

Cartesian Coordinates of Structures 1-14 (optimized with PW91 potential) published in JACS 2008, 130, 15002-15021:

Structure 1:

184

|    |              |              |              |    |              |              |              |
|----|--------------|--------------|--------------|----|--------------|--------------|--------------|
| O  | 84.993741447 | 24.382011398 | 4.240671196  | Cu | 78.405034000 | 24.763772000 | 4.178497000  |
| O  | 88.485125260 | 24.532308495 | 1.791168405  | C  | 76.690150878 | 24.113262980 | 6.875894598  |
| O  | 84.501949589 | 20.082945667 | 1.705431384  | C  | 75.972252544 | 24.905615881 | 5.848162636  |
| O  | 86.326495557 | 22.109234657 | 5.011100950  | C  | 74.721139160 | 25.445301437 | 5.930851407  |
| Fe | 79.100034000 | 28.054773000 | 1.364498000  | N  | 76.547203117 | 25.312524303 | 4.648061128  |
| C  | 82.228444672 | 26.845237509 | 2.002756649  | C  | 75.645000555 | 26.061889187 | 4.018441970  |
| C  | 78.279962419 | 25.135388265 | -0.193270533 | N  | 74.523379834 | 26.184920429 | 4.779187695  |
| C  | 75.964450151 | 29.272482540 | 0.682947413  | C  | 71.636441857 | 29.583443197 | 6.845892890  |
| C  | 79.728955915 | 30.757519904 | 3.299310257  | C  | 72.043103441 | 28.802282252 | 5.629748707  |
| N  | 80.683032208 | 28.691687132 | 2.399487272  | C  | 71.486822411 | 29.034877333 | 4.358901325  |
| C  | 81.896396830 | 28.064118539 | 2.558902067  | C  | 71.914432713 | 28.341850598 | 3.237818918  |
| C  | 82.748011607 | 28.829990479 | 3.440897467  | C  | 73.039168615 | 27.829878440 | 5.721661001  |
| C  | 82.018615518 | 29.919759552 | 3.835898993  | C  | 73.475893559 | 27.125964518 | 4.604964633  |
| C  | 80.742013735 | 29.822635125 | 3.167955345  | C  | 72.942161392 | 27.353785350 | 3.293709498  |
| C  | 82.415909684 | 30.983006264 | 4.798047360  | O  | 73.374347789 | 26.704124255 | 2.265413626  |
| O  | 79.336034000 | 22.138773000 | -0.333504000 | C  | 78.697821125 | 19.649475699 | 1.784480612  |
| C  | 84.129192208 | 28.475270370 | 3.876910235  | C  | 78.227158388 | 20.893133379 | 2.478269844  |
| C  | 84.196443864 | 27.932173770 | 5.321689965  | C  | 78.932145288 | 22.004093542 | 2.905220840  |
| C  | 85.642580336 | 27.614734229 | 5.656797447  | N  | 76.873195314 | 21.139685980 | 2.652451419  |
| O  | 86.403446986 | 28.573807984 | 5.959331518  | C  | 76.817240758 | 22.375792758 | 3.172002571  |
| O  | 86.032940272 | 26.394795476 | 5.551618295  | N  | 78.031788594 | 22.953651447 | 3.337806426  |
| N  | 77.500145589 | 27.402771129 | 0.341788805  | C  | 82.479351968 | 21.483310588 | 5.698910208  |
| C  | 77.357118552 | 26.162513077 | -0.234089910 | C  | 81.744485253 | 22.731340439 | 5.369324790  |
| C  | 76.053712164 | 26.033458955 | -0.848471014 | C  | 80.402785689 | 23.005610412 | 5.397361866  |
| C  | 75.388784308 | 27.205915735 | -0.604965482 | N  | 82.335179918 | 23.866710799 | 4.847683496  |
| C  | 76.297220996 | 28.039343002 | 0.153122265  | C  | 81.368697909 | 24.763449865 | 4.570569644  |
| C  | 75.596644911 | 24.830523620 | -1.596589191 | N  | 80.173320600 | 24.268392758 | 4.881986894  |
| N  | 78.068399261 | 29.701393027 | 1.849557848  | C  | 82.543111532 | 30.323515305 | -2.447422442 |
| C  | 76.784327495 | 30.034167522 | 1.492494653  | C  | 81.342845171 | 29.840896124 | -1.723794853 |
| C  | 76.377071105 | 31.271210169 | 2.113842644  | C  | 81.203833465 | 29.235463780 | -0.502964928 |
| C  | 77.448414627 | 31.693451893 | 2.869247356  | N  | 80.059817195 | 29.941546507 | -2.218214230 |
| C  | 78.493982613 | 30.700927162 | 2.684092617  | C  | 79.197567636 | 29.416913619 | -1.325428061 |
| C  | 75.055801606 | 31.926867971 | 1.930363885  | N  | 79.865179355 | 28.976848462 | -0.263729205 |
| C  | 77.597748730 | 32.882015427 | 3.684447212  | C  | 91.087407057 | 28.484140436 | 2.856650562  |
| C  | 76.610289871 | 33.590969356 | 4.256489276  | N  | 90.128293028 | 27.413739829 | 3.041660621  |
| N  | 80.078038129 | 26.338750808 | 0.931992636  | C  | 89.094398037 | 27.450442121 | 3.888395913  |
| C  | 79.539325390 | 25.211393104 | 0.375552247  | N  | 88.227998233 | 26.439402256 | 3.892334755  |
| C  | 80.501142996 | 24.127552428 | 0.409764164  | N  | 88.919053922 | 28.485750084 | 4.710563163  |
| C  | 81.654917662 | 24.649524114 | 0.972485942  | H  | 77.187468000 | 24.805656000 | 7.571399000  |
| C  | 81.363333094 | 26.016360836 | 1.300240295  | H  | 72.456487000 | 30.243740000 | 7.189745000  |
| C  | 80.354073077 | 22.729377737 | 0.041210015  | H  | 79.556552000 | 19.138576000 | 2.253324000  |
| C  | 82.944133083 | 23.963158253 | 1.265263860  | H  | 82.592179000 | 20.840344000 | 4.808238000  |
| C  | 83.986420235 | 24.128975580 | 0.146024963  | H  | 82.504144146 | 31.411404530 | -2.602011670 |
| C  | 85.332743328 | 23.575146488 | 0.564919511  | H  | 81.979777262 | 28.985152626 | 0.206059870  |
| O  | 85.884985411 | 22.692029839 | -0.181341375 | H  | 79.923118132 | 31.602269067 | 3.953896116  |
| O  | 85.863926825 | 24.022249040 | 1.621214281  | H  | 78.624865881 | 33.221540637 | 3.844643822  |
| C  | 73.994368201 | 27.569810148 | -1.031617191 | H  | 78.130002506 | 29.367339745 | -1.484441963 |
| O  | 73.203407225 | 28.102710023 | 0.038123510  | H  | 90.216240642 | 26.582209811 | 2.461296214  |
| C  | 73.976513323 | 28.606301414 | -2.149423298 | H  | 75.731035378 | 26.508391573 | 3.037991116  |

|   |              |              |              |   |              |              |              |
|---|--------------|--------------|--------------|---|--------------|--------------|--------------|
| H | 73.511837030 | 27.637766500 | 6.685038853  | H | 83.570718092 | 27.034491071 | 5.425204145  |
| H | 70.701370356 | 29.785588873 | 4.253816809  | H | 84.571606068 | 27.738571690 | 3.188775970  |
| H | 75.563440676 | 33.301483939 | 4.187002777  | H | 84.767010093 | 29.372355638 | 3.819626911  |
| H | 76.843654756 | 34.480443490 | 4.841190695  | H | 88.368573566 | 25.660792510 | 3.232893680  |
| H | 72.936152427 | 28.799723171 | -2.447419902 | H | 87.480528602 | 26.394741999 | 4.614666286  |
| H | 74.423999940 | 29.549948362 | -1.804226369 | H | 89.583922675 | 29.253127053 | 4.732669289  |
| H | 74.538742002 | 28.249759655 | -3.023956787 | H | 88.050056633 | 28.536433684 | 5.284832041  |
| H | 73.289550593 | 27.511600779 | 0.862911518  | H | 85.275683622 | 24.396163868 | 3.285952011  |
| H | 71.463626796 | 28.540608517 | 2.264363247  | H | 85.341138390 | 25.222515132 | 4.705194886  |
| H | 70.759327731 | 30.209165399 | 6.639491003  | H | 91.695123275 | 28.642369210 | 3.758313258  |
| H | 71.395098536 | 28.912530479 | 7.683030430  | H | 90.589753972 | 29.421735506 | 2.572920804  |
| H | 73.958102751 | 25.366574270 | 6.694234429  | C | 84.177325636 | 19.296613997 | -3.110908051 |
| H | 81.550139419 | 25.746891835 | 4.160000370  | C | 84.780697921 | 20.066460834 | -1.978204429 |
| H | 79.592634196 | 22.358841564 | 5.709273604  | O | 85.237833342 | 19.530105363 | -0.965088302 |
| H | 83.353466759 | 24.024947707 | 4.667549539  | O | 84.756478218 | 21.389929632 | -2.156318997 |
| H | 83.472890610 | 21.694643759 | 6.112896825  | C | 88.808576257 | 20.764092156 | -1.345159919 |
| H | 81.916472334 | 20.908466029 | 6.444384754  | C | 88.814805481 | 20.685270898 | 0.136728890  |
| H | 79.794704276 | 30.342698183 | -3.117539805 | C | 89.655309386 | 20.037743444 | 1.000692300  |
| H | 79.997732431 | 22.198283178 | 2.909290261  | N | 87.841180502 | 21.276067871 | 0.921723600  |
| H | 75.893798928 | 22.872026160 | 3.452871043  | C | 88.062842802 | 21.001967613 | 2.208086279  |
| H | 78.993369195 | 19.880974584 | 0.748631507  | N | 89.163913137 | 20.251430691 | 2.268442136  |
| H | 77.869915589 | 18.928804960 | 1.736702716  | H | 84.681485000 | 19.503926000 | -4.065239000 |
| H | 75.989530686 | 23.497307571 | 7.453767271  | H | 88.765971000 | 21.799802000 | -1.706250000 |
| H | 77.442574998 | 23.453749781 | 6.427781100  | H | 89.713164791 | 20.292532980 | -1.744215860 |
| H | 83.440785513 | 30.088872100 | -1.864421819 | H | 87.934836671 | 20.232545348 | -1.749480178 |
| H | 82.633156495 | 29.840605907 | -3.431327761 | H | 84.225281731 | 18.225935263 | -2.893315674 |
| H | 75.155685102 | 33.019067541 | 1.988831522  | H | 83.128486961 | 19.601784851 | -3.229189477 |
| H | 74.609986393 | 31.673826129 | 0.960698118  | H | 90.545872722 | 19.450101798 | 0.822711302  |
| H | 74.346716486 | 31.620056788 | 2.715969579  | H | 87.465313137 | 21.328796825 | 3.054633191  |
| H | 82.000731831 | 31.961226415 | 4.520786237  | H | 87.034190846 | 21.869889141 | 0.536895553  |
| H | 82.055156055 | 30.745410633 | 5.811683549  | H | 84.787440892 | 20.000952245 | 0.761314645  |
| H | 83.508844595 | 31.079022143 | 4.847707379  | H | 83.589025000 | 19.723529000 | 1.696373000  |
| H | 74.947781604 | 29.612601989 | 0.513004887  | H | 87.537089625 | 24.211538660 | 1.685496524  |
| H | 83.230534652 | 26.470047848 | 2.196898218  | H | 89.056548359 | 23.778116929 | 1.528017008  |
| H | 78.005631369 | 24.179477407 | -0.631390451 | H | 85.169747128 | 21.875601385 | -1.340834435 |
| H | 74.543937162 | 24.918784671 | -1.889006463 | H | 91.740917000 | 28.167083000 | 2.038155000  |
| H | 76.191205795 | 24.691671567 | -2.512312809 | H | 73.524682662 | 26.648258105 | -1.417669981 |
| H | 75.708268720 | 23.918247480 | -0.992728761 | H | 89.576659989 | 19.892507338 | 3.129824356  |
| H | 81.300905728 | 22.155658835 | 0.144514487  | O | 78.500704023 | 27.182175857 | 2.901843749  |
| H | 83.640222548 | 23.649241924 | -0.778664263 | H | 85.611387027 | 21.463648144 | 5.188223517  |
| H | 84.129818081 | 25.201293579 | -0.065552391 | H | 85.837041926 | 22.943376283 | 4.753157101  |
| H | 83.367357336 | 24.366800682 | 2.193113182  | H | 77.625559281 | 27.569968225 | 3.108274846  |
| H | 82.782630421 | 22.890907180 | 1.447874338  |   |              |              |              |
| H | 83.824252277 | 28.697363849 | 6.017915290  |   |              |              |              |

