 |
| C | 0.988659 | -0.532272 | -1.822914 |
| H | -0.759889 | -1.804796 | -1.159033 |
| H | 1.771794 | -0.514179 | -2.577354 |

DEC 13

1 2

| | | | |
|---|-----------|-----------|-----------|
| C | -3.197980 | -0.884255 | -1.535791 |
| C | -2.987868 | -2.054673 | -1.687303 |
| H | -3.410494 | 0.155887 | -1.407784 |
| H | -2.837054 | -3.099887 | -1.844161 |
| C | 1.190523 | -0.351668 | -1.289944 |
| C | 0.041591 | 0.442504 | -1.031462 |
| H | 2.246134 | -0.130634 | -1.137335 |
| H | -0.160658 | 1.479251 | -0.809330 |
| C | 4.385232 | 0.843176 | 0.034369 |
| C | 3.608305 | 1.755627 | 0.064899 |
| H | 5.092772 | 0.043670 | 0.000338 |
| H | 2.934920 | 2.585804 | 0.079206 |
| C | 0.866831 | 3.947957 | -1.741705 |
| C | 0.689395 | 4.194462 | -0.582712 |
| H | 1.033267 | 3.769321 | -2.780832 |
| H | 0.545476 | 4.434994 | 0.447776 |
| C | 4.043449 | -2.502070 | -1.857199 |
| C | 3.765439 | -2.747203 | -0.717945 |
| H | 4.317412 | -2.308334 | -2.870657 |
| H | 3.531308 | -2.975918 | 0.298781 |
| C | -0.405033 | -0.827714 | -0.565565 |
| C | 0.507825 | -1.594235 | -1.350445 |
| H | -0.933217 | -1.079296 | 0.353584 |
| H | 0.792808 | -2.629814 | -1.439844 |
| C | -2.754919 | 2.823086 | -0.320904 |
| C | -3.125650 | 2.042284 | 0.509470 |
| H | -2.440538 | 3.539133 | -1.048544 |
| H | -3.462383 | 1.355890 | 1.256348 |
| C | -2.768458 | -1.355426 | 2.148417 |
| C | -1.882425 | -0.760182 | 2.694153 |
| H | -3.569549 | -1.884255 | 1.680529 |
| H | -1.096522 | -0.231794 | 3.190199 |
| C | 1.088798 | 2.095147 | 2.782851 |
| C | 0.034708 | 2.268461 | 2.240332 |
| H | 2.020631 | 1.957494 | 3.285378 |
| H | -0.912276 | 2.442386 | 1.775165 |
| C | 1.287344 | -2.171341 | 2.274363 |
| C | 1.963078 | -1.230197 | 1.968175 |
| H | 0.691605 | -3.004343 | 2.576928 |
| H | 2.577578 | -0.394753 | 1.706783 |

DEC 14

1 2

| | | | |
|---|-----------|-----------|-----------|
| C | -0.627404 | 2.372758 | 1.366459 |
| C | 0.007846 | 1.696747 | 2.125059 |
| H | -1.206881 | 2.970127 | 0.696530 |
| H | 0.555394 | 1.087941 | 2.810323 |
| C | 0.790950 | 0.268654 | -1.318789 |
| C | 1.048819 | -0.100282 | -2.429390 |
| H | 0.532107 | 0.591279 | -0.331790 |
| H | 1.256405 | -0.446394 | -3.417915 |
| C | 2.348397 | 3.854098 | 0.344049 |
| C | 2.872146 | 4.677889 | -0.450824 |
| H | 1.801473 | 3.472625 | 1.191349 |
| H | 3.212251 | 5.613918 | -0.857980 |
| C | 4.396302 | 1.505754 | -1.924701 |
| C | 5.602307 | 0.961330 | -1.866173 |
| H | 3.663286 | 1.210482 | -2.670407 |
| H | 6.501982 | 1.054758 | -1.269880 |
| C | 6.006341 | 4.256945 | 1.849541 |
| C | 6.712416 | 3.291330 | 1.790671 |
| H | 5.399765 | 5.131528 | 1.926840 |
| H | 7.359502 | 2.442413 | 1.772614 |
| C | 2.318422 | 3.397991 | -4.588038 |
| C | 3.309641 | 2.928015 | -5.069684 |
| H | 1.420723 | 3.815711 | -4.185219 |
| H | 4.180872 | 2.517308 | -5.529950 |
| C | 6.235250 | 5.056126 | -1.773262 |
| C | 5.490778 | 4.895418 | -2.698458 |
| H | 6.916945 | 5.207822 | -0.965521 |
| H | 4.835499 | 4.756839 | -3.531858 |
| C | -0.557218 | 4.569657 | -2.032621 |
| C | -0.610248 | 3.395445 | -2.265701 |
| H | -0.543703 | 5.618860 | -1.837716 |
| H | -0.667010 | 2.349385 | -2.477018 |
| C | 2.833866 | 3.205001 | -0.996504 |
| C | 4.055144 | 2.530103 | -0.985985 |
| H | 2.087354 | 2.940796 | -1.737320 |
| H | 4.792405 | 2.810571 | -0.236626 |
| C | 3.374830 | 0.286795 | 1.289993 |
| C | 3.847057 | 1.080555 | 2.053605 |
| H | 2.958524 | -0.435901 | 0.622514 |
| H | 4.282026 | 1.770845 | 2.742724 |

DEC 15

1 2

| | | | |
|---|-----------|-----------|-----------|
| C | -1.261837 | 3.463647 | 2.025276 |
| C | -1.681155 | 3.593826 | 0.910604 |
| H | -0.900807 | 3.371047 | 3.025583 |
| H | -2.082109 | 3.728200 | -0.069584 |
| C | -3.959151 | 0.866032 | -0.916481 |
| C | -4.333775 | 1.408098 | 0.084683 |
| H | -3.646659 | 0.384599 | -1.818010 |
| H | -4.686546 | 1.901810 | 0.963504 |
| C | 2.270071 | 3.274080 | 0.708822 |
| C | 3.441553 | 3.066033 | 0.568314 |
| H | 1.231818 | 3.490787 | 0.846491 |
| H | 4.491371 | 2.906756 | 0.456532 |
| C | -1.137912 | 0.192159 | 1.363568 |
| C | 0.122872 | -0.080758 | 1.038380 |

| | | | |
|---|-----------|-----------|-----------|
| H | -2.036363 | 0.575209 | 0.886999 |
| H | 0.839945 | -0.480955 | 1.751997 |
| C | 3.352499 | -0.099289 | 2.626073 |
| C | 3.267594 | -1.294203 | 2.644982 |
| H | 3.430372 | 0.965772 | 2.618364 |
| H | 3.200193 | -2.359034 | 2.679044 |
| C | -3.361964 | -2.602714 | 0.240578 |
| C | -2.882446 | -3.662755 | -0.044746 |
| H | -3.830512 | -1.674194 | 0.483633 |
| H | -2.483090 | -4.621074 | -0.294258 |
| C | 0.684404 | -3.398451 | 0.472354 |
| C | 1.766931 | -3.581026 | -0.006350 |
| H | -0.286130 | -3.259702 | 0.896476 |
| H | 2.730215 | -3.774042 | -0.423215 |
| C | 2.300565 | 0.806934 | -1.980342 |
| C | 1.945637 | -0.349644 | -2.330812 |
| H | 2.704995 | 1.801930 | -2.046941 |
| H | 1.785761 | -1.197459 | -2.973746 |
| C | -1.310839 | -0.452527 | -3.473640 |
| C | -1.536326 | -1.294192 | -2.650412 |
| H | -1.125990 | 0.280566 | -4.227496 |
| H | -1.771784 | -2.047424 | -1.926992 |
| C | 0.532079 | 0.168565 | -0.300240 |
| C | 1.813963 | -0.094627 | -0.791833 |
| H | -0.199725 | 0.586025 | -0.989730 |
| H | 2.550157 | -0.522071 | -0.118905 |

DEC 16

1 2

| | | | |
|---|-----------|----------|-----------|
| C | -0.938110 | 2.179200 | 0.797943 |
| C | 0.139332 | 1.851158 | 0.388076 |
| H | -1.903646 | 2.472428 | 1.151596 |
| H | 1.103651 | 1.566729 | 0.028159 |
| C | 1.164724 | 3.060758 | -2.724310 |
| C | 1.233340 | 2.075190 | -3.401769 |
| H | 1.092252 | 3.936984 | -2.115423 |
| H | 1.281252 | 1.199952 | -4.008373 |
| C | 1.701725 | 3.246531 | 3.282604 |
| C | 2.608434 | 3.878340 | 3.745062 |
| H | 0.891661 | 2.692172 | 2.856465 |
| H | 3.412308 | 4.440372 | 4.162656 |
| C | 3.792990 | 1.910065 | -0.468124 |
| C | 3.868221 | 1.757255 | 0.717418 |
| H | 3.703927 | 2.053397 | -1.522407 |
| H | 3.925990 | 1.631730 | 1.775363 |
| C | -3.714576 | 1.717026 | -2.916402 |
| C | -2.617498 | 1.900702 | -2.472938 |
| H | -4.690500 | 1.546155 | -3.308507 |
| H | -1.641220 | 2.068354 | -2.071625 |
| C | -2.271483 | 1.813996 | 4.463212 |
| C | -1.922658 | 2.938948 | 4.247643 |
| H | -2.573861 | 0.810308 | 4.656632 |
| H | -1.611191 | 3.939128 | 4.036223 |
| C | 2.273707 | 5.188699 | 0.104189 |
| C | 1.767028 | 6.169697 | -0.360022 |
| H | 2.725756 | 4.310904 | 0.512669 |
| H | 1.306838 | 7.037733 | -0.774409 |
| C | -1.787835 | 6.075481 | 2.341815 |
| C | -0.602444 | 5.918317 | 2.418238 |
| H | -2.843846 | 6.201086 | 2.255635 |
| H | 0.453901 | 5.767705 | 2.472131 |
| C | -1.738164 | 5.225612 | -2.370492 |

| | | | |
|---|-----------|----------|-----------|
| C | -1.481074 | 5.320916 | -1.204432 |
| H | -1.966971 | 5.120788 | -3.406250 |
| H | -1.251803 | 5.396997 | -0.162862 |
| C | -4.195864 | 3.687710 | 0.483830 |
| C | -4.397928 | 3.523328 | 1.653149 |
| H | -3.995108 | 3.816612 | -0.557909 |
| H | -4.563570 | 3.362296 | 2.694460 |

DEC 17

1 2

| | | | |
|---|-----------|-----------|-----------|
| C | 1.590704 | 1.203729 | 1.532837 |
| C | 1.954112 | 0.844329 | 0.448452 |
| H | 1.287310 | 1.510965 | 2.511639 |
| H | 2.314645 | 0.530783 | -0.507941 |
| C | 0.393037 | 2.881545 | -2.567491 |
| C | -0.782179 | 3.246910 | -2.865664 |
| H | 1.464045 | 2.802464 | -2.667906 |
| H | -1.541899 | 3.752464 | -3.435895 |
| C | -0.367853 | 2.129201 | 4.438861 |
| C | 0.442821 | 2.938747 | 4.789783 |
| H | -1.075832 | 1.392881 | 4.123398 |
| H | 1.170559 | 3.644084 | 5.125525 |
| C | 3.921814 | 1.810027 | -2.517784 |
| C | 3.440463 | 0.929983 | -3.172576 |
| H | 4.363831 | 2.595239 | -1.944657 |
| H | 3.044114 | 0.141558 | -3.772909 |
| C | -0.906979 | 2.749547 | -0.355559 |
| C | -0.711286 | 2.256763 | -1.680442 |
| H | -1.335041 | 2.053567 | 0.366131 |
| H | -0.990467 | 1.221408 | -1.852025 |
| C | -4.142412 | 4.015394 | 3.229331 |
| C | -3.668916 | 3.466145 | 4.182617 |
| H | -4.595509 | 4.514462 | 2.401925 |
| H | -3.268187 | 2.985391 | 5.047591 |
| C | 2.932698 | 5.309160 | -0.887008 |
| C | 2.786460 | 4.348757 | -0.185711 |
| H | 3.083893 | 6.168085 | -1.502374 |
| H | 2.669711 | 3.483759 | 0.431987 |
| C | -0.612494 | 4.033522 | 0.093781 |
| C | -0.881855 | 4.352970 | 1.402269 |
| H | -0.158348 | 4.762875 | -0.567745 |
| H | -1.332770 | 3.604394 | 2.051223 |
| C | -2.792467 | 0.544381 | 2.098348 |
| C | -1.793105 | -0.075285 | 1.866563 |
| H | -3.689230 | 1.081438 | 2.318978 |
| H | -0.908129 | -0.638029 | 1.663585 |
| C | -0.958287 | 5.902131 | 3.228268 |
| C | -0.604414 | 5.641598 | 1.979786 |
| H | -1.456232 | 5.393190 | 4.044417 |
| H | -0.109105 | 6.392400 | 1.366959 |

DEC 18

1 2

| | | | |
|---|-----------|-----------|-----------|
| C | 1.101195 | -2.539866 | 0.384301 |
| C | -0.136675 | -2.756120 | 0.480297 |
| H | 2.166478 | -2.656343 | 0.524182 |
| H | -1.044532 | -3.247449 | 0.785785 |
| C | 0.271320 | -0.567753 | -4.172576 |
| C | 0.063300 | 0.523798 | -3.724337 |
| H | 0.455504 | -1.526208 | -4.605014 |
| H | -0.116437 | 1.506129 | -3.342735 |

| | | | |
|---|-----------|-----------|-----------|
| C | 0.111356 | 0.129690 | 1.456169 |
| C | 0.027557 | 1.421604 | 1.762623 |
| H | 0.197559 | -0.633253 | 2.224276 |
| H | -0.059640 | 2.358583 | 1.223928 |
| C | -3.173033 | -1.638734 | 1.720369 |
| C | -2.863204 | -2.033257 | 2.808589 |
| H | -3.465447 | -1.284063 | 0.755145 |
| H | -2.618208 | -2.394512 | 3.782963 |
| C | 4.721928 | -2.388990 | 0.656609 |
| C | 4.461165 | -2.563008 | 1.812552 |
| H | 4.979405 | -2.232126 | -0.367213 |
| H | 4.264319 | -2.728108 | 2.848222 |
| C | 0.684776 | 3.280298 | -1.281243 |
| C | -0.502085 | 3.430070 | -1.357276 |
| H | 1.744492 | 3.154888 | -1.226659 |
| H | -1.555591 | 3.578909 | -1.447075 |
| C | 2.957627 | 0.466525 | -1.529926 |
| C | 3.434838 | 0.626214 | -0.442228 |
| H | 2.538657 | 0.328696 | -2.503868 |
| H | 3.891145 | 0.760847 | 0.513502 |
| C | -2.994858 | 1.919242 | 2.723213 |
| C | -2.810411 | 3.076338 | 2.472671 |
| H | -3.175186 | 0.891265 | 2.953005 |
| H | -2.666888 | 4.116534 | 2.280489 |
| C | -2.838650 | 0.295906 | -1.738737 |
| C | -3.029655 | 0.944738 | -0.748986 |
| H | -2.681209 | -0.262537 | -2.635522 |
| H | -3.217804 | 1.523880 | 0.131250 |
| C | 0.203983 | -1.536309 | -0.427822 |
| C | 0.081807 | -0.232177 | 0.079925 |
| H | 0.146504 | -1.650335 | -1.504913 |
| H | -0.039519 | 0.577981 | -0.636528 |

DEC 19

1 2

| | | | |
|---|-----------|-----------|-----------|
| C | 0.304289 | 0.572754 | -0.941108 |
| C | -0.816923 | 1.408453 | -1.219894 |
| H | 0.349063 | -0.409064 | -0.476529 |
| H | -1.887110 | 1.292533 | -1.321659 |
| C | 4.247162 | -0.244111 | -1.106173 |
| C | 4.837809 | 0.738000 | -1.456564 |
| H | 3.737228 | -1.128206 | -0.786016 |
| H | 5.391319 | 1.594069 | -1.774082 |
| C | -1.856782 | -2.087527 | 0.045220 |
| C | -2.658955 | -1.636003 | -0.722765 |
| H | -1.148034 | -2.504868 | 0.727791 |
| H | -3.392781 | -1.240180 | -1.391882 |
| C | 1.263848 | 1.629384 | -0.921382 |
| C | 0.074016 | 2.351341 | -0.645724 |
| H | 2.318435 | 1.711381 | -0.708783 |
| H | -0.114087 | 3.161506 | 0.053431 |
| C | 1.353286 | -0.872285 | -3.309203 |
| C | 0.297738 | -1.401194 | -3.099645 |
| H | 2.299891 | -0.422666 | -3.517987 |
| H | -0.635759 | -1.890462 | -2.923683 |
| C | 3.685398 | 0.190948 | 3.640933 |
| C | 4.164438 | 0.270915 | 2.545824 |
| H | 3.284218 | 0.121169 | 4.627872 |
| H | 4.623215 | 0.335894 | 1.583215 |
| C | 1.663539 | -2.754052 | -0.023156 |
| C | 1.900148 | -2.176119 | 1.000246 |
| H | 1.464866 | -3.284906 | -0.928027 |

| | | | |
|---|-----------|-----------|-----------|
| H | 2.139751 | -1.680812 | 1.917087 |
| C | -4.490647 | 1.358342 | -1.332551 |
| C | -4.260150 | 1.444495 | -2.505463 |
| H | -4.713783 | 1.275850 | -0.289277 |
| H | -4.089701 | 1.532170 | -3.555552 |
| C | 0.407969 | 0.971264 | 2.420266 |
| C | -0.773421 | 0.797944 | 2.308822 |
| H | 1.460940 | 1.106230 | 2.556309 |
| H | -1.831832 | 0.645938 | 2.244378 |
| C | -4.484424 | 1.108914 | 2.486574 |
| C | -4.387586 | -0.014684 | 2.082738 |
| H | -4.590124 | 2.100099 | 2.868294 |
| H | -4.310680 | -1.020732 | 1.733742 |

DEC 20

1 2

| | | | |
|---|-----------|-----------|-----------|
| C | 0.976421 | 1.724873 | 1.123014 |
| C | 1.379431 | 2.158112 | 2.412161 |
| H | 1.128896 | 0.853432 | 0.505026 |
| H | 2.104920 | 1.742977 | 3.105590 |
| C | -0.629632 | 4.132568 | -4.688393 |
| C | -0.999645 | 3.048093 | -4.339831 |
| H | -0.311744 | 5.100676 | -5.006588 |
| H | -1.349150 | 2.080982 | -4.055912 |
| C | 0.951901 | 3.137894 | 0.910172 |
| C | 0.849720 | 3.468629 | 2.295720 |
| H | 1.329846 | 3.725913 | 0.076998 |
| H | 0.855147 | 4.379490 | 2.871619 |
| C | 4.517300 | 2.497271 | 1.283531 |
| C | 4.596405 | 3.371297 | 2.099717 |
| H | 4.467347 | 1.708350 | 0.562080 |
| H | 4.712275 | 4.135053 | 2.836590 |
| C | -2.054994 | 1.166185 | 3.047437 |
| C | -2.058491 | 2.213677 | 3.628203 |
| H | -2.083832 | 0.220764 | 2.553052 |
| H | -2.095999 | 3.133252 | 4.168841 |
| C | 3.180562 | 0.325458 | -1.347520 |
| C | 3.293449 | -0.639865 | -0.646782 |
| H | 3.098513 | 1.181340 | -1.982517 |
| H | 3.409165 | -1.519321 | -0.052942 |
| C | -1.699058 | 3.498671 | 0.129276 |
| C | -1.206009 | 4.058467 | -0.811631 |
| H | -2.162279 | 3.003655 | 0.956933 |
| H | -0.807001 | 4.573226 | -1.661733 |
| C | 2.201926 | 3.791215 | -2.470515 |
| C | 3.138364 | 4.057413 | -1.770254 |
| H | 1.376941 | 3.570073 | -3.118584 |
| H | 3.983414 | 4.298411 | -1.162988 |
| C | -0.717516 | 7.146252 | -2.659008 |
| C | 0.464347 | 6.991662 | -2.541442 |
| H | -1.767695 | 7.297883 | -2.774125 |
| H | 1.519001 | 6.865548 | -2.437245 |
| C | 1.210408 | 6.601515 | 0.794811 |
| C | 2.353776 | 6.471581 | 1.127943 |
| H | 0.199825 | 6.742691 | 0.478680 |
| H | 3.378384 | 6.398068 | 1.415374 |

EICO 1

1 2

| | | | |
|---|----------|----------|-----------|
| C | 4.391113 | 5.326055 | 10.246044 |
|---|----------|----------|-----------|

| | | | |
|---|----------|-----------|-----------|
| C | 5.531264 | 5.670584 | 10.385625 |
| H | 3.370684 | 5.020604 | 10.142717 |
| H | 6.552096 | 5.956146 | 10.524836 |
| C | 2.282537 | 9.658657 | 10.508928 |
| C | 3.118761 | 8.814731 | 10.661735 |
| H | 1.539687 | 10.416465 | 10.398312 |
| H | 3.861854 | 8.061492 | 10.813984 |
| C | 9.409128 | 6.587980 | 10.081143 |
| C | 9.005294 | 5.541360 | 9.660222 |
| H | 9.786230 | 7.508565 | 10.466582 |
| H | 8.643253 | 4.600645 | 9.301976 |
| C | 8.018680 | 1.994943 | 8.708727 |
| C | 6.951449 | 2.389837 | 9.084073 |
| H | 8.967666 | 1.625526 | 8.389279 |
| H | 5.998356 | 2.721925 | 9.438335 |
| C | 0.750191 | 4.504979 | 9.765383 |
| C | 0.871613 | 5.696221 | 9.721682 |
| H | 0.642307 | 3.444441 | 9.821773 |
| H | 0.982421 | 6.758381 | 9.701192 |
| C | 6.718708 | 8.551038 | 8.597122 |
| C | 6.008050 | 9.517082 | 8.603985 |
| H | 7.357784 | 7.693150 | 8.614348 |
| H | 5.376878 | 10.378633 | 8.632585 |
| C | 3.047046 | 3.492477 | 2.190247 |
| C | 4.194034 | 3.839192 | 2.187166 |
| H | 2.027920 | 3.174628 | 2.184438 |
| H | 5.218029 | 4.146701 | 2.167235 |
| C | 6.512785 | 1.828135 | 4.042106 |
| C | 6.765541 | 2.095396 | 5.182668 |
| H | 6.293509 | 1.564851 | 3.031463 |
| H | 6.989880 | 2.308943 | 6.206712 |
| C | 4.175039 | 8.241293 | 0.833838 |
| C | 3.705490 | 7.153803 | 1.019544 |
| H | 4.585657 | 9.207907 | 0.641990 |
| H | 3.296104 | 6.177252 | 1.176177 |
| C | 3.267477 | 1.720478 | 9.450078 |
| C | 3.370311 | 1.957795 | 10.619319 |
| H | 3.177579 | 1.505602 | 8.408912 |
| H | 3.463570 | 2.156137 | 11.663530 |
| C | 2.227904 | 7.457026 | 6.814134 |
| C | 3.182377 | 7.326021 | 7.527764 |
| H | 1.366147 | 7.544502 | 6.188040 |
| H | 4.017567 | 7.203592 | 8.186188 |
| C | 8.281084 | 9.185722 | 5.438159 |
| C | 8.319299 | 8.453345 | 4.489878 |
| H | 8.259588 | 9.833927 | 6.286614 |
| H | 8.369176 | 7.793310 | 3.650527 |
| C | 3.119675 | 10.958924 | 7.093245 |
| C | 3.427919 | 12.004419 | 6.594808 |
| H | 2.846343 | 10.031549 | 7.551399 |
| H | 3.688201 | 12.947632 | 6.167985 |
| C | 7.483833 | 5.694291 | 6.572071 |
| C | 6.436161 | 5.210694 | 6.897358 |
| H | 8.420409 | 6.132912 | 6.305076 |
| H | 5.506663 | 4.767307 | 7.187948 |
| C | 5.011165 | 6.975802 | 4.382151 |
| C | 4.004819 | 7.887724 | 3.962071 |
| H | 5.111328 | 5.907732 | 4.481752 |
| H | 2.940445 | 7.733196 | 3.800374 |
| C | 1.554030 | 10.000863 | 2.613492 |
| C | 1.504904 | 10.423358 | 3.733479 |
| H | 1.590698 | 9.633332 | 1.611944 |
| H | 1.462701 | 10.821857 | 4.723824 |

| | | | |
|---|-----------|-----------|----------|
| C | 3.491269 | 3.349056 | 5.905742 |
| C | 2.826703 | 3.917870 | 6.727042 |
| H | 4.092357 | 2.832674 | 5.186838 |
| H | 2.227563 | 4.415912 | 7.461378 |
| C | 7.572153 | 5.133312 | 2.849937 |
| C | 7.256678 | 5.862716 | 1.952380 |
| H | 7.838740 | 4.460790 | 3.637704 |
| H | 6.977333 | 6.496814 | 1.139702 |
| C | 0.532409 | 6.601576 | 3.437547 |
| C | 1.172805 | 5.764318 | 4.008597 |
| H | -0.055089 | 7.338585 | 2.936460 |
| H | 1.732721 | 5.015180 | 4.529562 |
| C | 4.722824 | 9.064947 | 4.308627 |
| C | 5.371603 | 8.117434 | 5.150930 |
| H | 4.509353 | 10.120615 | 4.342929 |
| H | 5.682343 | 8.196894 | 6.190899 |

EICO 2

1 2

| | | | |
|---|----------|-----------|-----------|
| C | 4.097708 | 5.526044 | 10.558401 |
| C | 5.128466 | 6.254277 | 10.579944 |
| H | 3.513609 | 4.620241 | 10.606098 |
| H | 6.171324 | 6.518969 | 10.655740 |
| C | 3.559532 | 7.476441 | 8.997945 |
| C | 3.801262 | 7.031571 | 10.313819 |
| H | 2.990136 | 8.396937 | 8.880819 |
| H | 3.377324 | 7.622288 | 11.119454 |
| C | 8.703017 | 7.118624 | 9.720121 |
| C | 8.361087 | 6.082483 | 9.224615 |
| H | 9.022922 | 8.036997 | 10.160295 |
| H | 8.059286 | 5.155802 | 8.785101 |
| C | 6.223424 | 3.874666 | 7.170562 |
| C | 5.855850 | 3.378837 | 8.198626 |
| H | 6.561969 | 4.289410 | 6.241887 |
| H | 5.525457 | 2.913098 | 9.100562 |
| C | 0.474518 | 5.911127 | 9.113283 |
| C | 0.339925 | 6.888460 | 8.433047 |
| H | 0.571615 | 5.027187 | 9.705054 |
| H | 0.204172 | 7.743717 | 7.805983 |
| C | 6.179629 | 9.374334 | 8.818597 |
| C | 5.700385 | 10.120605 | 9.624524 |
| H | 6.609301 | 8.714891 | 8.094352 |
| H | 5.282952 | 10.795669 | 10.338486 |
| C | 3.171474 | 3.438733 | 1.964627 |
| C | 4.339033 | 3.700316 | 2.029949 |
| H | 2.133279 | 3.202312 | 1.897813 |
| H | 5.379873 | 3.940929 | 2.084774 |
| C | 4.731017 | 0.880191 | 4.253957 |
| C | 5.164616 | 0.830440 | 5.369251 |
| H | 4.345929 | 0.930587 | 3.259691 |
| H | 5.553503 | 0.778251 | 6.360877 |
| C | 7.151302 | 6.346178 | 0.706606 |
| C | 5.963537 | 6.371715 | 0.553506 |
| H | 8.210754 | 6.333619 | 0.839520 |
| H | 4.905682 | 6.384666 | 0.414494 |
| C | 2.407479 | 2.759440 | 9.114274 |
| C | 2.284056 | 2.340734 | 10.230933 |
| H | 2.504488 | 3.115259 | 8.108267 |
| H | 2.160571 | 1.938035 | 11.211903 |
| C | 3.720823 | 7.424745 | 6.654665 |
| C | 4.006114 | 6.834900 | 7.813316 |
| H | 3.213316 | 8.322080 | 6.312188 |
| H | 4.561688 | 5.900471 | 7.854380 |

| | | | |
|---|-----------|-----------|-----------|
| C | 9.621459 | 7.848769 | 2.985327 |
| C | 10.383580 | 6.927748 | 2.910057 |
| H | 8.946850 | 8.675027 | 3.048955 |
| H | 11.071964 | 6.115472 | 2.842811 |
| C | 2.307856 | 10.850742 | 8.784022 |
| C | 1.497413 | 10.532732 | 9.607921 |
| H | 3.026073 | 11.137486 | 8.044120 |
| H | 0.769618 | 10.271699 | 10.344147 |
| C | 7.603756 | 7.504212 | 5.961931 |
| C | 6.638859 | 7.640177 | 5.262616 |
| H | 8.473084 | 7.375629 | 6.569409 |
| H | 5.801174 | 7.756131 | 4.605842 |
| C | 3.663868 | 8.162153 | 3.067214 |
| C | 3.454336 | 6.998444 | 3.268361 |
| H | 3.881347 | 9.191703 | 2.881556 |
| H | 3.277050 | 5.954873 | 3.422783 |
| C | 0.742306 | 8.896282 | 5.154556 |
| C | 0.424773 | 9.683855 | 6.000290 |
| H | 1.032688 | 8.214974 | 4.383805 |
| H | 0.138186 | 10.391720 | 6.746637 |
| C | 6.623812 | 10.706781 | 2.711658 |
| C | 6.583696 | 9.691214 | 2.077276 |
| H | 6.658112 | 11.622078 | 3.257908 |
| H | 6.548790 | 8.785912 | 1.507198 |
| C | 7.759852 | 4.525991 | 3.762334 |
| C | 7.417485 | 3.384656 | 3.893729 |
| H | 8.085666 | 5.536941 | 3.641399 |
| H | 7.102034 | 2.370606 | 4.011712 |
| C | 1.991151 | 4.575630 | 5.945527 |
| C | 2.893438 | 3.895567 | 5.543457 |
| H | 1.180109 | 5.161047 | 6.320320 |
| H | 3.680395 | 3.269030 | 5.177753 |
| C | 3.706402 | 11.035587 | 5.375528 |
| C | 4.791306 | 10.785197 | 5.818628 |
| H | 2.741064 | 11.255649 | 4.976130 |
| H | 5.764794 | 10.573496 | 6.202006 |