## Structure 2:

183

|    |              |              |             |   |              |              |             |
|----|--------------|--------------|-------------|---|--------------|--------------|-------------|
| C  | 81.090814897 | 24.691240163 | 4.741938823 | N | 76.321715131 | 24.931346261 | 4.700046561 |
| N  | 79.913643394 | 24.127856751 | 4.996475577 | C | 75.376995554 | 25.638671689 | 4.091282669 |
| C  | 80.201555387 | 22.871546115 | 5.505340109 | N | 74.192509449 | 25.500514441 | 4.742216344 |
| C  | 81.558743083 | 22.677818758 | 5.535447552 | C | 74.407394434 | 24.642441980 | 5.810964600 |
| N  | 82.101936217 | 23.846141402 | 5.048888523 | C | 75.734595100 | 24.289355354 | 5.782360690 |
| Cu | 78.131000000 | 24.537000000 | 4.280000000 | C | 73.059127871 | 26.346922161 | 4.535444063 |

|    |              |              |              |   |              |              |              |
|----|--------------|--------------|--------------|---|--------------|--------------|--------------|
| C  | 72.684412359 | 26.711646369 | 3.200344719  | C | 82.140492889 | 31.059957215 | 5.065689413  |
| C  | 71.608247846 | 27.643232617 | 3.130365750  | C | 79.465818549 | 30.782143993 | 3.544529597  |
| C  | 71.005290900 | 28.185236484 | 4.257697909  | C | 78.209467765 | 30.708474242 | 2.946345795  |
| C  | 71.411966586 | 27.825467750 | 5.549575468  | N | 77.831044958 | 29.751310522 | 2.045344402  |
| C  | 72.442688603 | 26.892605071 | 5.657437116  | C | 76.527044998 | 30.022730945 | 1.701991273  |
| C  | 76.528836322 | 23.449368304 | 6.736358854  | C | 76.061915635 | 31.197170049 | 2.396565996  |
| H  | 76.891041224 | 24.068604560 | 7.571851711  | C | 77.114010517 | 31.631105402 | 3.187544212  |
| O  | 73.293246305 | 26.249145620 | 2.151085639  | C | 77.179470786 | 32.694181045 | 4.170084591  |
| C  | 70.897620516 | 28.529108411 | 6.770915554  | C | 76.405911016 | 33.789450894 | 4.267133377  |
| H  | 71.578001000 | 29.361002000 | 7.011997000  | C | 74.681576610 | 31.742437274 | 2.292177931  |
| C  | 82.370615376 | 21.493648728 | 5.913386921  | C | 75.745988502 | 29.247335095 | 0.845839981  |
| H  | 82.535000000 | 20.841000000 | 5.044000000  | C | 75.449510321 | 24.893579790 | -1.642018633 |
| N  | 78.002077246 | 22.836944697 | 2.904734774  | C | 82.474500068 | 30.377689079 | -2.650905955 |
| C  | 76.861603342 | 22.453639287 | 2.351421015  | H | 82.482004000 | 31.468996000 | -2.549001000 |
| N  | 76.997382422 | 21.233271851 | 1.779898192  | O | 85.708062700 | 24.248668985 | 1.922367144  |
| C  | 78.291839911 | 20.793290625 | 1.972107583  | O | 85.815831088 | 28.520316842 | 6.597376928  |
| C  | 78.898469346 | 21.811620968 | 2.669535074  | H | 85.180693860 | 22.193311400 | -1.078376012 |
| C  | 78.771711836 | 19.492803683 | 1.426404976  | N | 87.577541556 | 26.710802957 | 4.180616622  |
| H  | 79.537998000 | 19.027000000 | 2.065000000  | C | 88.391060843 | 27.769791869 | 4.206900111  |
| O  | 73.014154997 | 27.925579770 | 0.157645984  | N | 88.117170406 | 28.807804792 | 4.998605932  |
| C  | 73.808241952 | 27.506404220 | -0.955317469 | N | 89.456268862 | 27.783854979 | 3.403277280  |
| C  | 73.723624819 | 28.590129369 | -2.025820182 | C | 90.404389829 | 28.869681457 | 3.293073173  |
| H  | 72.672429820 | 28.748966848 | -2.305025229 | H | 91.324001000 | 28.427991000 | 2.916002000  |
| C  | 75.221258954 | 27.205800398 | -0.553822816 | N | 87.833746727 | 21.446123329 | 1.113807129  |
| C  | 76.092922017 | 28.037600381 | 0.255036127  | C | 88.153409410 | 21.053966817 | 2.345994650  |
| N  | 77.307791570 | 27.422889326 | 0.414307673  | N | 89.297435623 | 20.375158480 | 2.263410651  |
| C  | 77.222603076 | 26.209871519 | -0.227683521 | C | 89.723891091 | 20.334744562 | 0.955542643  |
| C  | 75.922631799 | 26.068472244 | -0.854229995 | C | 88.795171612 | 21.016400667 | 0.218467081  |
| Fe | 79.022001000 | 28.208998000 | 1.279999000  | C | 88.706039992 | 21.309590783 | -1.230976104 |
| N  | 79.807393362 | 29.037550061 | -0.466790551 | H | 88.624998000 | 22.392991000 | -1.404997000 |
| C  | 81.145127308 | 29.275784945 | -0.711112762 | O | 86.960281985 | 22.647547452 | 4.995559151  |
| C  | 81.286923063 | 29.850325115 | -1.946209496 | O | 84.836461717 | 24.333688126 | 4.606806162  |
| N  | 80.005716518 | 29.958436106 | -2.441068560 | O | 84.809558350 | 21.779699435 | -1.961226947 |
| C  | 79.141335395 | 29.457821628 | -1.533619690 | C | 84.671592554 | 20.458650935 | -1.861507723 |
| C  | 78.210446859 | 25.233747705 | -0.226020154 | O | 84.922828952 | 19.821567108 | -0.833481602 |
| C  | 79.455048927 | 25.286608474 | 0.402446965  | C | 84.185497819 | 19.816234256 | -3.122453461 |
| N  | 79.935839791 | 26.350875131 | 1.110326841  | H | 84.926997000 | 19.944991000 | -3.924995000 |
| C  | 81.199936797 | 26.026209893 | 1.544567369  | O | 84.219256161 | 20.443705985 | 1.806333507  |
| C  | 81.529426511 | 24.698483744 | 1.134047645  | O | 88.173155127 | 24.230406131 | 3.037432869  |
| C  | 80.440505752 | 24.227575067 | 0.404684016  | H | 78.000660551 | 24.303955687 | -0.746515941 |
| C  | 80.363019958 | 22.933075708 | -0.218608392 | H | 83.011594230 | 26.492797251 | 2.545737357  |
| O  | 79.457488455 | 22.529401160 | -0.961711342 | H | 79.640702875 | 31.617021004 | 4.218502128  |
| C  | 82.810700360 | 24.004790895 | 1.428950268  | H | 74.725372720 | 29.579118221 | 0.673646634  |
| C  | 83.897082824 | 24.293867081 | 0.377239005  | H | 74.505959879 | 24.501152180 | -1.234575819 |
| C  | 85.240466401 | 23.780855831 | 0.848760470  | H | 75.265255697 | 25.163066836 | -2.692687972 |
| O  | 85.840773919 | 22.902161250 | 0.131497528  | H | 76.181386291 | 24.077163676 | -1.636714739 |
| C  | 82.021532105 | 26.872307508 | 2.303254875  | H | 81.225436342 | 22.266280177 | 0.000826122  |
| C  | 81.692135575 | 28.109553774 | 2.832738091  | H | 73.389192646 | 26.578975149 | -1.386759372 |
| N  | 80.494020778 | 28.755333094 | 2.622088026  | H | 74.136876504 | 29.537628430 | -1.650805296 |
| C  | 80.515807220 | 29.883187402 | 3.402719582  | H | 74.287181816 | 28.294448152 | -2.922704810 |
| C  | 81.777011825 | 29.980425929 | 4.108092761  | H | 77.958549668 | 32.569026295 | 4.927102311  |
| C  | 82.511565389 | 28.883310143 | 3.748066467  | H | 75.627258464 | 34.031900041 | 3.547029864  |
| C  | 83.847393806 | 28.496664872 | 4.281547999  | H | 76.558654745 | 34.488729711 | 5.089351604  |
| C  | 83.744939921 | 27.809131839 | 5.660909655  | H | 81.495877464 | 31.029528945 | 5.957881754  |
| C  | 85.141951776 | 27.538547291 | 6.181657442  | H | 82.022400897 | 32.054063734 | 4.609632390  |
| O  | 85.603813030 | 26.342149193 | 6.097224085  | H | 83.180700089 | 30.961002633 | 5.398880675  |

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|---|--------------|--------------|--------------|---|--------------|--------------|--------------|
| H | 74.435086531 | 32.371046577 | 3.155919410  | H | 84.473593324 | 29.395897470 | 4.390659869  |
| H | 73.941269984 | 30.931102774 | 2.238668446  | H | 84.372145669 | 27.835801703 | 3.573555929  |
| H | 74.564433925 | 32.355860548 | 1.382998403  | H | 83.221502872 | 28.480270750 | 6.357851333  |
| H | 81.913102267 | 29.028478926 | 0.012021416  | H | 83.169842389 | 26.876096434 | 5.582457935  |
| H | 83.388968771 | 29.980141535 | -2.197979125 | H | 87.002533930 | 22.056364621 | 0.830456182  |
| H | 82.462705964 | 30.121269666 | -3.717511844 | H | 87.606169449 | 21.263955080 | 3.255920703  |
| H | 79.745748807 | 30.356105407 | -3.343000187 | H | 89.783117357 | 19.959955801 | 3.058806160  |
| H | 78.070772008 | 29.413838696 | -1.681405875 | H | 90.636587459 | 19.832339762 | 0.665667097  |
| H | 75.481457024 | 26.236240987 | 3.195561826  | H | 89.597168792 | 20.934633802 | -1.745569669 |
| H | 73.605466097 | 24.369995125 | 6.485846882  | H | 87.821470189 | 20.826707163 | -1.670862981 |
| H | 75.906801086 | 22.650028400 | 7.160505242  | H | 90.618153654 | 29.300464753 | 4.278620234  |
| H | 77.427000000 | 22.984000000 | 6.282000000  | H | 90.054838551 | 29.656646986 | 2.610281774  |
| H | 71.278968325 | 27.951230596 | 2.137178998  | H | 89.567398026 | 26.991830781 | 2.773296319  |
| H | 70.213234649 | 28.927159523 | 4.134113822  | H | 88.728047123 | 29.618546809 | 5.022328418  |
| H | 69.894291428 | 28.943438008 | 6.607885567  | H | 87.341573740 | 28.734771362 | 5.686663899  |
| H | 70.864294386 | 27.860565209 | 7.641462048  | H | 87.903061571 | 25.836374787 | 3.717608371  |
| H | 72.817809441 | 26.621526354 | 6.645721806  | H | 86.924651955 | 26.585558921 | 4.975028609  |
| H | 75.928185711 | 23.001993741 | 2.360366378  | H | 84.007018790 | 18.750273175 | -2.955034487 |
| H | 76.257885638 | 20.718246694 | 1.302742622  | H | 83.259948258 | 20.305001893 | -3.454340981 |
| H | 79.921742131 | 21.870165932 | 3.021129739  | H | 73.149996636 | 27.251277246 | 0.923906186  |
| H | 79.199420259 | 19.621439890 | 0.420641088  | H | 83.454980994 | 19.832225350 | 1.863779679  |
| H | 77.937028555 | 18.784283641 | 1.344284646  | H | 84.528611794 | 20.328131041 | 0.871278821  |
| H | 79.423516335 | 22.175858412 | 5.794381405  | H | 87.923926355 | 23.653820799 | 3.811900281  |
| H | 83.348687257 | 21.788351796 | 6.313533445  | H | 87.340223302 | 24.182931861 | 2.482473471  |
| H | 81.847860431 | 20.904221392 | 6.676157063  | H | 87.284040805 | 22.739952219 | 5.918086584  |
| H | 83.119444229 | 24.032107622 | 4.913515415  | H | 86.138809185 | 23.223602133 | 4.957163896  |
| H | 83.183524401 | 24.332970644 | 2.407335642  | H | 85.072021439 | 25.181489036 | 5.126865495  |
| H | 82.667239556 | 22.916529242 | 1.507425099  | H | 85.066113049 | 24.471536813 | 3.649981369  |
| H | 83.991137318 | 25.383132381 | 0.236073674  | H | 81.236945978 | 25.688027112 | 4.350679264  |
| H | 83.622408917 | 23.853388235 | -0.590576945 |   |              |              |              |

### Structure 3:

189

|    |              |              |             |   |              |              |              |
|----|--------------|--------------|-------------|---|--------------|--------------|--------------|
| C  | 81.101870513 | 24.656880219 | 4.590707968 | C | 70.866729417 | 28.548992912 | 6.780898415  |
| N  | 79.925025213 | 24.124298576 | 4.905695664 | H | 71.578000000 | 29.361002000 | 7.011997000  |
| C  | 80.207998560 | 22.901503726 | 5.491099259 | C | 82.361874151 | 21.507209356 | 5.904414663  |
| C  | 81.561519677 | 22.690555095 | 5.499834486 | H | 82.535000000 | 20.841000000 | 5.044000000  |
| N  | 82.107574170 | 23.821005760 | 4.930632953 | N | 77.773920428 | 22.442458463 | 3.480923086  |
| Cu | 78.131000000 | 24.537000000 | 4.280000000 | C | 76.616232656 | 22.056219549 | 2.966109667  |
| N  | 76.290019134 | 24.887264959 | 4.894154656 | N | 76.779780825 | 20.941440024 | 2.211904387  |
| C  | 75.356772101 | 25.610997067 | 4.307660210 | C | 78.110025214 | 20.582538494 | 2.239345678  |
| N  | 74.153065950 | 25.423627280 | 4.903762361 | C | 78.708005686 | 21.532338203 | 3.031291439  |
| C  | 74.351499750 | 24.512176921 | 5.939370522 | C | 78.662572355 | 19.406501849 | 1.521737499  |
| C  | 75.673061174 | 24.180931524 | 5.920690767 | H | 79.538000000 | 19.026998000 | 2.065001000  |
| C  | 73.032317157 | 26.268676669 | 4.663750199 | O | 73.189888244 | 27.788049053 | 0.191517963  |
| C  | 72.681564995 | 26.637911170 | 3.354928034 | C | 73.909216441 | 27.522932727 | -1.053787924 |
| C  | 71.651916376 | 27.576665442 | 3.190092811 | C | 73.670459780 | 28.654707740 | -2.044502481 |
| C  | 71.029244526 | 28.154268193 | 4.291317726 | H | 72.593411728 | 28.755613657 | -2.243456649 |
| C  | 71.391821150 | 27.807581357 | 5.589826242 | C | 75.349056029 | 27.292837809 | -0.729953075 |
| C  | 72.387731488 | 26.839392778 | 5.756822139 | C | 76.212126498 | 28.114664797 | 0.087857944  |
| C  | 76.482725996 | 23.264178319 | 6.786712725 | N | 77.466120614 | 27.552515356 | 0.182244714  |
| H  | 76.748708880 | 23.758810569 | 7.732407783 | C | 77.420860234 | 26.420105658 | -0.597594597 |
| O  | 73.346566181 | 26.097009614 | 2.301624662 | C | 76.106354808 | 26.242831227 | -1.174351567 |