EICO 3

1 2

| | | | |
|---|----------|-----------|-----------|
| C | 4.383527 | 5.882568 | 9.918952 |
| C | 5.327195 | 6.621878 | 9.978605 |
| H | 3.571448 | 5.189677 | 9.859339 |
| H | 6.186791 | 7.257973 | 10.041424 |
| C | 1.765158 | 8.011988 | 8.723959 |
| C | 2.893248 | 8.388661 | 9.327193 |
| H | 1.085917 | 7.320596 | 9.217223 |
| H | 3.749396 | 9.028484 | 9.138029 |
| C | 8.597239 | 8.604923 | 9.811378 |
| C | 8.629174 | 7.522248 | 9.298927 |
| H | 8.582011 | 9.569302 | 10.266491 |
| H | 8.649805 | 6.555745 | 8.840384 |
| C | 8.887068 | 4.285849 | 7.601867 |
| C | 7.853985 | 3.802448 | 7.969526 |
| H | 9.802205 | 4.731247 | 7.275097 |
| H | 6.934162 | 3.357227 | 8.282987 |
| C | 0.966623 | 4.067459 | 9.157673 |
| C | 1.336950 | 4.469397 | 8.090616 |
| H | 0.646727 | 3.688656 | 10.103467 |
| H | 1.676258 | 4.808341 | 7.134022 |
| C | 5.847404 | 9.803785 | 7.895216 |
| C | 5.428614 | 10.826976 | 8.358754 |
| H | 6.253154 | 8.904211 | 7.478753 |
| H | 5.086907 | 11.751823 | 8.767558 |

| | | | |
|---|-----------|-----------|-----------|
| C | -0.140639 | 4.928531 | 4.729762 |
| C | 0.678922 | 4.224424 | 4.212243 |
| H | -0.886663 | 5.538097 | 5.191104 |
| H | 1.391872 | 3.578389 | 3.749297 |
| C | 1.814344 | 1.502528 | 6.091804 |
| C | 2.779963 | 0.962561 | 5.632490 |
| H | 0.945201 | 1.967334 | 6.500839 |
| H | 3.637740 | 0.473863 | 5.226302 |
| C | 6.466517 | 7.045747 | 2.035667 |
| C | 6.032334 | 6.019858 | 2.476157 |
| H | 6.855771 | 7.957527 | 1.641076 |
| H | 5.670157 | 5.096912 | 2.875885 |
| C | 4.308530 | 2.244071 | 8.899842 |
| C | 4.920135 | 2.533197 | 9.888469 |
| H | 3.758164 | 1.964786 | 8.026918 |
| H | 5.468304 | 2.784558 | 10.768673 |
| C | 3.411139 | 6.307129 | 5.377430 |
| C | 3.962736 | 6.230799 | 6.439806 |
| H | 2.935858 | 6.366136 | 4.419919 |
| H | 4.465146 | 6.143801 | 7.381578 |
| C | 11.543854 | 7.112723 | 7.300915 |
| C | 11.336512 | 6.686044 | 6.201236 |
| H | 11.731886 | 7.496472 | 8.278263 |
| H | 11.146295 | 6.294183 | 5.225841 |
| C | 2.087960 | 9.389242 | 6.616186 |
| C | 1.372215 | 8.522784 | 7.455778 |
| H | 3.102282 | 9.684675 | 6.868977 |
| H | 0.381208 | 8.224300 | 7.110750 |
| C | 7.994912 | 7.716060 | 5.906010 |
| C | 7.304456 | 6.743392 | 5.786331 |
| H | 8.638053 | 8.559889 | 6.025169 |
| H | 6.719040 | 5.855511 | 5.674703 |
| C | 2.687608 | 7.527293 | 2.101279 |
| C | 1.562249 | 7.125805 | 2.198832 |
| H | 3.698913 | 7.861919 | 2.012039 |
| H | 0.567303 | 6.744938 | 2.264602 |
| C | 1.203281 | 10.375457 | 5.775534 |
| C | 1.673603 | 9.413201 | 5.109376 |
| H | 0.702885 | 11.309047 | 5.961011 |
| H | 1.914242 | 8.828429 | 4.233968 |
| C | 6.441430 | 3.214655 | 4.861382 |
| C | 5.260748 | 3.274841 | 5.058142 |
| H | 7.496887 | 3.174412 | 4.694962 |
| H | 4.212090 | 3.309251 | 5.249944 |
| C | 9.401621 | 4.825647 | 3.546917 |
| C | 10.169026 | 3.967651 | 3.878345 |
| H | 8.711666 | 5.584707 | 3.247406 |
| H | 10.858809 | 3.204943 | 4.162735 |
| C | -1.630912 | 6.474319 | 7.602845 |
| C | -2.223572 | 7.370049 | 7.071629 |
| H | -1.113192 | 5.662091 | 8.067979 |
| H | -2.783614 | 8.153385 | 6.611210 |
| C | 4.584543 | 10.372627 | 3.807242 |
| C | 5.085336 | 9.389072 | 4.274490 |
| H | 4.159645 | 11.254586 | 3.383380 |
| H | 5.560811 | 8.517045 | 4.672795 |

EICO 4

1 2

| | | | |
|---|----------|----------|----------|
| C | 2.087491 | 2.675779 | 2.720306 |
| C | 2.909777 | 2.415285 | 1.887698 |
| H | 1.361672 | 2.896440 | 3.471350 |
| H | 3.663173 | 2.181486 | 1.163757 |

| | | | |
|---|-----------|-----------|-----------|
| C | 5.777396 | 2.233062 | -0.217792 |
| C | 5.831221 | 1.037237 | -0.169024 |
| H | 5.745546 | 3.301398 | -0.240768 |
| H | 5.914348 | -0.026914 | -0.128240 |
| C | -1.012693 | 2.648055 | 0.632446 |
| C | -2.059756 | 2.069498 | 0.722497 |
| H | -0.091034 | 3.184051 | 0.539333 |
| H | -3.006295 | 1.574362 | 0.786366 |
| C | 0.706910 | -4.466365 | 0.387615 |
| C | 1.777965 | -4.181767 | -0.069249 |
| H | -0.245515 | -4.732342 | 0.796517 |
| H | 2.747413 | -3.950649 | -0.454757 |
| C | -4.242276 | -1.157108 | 2.381113 |
| C | -3.893596 | -0.760828 | 3.457247 |
| H | -4.562932 | -1.524023 | 1.427960 |
| H | -3.592091 | -0.411048 | 4.419434 |
| C | -0.912447 | 1.136736 | 4.010865 |
| C | -0.203698 | 0.300248 | 4.493908 |
| H | -1.538829 | 1.882840 | 3.574048 |
| H | 0.429007 | -0.441696 | 4.928233 |
| C | 4.747755 | 5.436380 | 1.267799 |
| C | 5.059275 | 5.985770 | 0.250218 |
| H | 4.471117 | 4.958430 | 2.181311 |
| H | 5.340670 | 6.495333 | -0.644294 |
| C | 2.822779 | -0.995683 | 2.983197 |
| C | 2.362411 | -2.066767 | 2.703193 |
| H | 3.217464 | -0.035855 | 3.237567 |
| H | 1.963964 | -3.023700 | 2.442951 |
| C | -5.128122 | 1.625686 | -1.124255 |
| C | -5.633773 | 1.226660 | -0.114185 |
| H | -4.689015 | 1.997499 | -2.024528 |
| H | -6.102099 | 0.880035 | 0.780289 |
| C | -2.611563 | 3.894923 | -2.453407 |
| C | -2.352682 | 3.427733 | -3.525788 |
| H | -2.842703 | 4.317150 | -1.500709 |
| H | -2.119709 | 3.026216 | -4.486870 |
| C | 0.225451 | -0.439791 | 0.693386 |
| C | 0.862155 | -0.556546 | -0.547063 |
| H | 0.673883 | 0.239375 | 1.417399 |
| H | 0.431692 | -1.194815 | -1.311990 |
| C | 1.906564 | 4.453936 | -1.041470 |
| C | 0.963897 | 4.234990 | -1.749475 |
| H | 2.742606 | 4.687716 | -0.416234 |
| H | 0.115318 | 4.055335 | -2.375512 |
| C | 1.422652 | 2.094211 | -4.390763 |
| C | 0.583373 | 1.247959 | -4.272699 |
| H | 2.167761 | 2.849411 | -4.504943 |
| H | -0.171189 | 0.498969 | -4.172946 |
| C | -2.140360 | 0.046082 | -2.388995 |
| C | -2.258520 | -0.973471 | -3.008716 |
| H | -2.034404 | 0.970166 | -1.860456 |
| H | -2.360364 | -1.885623 | -3.555062 |
| C | 2.410657 | -0.319288 | -0.556269 |
| C | 1.749570 | 0.657611 | -0.998859 |
| H | 3.267909 | -0.922694 | -0.307379 |
| H | 1.561617 | 1.617966 | -1.452706 |
| C | 5.113756 | -2.679020 | 0.378225 |
| C | 5.321501 | -2.679508 | -0.802063 |
| H | 4.934286 | -2.681863 | 1.431527 |
| H | 5.532214 | -2.691438 | -1.848721 |
| C | -1.279565 | -4.697897 | -2.440821 |
| C | -2.421843 | -4.398225 | -2.237308 |
| H | -0.267408 | -4.984635 | -2.618921 |

| | | | |
|---|-----------|-----------|-----------|
| H | -3.438155 | -4.124140 | -2.048123 |
| C | -2.866942 | -4.560011 | 1.993325 |
| C | -2.737340 | -5.442379 | 1.192933 |
| H | -3.006645 | -3.781314 | 2.711426 |
| H | -2.626906 | -6.232563 | 0.483531 |
| C | -5.211771 | -2.194012 | -1.032417 |
| C | -5.320879 | -3.208579 | -0.403807 |
| H | -5.130651 | -1.276900 | -1.574320 |
| H | -5.417527 | -4.109811 | 0.160357 |
| C | -0.961074 | -1.123218 | 1.105265 |
| C | -1.562700 | -2.032360 | 0.347483 |
| H | -1.369502 | -0.869020 | 2.081016 |
| H | -1.478195 | -2.551719 | -0.599621 |

EICO 5

1 2

| | | | |
|---|----------|-----------|-----------|
| C | 4.735817 | 3.868728 | 11.436110 |
| C | 5.782041 | 4.210202 | 10.962240 |
| H | 3.810483 | 3.554744 | 11.866213 |
| H | 6.711068 | 4.521198 | 10.535625 |
| C | 4.531175 | 8.585745 | 9.877637 |
| C | 4.869102 | 7.663723 | 10.565125 |
| H | 4.211919 | 9.413369 | 9.280404 |
| H | 5.156550 | 6.841495 | 11.184117 |
| C | 7.669655 | 6.291848 | 8.454926 |
| C | 7.640438 | 5.211739 | 7.935071 |
| H | 7.713605 | 7.262848 | 8.901009 |
| H | 7.614271 | 4.251415 | 7.467412 |
| C | 4.365004 | 4.675407 | 6.673847 |
| C | 4.273981 | 3.855773 | 7.717749 |
| H | 4.346087 | 4.309347 | 5.650779 |
| H | 4.300237 | 3.934408 | 8.798776 |
| C | 3.481750 | 1.639447 | 4.580774 |
| C | 2.864674 | 1.581638 | 5.607084 |
| H | 4.005670 | 1.697647 | 3.650994 |
| H | 2.310822 | 1.529187 | 6.520157 |
| C | 8.414296 | 9.881472 | 7.869262 |
| C | 7.682326 | 10.040172 | 8.804267 |
| H | 9.073605 | 9.747647 | 7.039944 |
| H | 7.048638 | 10.189055 | 9.650042 |
| C | 3.374728 | 3.643473 | 1.490085 |
| C | 4.557429 | 3.733141 | 1.659311 |
| H | 2.323786 | 3.556738 | 1.325678 |
| H | 5.613606 | 3.806193 | 1.799939 |
| C | 5.932132 | 1.358854 | 7.548541 |
| C | 6.643412 | 1.541126 | 8.496021 |
| H | 5.292600 | 1.173472 | 6.712045 |
| H | 7.271792 | 1.675755 | 9.347980 |
| C | 8.071558 | 6.278627 | 1.123086 |
| C | 6.942106 | 6.359611 | 0.732010 |
| H | 9.080383 | 6.201136 | 1.462768 |
| H | 5.935702 | 6.432205 | 0.383391 |
| C | 1.494767 | 2.916981 | 9.072020 |
| C | 2.146374 | 1.943156 | 9.322815 |
| H | 0.914531 | 3.788225 | 8.859095 |
| H | 2.722039 | 1.073394 | 9.551445 |
| C | 1.322933 | 6.514469 | 7.612221 |
| C | 1.648119 | 6.864689 | 8.711722 |
| H | 1.040301 | 6.193210 | 6.631267 |
| H | 1.945445 | 7.175133 | 9.689096 |
| C | 8.322278 | 8.360520 | 4.263941 |
| C | 8.560745 | 7.524661 | 5.089640 |
| H | 8.124472 | 9.103005 | 3.519218 |

| | | | |
|---|----------|-----------|----------|
| H | 8.768802 | 6.778685 | 5.825672 |
| C | 2.706034 | 11.363482 | 7.721660 |
| C | 2.046463 | 10.835004 | 8.569682 |
| H | 3.276540 | 11.858727 | 6.968121 |
| H | 1.448965 | 10.385652 | 9.330884 |
| C | 4.669889 | 7.024247 | 5.920150 |
| C | 4.517525 | 6.065389 | 6.926111 |
| H | 4.714609 | 6.701832 | 4.884572 |
| H | 4.507721 | 6.406970 | 7.959364 |
| C | 4.480129 | 8.345901 | 2.390612 |
| C | 3.847301 | 7.329379 | 2.453635 |
| H | 5.058396 | 9.241301 | 2.302338 |
| H | 3.291337 | 6.417267 | 2.503817 |
| C | 1.355597 | 9.393031 | 4.246190 |
| C | 0.675923 | 9.536502 | 5.222517 |
| H | 1.964325 | 9.258247 | 3.378003 |
| H | 0.068576 | 9.683822 | 6.087605 |
| C | 7.230579 | 11.089911 | 1.684151 |
| C | 7.413702 | 10.017696 | 1.182423 |
| H | 7.081763 | 12.059493 | 2.103308 |
| H | 7.578386 | 9.059318 | 0.738317 |
| C | 7.030613 | 4.556350 | 4.125516 |
| C | 7.085469 | 3.477672 | 4.644860 |
| H | 7.004987 | 5.509548 | 3.640809 |
| H | 7.153101 | 2.517148 | 5.106206 |
| C | 0.979090 | 5.837215 | 4.068546 |
| C | 1.483877 | 4.768814 | 4.270727 |
| H | 0.524854 | 6.788963 | 3.896829 |
| H | 1.917740 | 3.805389 | 4.439330 |
| C | 4.079804 | 8.448310 | 6.221630 |
| C | 5.334781 | 8.381517 | 6.318526 |
| H | 3.088368 | 8.870692 | 6.183634 |
| H | 6.348157 | 8.720975 | 6.452508 |

EICO 6

1 2

| | | | |
|---|-----------|-----------|-----------|
| C | 2.666329 | 4.942673 | -0.660032 |
| C | 3.482394 | 5.053090 | 0.210251 |
| H | 1.937893 | 4.857911 | -1.435766 |
| H | 4.215046 | 5.147775 | 0.981537 |
| C | 4.284071 | 0.212632 | -0.902971 |
| C | 4.096455 | 1.339739 | -0.539198 |
| H | 4.443935 | -0.788026 | -1.243588 |
| H | 3.943345 | 2.349374 | -0.220430 |
| C | 5.943139 | 3.016221 | 2.168414 |
| C | 4.933143 | 2.986831 | 2.811180 |
| H | 6.850753 | 3.044303 | 1.608164 |
| H | 4.034726 | 2.951290 | 3.386375 |
| C | 1.104315 | 1.908579 | 2.866657 |
| C | 1.309713 | 2.793868 | 2.084493 |
| H | 0.941501 | 1.109844 | 3.556932 |
| H | 1.528576 | 3.585314 | 1.397355 |
| C | -4.867398 | 2.159109 | -2.387463 |
| C | -4.000691 | 2.929207 | -2.691048 |
| H | -5.639505 | 1.469908 | -2.122727 |
| H | -3.233318 | 3.619669 | -2.964109 |
| C | 4.036039 | -0.378837 | 2.967396 |
| C | 3.416888 | -0.968795 | 3.806835 |
| H | 4.592468 | 0.165016 | 2.233834 |
| H | 2.882890 | -1.486733 | 4.572189 |
| C | -5.305848 | -1.368150 | -1.472643 |
| C | -5.525237 | -0.970698 | -0.363698 |
| H | -5.109221 | -1.715520 | -2.462883 |

| | | | |
|---|-----------|-----------|-----------|
| H | -5.712098 | -0.622882 | 0.629274 |
| C | -3.220111 | 3.419581 | 1.001840 |
| C | -2.390045 | 3.521923 | 1.860463 |
| H | -3.956286 | 3.343729 | 0.229878 |
| H | -1.650663 | 3.622844 | 2.625003 |
| C | -4.164503 | 0.378726 | 2.960041 |
| C | -4.374571 | -0.781090 | 3.176419 |
| H | -3.985283 | 1.415137 | 2.769620 |
| H | -4.563642 | -1.814257 | 3.368103 |
| C | -0.164483 | 3.175284 | -2.508068 |
| C | -0.646580 | 3.579794 | -1.487600 |
| H | 0.274341 | 2.804576 | -3.408935 |
| H | -1.091014 | 3.937437 | -0.583159 |
| C | 1.039866 | 0.163986 | -4.133575 |
| C | 2.071029 | 0.606816 | -3.712610 |
| H | 0.115431 | -0.225319 | -4.502641 |
| H | 2.990127 | 0.994180 | -3.328901 |
| C | 0.097221 | -2.081546 | 3.083843 |
| C | -0.810064 | -1.393085 | 3.458305 |
| H | 0.899558 | -2.705125 | 2.747911 |
| H | -1.637415 | -0.799846 | 3.784728 |
| C | 2.140947 | -4.286867 | 0.958744 |
| C | 3.055043 | -3.799937 | 1.561657 |
| H | 1.336147 | -4.725447 | 0.408974 |
| H | 3.866851 | -3.366853 | 2.104289 |
| C | -1.060000 | 0.440812 | 0.301178 |
| C | 0.514938 | 0.137219 | -0.380503 |
| H | -0.807815 | 1.161207 | 1.081798 |
| H | 0.672088 | 1.052219 | -0.956047 |
| C | -2.912898 | -3.962094 | 1.829497 |
| C | -3.816082 | -3.806902 | 1.057046 |
| H | -2.119654 | -4.098166 | 2.531288 |
| H | -4.626960 | -3.660826 | 0.376810 |
| C | -0.942781 | -4.370308 | -1.371574 |
| C | -0.040392 | -4.461336 | -2.155802 |
| H | -1.750107 | -4.313896 | -0.671425 |
| H | 0.771509 | -4.550368 | -2.845114 |
| C | -2.048435 | -0.598339 | 0.280714 |
| C | -2.185681 | 0.389486 | -0.582018 |
| H | -2.419942 | -1.510338 | 0.723313 |
| H | -2.750885 | 0.876729 | -1.361200 |
| C | -2.190063 | -1.545637 | -3.601188 |
| C | -2.685530 | -0.525152 | -3.987561 |
| H | -1.755778 | -2.462589 | -3.263096 |
| H | -3.140739 | 0.380398 | -4.325427 |
| C | 0.908310 | -1.210327 | -0.665782 |
| C | 1.427444 | -0.634451 | 0.403197 |
| H | 0.853291 | -2.060798 | -1.325609 |
| H | 2.093636 | -0.662223 | 1.251885 |
| C | 3.531151 | -3.417355 | -2.191265 |
| C | 3.240513 | -2.715987 | -3.118425 |
| H | 3.793113 | -4.041304 | -1.365424 |
| H | 2.988574 | -2.085959 | -3.942840 |

EICO 7

12

| | | | |
|---|-----------|-----------|-----------|
| C | -0.777027 | -0.966651 | 1.523574 |
| C | -1.306225 | 0.238294 | 0.980172 |
| H | -1.001414 | -2.000986 | 1.275560 |
| H | -2.155261 | 0.515645 | 0.375657 |
| C | -4.495740 | -0.679357 | -0.454264 |
| C | -4.625971 | 0.453774 | -0.824221 |
| H | -4.382899 | -1.695823 | -0.143274 |

| | | | |
|---|-----------|-----------|-----------|
| H | -4.765561 | 1.465304 | -1.144183 |
| C | 0.868897 | -1.700080 | -1.408556 |
| C | 1.732368 | -1.931825 | -0.608976 |
| H | 0.117520 | -1.501719 | -2.144427 |
| H | 2.522734 | -2.120393 | 0.086454 |
| C | -5.212217 | 4.210976 | -0.346138 |
| C | -5.142559 | 4.087095 | -1.535563 |
| H | -5.285350 | 4.338673 | 0.710910 |
| H | -5.093996 | 3.984054 | -2.597456 |
| C | 4.133931 | -0.757976 | 2.062635 |
| C | 3.918024 | -1.854067 | 2.497684 |
| H | 4.358480 | 0.208391 | 1.663221 |
| H | 3.738948 | -2.836732 | 2.874314 |
| C | 0.942258 | -3.545052 | 3.417780 |
| C | 0.687135 | -4.108633 | 2.391494 |
| H | 1.172151 | -3.041815 | 4.332484 |
| H | 0.459707 | -4.621085 | 1.482277 |
| C | -2.736296 | -3.940573 | 0.760821 |
| C | -2.327832 | -3.669781 | -0.333105 |
| H | -3.115568 | -4.195464 | 1.725430 |
| H | -1.989844 | -3.432685 | -1.320031 |
| C | -3.213284 | 2.492906 | 2.765237 |
| C | -4.177149 | 1.959185 | 2.293212 |
| H | -2.356033 | 2.970075 | 3.188666 |
| H | -5.034371 | 1.482185 | 1.870861 |
| C | 4.285370 | -1.308740 | -2.896301 |
| C | 5.162452 | -0.706413 | -2.344440 |
| H | 3.517538 | -1.858429 | -3.397963 |
| H | 5.947575 | -0.179469 | -1.846510 |
| C | 1.801688 | -3.590153 | -4.842725 |
| C | 1.575032 | -2.462327 | -5.176132 |
| H | 2.013748 | -4.597486 | -4.562744 |
| H | 1.376034 | -1.454136 | -5.467104 |
| C | 0.400311 | -0.381434 | 2.063133 |
| C | 0.069415 | 0.573903 | 1.060402 |
| H | 1.306093 | -0.734612 | 2.528978 |
| H | 0.717629 | 1.095713 | 0.360813 |
| C | -2.421003 | -1.500706 | -3.281614 |
| C | -1.707945 | -2.234852 | -3.906098 |
| H | -3.071359 | -0.850357 | -2.736145 |
| H | -1.063725 | -2.875374 | -4.469308 |
| C | 0.366521 | 0.950884 | -4.110743 |
| C | 1.552672 | 0.987922 | -3.942544 |
| H | -0.689593 | 0.913411 | -4.273337 |
| H | 2.612944 | 1.012417 | -3.814295 |
| C | 3.091890 | 1.517392 | -0.600615 |
| C | 2.934085 | 2.496071 | 0.074380 |
| H | 3.259736 | 0.642503 | -1.196449 |
| H | 2.804207 | 3.365410 | 0.680209 |
| C | -1.570047 | 3.276013 | -0.798171 |
| C | -0.520272 | 3.033497 | -1.324932 |
| H | -2.519167 | 3.506536 | -0.361212 |
| H | 0.406078 | 2.816220 | -1.813653 |
| C | -3.808374 | 1.567976 | -4.475438 |
| C | -3.081123 | 2.330667 | -3.905913 |
| H | -4.453444 | 0.894790 | -4.994809 |
| H | -2.429653 | 3.008346 | -3.399152 |
| C | 0.660518 | 2.832750 | 3.246718 |
| C | 0.295176 | 3.486919 | 2.310793 |
| H | 0.986539 | 2.254778 | 4.085419 |
| H | -0.028796 | 4.070419 | 1.476346 |
| C | 6.651251 | 1.635609 | 0.198196 |
| C | 7.079260 | 0.608955 | 0.641385 |

| | | | |
|---|-----------|-----------|-----------|
| H | 6.280492 | 2.553857 | -0.197726 |
| H | 7.469501 | -0.300865 | 1.039146 |
| C | 1.949837 | -0.272227 | 5.323230 |
| C | 0.761052 | -0.350340 | 5.453095 |
| H | 3.010227 | -0.206448 | 5.215126 |
| H | -0.297072 | -0.429200 | 5.577792 |
| C | -2.784750 | -1.130196 | 3.855629 |
| C | -2.251657 | -2.189881 | 4.029686 |
| H | -3.262405 | -0.184424 | 3.708291 |
| H | -1.780663 | -3.134326 | 4.192716 |

EICO 8

1 2

| | | | |
|---|-----------|-----------|-----------|
| C | 6.054438 | 1.544232 | -1.041290 |
| C | 5.947956 | 2.507498 | -0.335860 |
| H | 6.165576 | 0.688896 | -1.676334 |
| H | 5.858834 | 3.363529 | 0.296104 |
| C | 2.883289 | 4.658076 | 1.192244 |
| C | 3.322545 | 3.756337 | 1.848579 |
| H | 2.485324 | 5.465998 | 0.617223 |
| H | 3.700242 | 2.952586 | 2.441515 |
| C | 0.280311 | 5.535341 | -1.333926 |
| C | 1.318078 | 5.604810 | -1.929265 |
| H | -0.653264 | 5.478206 | -0.818718 |
| H | 2.225806 | 5.692967 | -2.486434 |
| C | 2.472396 | 2.226726 | -1.472118 |
| C | 2.969763 | 1.859745 | -2.568149 |
| H | 2.871185 | 2.690081 | -0.574166 |
| H | 3.215061 | 1.473156 | -3.543344 |
| C | -2.641135 | 3.166017 | -1.145355 |
| C | -2.242084 | 3.119964 | -0.015369 |
| H | -3.008755 | 3.188065 | -2.150379 |
| H | -1.890747 | 3.076871 | 0.994780 |
| C | -0.024829 | 2.687811 | 2.825410 |
| C | -0.913264 | 2.081306 | 3.354758 |
| H | 0.773372 | 3.238498 | 2.375260 |
| H | -1.697136 | 1.542172 | 3.847179 |
| C | 2.101503 | -1.481426 | -2.743333 |
| C | 2.326948 | -1.820754 | -1.616019 |
| H | 1.923687 | -1.185104 | -3.755057 |
| H | 2.531379 | -2.147773 | -0.617975 |
| C | 2.899841 | -3.519503 | 1.697571 |
| C | 2.591725 | -4.357612 | 0.899382 |
| H | 3.178215 | -2.782625 | 2.417745 |
| H | 2.331064 | -5.117301 | 0.196577 |
| C | 0.852961 | 2.056683 | -1.386791 |
| C | 0.496063 | 0.978404 | -0.860614 |
| H | 0.339032 | 2.927644 | -1.781616 |
| H | 0.287070 | 0.028677 | -0.396511 |
| C | -1.181756 | -1.005897 | 1.516218 |
| C | -0.381302 | -1.875330 | 1.315422 |
| H | -1.917034 | -0.253192 | 1.701130 |
| H | 0.333260 | -2.657446 | 1.167556 |
| C | 2.325581 | 0.216842 | 1.830362 |
| C | 3.357717 | 0.255928 | 1.220835 |
| H | 1.407387 | 0.184034 | 2.377583 |
| H | 4.283993 | 0.313521 | 0.690765 |
| C | 5.728181 | -1.401981 | -3.317263 |
| C | 6.597597 | -0.773742 | -3.851491 |
| H | 4.947545 | -1.964662 | -2.854041 |
| H | 7.380795 | -0.224078 | -4.325101 |
| C | -2.304730 | -0.289185 | -1.904182 |

| | | | |
|---|-----------|-----------|-----------|
| C | -1.642353 | -0.841240 | -2.736871 |
| H | -2.913297 | 0.180592 | -1.160208 |
| H | -1.070128 | -1.361111 | -3.472201 |
| C | 3.563456 | 5.696430 | -5.007790 |
| C | 2.668628 | 6.489300 | -5.084034 |
| H | 4.371107 | 4.998104 | -4.956706 |
| H | 1.883820 | 7.208537 | -5.157246 |
| C | -4.047562 | 1.806688 | -4.297152 |
| C | -3.790313 | 2.888392 | -4.742172 |
| H | -4.282332 | 0.840490 | -3.909695 |
| H | -3.569012 | 3.846002 | -5.157694 |
| C | 3.421288 | -0.043306 | -5.780783 |
| C | 2.417255 | 0.564630 | -6.026333 |
| H | 4.321209 | -0.580366 | -5.566797 |
| H | 1.524755 | 1.108859 | -6.246721 |
| C | -4.799627 | 0.828533 | 0.849626 |
| C | -4.698999 | -0.359809 | 0.964131 |
| H | -4.897060 | 1.885582 | 0.737146 |
| H | -4.623839 | -1.419340 | 1.071719 |
| C | 6.015975 | 2.951499 | -4.231918 |
| C | 5.567199 | 2.630494 | -5.295554 |
| H | 6.426290 | 3.234457 | -3.287659 |
| H | 5.176800 | 2.347455 | -6.247964 |
| C | -3.818913 | 0.056522 | 4.532799 |
| C | -2.973534 | -0.297349 | 5.303880 |
| H | -4.581956 | 0.359439 | 3.849733 |
| H | -2.235673 | -0.617009 | 6.005905 |
| C | -0.275798 | 2.528394 | -4.469582 |
| C | 0.585718 | 3.329893 | -4.701453 |
| H | -1.069521 | 1.839821 | -4.270588 |
| H | 1.343989 | 4.053655 | -4.919507 |