|    |              |              |              |   |              |              |              |
|----|--------------|--------------|--------------|---|--------------|--------------|--------------|
| Fe | 79.022001000 | 28.208997000 | 1.279999000  | C | 88.710636450 | 21.314328297 | -1.203121116 |
| N  | 79.791399294 | 29.117337677 | -0.350036839 | H | 88.625001000 | 22.392995000 | -1.404995000 |
| C  | 81.131307882 | 29.286395380 | -0.641112464 | O | 86.868187020 | 22.649315273 | 5.046858806  |
| C  | 81.257029949 | 29.899713678 | -1.859645136 | O | 84.791101124 | 24.354787965 | 4.545419761  |
| N  | 79.965465396 | 30.097493201 | -2.296815891 | O | 84.821564068 | 21.800652558 | -1.973238211 |
| C  | 79.108807507 | 29.617544917 | -1.373272503 | C | 84.719429890 | 20.477267284 | -1.854625786 |
| C  | 78.435215318 | 25.486387494 | -0.694967043 | O | 85.007517960 | 19.866201888 | -0.820415647 |
| C  | 79.623559588 | 25.523070730 | 0.018513464  | C | 84.219569336 | 19.803297123 | -3.093752059 |
| N  | 80.042578010 | 26.552277054 | 0.819560130  | H | 84.927003000 | 19.944993000 | -3.924993000 |
| C  | 81.264038494 | 26.175996501 | 1.329986450  | O | 84.178193508 | 20.525136401 | 1.780259896  |
| C  | 81.600930894 | 24.852428784 | 0.905903725  | O | 88.148747067 | 24.197028265 | 3.118370321  |
| C  | 80.577973265 | 24.439115051 | 0.068838178  | H | 78.276065166 | 24.607137710 | -1.311613235 |
| C  | 80.501237601 | 23.143633540 | -0.560372686 | H | 83.034225574 | 26.550785389 | 2.435388339  |
| O  | 79.602825497 | 22.750391658 | -1.313183460 | H | 79.728646268 | 31.738586627 | 3.946363982  |
| C  | 82.834817821 | 24.121167936 | 1.290473003  | H | 74.798663085 | 29.604938790 | 0.557549874  |
| C  | 83.973331523 | 24.366456980 | 0.286597700  | H | 74.710894912 | 24.697343587 | -1.664859374 |
| C  | 85.280746193 | 23.816719726 | 0.812491968  | H | 75.504962540 | 25.430656494 | -3.070208607 |
| O  | 85.883422828 | 22.929182847 | 0.110831992  | H | 76.394928207 | 24.291649748 | -2.044057095 |
| C  | 82.069697932 | 26.960597273 | 2.146271140  | H | 81.345469364 | 22.464832459 | -0.314824584 |
| C  | 81.738802524 | 28.202681413 | 2.643189618  | H | 73.507754758 | 26.592954527 | -1.484258140 |
| N  | 80.565962178 | 28.862122745 | 2.370983714  | H | 74.056687365 | 29.609861500 | -1.661111955 |
| C  | 80.592449143 | 29.993317767 | 3.139518023  | H | 74.176411108 | 28.428815737 | -2.994619087 |
| C  | 81.818939330 | 30.070285059 | 3.902599673  | H | 78.027382287 | 32.579636104 | 4.742354616  |
| C  | 82.540464649 | 28.954989056 | 3.585553495  | H | 75.641724965 | 34.006500414 | 3.416886568  |
| C  | 83.841783943 | 28.534033340 | 4.174229521  | H | 76.539310066 | 34.430810689 | 4.988523102  |
| C  | 83.676922590 | 27.846952547 | 5.548482950  | H | 81.463448943 | 31.064865390 | 5.762125883  |
| C  | 85.055235233 | 27.560874140 | 6.112219684  | H | 82.026384189 | 32.135566955 | 4.464482354  |
| O  | 85.499387634 | 26.355839813 | 6.065467275  | H | 83.167069368 | 31.028929787 | 5.263090769  |
| C  | 82.139690381 | 31.130490824 | 4.895089794  | H | 74.492965141 | 32.245673460 | 3.110902792  |
| C  | 79.564575778 | 30.908817571 | 3.265173126  | H | 74.037283650 | 30.868802523 | 2.090058204  |
| C  | 78.326703750 | 30.816884230 | 2.655826383  | H | 74.555548823 | 32.392888460 | 1.342802056  |
| N  | 77.965549643 | 29.860054190 | 1.749977276  | H | 81.913797482 | 28.971681681 | 0.036163117  |
| C  | 76.637343921 | 30.089601294 | 1.481251809  | H | 83.355300361 | 29.970869807 | -2.151063358 |
| C  | 76.148685271 | 31.236416363 | 2.206521117  | H | 82.405514566 | 30.076058269 | -3.659232619 |
| C  | 77.206010634 | 31.695660253 | 2.957263817  | H | 79.691848606 | 30.529169610 | -3.178926625 |
| C  | 77.248074946 | 32.714560047 | 3.987226333  | H | 78.034596527 | 29.641428253 | -1.484503228 |
| C  | 76.425167838 | 33.767455507 | 4.131768674  | H | 75.493870052 | 26.276390990 | 3.470527294  |
| C  | 74.737446767 | 31.708164089 | 2.185893890  | H | 73.525588255 | 24.193306153 | 6.570673525  |
| C  | 75.830838704 | 29.297894721 | 0.685608555  | H | 75.927014012 | 22.349259030 | 7.028735124  |
| C  | 75.663656269 | 25.107612522 | -2.029655381 | H | 77.427000000 | 22.984001000 | 6.282000000  |
| C  | 82.443124824 | 30.374442726 | -2.602973547 | H | 71.351921707 | 27.856680831 | 2.183482051  |
| H  | 82.482002000 | 31.468994000 | -2.549003000 | H | 70.257517298 | 28.909808000 | 4.126838834  |
| O  | 85.716537517 | 24.266655989 | 1.906876279  | H | 69.885869435 | 28.995579579 | 6.576838665  |
| O  | 85.732203746 | 28.540469431 | 6.527576249  | H | 70.791205620 | 27.902743978 | 7.663472965  |
| H  | 85.207160116 | 22.221366454 | -1.101987304 | H | 72.720711210 | 26.572333496 | 6.757071405  |
| N  | 87.584304436 | 26.699276437 | 4.244099380  | H | 75.660184440 | 22.546025274 | 3.096147904  |
| C  | 88.400172390 | 27.755818496 | 4.261521617  | H | 76.039335910 | 20.450962756 | 1.710772032  |
| N  | 88.120033151 | 28.803165408 | 5.038382092  | H | 79.753999043 | 21.612588762 | 3.301005922  |
| N  | 89.479295894 | 27.751560859 | 3.474620946  | H | 78.973121294 | 19.663519977 | 0.498428061  |
| C  | 90.408656557 | 28.851851489 | 3.334604767  | H | 77.922707986 | 18.598446233 | 1.457818133  |
| H  | 91.324000000 | 28.427995000 | 2.916003000  | H | 79.426166461 | 22.234926471 | 5.830963330  |
| N  | 87.839665644 | 21.463804625 | 1.143456186  | H | 83.336655144 | 21.800296875 | 6.315462857  |
| C  | 88.158408151 | 21.075406978 | 2.376561718  | H | 81.823101426 | 20.932531174 | 6.666913814  |
| N  | 89.307697472 | 20.405099241 | 2.298186969  | H | 83.128447023 | 24.004343376 | 4.790156363  |
| C  | 89.737863035 | 20.367081882 | 0.991382895  | H | 83.165473255 | 24.451640581 | 2.282360165  |
| C  | 88.806166811 | 21.041263903 | 0.250842087  | H | 82.648098846 | 23.040132264 | 1.376596145  |

|   |              |              |              |   |              |              |              |
|---|--------------|--------------|--------------|---|--------------|--------------|--------------|
| H | 84.105024169 | 25.450695866 | 0.139968882  | H | 84.082320788 | 18.734299950 | -2.908117152 |
| H | 83.722727228 | 23.926075034 | -0.687352730 | H | 83.266684772 | 20.255846037 | -3.399101060 |
| H | 84.481969084 | 29.418528982 | 4.310379995  | H | 73.236961450 | 26.686585598 | 1.486922808  |
| H | 84.380089923 | 27.863211807 | 3.486708315  | H | 83.474978799 | 19.846210358 | 1.852810201  |
| H | 83.141095678 | 28.525978592 | 6.228452450  | H | 84.530377390 | 20.388102899 | 0.863946298  |
| H | 83.090878884 | 26.922823825 | 5.452223760  | H | 87.859195406 | 23.638320942 | 3.892141752  |
| H | 87.010990945 | 22.071958163 | 0.852258486  | H | 87.334268222 | 24.176140865 | 2.537917942  |
| H | 87.603312761 | 21.275858532 | 3.283707870  | H | 87.167448694 | 22.764640400 | 5.975329294  |
| H | 89.793104754 | 19.993484951 | 3.095520852  | H | 86.057988188 | 23.236124105 | 4.968225557  |
| H | 90.655888098 | 19.871745146 | 0.705618109  | H | 85.008769236 | 25.202669086 | 5.076336193  |
| H | 89.599293900 | 20.928913387 | -1.713924025 | H | 85.054248418 | 24.486588986 | 3.595513992  |
| H | 87.825715260 | 20.819539298 | -1.628464438 | H | 81.246146460 | 25.626230325 | 4.134472012  |
| H | 90.647377573 | 29.282809433 | 4.314653133  | O | 78.421442414 | 27.515998907 | 2.808262551  |
| H | 90.025283942 | 29.637752955 | 2.668358466  | O | 77.130807941 | 27.599485179 | 3.059891892  |
| H | 89.584017357 | 26.955480580 | 2.845553301  | O | 77.223586573 | 24.880477810 | 2.124075780  |
| H | 88.710722096 | 29.629166183 | 5.033524233  | H | 77.207458534 | 25.833560464 | 1.894933152  |
| H | 87.308337974 | 28.753189528 | 5.684830007  | H | 77.859673362 | 24.489360045 | 1.487056768  |
| H | 87.901388950 | 25.816703547 | 3.790264878  | H | 72.253783496 | 27.940944395 | -0.065825762 |
| H | 86.902851060 | 26.595913400 | 5.016894623  |   |              |              |              |