EICO 9

1 2

| | | | |
|---|-----------|-----------|-----------|
| C | -2.687351 | -1.477175 | 1.187204 |
| C | -3.201214 | -0.420696 | 0.950312 |
| H | -2.229995 | -2.419566 | 1.403880 |
| H | -3.673890 | 0.519051 | 0.771442 |
| C | 0.327557 | 4.346748 | -2.849752 |
| C | 0.783381 | 4.647702 | -1.782693 |
| H | -0.074893 | 4.082640 | -3.803394 |
| H | 1.183826 | 4.930433 | -0.830892 |
| C | -4.827586 | -3.789577 | 0.020583 |
| C | -4.450270 | -4.605499 | -0.771678 |
| H | -5.168528 | -3.075536 | 0.739696 |
| H | -4.139464 | -5.339941 | -1.480551 |
| C | -2.103862 | 4.990183 | 0.441264 |
| C | -2.204360 | 4.248139 | 1.377423 |
| H | -2.017999 | 5.657073 | -0.388173 |
| H | -2.305634 | 3.591365 | 2.215632 |
| C | -0.076716 | 0.996175 | -1.594622 |
| C | 0.241450 | 0.006580 | -0.661457 |
| H | 0.701175 | 1.441701 | -2.206763 |
| H | -0.588340 | -0.406204 | -0.089980 |
| C | -0.682075 | -2.443770 | -2.655221 |
| C | -1.729890 | -2.541204 | -2.078944 |
| H | 0.256903 | -2.363692 | -3.163786 |
| H | -2.665269 | -2.643852 | -1.567602 |
| C | 0.454290 | 1.965540 | 2.068376 |
| C | -0.269700 | 1.049682 | 2.341997 |
| H | 1.094204 | 2.794773 | 1.851609 |
| H | -0.913189 | 0.235284 | 2.598858 |

| | | | |
|---|-----------|-----------|-----------|
| C | 2.537375 | 5.251055 | 1.544028 |
| C | 1.374406 | 5.452076 | 1.749119 |
| H | 3.580726 | 5.097694 | 1.381127 |
| H | 0.337915 | 5.632227 | 1.935118 |
| C | 0.166736 | -3.709470 | 0.724280 |
| C | 0.271628 | -3.459121 | 1.891618 |
| H | 0.053130 | -3.934284 | -0.313479 |
| H | 0.337321 | -3.248483 | 2.936890 |
| C | -1.540265 | 1.001932 | -2.142312 |
| C | -1.335597 | 1.870709 | -1.252849 |
| H | -2.067662 | 0.456582 | -2.908543 |
| H | -1.515876 | 2.705360 | -0.592832 |
| C | 2.458911 | -1.507382 | -4.338218 |
| C | 2.972401 | -2.144854 | -3.462153 |
| H | 1.996602 | -0.949193 | -5.123326 |
| H | 3.431564 | -2.715212 | -2.682267 |
| C | 2.621511 | -0.105946 | -1.044808 |
| C | 1.546135 | -0.520231 | -0.389926 |
| H | 2.923023 | 0.594386 | -1.816183 |
| H | 1.628664 | -1.292050 | 0.371730 |
| C | -3.687960 | 1.512731 | 3.872217 |
| C | -4.504940 | 2.268228 | 3.427945 |
| H | -2.975217 | 0.831869 | 4.286816 |
| H | -5.236555 | 2.949615 | 3.054716 |
| C | 0.723675 | 1.535657 | -5.161154 |
| C | -0.364379 | 1.108644 | -5.426777 |
| H | 1.700917 | 1.908154 | -4.938096 |
| H | -1.332398 | 0.729295 | -5.675374 |
| C | 4.739104 | -2.686267 | -0.205569 |
| C | 3.811066 | -3.347358 | 0.163527 |
| H | 5.585084 | -2.116383 | -0.517854 |
| H | 2.991233 | -3.935507 | 0.513636 |
| C | 4.194044 | 1.718882 | -3.756886 |
| C | 3.636488 | 2.688130 | -3.325674 |
| H | 4.699412 | 0.862449 | -4.146240 |
| H | 3.136680 | 3.559413 | -2.960389 |
| C | -0.951395 | -1.185179 | 4.985643 |
| C | -1.940390 | -1.726163 | 4.577439 |
| H | -0.077125 | -0.704516 | 5.364687 |
| H | -2.832191 | -2.207637 | 4.231913 |
| C | -2.475967 | -5.193935 | 3.939562 |
| C | -2.886692 | -5.181321 | 2.814786 |
| H | -2.112314 | -5.216689 | 4.942342 |
| H | -3.262335 | -5.179141 | 1.814478 |
| C | -5.502779 | -2.964157 | 3.644078 |
| C | -5.474121 | -1.773305 | 3.517662 |
| H | -5.527193 | -4.023802 | 3.766876 |
| H | -5.447916 | -0.710111 | 3.422830 |
| C | -3.424209 | -0.890186 | -4.768370 |
| C | -3.981778 | 0.162233 | -4.896687 |
| H | -2.938104 | -1.833636 | -4.651708 |
| H | -4.498563 | 1.086572 | -5.028596 |

EICO 10

1 2

| | | | |
|---|-----------|----------|-----------|
| C | -3.142912 | 3.168362 | 0.485010 |
| C | -2.606800 | 3.383133 | -0.566302 |
| H | -3.639967 | 2.983453 | 1.414932 |
| H | -2.131668 | 3.596822 | -1.502230 |
| C | 2.074852 | 1.456009 | -2.073546 |
| C | 1.621941 | 1.932028 | -1.071561 |
| H | 2.499150 | 1.039081 | -2.959378 |
| H | 1.241567 | 2.361255 | -0.168881 |

| | | | |
|---|------------|-----------|-----------|
| C | -1.891706 | -1.521363 | -1.480535 |
| C | -2.739113 | -0.535231 | -1.066621 |
| H | -2.266938 | -2.542167 | -1.526848 |
| H | -2.416351 | 0.499276 | -1.001444 |
| C | -5.048086 | 0.024156 | -0.311556 |
| C | -4.057117 | -0.880614 | -0.732598 |
| H | -4.791523 | 1.077158 | -0.235280 |
| H | -4.337781 | -1.930064 | -0.799670 |
| C | -8.168348 | -3.549384 | 0.143899 |
| C | -7.324448 | -4.380896 | 0.323928 |
| H | -8.923683 | -2.807201 | -0.005659 |
| H | -6.573954 | -5.124508 | 0.476373 |
| C | -7.703043 | 2.657853 | -0.529153 |
| C | -6.688314 | 3.202172 | -0.861572 |
| H | -8.605059 | 2.164933 | -0.234807 |
| H | -5.782099 | 3.688034 | -1.151488 |
| C | -8.621604 | 0.988453 | -3.497859 |
| C | -8.413375 | -0.143114 | -3.832856 |
| H | -8.805502 | 2.000867 | -3.212588 |
| H | -8.222736 | -1.146454 | -4.144511 |
| C | -4.881751 | 1.373055 | -3.609477 |
| C | -3.710149 | 1.577702 | -3.755956 |
| H | -5.930228 | 1.192858 | -3.503443 |
| H | -2.674228 | 1.792319 | -3.904161 |
| C | 0.868902 | 3.349782 | 2.443593 |
| C | 0.111678 | 4.102131 | 1.900181 |
| H | 1.545168 | 2.683952 | 2.931751 |
| H | -0.558838 | 4.778479 | 1.419120 |
| C | -5.995999 | -2.845218 | -2.876964 |
| C | -5.369069 | -2.169543 | -3.643446 |
| H | -6.556917 | -3.435900 | -2.183207 |
| H | -4.819814 | -1.559276 | -4.326770 |
| C | -7.652966 | -1.024754 | 3.955613 |
| C | -7.984253 | -2.064464 | 3.460017 |
| H | -7.357495 | -0.099839 | 4.400788 |
| H | -8.282289 | -2.991354 | 3.020337 |
| C | -10.208370 | -0.265343 | -0.422161 |
| C | -9.843094 | -0.306469 | 0.718393 |
| H | -10.540589 | -0.224893 | -1.436081 |
| H | -9.527974 | -0.356754 | 1.738489 |
| C | -0.513852 | -1.296160 | -1.861656 |
| C | 0.238491 | -2.292544 | -2.289642 |
| H | -0.108755 | -0.288401 | -1.777728 |
| H | 0.150169 | -3.356617 | -2.470742 |
| C | -3.772035 | -4.872622 | -0.937341 |
| C | -3.566624 | -4.439517 | 0.161027 |
| H | -3.957030 | -5.269834 | -1.910679 |
| H | -3.391116 | -4.049759 | 1.141269 |
| C | -6.171398 | -0.554063 | 0.601169 |
| C | -6.530110 | -0.357486 | -0.593050 |
| H | -6.271726 | -0.800373 | 1.644067 |
| H | -7.198134 | -0.284244 | -1.435114 |
| C | -5.860081 | 2.128300 | 2.667907 |
| C | -4.994111 | 1.613066 | 3.317783 |
| H | -6.616455 | 2.598187 | 2.077317 |
| H | -4.209679 | 1.175120 | 3.899229 |
| C | -4.193567 | -2.157749 | 3.107478 |
| C | -3.161976 | -1.705220 | 2.696669 |
| H | -5.115812 | -2.540497 | 3.487845 |
| H | -2.233223 | -1.296092 | 2.355551 |
| C | -0.470628 | 0.393432 | 1.442857 |
| C | 0.254769 | -0.559594 | 1.422809 |
| H | -1.092771 | 1.261614 | 1.464499 |

| | | | |
|---|-----------|-----------|-----------|
| H | 0.914659 | -1.397970 | 1.409197 |
| C | -0.464455 | 3.787860 | -3.529181 |
| C | -1.416488 | 4.302969 | -4.042494 |
| H | 0.392498 | 3.340591 | -3.071790 |
| H | -2.252759 | 4.771326 | -4.511721 |
| C | -1.860750 | 0.552676 | 5.102533 |
| C | -1.574580 | 1.627824 | 4.659443 |
| H | -2.106543 | -0.404036 | 5.505874 |
| H | -1.299365 | 2.585864 | 4.275562 |

EICO 11

1 2

| | | | |
|---|-----------|-----------|-----------|
| C | -2.294194 | 3.237806 | -3.505799 |
| C | -1.626432 | 4.028147 | -2.900106 |
| H | -2.882130 | 2.527964 | -4.049287 |
| H | -1.016702 | 4.727397 | -2.371951 |
| C | 1.054697 | 3.197221 | -0.268344 |
| C | 0.396807 | 3.982421 | 0.353791 |
| H | 1.647611 | 2.505523 | -0.825404 |
| H | -0.173435 | 4.702437 | 0.901306 |
| C | -2.688242 | -2.650807 | -0.197451 |
| C | -1.873912 | -2.032105 | 0.427429 |
| H | -3.395524 | -3.201741 | -0.779526 |
| H | -1.143111 | -1.483933 | 0.982737 |
| C | -4.840063 | 0.915496 | -1.884465 |
| C | -3.836919 | 0.275833 | -2.039620 |
| H | -5.742068 | 1.475047 | -1.744425 |
| H | -2.931620 | -0.276756 | -2.177375 |
| C | -6.724360 | -1.589490 | -0.379962 |
| C | -7.703187 | -1.813821 | 0.273699 |
| H | -5.859722 | -1.387920 | -0.975165 |
| H | -8.576663 | -2.016518 | 0.852150 |
| C | -8.198209 | 2.667040 | -1.404163 |
| C | -8.397913 | 1.505587 | -1.624232 |
| H | -8.023110 | 3.705043 | -1.226096 |
| H | -8.574308 | 0.473003 | -1.833640 |
| C | -6.039090 | 3.184556 | -4.484133 |
| C | -5.300287 | 3.876811 | -5.124173 |
| H | -6.710621 | 2.568780 | -3.926877 |
| H | -4.648494 | 4.493659 | -5.701494 |
| C | -3.589356 | 0.112985 | -5.406188 |
| C | -2.408695 | -0.080993 | -5.340507 |
| H | -4.642196 | 0.289242 | -5.466498 |
| H | -1.355569 | -0.246742 | -5.292663 |
| C | -2.676407 | 2.524835 | 1.675887 |
| C | -2.639599 | 2.647923 | 0.352816 |
| H | -2.185125 | 3.263188 | 2.305465 |
| H | -2.988242 | 2.165708 | -0.553930 |
| C | -7.786959 | 0.096283 | -4.935460 |
| C | -7.113363 | -0.693851 | -4.337949 |
| H | -8.391401 | 0.789406 | -5.476807 |
| H | -6.515173 | -1.418122 | -3.827762 |
| C | -1.252388 | 2.926910 | 4.947837 |
| C | -2.278615 | 3.298624 | 5.441729 |
| H | -0.334625 | 2.583202 | 4.523706 |
| H | -3.182863 | 3.629668 | 5.902044 |
| C | -0.297407 | 0.637347 | -2.177037 |
| C | 0.061632 | -0.464348 | -1.870117 |
| H | -0.619386 | 1.616487 | -2.466677 |
| H | 0.381267 | -1.448038 | -1.607444 |
| C | -4.420942 | -2.995533 | -3.453100 |
| C | -5.219017 | -3.651841 | -2.846409 |
| H | -3.725189 | -2.412259 | -4.018097 |

| | | | |
|---|-----------|-----------|-----------|
| H | -5.935518 | -4.242826 | -2.320552 |
| C | -4.176480 | -0.901837 | 2.582499 |
| C | -5.242044 | -0.230535 | 2.539562 |
| H | -3.535729 | -1.744491 | 2.769672 |
| H | -6.291127 | -0.007185 | 2.655627 |
| C | 0.032593 | 0.594376 | 2.276503 |
| C | -0.157851 | -0.132591 | 3.210289 |
| H | 0.215371 | 1.252900 | 1.452853 |
| H | -0.293740 | -0.779175 | 4.048805 |
| C | -4.953223 | 4.494016 | -1.247735 |
| C | -5.321527 | 4.428128 | -0.108086 |
| H | -4.637285 | 4.538912 | -2.268758 |
| H | -5.652041 | 4.374551 | 0.907443 |
| C | -2.485753 | 6.058939 | 1.668141 |
| C | -1.840982 | 6.087386 | 2.678028 |
| H | -3.067988 | 6.038064 | 0.771565 |
| H | -1.268569 | 6.127351 | 3.578645 |
| C | -8.783725 | 0.764770 | 3.242385 |
| C | -8.589678 | 1.098343 | 2.107484 |
| H | -8.987485 | 0.471618 | 4.248485 |
| H | -8.440468 | 1.393238 | 1.088893 |
| C | -6.040462 | 3.405846 | 3.495193 |
| C | -5.088726 | 4.134493 | 3.467522 |
| H | -6.907521 | 2.779985 | 3.516276 |
| H | -4.251022 | 4.798752 | 3.428569 |
| C | -4.060128 | 0.410932 | 1.735511 |
| C | -3.375500 | 1.472973 | 2.338726 |
| H | -4.076979 | 0.328970 | 0.653317 |
| H | -3.360502 | 1.502126 | 3.427958 |

EICO 12

1 2

| | | | |
|---|-----------|-----------|-----------|
| C | 1.274121 | 1.804850 | 2.573489 |
| C | 1.887357 | 0.848480 | 2.956643 |
| H | 0.719043 | 2.655130 | 2.235424 |
| H | 2.442580 | 0.007124 | 3.315163 |
| C | -1.901341 | 0.154523 | -0.102251 |
| C | -1.111926 | 0.114288 | 0.884160 |
| H | -2.848071 | 0.049151 | -0.607908 |
| H | -0.771180 | -0.055346 | 1.890229 |
| C | -5.115329 | -1.305498 | -1.131424 |
| C | -5.478875 | -0.399950 | -0.435699 |
| H | -4.802398 | -2.118274 | -1.748971 |
| H | -5.798662 | 0.408448 | 0.186141 |
| C | -4.475843 | 1.834555 | 2.371927 |
| C | -4.927024 | 2.744360 | 1.736668 |
| H | -4.085428 | 1.023272 | 2.947498 |
| H | -5.332653 | 3.563651 | 1.185839 |
| C | -3.296967 | -4.129851 | -0.116760 |
| C | -2.479746 | -4.396062 | -0.952225 |
| H | -4.052077 | -3.918718 | 0.612111 |
| H | -1.771806 | -4.677721 | -1.699245 |
| C | 4.025490 | -1.689088 | 0.343538 |
| C | 4.224536 | -0.507876 | 0.285966 |
| H | 3.868027 | -2.746171 | 0.412535 |
| H | 4.418281 | 0.544121 | 0.263690 |
| C | -1.483718 | 3.838809 | 1.083220 |
| C | -0.575253 | 4.320525 | 0.467682 |
| H | -2.308812 | 3.425057 | 1.623402 |
| H | 0.226859 | 4.755721 | -0.086483 |
| C | 0.422832 | -1.567409 | -1.108465 |
| C | 1.470192 | -2.244084 | -1.675130 |

| | | | |
|---|-----------|-----------|-----------|
| H | -0.384309 | -2.110362 | -0.629738 |
| H | 2.275817 | -1.678248 | -2.137684 |
| C | -0.476669 | 0.670914 | -0.426135 |
| C | 0.453881 | -0.173615 | -1.083380 |
| H | -0.313770 | 1.740377 | -0.503482 |
| H | 1.288193 | 0.319789 | -1.582222 |
| C | 3.439264 | -5.373766 | 1.218968 |
| C | 4.615395 | -5.143009 | 1.214958 |
| H | 2.393870 | -5.597486 | 1.222220 |
| H | 5.664509 | -4.945467 | 1.210687 |
| C | -0.103450 | -6.704378 | 0.073241 |
| C | 0.747049 | -7.011280 | -0.713079 |
| H | -0.873764 | -6.454717 | 0.767888 |
| H | 1.511220 | -7.298297 | -1.404108 |
| C | 1.589056 | -3.678780 | -1.661346 |
| C | 2.644458 | -4.275772 | -2.190693 |
| H | 0.810869 | -4.263126 | -1.171999 |
| H | 3.575843 | -4.016440 | -2.680673 |
| C | 4.160744 | -7.327384 | -1.845808 |
| C | 3.980902 | -7.721924 | -2.962615 |
| H | 4.317369 | -6.975306 | -0.848634 |
| H | 3.829017 | -8.088641 | -3.952977 |
| C | -0.109273 | -3.291214 | 1.911259 |
| C | 0.997217 | -3.039605 | 2.298407 |
| H | -1.098662 | -3.509079 | 1.570338 |
| H | 1.980444 | -2.829402 | 2.664767 |
| C | -2.777519 | -1.683714 | 3.511692 |
| C | -3.572050 | -1.617005 | 2.617309 |
| H | -2.072957 | -1.756455 | 4.309925 |
| H | -4.294494 | -1.566432 | 1.830820 |
| C | 4.610969 | 2.913392 | 1.496487 |
| C | 5.391353 | 3.173551 | 0.625333 |
| H | 3.916136 | 2.682269 | 2.275200 |
| H | 6.098283 | 3.423106 | -0.134548 |
| C | -6.666945 | -3.526699 | 1.377833 |
| C | -6.150140 | -3.839499 | 2.411605 |
| H | -7.144416 | -3.247470 | 0.465742 |
| H | -5.704680 | -4.115019 | 3.340891 |
| C | 2.342401 | 3.020154 | -1.494729 |
| C | 1.611123 | 3.081113 | -2.441938 |
| H | 3.009669 | 2.994140 | -0.658179 |
| H | 0.970345 | 3.157449 | -3.291883 |
| C | 6.235511 | -4.467848 | -2.212213 |
| C | 6.242340 | -3.338295 | -1.813512 |
| H | 6.230497 | -5.474768 | -2.567677 |
| H | 6.258568 | -2.333687 | -1.454521 |
| C | 4.326318 | -1.843105 | 3.838615 |
| C | 3.626997 | -2.154460 | 4.759721 |
| H | 4.953345 | -1.563171 | 3.021523 |
| H | 3.025321 | -2.438932 | 5.593718 |

EICO 13

1 2

| | | | |
|---|----------|----------|-----------|
| C | 6.054438 | 1.544232 | -1.041290 |
| C | 5.947956 | 2.507498 | -0.335860 |
| H | 6.165576 | 0.688896 | -1.676334 |
| H | 5.858834 | 3.363529 | 0.296104 |
| C | 2.883289 | 4.658076 | 1.192244 |
| C | 3.322545 | 3.756337 | 1.848579 |
| H | 2.485324 | 5.465998 | 0.617223 |
| H | 3.700242 | 2.952586 | 2.441515 |
| C | 0.280311 | 5.535341 | -1.333926 |

| | | | |
|---|-----------|-----------|-----------|
| C | 1.318078 | 5.604810 | -1.929265 |
| H | -0.653264 | 5.478206 | -0.818718 |
| H | 2.225806 | 5.692967 | -2.486434 |
| C | 2.472396 | 2.226726 | -1.472118 |
| C | 2.969763 | 1.859745 | -2.568149 |
| H | 2.871185 | 2.690081 | -0.574166 |
| H | 3.215061 | 1.473156 | -3.543344 |
| C | -2.641135 | 3.166017 | -1.145355 |
| C | -2.242084 | 3.119964 | -0.015369 |
| H | -3.008755 | 3.188065 | -2.150379 |
| H | -1.890747 | 3.076871 | 0.994780 |
| C | -0.024829 | 2.687811 | 2.825410 |
| C | -0.913264 | 2.081306 | 3.354758 |
| H | 0.773372 | 3.238498 | 2.375260 |
| H | -1.697136 | 1.542172 | 3.847179 |
| C | 2.101503 | -1.481426 | -2.743333 |
| C | 2.326948 | -1.820754 | -1.616019 |
| H | 1.923687 | -1.185104 | -3.755057 |
| H | 2.531379 | -2.147773 | -0.617975 |
| C | 2.899841 | -3.519503 | 1.697571 |
| C | 2.591725 | -4.357612 | 0.899382 |
| H | 3.178215 | -2.782625 | 2.417745 |
| H | 2.331064 | -5.117301 | 0.196577 |
| C | 0.852961 | 2.056683 | -1.386791 |
| C | 0.496063 | 0.978404 | -0.860614 |
| H | 0.339032 | 2.927644 | -1.781616 |
| H | 0.287070 | 0.028677 | -0.396511 |
| C | -1.181756 | -1.005897 | 1.516218 |
| C | -0.381302 | -1.875330 | 1.315422 |
| H | -1.917034 | -0.253192 | 1.701130 |
| H | 0.333260 | -2.657446 | 1.167556 |
| C | 2.325581 | 0.216842 | 1.830362 |
| C | 3.357717 | 0.255928 | 1.220835 |
| H | 1.407387 | 0.184034 | 2.377583 |
| H | 4.283993 | 0.313521 | 0.690765 |
| C | 5.728181 | -1.401981 | -3.317263 |
| C | 6.597597 | -0.773742 | -3.851491 |
| H | 4.947545 | -1.964662 | -2.854041 |
| H | 7.380795 | -0.224078 | -4.325101 |
| C | -2.304730 | -0.289185 | -1.904182 |
| C | -1.642353 | -0.841240 | -2.736871 |
| H | -2.913297 | 0.180592 | -1.160208 |
| H | -1.070128 | -1.361111 | -3.472201 |
| C | 3.563456 | 5.696430 | -5.007790 |
| C | 2.668628 | 6.489300 | -5.084034 |
| H | 4.371107 | 4.998104 | -4.956706 |
| H | 1.883820 | 7.208537 | -5.157246 |
| C | -4.047562 | 1.806688 | -4.297152 |
| C | -3.790313 | 2.888392 | -4.742172 |
| H | -4.282332 | 0.840490 | -3.909695 |
| H | -3.569012 | 3.846002 | -5.157694 |
| C | 3.421288 | -0.043306 | -5.780783 |
| C | 2.417255 | 0.564630 | -6.026333 |
| H | 4.321209 | -0.580366 | -5.566797 |
| H | 1.524755 | 1.108859 | -6.246721 |
| C | -4.799627 | 0.828533 | 0.849626 |
| C | -4.698999 | -0.359809 | 0.964131 |
| H | -4.897060 | 1.885582 | 0.737146 |
| H | -4.623839 | -1.419340 | 1.071719 |
| C | 6.015975 | 2.951499 | -4.231918 |
| C | 5.567199 | 2.630494 | -5.295554 |
| H | 6.426290 | 3.234457 | -3.287659 |
| H | 5.176800 | 2.347455 | -6.247964 |

| | | | |
|---|-----------|-----------|-----------|
| C | -3.818913 | 0.056522 | 4.532799 |
| C | -2.973534 | -0.297349 | 5.303880 |
| H | -4.581956 | 0.359439 | 3.849733 |
| H | -2.235673 | -0.617009 | 6.005905 |
| C | -0.275798 | 2.528394 | -4.469582 |
| C | 0.585718 | 3.329893 | -4.701453 |
| H | -1.069521 | 1.839821 | -4.270588 |
| H | 1.343989 | 4.053655 | -4.919507 |

EICO 14

1 2

| | | | |
|---|-----------|-----------|-----------|
| C | 0.313260 | 1.750717 | 0.969247 |
| C | 0.945102 | 1.526412 | 1.962830 |
| H | -0.265934 | 1.942135 | 0.093111 |
| H | 1.501647 | 1.330939 | 2.856503 |
| C | 2.775410 | 0.674568 | -1.800242 |
| C | 3.622496 | -0.172159 | -1.780175 |
| H | 2.020707 | 1.430650 | -1.816744 |
| H | 4.362358 | -0.940331 | -1.741284 |
| C | 1.580465 | 4.665752 | 3.343970 |
| C | 2.655969 | 5.044718 | 3.711941 |
| H | 0.621896 | 4.318791 | 3.026210 |
| H | 3.613116 | 5.371075 | 4.056019 |
| C | 3.744491 | 3.251024 | 0.668824 |
| C | 4.972482 | 2.952793 | 0.560197 |
| H | 2.690121 | 3.059833 | 0.792380 |
| H | 5.820479 | 2.289655 | 0.495481 |
| C | 2.910761 | 1.646769 | 5.161542 |
| C | 3.479550 | 0.719239 | 4.659773 |
| H | 2.403795 | 2.467576 | 5.618148 |
| H | 3.986138 | -0.109123 | 4.214928 |
| C | 4.315711 | 2.467301 | -4.471347 |
| C | 4.394390 | 3.666667 | -3.916027 |
| H | 4.290275 | 1.433550 | -4.149177 |
| H | 4.398378 | 4.564186 | -4.531549 |
| C | 4.637909 | 5.041125 | -1.896216 |
| C | 4.494068 | 3.808032 | -2.487776 |
| H | 4.676933 | 5.906583 | -2.549546 |
| H | 4.464567 | 2.899274 | -1.896429 |
| C | 2.026631 | 6.942401 | 0.466524 |
| C | 2.113226 | 7.267045 | -0.684620 |
| H | 1.944401 | 6.658796 | 1.494459 |
| H | 2.187790 | 7.556536 | -1.712040 |
| C | 4.699198 | 4.463872 | 0.626874 |
| C | 4.773098 | 5.302111 | -0.529063 |
| H | 4.908389 | 4.968482 | 1.565377 |
| H | 4.962170 | 6.350272 | -0.304414 |
| C | 6.661077 | 4.425987 | 3.695115 |
| C | 5.889171 | 3.544404 | 3.948562 |
| H | 7.354257 | 5.207923 | 3.474645 |
| H | 5.193707 | 2.766352 | 4.189246 |
| C | 7.635596 | 2.509363 | -5.508045 |
| C | 7.436836 | 1.554718 | -6.203390 |
| H | 7.817932 | 3.369704 | -4.901159 |
| H | 7.276792 | 0.703630 | -6.826340 |
| C | 7.924851 | 6.490732 | 0.226598 |
| C | 8.144192 | 5.322299 | 0.379402 |
| H | 7.738006 | 7.533103 | 0.086660 |
| H | 8.354581 | 4.283279 | 0.523787 |
| C | 0.492517 | 3.359827 | -2.781594 |
| C | 0.860949 | 4.102203 | -1.915570 |
| H | 0.151304 | 2.705347 | -3.553211 |
| H | 1.171023 | 4.795714 | -1.161342 |

| | | | |
|---|----------|-----------|-----------|
| C | 5.109347 | 9.039908 | -1.311269 |
| C | 5.847101 | 8.507324 | -2.091543 |
| H | 4.452039 | 9.523964 | -0.623270 |
| H | 6.503508 | 8.033459 | -2.791183 |
| C | 3.032477 | 7.432648 | -4.469146 |
| C | 2.201342 | 6.595213 | -4.256840 |
| H | 3.771941 | 8.175816 | -4.683808 |
| H | 1.458961 | 5.851568 | -4.063577 |
| C | 5.568491 | -0.619060 | 1.703087 |
| C | 4.423093 | -0.384343 | 1.442350 |
| H | 6.588931 | -0.833021 | 1.930229 |
| H | 3.403057 | -0.186690 | 1.195378 |
| C | 5.942178 | 9.606431 | -5.504482 |
| C | 5.856681 | 8.844153 | -6.424185 |
| H | 6.024575 | 10.299871 | -4.697418 |
| H | 5.789842 | 8.179316 | -7.256942 |
| C | 7.256117 | 5.990663 | -4.446652 |
| C | 7.804864 | 5.766585 | -3.404735 |
| H | 6.768910 | 6.188363 | -5.377408 |
| H | 8.290411 | 5.591334 | -2.468955 |
| C | 8.248503 | 1.845035 | 1.592179 |
| C | 8.628380 | 1.455135 | 0.524679 |
| H | 7.908921 | 2.199604 | 2.542247 |
| H | 8.988182 | 1.094068 | -0.412975 |
| C | 4.423117 | 5.518933 | -7.209231 |
| C | 5.332732 | 4.744662 | -7.302966 |
| H | 3.601247 | 6.195204 | -7.128112 |
| H | 6.132582 | 4.040657 | -7.383930 |