#### Structure 4:

188

|    |              |              |             |    |              |              |              |
|----|--------------|--------------|-------------|----|--------------|--------------|--------------|
| C  | 81.086365796 | 24.618099429 | 4.640537840 | O  | 73.126931403 | 27.811120718 | 0.165384650  |
| N  | 79.927373570 | 24.071979849 | 4.997308352 | C  | 73.876748666 | 27.514899449 | -1.058634350 |
| C  | 80.235318888 | 22.857812790 | 5.581923783 | C  | 73.677894038 | 28.641414793 | -2.062759861 |
| C  | 81.592135042 | 22.669308948 | 5.560207184 | H  | 72.607127394 | 28.754088212 | -2.289525379 |
| N  | 82.108000853 | 23.802437605 | 4.966174371 | C  | 75.301362440 | 27.257825401 | -0.689334882 |
| Cu | 78.131000000 | 24.537000000 | 4.280000000 | C  | 76.190425420 | 28.117824532 | 0.064051880  |
| N  | 76.287631549 | 24.861217902 | 4.719502574 | N  | 77.427350581 | 27.540290071 | 0.199094694  |
| C  | 75.391141010 | 25.648587703 | 4.148974408 | C  | 77.332562231 | 26.323558370 | -0.432219958 |
| N  | 74.200844936 | 25.516524177 | 4.783885342 | C  | 76.014118650 | 26.133744522 | -1.000724068 |
| C  | 74.367996155 | 24.594926334 | 5.807345306 | Fe | 79.021999000 | 28.208999000 | 1.279999000  |
| C  | 75.676653195 | 24.185854382 | 5.765721215 | N  | 79.742040686 | 29.145675803 | -0.289339276 |
| C  | 73.070647453 | 26.358057269 | 4.579224919 | C  | 81.081120123 | 29.275330058 | -0.606741022 |
| C  | 72.646500080 | 26.680163858 | 3.278311077 | C  | 81.202774941 | 29.942709578 | -1.797951485 |
| C  | 71.575725606 | 27.567560652 | 3.143698724 | N  | 79.910113871 | 30.211102781 | -2.190825700 |
| C  | 70.973927954 | 28.140457910 | 4.259511639 | C  | 79.055044223 | 29.723449333 | -1.268194963 |
| C  | 71.408844098 | 27.835821499 | 5.551643014 | C  | 78.318675124 | 25.359490624 | -0.452026794 |
| C  | 72.454734863 | 26.924685196 | 5.689039435 | C  | 79.549938930 | 25.456245417 | 0.170107610  |
| C  | 76.425735604 | 23.255154114 | 6.667221838 | N  | 80.023764955 | 26.549371924 | 0.843890176  |
| H  | 76.581159445 | 23.724958974 | 7.649774767 | C  | 81.258297018 | 26.190744123 | 1.336369071  |
| O  | 73.285046572 | 26.124851614 | 2.217958251 | C  | 81.575126430 | 24.840331115 | 0.986559114  |
| C  | 70.875724326 | 28.551007066 | 6.755333779 | C  | 80.504904708 | 24.372598889 | 0.244200228  |
| H  | 71.578000000 | 29.361000000 | 7.012001000 | C  | 80.403388461 | 23.037727505 | -0.289451913 |
| C  | 82.416982048 | 21.492064047 | 5.923776045 | O  | 79.497172320 | 22.594087154 | -1.007089434 |
| H  | 82.535000000 | 20.841000000 | 5.044000000 | C  | 82.825216229 | 24.129535916 | 1.361583152  |
| N  | 77.892099778 | 22.703037662 | 3.249653895 | C  | 83.927895266 | 24.302385651 | 0.306414751  |
| C  | 76.753584551 | 22.328512041 | 2.680297820 | C  | 85.260002234 | 23.780907802 | 0.807563667  |
| N  | 76.931962498 | 21.173442358 | 2.005223099 | O  | 85.891928380 | 22.939854034 | 0.079518383  |
| C  | 78.245038610 | 20.767892731 | 2.138480621 | C  | 82.070894200 | 26.997406994 | 2.123141676  |
| C  | 78.828005150 | 21.741658113 | 2.912491178 | C  | 81.713069584 | 28.221616917 | 2.641655735  |
| C  | 78.759577587 | 19.535785941 | 1.475674221 | N  | 80.505796826 | 28.844764030 | 2.411691992  |
| H  | 79.537999000 | 19.027000000 | 2.064998000 | C  | 80.533248002 | 29.980204431 | 3.180668223  |

|   |              |              |              |   |              |              |              |
|---|--------------|--------------|--------------|---|--------------|--------------|--------------|
| C | 81.781826794 | 30.089543360 | 3.900805260  | H | 77.925235707 | 32.603632363 | 4.767533398  |
| C | 82.520488510 | 28.992719831 | 3.562024877  | H | 75.632197351 | 34.028879918 | 3.285100529  |
| C | 83.836692237 | 28.590200805 | 4.131293268  | H | 76.476754325 | 34.509011156 | 4.870697639  |
| C | 83.681667452 | 27.878630804 | 5.493933146  | H | 81.468393912 | 31.106320349 | 5.761670909  |
| C | 85.056003757 | 27.593824080 | 6.066246544  | H | 81.974431904 | 32.164926336 | 4.432019885  |
| O | 85.496936981 | 26.387979688 | 6.032593540  | H | 83.155796291 | 31.086973040 | 5.208543368  |
| C | 82.115147677 | 31.167073905 | 4.872424515  | H | 74.425332281 | 32.199217289 | 3.090705774  |
| C | 79.491594083 | 30.875519286 | 3.333366626  | H | 73.998594501 | 30.957151053 | 1.895365326  |
| C | 78.253494307 | 30.767913613 | 2.731870746  | H | 74.606591010 | 32.536569242 | 1.358848760  |
| N | 77.903611703 | 29.799000620 | 1.827919867  | H | 81.865857858 | 28.894233302 | 0.032782401  |
| C | 76.598495768 | 30.077523968 | 1.487028193  | H | 83.297556800 | 29.949125136 | -2.117822342 |
| C | 76.107938795 | 31.237989391 | 2.193210831  | H | 82.331894345 | 30.048251134 | -3.613338172 |
| C | 77.146836262 | 31.673881511 | 2.983792432  | H | 79.632691512 | 30.704566803 | -3.038502311 |
| C | 77.177329447 | 32.726080736 | 3.979219706  | H | 77.980227152 | 29.797500748 | -1.345845802 |
| C | 76.379176453 | 33.805474443 | 4.044096342  | H | 75.561287586 | 26.306937377 | 3.307992608  |
| C | 74.714815025 | 31.755485430 | 2.127885882  | H | 73.547835267 | 24.323686544 | 6.459562283  |
| C | 75.812828643 | 29.314404969 | 0.644741603  | H | 75.864630599 | 22.325326394 | 6.826721374  |
| C | 75.544621460 | 24.932443779 | -1.748502440 | H | 77.427000000 | 22.984000000 | 6.282000000  |
| C | 82.392973344 | 30.374221208 | -2.565783182 | H | 71.213958465 | 27.810248475 | 2.145342334  |
| H | 82.481997000 | 31.468999000 | -2.549004000 | H | 70.158495762 | 28.851148977 | 4.117269126  |
| O | 85.693389713 | 24.224378979 | 1.907945203  | H | 69.892496236 | 28.994125678 | 6.558202077  |
| O | 85.733344158 | 28.575188147 | 6.479447977  | H | 70.800041220 | 27.882829652 | 7.622294676  |
| H | 85.262444912 | 22.252483419 | -1.115054059 | H | 72.841425025 | 26.687467617 | 6.679759716  |
| N | 87.578152258 | 26.690354849 | 4.194636760  | H | 75.803852305 | 22.843561024 | 2.741374934  |
| C | 88.394401530 | 27.745665770 | 4.224401675  | H | 76.206321758 | 20.681578250 | 1.484088153  |
| N | 88.135921191 | 28.774221470 | 5.034422108  | H | 79.854926564 | 21.811776474 | 3.247034761  |
| N | 89.463230807 | 27.761089527 | 3.424110428  | H | 79.179569877 | 19.770775398 | 0.486368022  |
| C | 90.409159719 | 28.851516248 | 3.330181280  | H | 77.940062949 | 18.820354175 | 1.327722603  |
| H | 91.324000000 | 28.428000000 | 2.915991000  | H | 79.473042790 | 22.182258466 | 5.949938556  |
| N | 87.904097466 | 21.383106604 | 1.116062260  | H | 83.413086011 | 21.784332574 | 6.278111805  |
| C | 88.262103703 | 20.914551539 | 2.333321607  | H | 81.922285496 | 20.908891737 | 6.709368948  |
| N | 89.390133310 | 20.217967638 | 2.259987184  | H | 83.125701722 | 23.999230711 | 4.802806700  |
| C | 89.763835447 | 20.252925915 | 0.929051858  | H | 83.198615933 | 24.519622122 | 2.315778883  |
| C | 88.848526018 | 20.976919152 | 0.200787350  | H | 82.645112329 | 23.055628490 | 1.520709242  |
| C | 88.745257744 | 21.310388067 | -1.244774166 | H | 84.062220250 | 25.375249281 | 0.088907702  |
| H | 88.624997000 | 22.392997000 | -1.405005000 | H | 83.641987947 | 23.808297659 | -0.631665933 |
| O | 86.923531007 | 22.719251043 | 5.106589093  | H | 84.462378991 | 29.483523437 | 4.279957330  |
| O | 84.786320805 | 24.361923813 | 4.553670617  | H | 84.383726329 | 27.939130103 | 3.431458019  |
| O | 84.907470851 | 21.823087448 | -2.009126693 | H | 83.135561191 | 28.541190947 | 6.182313742  |
| C | 84.689009591 | 20.519896302 | -1.863067655 | H | 83.104428571 | 26.950861782 | 5.379525805  |
| O | 84.864813860 | 19.913012217 | -0.800658690 | H | 87.089610354 | 21.991634390 | 0.872103301  |
| C | 84.195657337 | 19.848906620 | -3.108991911 | H | 87.694886286 | 21.110729239 | 3.235092196  |
| H | 84.926997000 | 19.944997000 | -3.925002000 | H | 90.662202373 | 19.758159831 | 0.575562465  |
| O | 84.057423096 | 20.646396049 | 1.785522939  | H | 89.646564618 | 20.977157467 | -1.772195931 |
| O | 88.149847462 | 24.195725876 | 3.069875276  | H | 87.878836371 | 20.811302642 | -1.702677421 |
| H | 78.114437503 | 24.416393029 | -0.949294716 | H | 90.639008681 | 29.248174311 | 4.326179140  |
| H | 83.051284090 | 26.610712228 | 2.391043756  | H | 90.044907869 | 29.661313549 | 2.682544735  |
| H | 79.655811610 | 31.713019222 | 4.005770681  | H | 89.564998883 | 26.984242424 | 2.774579953  |
| H | 74.791437520 | 29.640904081 | 0.482117375  | H | 88.684673977 | 29.627196062 | 4.984893266  |
| H | 74.540239967 | 24.632145840 | -1.418071060 | H | 87.304512284 | 28.737546980 | 5.658084282  |
| H | 75.489174988 | 25.130959213 | -2.829916034 | H | 87.893518553 | 25.803011145 | 3.742239191  |
| H | 76.212717190 | 24.075445726 | -1.605477655 | H | 86.891444499 | 26.590162243 | 4.962774034  |
| H | 81.248251366 | 22.373438559 | -0.007214753 | H | 84.002881153 | 18.790605858 | -2.911085174 |
| H | 73.465984683 | 26.589212524 | -1.487647856 | H | 83.271423670 | 20.338938966 | -3.443912927 |
| H | 74.063869546 | 29.595036555 | -1.676363924 | H | 73.167287913 | 26.719035409 | 1.402005509  |
| H | 74.205330465 | 28.402949147 | -2.997718568 | H | 83.352969331 | 19.967351036 | 1.845012255  |

|   |              |              |             |   |              |              |              |
|---|--------------|--------------|-------------|---|--------------|--------------|--------------|
| H | 84.425126862 | 20.503732613 | 0.875889974 | H | 81.194820396 | 25.573890025 | 4.146464283  |
| H | 87.885506521 | 23.635972750 | 3.853331838 | O | 78.163726668 | 27.195972427 | 2.741297854  |
| H | 87.323305848 | 24.145084460 | 2.505906026 | O | 78.887510178 | 26.364591638 | 3.520594506  |
| H | 87.248629869 | 22.930345396 | 6.009073649 | H | 72.205483791 | 28.009215547 | -0.117270381 |
| H | 86.102378108 | 23.284093395 | 5.001047528 | H | 90.158236579 | 19.483881278 | 3.623833550  |
| H | 85.002907695 | 25.223099705 | 5.059955970 | O | 90.579960200 | 19.072748934 | 4.450785383  |
| H | 85.044703129 | 24.465061682 | 3.597741828 | H | 91.402350642 | 18.662928686 | 4.111595531  |

Structure 5:

185

|    |              |              |              |   |              |              |              |
|----|--------------|--------------|--------------|---|--------------|--------------|--------------|
| C  | 81.082149063 | 24.611972427 | 4.669853643  | C | 81.214574892 | 29.934317464 | -1.811182899 |
| N  | 79.924478723 | 24.065663883 | 5.029640721  | N | 79.921064469 | 30.173627354 | -2.220088676 |
| C  | 80.235803628 | 22.849659696 | 5.607657735  | C | 79.067081700 | 29.688778071 | -1.294565571 |
| C  | 81.592629006 | 22.660058240 | 5.579219495  | C | 78.304624274 | 25.372334609 | -0.467931033 |
| N  | 82.106305269 | 23.793081529 | 4.986509551  | C | 79.535865128 | 25.457626745 | 0.158823772  |
| Cu | 78.131000000 | 24.537000000 | 4.280000000  | N | 80.013628913 | 26.544729577 | 0.834117764  |
| N  | 76.275795571 | 24.825974936 | 4.695186163  | C | 81.246916336 | 26.181730276 | 1.326986303  |
| C  | 75.360180960 | 25.573801953 | 4.093725621  | C | 81.558334008 | 24.834415629 | 0.971665074  |
| N  | 74.176961690 | 25.463334452 | 4.744193673  | C | 80.486339168 | 24.370190746 | 0.227588825  |
| C  | 74.363164813 | 24.584726597 | 5.802482404  | C | 80.377279439 | 23.039202990 | -0.312603647 |
| C  | 75.678436956 | 24.188755842 | 5.769539017  | O | 79.468805467 | 22.601963144 | -1.031542447 |
| C  | 73.059963997 | 26.328214971 | 4.533173120  | C | 82.808287334 | 24.120970490 | 1.342519443  |
| C  | 72.705608691 | 26.707172250 | 3.196607080  | C | 83.926821178 | 24.336678179 | 0.309765619  |
| C  | 71.626761805 | 27.636382616 | 3.125377109  | C | 85.243378555 | 23.793646575 | 0.819939410  |
| C  | 71.021263296 | 28.177395048 | 4.251492102  | O | 85.845463633 | 22.909455224 | 0.112400276  |
| C  | 71.421967322 | 27.815876646 | 5.547088396  | C | 82.062190884 | 26.980865146 | 2.119578132  |
| C  | 72.441904408 | 26.872055154 | 5.655012761  | C | 81.710899556 | 28.203992589 | 2.646600382  |
| C  | 76.452549403 | 23.307202022 | 6.699885438  | N | 80.511574672 | 28.838223046 | 2.413178150  |
| H  | 76.673862959 | 23.842917714 | 7.635412728  | C | 80.530923473 | 29.955446893 | 3.207288077  |
| O  | 73.332007402 | 26.258917039 | 2.151630587  | C | 81.770055441 | 30.046657935 | 3.943946840  |
| C  | 70.905182635 | 28.520322782 | 6.767649844  | C | 82.511597203 | 28.955901910 | 3.589539185  |
| H  | 71.578000000 | 29.361000000 | 7.012000000  | C | 83.826935799 | 28.548626045 | 4.158949652  |
| C  | 82.422054890 | 21.482406970 | 5.930524852  | C | 83.679609986 | 27.844438093 | 5.526492248  |
| H  | 82.535000000 | 20.841000000 | 5.044000000  | C | 85.060312582 | 27.563430646 | 6.084175353  |
| N  | 77.897999785 | 22.700272262 | 3.222865215  | O | 85.507567429 | 26.359581010 | 6.036770849  |
| C  | 76.751281248 | 22.317785324 | 2.678417075  | C | 82.089829685 | 31.099554673 | 4.946394349  |
| N  | 76.915860184 | 21.152004535 | 2.016483028  | C | 79.487503531 | 30.847429488 | 3.372160838  |
| C  | 78.230123652 | 20.747572850 | 2.135271473  | C | 78.253319255 | 30.751841698 | 2.762591006  |
| C  | 78.825423749 | 21.732301923 | 2.886855805  | N | 77.909340098 | 29.805580601 | 1.831108514  |
| C  | 78.736505886 | 19.507322456 | 1.485092358  | C | 76.604211189 | 30.083319156 | 1.498944966  |
| H  | 79.538000000 | 19.027000000 | 2.064999000  | C | 76.106838847 | 31.223746987 | 2.231511524  |
| O  | 73.106851352 | 27.952980079 | 0.150505527  | C | 77.140865289 | 31.645356022 | 3.037286706  |
| C  | 73.850738548 | 27.544981872 | -1.002469099 | C | 77.172229430 | 32.660660352 | 4.071839759  |
| C  | 73.650264178 | 28.610913341 | -2.074475266 | C | 76.376914770 | 33.736290312 | 4.195927135  |
| H  | 72.576473456 | 28.721383047 | -2.282651458 | C | 74.706847478 | 31.721323370 | 2.159415540  |
| C  | 75.298454434 | 27.288183402 | -0.694191498 | C | 75.817165631 | 29.329487877 | 0.649365511  |
| C  | 76.194876971 | 28.136413513 | 0.064118757  | C | 75.521311821 | 24.967115773 | -1.758202387 |
| N  | 77.431128049 | 27.555612760 | 0.192792582  | C | 82.402881186 | 30.374309105 | -2.575209684 |
| C  | 77.327883177 | 26.342579380 | -0.446563287 | H | 82.481999000 | 31.468999000 | -2.549002000 |
| C  | 76.007925550 | 26.165980260 | -1.016583396 | O | 85.691645114 | 24.244682698 | 1.908639969  |
| Fe | 79.022000000 | 28.208999000 | 1.280000000  | O | 85.738381769 | 28.544614043 | 6.494390772  |
| N  | 79.755536661 | 29.145980569 | -0.297762950 | H | 85.177302769 | 22.215612688 | -1.101056211 |
| C  | 81.094192361 | 29.291845128 | -0.607329573 | N | 87.562510382 | 26.714436187 | 4.179741261  |