EICO 15

1 2

| | | | |
|---|-----------|-----------|-----------|
| C | 0.370610 | -1.822845 | -0.098315 |
| C | 1.209463 | -1.373274 | 0.629092 |
| H | -0.385055 | -2.247443 | -0.721042 |
| H | 1.965653 | -0.985370 | 1.276993 |
| C | 2.010948 | 2.776014 | -3.702702 |
| C | 2.598712 | 1.815378 | -2.882811 |
| H | 1.283153 | 2.465641 | -4.445474 |
| H | 3.325353 | 2.144181 | -2.141574 |
| C | 0.288494 | 1.535951 | 4.111778 |
| C | 0.279604 | 2.710989 | 3.879355 |
| H | 0.271074 | 0.491077 | 4.326486 |
| H | 0.276548 | 3.761035 | 3.680902 |
| C | 0.923451 | 2.079738 | -0.043083 |
| C | 1.471505 | 3.114675 | 0.212999 |
| H | 0.438716 | 1.145297 | -0.225216 |
| H | 1.943229 | 4.034734 | 0.483697 |
| C | 3.690091 | 3.145934 | 2.850234 |
| C | 4.622382 | 3.767244 | 2.422376 |
| H | 2.848467 | 2.605403 | 3.229730 |
| H | 5.452924 | 4.331007 | 2.051539 |
| C | 6.802383 | 6.498378 | -3.394930 |
| C | 6.747447 | 5.300444 | -3.399890 |
| H | 6.876422 | 7.563728 | -3.380095 |
| H | 6.734065 | 4.230262 | -3.386763 |
| C | 7.357437 | 5.790145 | 0.354241 |
| C | 7.596433 | 5.859888 | 1.526096 |
| H | 7.158036 | 5.739842 | -0.693955 |
| H | 7.803082 | 5.935022 | 2.570577 |
| C | 0.680443 | 6.253118 | 2.311527 |
| C | 1.691405 | 6.080031 | 2.932272 |
| H | -0.216642 | 6.414243 | 1.756436 |

| | | | |
|---|-----------|-----------|-----------|
| H | 2.591074 | 5.926484 | 3.490240 |
| C | 1.923764 | 4.236162 | -3.115630 |
| C | 2.829636 | 4.090942 | -3.976580 |
| H | 1.255306 | 4.727653 | -2.423911 |
| H | 3.600008 | 4.362058 | -4.682332 |
| C | 3.753046 | 6.629807 | -1.380220 |
| C | 3.160011 | 6.636261 | -0.338209 |
| H | 4.307695 | 6.622764 | -2.293095 |
| H | 2.626567 | 6.658023 | 0.591066 |
| C | 5.335884 | 7.291972 | 3.870421 |
| C | 5.202391 | 6.325791 | 4.565450 |
| H | 5.466623 | 8.155461 | 3.257909 |
| H | 5.061985 | 5.466860 | 5.183267 |
| C | 2.859024 | -0.390979 | -2.060575 |
| C | 2.307860 | 0.418550 | -2.957995 |
| H | 3.516117 | -0.313291 | -1.197417 |
| H | 1.633035 | 0.049672 | -3.727621 |
| C | 5.109655 | 3.373618 | -0.857572 |
| C | 5.790039 | 2.394727 | -0.983529 |
| H | 4.526151 | 4.262186 | -0.733191 |
| H | 6.429393 | 1.544084 | -1.067644 |
| C | 2.509611 | 1.690147 | -7.042406 |
| C | 1.448665 | 2.128745 | -7.386928 |
| H | 3.456775 | 1.290468 | -6.749980 |
| H | 0.503595 | 2.501765 | -7.717563 |
| C | 4.191700 | 4.918279 | -7.245457 |
| C | 5.085202 | 5.448826 | -6.648205 |
| H | 3.403699 | 4.445720 | -7.790052 |
| H | 5.884776 | 5.922893 | -6.121670 |
| C | 5.703008 | 2.182058 | -5.253308 |
| C | 5.802715 | 1.303893 | -4.444209 |
| H | 5.622140 | 2.964471 | -5.980195 |
| H | 5.925892 | 0.516845 | -3.733719 |
| C | 2.255990 | 4.340743 | 6.323272 |
| C | 2.460938 | 5.510311 | 6.477293 |
| H | 2.051903 | 3.301238 | 6.196966 |
| H | 2.643530 | 6.551672 | 6.620703 |
| C | -0.815785 | 5.465553 | -1.022991 |
| C | -0.248974 | 6.485668 | -1.291056 |
| H | -1.326236 | 4.562942 | -0.773578 |
| H | 0.247372 | 7.400746 | -1.524284 |
| C | 9.080960 | 2.273519 | -2.883885 |
| C | 9.012247 | 2.880947 | -1.854234 |
| H | 9.163725 | 1.741722 | -3.804578 |
| H | 8.960609 | 3.425309 | -0.937161 |
| C | 4.823738 | -1.060051 | 0.945438 |
| C | 4.681884 | 0.104721 | 1.191663 |
| H | 4.960695 | -2.101755 | 0.756788 |
| H | 4.577970 | 1.143871 | 1.430935 |

EICO 16

1 2

| | | | |
|---|-----------|-----------|-----------|
| C | 0.645105 | 2.476644 | -1.174737 |
| C | 1.360523 | 2.207590 | 0.021497 |
| H | -0.311249 | 2.089668 | -1.523909 |
| H | 1.356633 | 1.462988 | 0.801253 |
| C | 1.117189 | 0.669680 | -3.804541 |
| C | 1.197376 | -0.093144 | -2.883926 |
| H | 1.054936 | 1.325008 | -4.644552 |
| H | 1.277523 | -0.790995 | -2.076441 |
| C | 0.448477 | 4.017223 | 3.303197 |
| C | 1.497889 | 4.594216 | 3.363676 |

| | | | |
|---|-----------|-----------|-----------|
| H | -0.497586 | 3.519776 | 3.280763 |
| H | 2.424008 | 5.123163 | 3.423968 |
| C | 4.058788 | 0.834969 | -0.918632 |
| C | 4.638731 | 1.790298 | -1.350262 |
| H | 3.556013 | -0.028220 | -0.538106 |
| H | 5.165362 | 2.636811 | -1.730313 |
| C | -2.899655 | 1.433336 | -1.848169 |
| C | -2.272861 | 0.611491 | -2.455551 |
| H | -3.481038 | 2.146012 | -1.304983 |
| H | -1.726680 | -0.114956 | -3.015465 |
| C | -3.307472 | 2.692015 | 4.018633 |
| C | -2.853463 | 3.700801 | 4.482268 |
| H | -3.729113 | 1.804270 | 3.598986 |
| H | -2.442260 | 4.599130 | 4.893200 |
| C | 1.306824 | 7.328423 | -0.359984 |
| C | 0.629573 | 7.022481 | 0.581100 |
| H | 1.899537 | 7.639021 | -1.191317 |
| H | 0.005909 | 6.773063 | 1.417298 |
| C | -1.894996 | 4.804746 | -0.261396 |
| C | -2.131972 | 4.017339 | 0.610880 |
| H | -1.700132 | 5.532959 | -1.017113 |
| H | -2.371552 | 3.333183 | 1.397684 |
| C | -0.827560 | 0.512985 | 2.417935 |
| C | -1.372978 | 0.475310 | 1.350013 |
| H | -0.357363 | 0.538597 | 3.380586 |
| H | -1.871266 | 0.435356 | 0.403716 |
| C | 2.079467 | 7.588435 | 5.059779 |
| C | 2.198838 | 8.188350 | 4.030174 |
| H | 1.957550 | 7.058946 | 5.979141 |
| H | 2.303269 | 8.739497 | 3.122710 |
| C | -5.593586 | 5.414787 | 2.430667 |
| C | -5.607919 | 5.771027 | 1.287220 |
| H | -5.579943 | 5.098748 | 3.450388 |
| H | -5.640290 | 6.097941 | 0.272112 |
| C | 4.101610 | 5.163080 | 0.901134 |
| C | 4.286051 | 4.008707 | 1.167047 |
| H | 3.945676 | 6.196348 | 0.684836 |
| H | 4.457062 | 2.981084 | 1.408087 |
| C | 2.842501 | 1.244110 | 3.067872 |
| C | 3.460615 | 0.334542 | 2.589453 |
| H | 2.298076 | 2.059029 | 3.496272 |
| H | 4.026946 | -0.473376 | 2.173907 |
| C | 2.326621 | -2.361115 | -0.181978 |
| C | 1.475347 | -1.805456 | 0.452891 |
| H | 3.091142 | -2.866185 | -0.730477 |
| H | 0.710386 | -1.332283 | 1.031245 |
| C | 1.478708 | 3.620490 | -0.052141 |
| C | 1.297262 | 3.710084 | -1.460840 |
| H | 1.346604 | 4.367184 | 0.725018 |
| H | 1.169523 | 4.508999 | -2.172737 |
| C | 6.001871 | -1.648043 | 0.608591 |
| C | 5.549320 | -2.528300 | 1.282569 |
| H | 6.415211 | -0.868700 | 0.008009 |
| H | 5.163771 | -3.321041 | 1.883721 |
| C | -2.307178 | 6.839176 | 2.975022 |
| C | -1.326869 | 7.080939 | 3.621083 |
| H | -3.189940 | 6.618519 | 2.414333 |
| H | -0.444592 | 7.297245 | 4.184499 |
| C | -0.282417 | 1.385339 | 5.881555 |
| C | 0.813825 | 0.901714 | 5.888161 |
| H | -1.262149 | 1.812540 | 5.880627 |
| H | 1.786180 | 0.461752 | 5.908280 |
| C | -0.759840 | 5.933178 | 7.025788 |

| | | | |
|---|-----------|-----------|----------|
| C | -0.106911 | 4.964725 | 6.760612 |
| H | -1.340412 | 6.793474 | 7.273659 |
| H | 0.471137 | 4.096507 | 6.532158 |
| C | -5.193057 | 2.020772 | 1.129049 |
| C | -4.974318 | 0.854191 | 0.965719 |
| H | -5.403090 | 3.058875 | 1.281645 |
| H | -4.805927 | -0.188425 | 0.814754 |

EICO 17

1 2

| | | | |
|---|-----------|-----------|-----------|
| C | 3.299736 | -3.567357 | -3.897705 |
| C | 3.148922 | -2.878274 | -4.866141 |
| C | 2.219708 | -0.549817 | -1.995488 |
| C | 1.770038 | 0.326336 | -2.679858 |
| C | 0.539009 | 1.851941 | -0.046855 |
| C | -0.747291 | 1.328715 | -0.167072 |
| C | -1.045648 | 0.049629 | 0.703414 |
| C | -0.877911 | -0.197678 | -0.516871 |
| C | 0.852212 | 3.234954 | -0.239215 |
| C | 2.110384 | 3.621312 | -0.072747 |
| C | 0.627473 | 1.631346 | 3.303757 |
| C | 1.289625 | 0.645402 | 3.139041 |
| C | -3.574072 | 0.280290 | -2.578639 |
| C | -3.102538 | -0.451016 | -3.402673 |
| C | -1.187726 | -3.313540 | -2.357051 |
| C | -0.184826 | -3.017620 | -2.945169 |
| C | 4.312247 | 1.098306 | 1.364550 |
| C | 4.463083 | 0.899824 | 0.191694 |
| C | -2.431005 | -6.136824 | -0.007627 |
| C | -1.282685 | -6.187361 | 0.327803 |
| C | 0.426008 | -3.156634 | 0.953013 |
| C | 0.859878 | -3.090178 | 2.068392 |
| C | -0.884587 | 2.585892 | -3.684595 |
| C | -0.062955 | 3.453500 | -3.773737 |
| C | 5.652008 | -0.586592 | -3.139582 |
| C | 6.540683 | 0.086311 | -2.700623 |
| C | 4.860629 | -2.732976 | -0.488695 |
| C | 3.893060 | -3.310740 | -0.079821 |
| C | 2.590841 | -6.349331 | -1.135097 |
| C | 1.583756 | -5.961968 | -1.655210 |
| C | 4.050810 | -1.868849 | 3.242776 |
| C | 3.756060 | -1.675342 | 4.387971 |
| C | -4.291499 | 1.067535 | 1.008254 |
| C | -4.279689 | 2.189149 | 0.585236 |
| C | -3.903341 | -2.355057 | -0.073481 |
| C | -3.261608 | -2.912736 | 0.770971 |
| C | -2.266100 | 3.852360 | 3.164372 |
| C | -1.520652 | 4.726775 | 3.503436 |
| C | -2.372080 | 5.161947 | -0.187403 |
| C | -2.437028 | 4.952193 | -1.365521 |
| H | 3.427206 | -4.194405 | -3.041177 |
| H | 3.027251 | -2.279895 | -5.741075 |
| H | 0.717473 | -2.782218 | -3.471079 |
| H | -2.071213 | -3.582443 | -1.818107 |
| H | 0.047453 | -3.235339 | -0.044137 |
| H | 1.265254 | -3.043326 | 3.055353 |
| H | -0.837292 | -0.768064 | -1.429882 |
| H | -1.233279 | -0.109558 | 1.749502 |
| H | 5.719959 | -2.221986 | -0.865808 |
| H | 3.032149 | -3.827309 | 0.285660 |
| H | 4.198372 | 1.260418 | 2.413684 |
| H | 4.624389 | 0.714927 | -0.850122 |
| H | 1.363241 | 1.103350 | -3.291509 |

| | | | |
|---|-----------|-----------|-----------|
| H | 2.648502 | -1.330910 | -1.400839 |
| H | -4.324985 | 0.063166 | 1.372214 |
| H | -4.273437 | 3.189596 | 0.208461 |
| H | -2.693011 | -1.112252 | -4.134363 |
| H | -4.007888 | 0.914149 | -1.834963 |
| H | 0.058403 | 3.927651 | -0.512474 |
| H | 3.056203 | 3.155288 | 0.188490 |
| H | 4.872822 | -1.201633 | -3.537396 |
| H | 7.342395 | 0.682969 | -2.326946 |
| H | -2.944865 | 3.081716 | 2.868157 |
| H | -0.871325 | 5.511043 | 3.823940 |
| H | -0.258238 | -6.248385 | 0.620299 |
| H | -3.457381 | -6.108180 | -0.296203 |
| H | -1.568697 | 1.995359 | -0.415360 |
| H | 1.350592 | 1.177830 | 0.216122 |
| H | -1.624393 | 1.815452 | -3.618979 |
| H | 0.660248 | 4.232313 | -3.872563 |
| H | -2.320292 | 5.348258 | 0.863737 |
| H | -2.486295 | 4.783211 | -2.418400 |
| H | 4.323265 | -2.047099 | 2.223861 |
| H | 3.513981 | -1.508020 | 5.413634 |
| H | -4.472178 | -1.868407 | -0.834665 |
| H | -2.690670 | -3.436812 | 1.506129 |
| H | 0.681472 | -5.629976 | -2.120410 |
| H | 3.488070 | -6.707811 | -0.682328 |
| H | 0.027313 | 2.502241 | 3.463809 |
| H | 1.896972 | -0.227352 | 3.019810 |