|   |              |              |              |   |              |              |              |
|---|--------------|--------------|--------------|---|--------------|--------------|--------------|
| C | 88.376732042 | 27.772884530 | 4.200374161  | H | 71.299201731 | 27.945795507 | 2.131529308  |
| N | 88.089872476 | 28.822961053 | 4.971065857  | H | 70.230206449 | 28.920197460 | 4.126098660  |
| N | 89.457015553 | 27.770477375 | 3.415588103  | H | 69.898367804 | 28.926228689 | 6.604441488  |
| C | 90.392958942 | 28.865159615 | 3.278575156  | H | 70.875895535 | 27.852163021 | 7.638529811  |
| H | 91.324000000 | 28.428000000 | 2.915998000  | H | 72.807155175 | 26.589162740 | 6.643426594  |
| N | 87.807269867 | 21.450364109 | 1.137618215  | H | 75.801854122 | 22.832458789 | 2.751805936  |
| C | 88.132807224 | 21.072192873 | 2.372070283  | H | 76.180613955 | 20.651638139 | 1.517343184  |
| N | 89.291410821 | 20.417809278 | 2.295291241  | H | 79.856547676 | 21.804925471 | 3.208831090  |
| C | 89.721103286 | 20.379673384 | 0.988048235  | H | 79.124190227 | 19.722655549 | 0.478336844  |
| C | 88.779521155 | 21.037978686 | 0.245782975  | H | 77.923428935 | 18.777178070 | 1.379769321  |
| C | 88.682330662 | 21.312804030 | -1.207743889 | H | 79.474110198 | 22.173769354 | 5.976645812  |
| H | 88.625000000 | 22.393000000 | -1.405001000 | H | 83.419536495 | 21.775734052 | 6.280611533  |
| O | 86.905992507 | 22.669147053 | 5.031443008  | H | 81.934425435 | 20.891321274 | 6.714430881  |
| O | 84.787582271 | 24.340845077 | 4.554051852  | H | 83.120914220 | 23.985993085 | 4.815434991  |
| O | 84.799555813 | 21.797116648 | -1.978992824 | H | 83.161980078 | 24.481353001 | 2.316138585  |
| C | 84.689458369 | 20.474795558 | -1.863207161 | H | 82.628449212 | 23.042530398 | 1.463721037  |
| O | 84.967292992 | 19.858213887 | -0.829616876 | H | 84.062240479 | 25.416641046 | 0.137028393  |
| C | 84.201141986 | 19.806106700 | -3.109543214 | H | 83.654484621 | 23.876950031 | -0.649452002 |
| H | 84.927001000 | 19.945000000 | -3.925000000 | H | 84.456786284 | 29.440121727 | 4.300781109  |
| O | 84.253750256 | 20.404549857 | 1.828562318  | H | 84.368614510 | 27.892427188 | 3.459788098  |
| O | 88.151486303 | 24.214759469 | 3.068096604  | H | 83.140999474 | 28.510132183 | 6.217454470  |
| H | 78.093226956 | 24.432571800 | -0.968667057 | H | 83.101294066 | 26.916192514 | 5.421757855  |
| H | 83.038294368 | 26.585174759 | 2.389187175  | H | 86.972423903 | 22.051533682 | 0.845352103  |
| H | 79.646559074 | 31.667611505 | 4.066537291  | H | 87.578779909 | 21.273168964 | 3.279905154  |
| H | 74.787263935 | 29.638502292 | 0.501244320  | H | 89.783391682 | 20.017135807 | 3.094172878  |
| H | 74.575225902 | 24.603912936 | -1.330341677 | H | 90.644628275 | 19.895010720 | 0.703550253  |
| H | 75.332486951 | 25.198134826 | -2.817768124 | H | 89.557448604 | 20.905292627 | -1.724664622 |
| H | 76.241222732 | 24.141200971 | -1.724671632 | H | 87.781666155 | 20.843035285 | -1.627654700 |
| H | 81.220667924 | 22.369269517 | -0.036987339 | H | 90.596289280 | 29.324808541 | 4.253195832  |
| H | 73.437624766 | 26.598431104 | -1.396332894 | H | 90.034466696 | 29.629663389 | 2.575050290  |
| H | 74.044770486 | 29.580275569 | -1.736499408 | H | 89.567509068 | 26.972569796 | 2.792844230  |
| H | 74.164992914 | 28.329497627 | -3.004446295 | H | 88.691934179 | 29.640305493 | 4.986276143  |
| H | 77.926525667 | 32.505243513 | 4.848717535  | H | 87.291092647 | 28.763199664 | 5.633569446  |
| H | 75.619913995 | 33.999518619 | 3.459746444  | H | 87.886797700 | 25.832377265 | 3.729227401  |
| H | 76.485358060 | 34.396102015 | 5.056667945  | H | 86.890342445 | 26.602227546 | 4.959689466  |
| H | 81.429911962 | 31.015597595 | 5.824360863  | H | 84.053151346 | 18.737884580 | -2.927173483 |
| H | 81.955096195 | 32.108377845 | 4.530219472  | H | 83.257823524 | 20.266343701 | -3.431886924 |
| H | 83.125920340 | 31.010778691 | 5.296038760  | H | 73.239523748 | 27.266325971 | 0.901285364  |
| H | 74.445905943 | 32.293035781 | 3.058311201  | H | 83.456304477 | 19.835556054 | 1.855225405  |
| H | 73.995299713 | 30.888950273 | 2.070122646  | H | 84.558022052 | 20.324668678 | 0.888843676  |
| H | 74.557196106 | 32.378078528 | 1.287465517  | H | 87.884972665 | 23.664565572 | 3.856619493  |
| H | 81.879763639 | 28.938479054 | 0.047731348  | H | 87.323206420 | 24.175820057 | 2.506028716  |
| H | 83.309314269 | 29.953027609 | -2.126927564 | H | 87.186618798 | 22.744560448 | 5.972703386  |
| H | 82.345256993 | 30.054377181 | -3.624861672 | H | 86.088632256 | 23.247171691 | 4.965773119  |
| H | 79.642383422 | 30.641737182 | -3.081741325 | H | 85.008979440 | 25.195830548 | 5.071672204  |
| H | 77.991725652 | 29.737858639 | -1.385332353 | H | 85.036676795 | 24.468201921 | 3.599260165  |
| H | 75.494269893 | 26.182553660 | 3.210013821  | H | 81.187757192 | 25.568796736 | 4.177345062  |
| H | 73.552253511 | 24.329637046 | 6.472936468  | O | 78.245721380 | 27.242421309 | 2.749459640  |
| H | 75.880550961 | 22.406532835 | 6.958878060  | O | 78.918223373 | 26.342582279 | 3.488960105  |
| H | 77.427000000 | 22.984000000 | 6.282000000  |   |              |              |              |

## Structure 6:

186

|    |              |              |              |   |              |              |              |
|----|--------------|--------------|--------------|---|--------------|--------------|--------------|
| C  | 81.095145928 | 24.647008471 | 4.720498009  | C | 80.388254137 | 23.034471020 | -0.357666169 |
| N  | 79.926083758 | 24.077015991 | 5.009773466  | O | 79.452692983 | 22.600457164 | -1.035272701 |
| C  | 80.226595007 | 22.838685404 | 5.543733439  | C | 82.834719883 | 24.109452340 | 1.290710340  |
| C  | 81.585815370 | 22.661242952 | 5.559446985  | C | 83.963242704 | 24.365550411 | 0.279231772  |
| N  | 82.111930337 | 23.820430939 | 5.034523923  | C | 85.269570909 | 23.814329305 | 0.804138355  |
| Cu | 78.131000000 | 24.537000000 | 4.280000000  | O | 85.858390220 | 22.906820320 | 0.115380138  |
| N  | 76.276236914 | 24.839513555 | 4.716441855  | C | 82.086077596 | 26.975160091 | 2.095653432  |
| C  | 75.358988832 | 25.580900610 | 4.120926929  | C | 81.723650710 | 28.198577495 | 2.621876240  |
| N  | 74.181410973 | 25.482648898 | 4.794817067  | N | 80.525207890 | 28.834131587 | 2.383740517  |
| C  | 74.381149764 | 24.618054051 | 5.863912553  | C | 80.531632008 | 29.950354734 | 3.175868065  |
| C  | 75.688187827 | 24.208918445 | 5.806301874  | C | 81.764034416 | 30.041969257 | 3.919708246  |
| C  | 73.073510782 | 26.336896398 | 4.592955941  | C | 82.513341532 | 28.953270294 | 3.568643597  |
| C  | 72.709883545 | 26.714866877 | 3.245603238  | C | 83.828353543 | 28.556999240 | 4.141925695  |
| C  | 71.629315222 | 27.648405754 | 3.147354994  | C | 83.678810629 | 27.871108132 | 5.518079260  |
| C  | 71.017557015 | 28.182943472 | 4.259907619  | C | 85.058875616 | 27.598578251 | 6.082806635  |
| C  | 71.420643980 | 27.822653388 | 5.562934326  | O | 85.507692851 | 26.394888990 | 6.044183358  |
| C  | 72.437632530 | 26.876874461 | 5.699586766  | C | 82.079699100 | 31.098242770 | 4.918895849  |
| C  | 76.459328576 | 23.306116237 | 6.714194299  | C | 79.489769883 | 30.848706855 | 3.326648810  |
| H  | 76.691463954 | 23.824377341 | 7.656512603  | C | 78.262623549 | 30.771110530 | 2.701798828  |
| O  | 73.326476258 | 26.254887008 | 2.219985953  | N | 77.920769531 | 29.835806126 | 1.764789905  |
| C  | 70.889825557 | 28.529327087 | 6.766939329  | C | 76.613107967 | 30.097296067 | 1.439658503  |
| H  | 71.578000000 | 29.361001000 | 7.012000000  | C | 76.111874728 | 31.236823292 | 2.175784941  |
| C  | 82.409333066 | 21.485540263 | 5.925145589  | C | 77.145352854 | 31.662046657 | 2.976879170  |
| H  | 82.535000000 | 20.841000000 | 5.044000000  | C | 77.165142905 | 32.680608306 | 4.007321567  |
| N  | 77.943166657 | 22.796178952 | 3.111917437  | C | 76.369683604 | 33.758504843 | 4.094022685  |
| C  | 76.786226073 | 22.378378758 | 2.612461583  | C | 74.708151864 | 31.725496971 | 2.120267540  |
| N  | 76.952330958 | 21.189875609 | 1.995641880  | C | 75.826031673 | 29.334197511 | 0.601135273  |
| C  | 78.273145292 | 20.803386766 | 2.096124875  | C | 75.545122018 | 24.963667218 | -1.801714663 |
| C  | 78.876425317 | 21.825064316 | 2.791468122  | C | 82.400889845 | 30.375228719 | -2.607967253 |
| C  | 78.763088236 | 19.539533224 | 1.472738126  | H | 82.482002000 | 31.468999000 | -2.548999000 |
| H  | 79.538000000 | 19.027000000 | 2.065000000  | O | 85.713357590 | 24.277491555 | 1.890086220  |
| O  | 73.111836332 | 27.954427848 | 0.104139451  | O | 85.730692603 | 28.584520309 | 6.490310276  |
| C  | 73.861779333 | 27.531009766 | -1.047614124 | H | 85.190503610 | 22.205689829 | -1.103887770 |
| C  | 73.659093955 | 28.585437331 | -2.127860521 | N | 87.567251174 | 26.712233324 | 4.191541532  |
| H  | 72.585765352 | 28.688348161 | -2.340554116 | C | 88.383250022 | 27.769712416 | 4.212291291  |
| C  | 75.306846851 | 27.279499544 | -0.729055970 | N | 88.099092263 | 28.820761606 | 4.981970985  |
| C  | 76.201974535 | 28.135687682 | 0.022678282  | N | 89.465987444 | 27.765097238 | 3.431892876  |
| N  | 77.439146300 | 27.558091139 | 0.146648160  | C | 90.398224322 | 28.862571558 | 3.296058353  |
| C  | 77.342618586 | 26.342967892 | -0.480291126 | H | 91.324001000 | 28.427997000 | 2.916001000  |
| C  | 76.021831634 | 26.159497534 | -1.049405169 | N | 87.824010764 | 21.453446725 | 1.133086304  |
| Fe | 79.022001000 | 28.209000000 | 1.280001000  | C | 88.146199842 | 21.076746700 | 2.369062563  |
| N  | 79.768505066 | 29.114927431 | -0.331941763 | N | 89.307423351 | 20.427195631 | 2.298189116  |
| C  | 81.105881867 | 29.253154642 | -0.651933637 | C | 89.742002682 | 20.388680655 | 0.992536145  |
| C  | 81.219693893 | 29.918972748 | -1.843452716 | C | 88.801036761 | 21.042733137 | 0.245851161  |
| N  | 79.924153275 | 30.177369448 | -2.234181304 | C | 88.709208968 | 21.314783977 | -1.208257845 |
| C  | 79.076092908 | 29.687929997 | -1.310706188 | H | 88.624999000 | 22.392997000 | -1.404999000 |
| C  | 78.318595343 | 25.369981200 | -0.494679398 | O | 86.852797772 | 22.681733157 | 5.063352394  |
| C  | 79.548601718 | 25.445784849 | 0.136226911  | O | 84.776131845 | 24.390524783 | 4.545320489  |
| N  | 80.022868848 | 26.523876552 | 0.842825955  | O | 84.824666832 | 21.789281851 | -1.985719063 |
| C  | 81.279448862 | 26.171184878 | 1.299770228  | C | 84.661204829 | 20.472425343 | -1.863493797 |
| C  | 81.586433157 | 24.827402705 | 0.924577999  | O | 84.879150542 | 19.855147185 | -0.816090408 |
| C  | 80.506584185 | 24.368954045 | 0.187557134  | C | 84.187525037 | 19.813858581 | -3.120874478 |