EICO 18

1 2

| | | | |
|---|-----------|-----------|-----------|
| C | -0.708345 | 0.234353 | -2.769899 |
| C | -0.759562 | 1.338771 | -3.497611 |
| H | -0.633149 | -0.743675 | -3.241610 |
| H | -0.845723 | 2.413053 | -3.377358 |
| C | 2.691514 | 1.042517 | -2.123272 |
| C | 2.715565 | 1.407496 | -0.982839 |
| H | 2.683058 | 0.720609 | -3.140335 |
| H | 2.752227 | 1.718217 | 0.037942 |
| C | -4.212591 | 0.457688 | 1.074575 |
| C | -4.709866 | -0.633348 | 1.069044 |
| H | -3.818910 | 1.452401 | 1.094939 |
| H | -5.160175 | -1.602260 | 1.069341 |
| C | -0.014620 | 3.997501 | -0.733022 |
| C | -1.160380 | 4.119127 | -0.398510 |
| H | 1.005142 | 3.931297 | -1.050195 |
| H | -2.179287 | 4.248766 | -0.094527 |
| C | -3.259447 | -2.829093 | -2.856761 |
| C | -3.583887 | -1.983079 | -2.072567 |
| H | -2.987149 | -3.580936 | -3.563797 |
| H | -3.886341 | -1.236563 | -1.368395 |
| C | 1.852709 | 0.611155 | 2.743355 |
| C | 2.372945 | -0.210717 | 2.044020 |
| H | 1.389735 | 1.338823 | 3.373026 |
| H | 2.856961 | -0.931740 | 1.423426 |
| C | -0.791913 | -0.831301 | -0.543820 |
| C | -0.788207 | 0.293114 | -1.337465 |
| H | -0.723555 | -1.814812 | -0.998555 |
| H | -0.867400 | 1.277438 | -0.877936 |
| C | -4.151718 | 1.809853 | -2.544935 |
| C | -3.658761 | 2.902381 | -2.517033 |
| H | -4.632184 | 0.856153 | -2.587332 |
| H | -3.249968 | 3.890760 | -2.500718 |
| C | -1.067014 | 2.668228 | 2.741261 |

| | | | |
|---|-----------|-----------|-----------|
| C | -1.622357 | 2.031851 | 3.591222 |
| H | -0.584690 | 3.244836 | 1.980327 |
| H | -2.121681 | 1.483105 | 4.358117 |
| C | -0.694601 | -1.674466 | 3.189321 |
| C | -1.942541 | -1.665259 | 2.964355 |
| H | 0.198450 | -1.660830 | 3.788913 |
| H | -2.992689 | -1.625160 | 3.191694 |
| C | -6.891644 | -0.966517 | -2.290813 |
| C | -7.110613 | 0.123742 | -1.846067 |
| H | -6.712547 | -1.938477 | -2.691223 |
| H | -7.313870 | 1.102256 | -1.468137 |
| C | 2.736289 | 5.750400 | -2.248402 |
| C | 3.333661 | 4.723786 | -2.405681 |
| H | 2.203638 | 6.668795 | -2.120759 |
| H | 3.878897 | 3.816193 | -2.535828 |
| C | -5.072266 | 4.297686 | -5.578608 |
| C | -5.019369 | 5.380248 | -5.069005 |
| H | -5.128872 | 3.338469 | -6.041514 |
| H | -4.969764 | 6.342255 | -4.608909 |
| C | -3.900561 | -4.431184 | 2.016957 |
| C | -3.728380 | -4.137091 | 0.868774 |
| H | -4.062780 | -4.720321 | 3.031106 |
| H | -3.589498 | -3.888803 | -0.161407 |
| C | -1.067205 | -1.838829 | 1.705191 |
| C | -0.953221 | -0.719703 | 0.830059 |
| H | -1.005041 | -2.827305 | 1.255103 |
| H | -1.025226 | 0.272270 | 1.275766 |
| C | -1.353857 | 4.827641 | -4.694945 |
| C | -0.239843 | 4.874402 | -4.254837 |
| H | -2.349213 | 4.795118 | -5.086443 |
| H | 0.757158 | 4.923933 | -3.871226 |
| C | -4.155788 | 4.206280 | 1.787357 |
| C | -4.739066 | 3.907348 | 0.784139 |
| H | -3.644421 | 4.475639 | 2.684091 |
| H | -5.274970 | 3.648294 | -0.104701 |
| C | -3.137559 | 6.615351 | -2.035305 |
| C | -4.257038 | 6.387380 | -1.672686 |
| H | -2.139164 | 6.832293 | -2.351500 |
| H | -5.256690 | 6.192144 | -1.351402 |
| C | -7.742267 | 4.089979 | -1.213993 |
| C | -7.081326 | 3.991453 | -2.208418 |
| H | -8.344202 | 4.187423 | -0.338315 |
| H | -6.495110 | 3.918358 | -3.099740 |
| C | 0.070456 | 8.408181 | -1.893721 |
| C | 0.143324 | 8.216305 | -3.073463 |
| H | -0.002567 | 8.595646 | -0.846036 |
| H | 0.202504 | 8.053621 | -4.126494 |

EICO 19

1 2

| | | | |
|---|-----------|-----------|-----------|
| C | 0.907530 | 2.035990 | 2.755430 |
| C | 0.070405 | 1.191735 | 2.600809 |
| C | -3.002042 | 2.687627 | 2.299169 |
| C | -3.868638 | 2.426698 | 1.513551 |
| C | -6.115687 | -0.236793 | 1.500286 |
| C | -5.975275 | -0.798847 | 0.451968 |
| C | 1.855924 | -1.854202 | 2.816392 |
| C | 1.960267 | -2.868998 | 2.186775 |
| C | -1.582715 | 2.896751 | -1.134541 |
| C | -1.272985 | 3.302359 | -2.219272 |
| C | 1.521259 | 1.297917 | -1.171907 |
| C | 2.437528 | 1.778044 | -0.460113 |
| C | 2.191117 | 0.253414 | -0.174868 |

| | | | |
|---|-----------|-----------|-----------|
| C | 2.983671 | -0.722244 | -0.769899 |
| C | 3.767397 | -0.564634 | -1.960427 |
| C | 4.396438 | -1.626376 | -2.442489 |
| C | 0.511755 | -2.217405 | -2.409962 |
| C | 0.036777 | -2.277595 | -1.310637 |
| C | -0.468513 | 0.495023 | -4.136767 |
| C | 0.491058 | 0.893248 | -4.734567 |
| C | 5.910846 | 1.492395 | -0.062770 |
| C | 5.946454 | 2.434431 | -0.801988 |
| C | -3.224154 | -1.133367 | -2.029841 |
| C | -3.577650 | 0.006635 | -2.147076 |
| C | -2.383708 | -1.198368 | 1.387335 |
| C | -1.783396 | -1.985206 | 2.063966 |
| C | 5.459115 | -2.040750 | 1.494953 |
| C | 6.391651 | -1.971057 | 0.745778 |
| C | -2.320403 | -4.767227 | -1.540806 |
| C | -2.879497 | -4.548427 | -0.504041 |
| C | 3.920790 | -4.695107 | -0.383366 |
| C | 2.857579 | -4.636947 | -0.933553 |
| C | -4.911368 | -3.814158 | 2.522291 |
| C | -4.672634 | -4.967251 | 2.739614 |
| C | -5.252075 | 3.331026 | -1.698073 |
| C | -6.113234 | 2.510121 | -1.559830 |
| C | 3.024808 | 4.755806 | 1.456430 |
| C | 4.122140 | 4.304864 | 1.627643 |
| C | -0.644575 | 5.347680 | 1.423143 |
| C | -0.338444 | 5.766164 | 2.502606 |
| H | 1.644283 | 2.797188 | 2.894668 |
| H | -0.683586 | 0.442913 | 2.467662 |
| H | -2.231653 | 2.936671 | 2.994567 |
| H | -4.645524 | 2.217123 | 0.809912 |
| H | 1.645958 | -0.007938 | 0.724371 |
| H | 3.001184 | -1.705989 | -0.303034 |
| H | -0.929509 | 4.984035 | 0.460316 |
| H | -0.077121 | 6.150460 | 3.463075 |
| H | 5.107806 | 3.923156 | 1.774020 |
| H | 2.045712 | 5.169311 | 1.331071 |
| H | -1.005167 | 3.651182 | -3.191868 |
| H | -1.883520 | 2.556888 | -0.164196 |
| H | 0.904623 | -2.148862 | -3.400006 |
| H | -0.420328 | -2.326768 | -0.343423 |
| H | -1.264217 | -2.688049 | 2.677069 |
| H | -2.944322 | -0.509818 | 0.792068 |
| H | 5.998813 | 3.280619 | -1.450455 |
| H | 5.900337 | 0.648170 | 0.592931 |
| H | 4.866145 | -4.759170 | 0.109077 |
| H | 1.905086 | -4.589258 | -1.414893 |
| H | -1.831681 | -4.973429 | -2.465656 |
| H | -3.388543 | -4.372234 | 0.421102 |
| H | 2.063558 | -3.778832 | 1.635517 |
| H | 1.745357 | -0.954144 | 3.382084 |
| H | -4.489217 | 4.067419 | -1.818271 |
| H | -6.887315 | 1.786184 | -1.433412 |
| H | -3.917200 | 1.015627 | -2.249278 |
| H | -2.930896 | -2.155454 | -1.909433 |
| H | -6.247067 | 0.263553 | 2.433623 |
| H | -5.845136 | -1.298531 | -0.482078 |
| H | 3.078879 | 2.521823 | -0.011817 |
| H | 0.717526 | 1.207661 | -1.885014 |
| H | -5.136170 | -2.789086 | 2.323558 |
| H | -4.475798 | -5.996074 | 2.939589 |
| H | 7.237928 | -1.907982 | 0.098007 |
| H | 4.632745 | -2.117706 | 2.169154 |

| | | | |
|---|-----------|-----------|-----------|
| H | 3.835439 | 0.406821 | -2.441459 |
| H | 4.496691 | -2.676400 | -2.187009 |
| H | 1.326364 | 1.248564 | -5.295141 |
| H | -1.330095 | 0.139243 | -3.608529 |

EICO 20

1 2

| | | | |
|---|-----------|-----------|-----------|
| C | 1.214620 | 0.117598 | 1.985352 |
| C | 2.365369 | 0.410388 | 1.821200 |
| H | 0.190735 | -0.150620 | 2.125994 |
| H | 3.393377 | 0.668576 | 1.676506 |
| C | 2.754378 | 5.477007 | -4.724234 |
| C | 3.026354 | 4.308922 | -4.705217 |
| H | 2.510664 | 6.518431 | -4.771567 |
| H | 3.262663 | 3.266004 | -4.708154 |
| C | 2.372581 | 6.969178 | 4.413930 |
| C | 1.501803 | 6.224464 | 4.765270 |
| H | 3.143495 | 7.650127 | 4.129981 |
| H | 0.724772 | 5.566247 | 5.095715 |
| C | 5.356385 | 2.568079 | 0.982667 |
| C | 5.267851 | 2.615781 | 2.177639 |
| H | 5.447521 | 2.521366 | -0.083402 |
| H | 5.194148 | 2.643868 | 3.242989 |
| C | -1.992303 | 2.100403 | 1.545989 |
| C | -1.760228 | 2.112942 | 2.721805 |
| H | -2.222944 | 2.088372 | 0.503774 |
| H | -1.568929 | 2.137017 | 3.774085 |
| C | 4.811187 | 1.864899 | -2.600123 |
| C | 5.898674 | 2.356249 | -2.704695 |
| H | 3.839175 | 1.426535 | -2.538094 |
| H | 6.869532 | 2.788414 | -2.802375 |
| C | 1.318794 | 3.885260 | 2.309596 |
| C | 0.554003 | 4.736897 | 1.467135 |
| H | 1.194533 | 2.925430 | 2.784166 |
| H | -0.339071 | 4.531259 | 0.881302 |
| C | 1.484109 | 3.483745 | -1.619993 |
| C | 1.375198 | 2.451057 | -1.019392 |
| H | 1.582136 | 4.398220 | -2.168098 |
| H | 1.293838 | 1.528928 | -0.483204 |
| C | 0.679472 | 7.224845 | -1.918145 |
| C | 1.864817 | 7.396540 | -1.860729 |
| H | -0.379194 | 7.093802 | -2.002458 |
| H | 2.920350 | 7.553531 | -1.817824 |
| C | 1.584941 | 5.688562 | 1.226585 |
| C | 2.328392 | 4.519928 | 1.537632 |
| H | 1.704460 | 6.544275 | 0.579700 |
| H | 3.212532 | 4.101147 | 1.060373 |
| C | -1.663151 | 3.181537 | -4.666257 |
| C | -0.613753 | 3.749377 | -4.779428 |
| H | -2.601284 | 2.678439 | -4.587853 |
| H | 0.328273 | 4.242887 | -4.902406 |
| C | 1.634930 | 0.886074 | -4.542711 |
| C | 2.644007 | 0.310006 | -4.833372 |
| H | 0.727279 | 1.396928 | -4.306933 |
| H | 3.536652 | -0.210138 | -5.100334 |
| C | -2.444607 | 5.333619 | -0.593411 |
| C | -1.850115 | 4.576041 | -1.307152 |
| H | -2.981951 | 6.017082 | 0.026159 |
| H | -1.333049 | 3.919241 | -1.973644 |
| C | 3.173355 | 3.069850 | 5.260362 |
| C | 3.056225 | 1.902320 | 5.016997 |
| H | 3.274928 | 4.109357 | 5.486003 |

| | | | |
|---|-----------|-----------|-----------|
| H | 2.959050 | 0.860207 | 4.805330 |
| C | -2.063808 | 5.650379 | 2.844973 |
| C | -1.460648 | 6.669102 | 3.032188 |
| H | -2.601602 | 4.741891 | 2.679089 |
| H | -0.932839 | 7.578541 | 3.218279 |
| C | -1.306959 | 3.957624 | 5.894525 |
| C | -0.339644 | 3.269359 | 6.056102 |
| H | -2.169931 | 4.573404 | 5.770902 |
| H | 0.528037 | 2.667647 | 6.217305 |
| C | 5.139849 | 5.849926 | -0.368390 |
| C | 4.651217 | 5.410772 | -1.370692 |
| H | 5.608641 | 6.231158 | 0.510937 |
| H | 4.242452 | 5.022603 | -2.280229 |
| C | -0.129828 | 10.745012 | -2.475349 |
| C | -0.979502 | 11.257012 | -1.804810 |
| H | 0.624189 | 10.293560 | -3.082834 |
| H | -1.728332 | 11.730528 | -1.211304 |
| C | -2.260396 | 8.184039 | -3.780344 |
| C | -2.292383 | 7.041424 | -4.139911 |
| H | -2.218451 | 9.202681 | -3.459596 |
| H | -2.326764 | 6.024393 | -4.463676 |
| C | 2.127124 | 9.182538 | -5.512389 |
| C | 1.044639 | 8.702011 | -5.332628 |
| H | 3.083776 | 9.619018 | -5.692542 |
| H | 0.072243 | 8.285789 | -5.174343 |