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| H | 84.926999000 | 19.944998000 | -3.924999000 | H | 77.926858956 | 18.837814663 | 1.355008989  |
| O | 84.142466948 | 20.564365420 | 1.793702833  | H | 79.457819961 | 22.144308696 | 5.859206675  |
| O | 88.140569376 | 24.197484173 | 3.101169971  | H | 83.400840682 | 21.781410457 | 6.288538931  |
| H | 78.110219913 | 24.433664197 | -1.002549510 | H | 81.910250939 | 20.897227430 | 6.704078807  |
| H | 83.065540662 | 26.588179165 | 2.364944046  | H | 83.128755816 | 24.021619138 | 4.875721351  |
| H | 79.645068100 | 31.663990785 | 4.027847143  | H | 83.171281315 | 24.444018855 | 2.280287786  |
| H | 74.795692764 | 29.641710457 | 0.452937799  | H | 82.662957632 | 23.026300236 | 1.377356362  |
| H | 74.568794459 | 24.629434796 | -1.422080180 | H | 84.091347282 | 25.450503486 | 0.136616622  |
| H | 75.419544131 | 25.192222621 | -2.871666469 | H | 83.708214981 | 23.926070603 | -0.694334598 |
| H | 76.241578913 | 24.120804630 | -1.723458642 | H | 84.454173525 | 29.453441807 | 4.271832364  |
| H | 81.246638800 | 22.369467634 | -0.120372477 | H | 84.373461410 | 27.895198903 | 3.450971119  |
| H | 73.446262495 | 26.580445752 | -1.424937381 | H | 83.136522637 | 28.544262595 | 6.198548018  |
| H | 74.050013620 | 29.559588807 | -1.800369818 | H | 83.103264460 | 26.940069497 | 5.425174403  |
| H | 74.177741643 | 28.293987162 | -3.052222181 | H | 86.989375550 | 22.055645041 | 0.840802632  |
| H | 77.899246900 | 32.527110746 | 4.803511176  | H | 87.585804189 | 21.272316994 | 3.273545349  |
| H | 75.637305287 | 34.010327047 | 3.328997073  | H | 89.797738559 | 20.027094685 | 3.098453970  |
| H | 76.452239054 | 34.431485247 | 4.947372169  | H | 90.667509841 | 19.905685540 | 0.711648091  |
| H | 81.420193807 | 31.011554964 | 5.796543517  | H | 89.599689601 | 20.931114809 | -1.717165119 |
| H | 81.938475085 | 32.104019443 | 4.498309453  | H | 87.825789091 | 20.821196680 | -1.637957023 |
| H | 83.116307117 | 31.015615665 | 5.266862417  | H | 90.613813751 | 29.311718674 | 4.273144848  |
| H | 74.437631847 | 32.231989265 | 3.055726421  | H | 90.031875964 | 29.633527543 | 2.603769291  |
| H | 74.003859218 | 30.896198840 | 1.967888398  | H | 89.580190334 | 26.966218961 | 2.810808958  |
| H | 74.561674673 | 32.441796104 | 1.296690814  | H | 88.693447787 | 29.644391231 | 4.981551090  |
| H | 81.895799969 | 28.885383305 | -0.010584897 | H | 87.292380581 | 28.773047780 | 5.635154373  |
| H | 83.311394036 | 29.938543118 | -2.184319060 | H | 87.895189071 | 25.825006336 | 3.754422038  |
| H | 82.327909732 | 30.087573603 | -3.665630861 | H | 86.894629621 | 26.607680415 | 4.971709430  |
| H | 79.640756915 | 30.665717913 | -3.083458109 | H | 84.018897384 | 18.747632673 | -2.945727484 |
| H | 78.001250519 | 29.756211519 | -1.389777875 | H | 83.256403545 | 20.289615786 | -3.456827927 |
| H | 75.492659161 | 26.201940458 | 3.246141338  | H | 73.235077708 | 27.278356926 | 0.839682211  |
| H | 73.579166304 | 24.371045639 | 6.547357366  | H | 83.443373947 | 19.885266471 | 1.892991751  |
| H | 75.879102991 | 22.407473085 | 6.960363034  | H | 84.465966594 | 20.418723237 | 0.868173829  |
| H | 77.427000000 | 22.984000000 | 6.282000000  | H | 87.844036261 | 23.649681792 | 3.880684698  |
| H | 71.313880114 | 27.942948245 | 2.146464448  | H | 87.325114722 | 24.176326778 | 2.520333581  |
| H | 70.220768650 | 28.918037134 | 4.135233618  | H | 87.175014134 | 22.833175541 | 5.978484729  |
| H | 69.894713428 | 28.952130936 | 6.583534103  | H | 86.046693579 | 23.272221427 | 4.979690938  |
| H | 70.848369258 | 27.865639612 | 7.639743295  | H | 85.003955370 | 25.238987418 | 5.073774667  |
| H | 72.786259108 | 26.607128022 | 6.696176862  | H | 85.035724062 | 24.517167849 | 3.594787285  |
| H | 75.831707360 | 22.881530964 | 2.688529053  | H | 81.226086537 | 25.641367314 | 4.315850808  |
| H | 76.210915732 | 20.660815164 | 1.536046712  | O | 78.175017702 | 27.462145375 | 2.682150002  |
| H | 79.913253437 | 21.920052115 | 3.087140860  | O | 78.949780996 | 26.375125504 | 3.434487186  |
| H | 79.174958574 | 19.733776539 | 0.471303257  | H | 79.466886534 | 26.025450459 | 2.667977135  |

## Structure 7:

188

|    |              |              |             |   |              |              |             |
|----|--------------|--------------|-------------|---|--------------|--------------|-------------|
| C  | 80.951539322 | 24.626606051 | 4.890019816 | C | 74.396003233 | 24.592941096 | 5.987900781 |
| N  | 79.807521133 | 24.061968704 | 5.286241098 | C | 75.718833421 | 24.226190734 | 5.996843851 |
| C  | 80.153450571 | 22.816186783 | 5.779286551 | C | 73.140276941 | 26.352792018 | 4.710553485 |
| C  | 81.506310210 | 22.622730903 | 5.658691951 | C | 72.830994684 | 26.749708720 | 3.338064471 |
| N  | 81.990308336 | 23.789889820 | 5.094583017 | C | 71.761974697 | 27.697304903 | 3.182158616 |
| Cu | 78.131000000 | 24.537000000 | 4.280000000 | C | 71.095395069 | 28.218761106 | 4.257823900 |
| N  | 76.362073827 | 24.949904485 | 4.986352101 | C | 71.430972809 | 27.838725000 | 5.580053651 |
| C  | 75.454579302 | 25.691960488 | 4.371439731 | C | 72.433198155 | 26.871182972 | 5.776062826 |
| N  | 74.238229747 | 25.515822938 | 4.954474474 | C | 76.500208969 | 23.273248621 | 6.815992341 |

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|----|--------------|--------------|--------------|---|--------------|--------------|--------------|
| H  | 76.788971224 | 23.728250379 | 7.776961748  | C | 77.148149944 | 31.691230743 | 2.953882289  |
| O  | 73.474343092 | 26.283776841 | 2.349773064  | C | 77.145859363 | 32.675378743 | 4.012369249  |
| C  | 70.867309163 | 28.550212286 | 6.750379581  | C | 76.337158625 | 33.738627071 | 4.141060505  |
| H  | 71.578000000 | 29.361001000 | 7.011999000  | C | 74.708930403 | 31.713607065 | 2.087084425  |
| C  | 82.363195928 | 21.447797034 | 5.950311187  | C | 75.869492791 | 29.362454661 | 0.552178961  |
| H  | 82.535000000 | 20.841000000 | 5.044000000  | C | 75.608742535 | 24.995709990 | -1.866444736 |
| N  | 77.744869789 | 22.315884490 | 3.699120716  | C | 82.486241185 | 30.375697956 | -2.612207058 |
| C  | 76.653001751 | 22.100671443 | 2.981422013  | H | 82.482002000 | 31.468996000 | -2.549000000 |
| N  | 76.828906874 | 21.053947699 | 2.139845790  | O | 85.652250056 | 24.226598470 | 1.983325383  |
| C  | 78.106270077 | 20.561261839 | 2.315450943  | O | 85.712277564 | 28.561800980 | 6.567127526  |
| C  | 78.657892408 | 21.361805517 | 3.286274785  | H | 85.281506020 | 22.229519280 | -1.060542873 |
| C  | 78.663273275 | 19.427904046 | 1.540008577  | N | 87.578808036 | 26.732516544 | 4.289225452  |
| H  | 79.537999000 | 19.027000000 | 2.065002000  | C | 88.398636280 | 27.781842185 | 4.298747777  |
| O  | 73.166767493 | 27.939252703 | 0.066792783  | N | 88.114480031 | 28.845502883 | 5.058472056  |
| C  | 73.920551678 | 27.552499269 | -1.103341638 | N | 89.482018413 | 27.765063230 | 3.516590526  |
| C  | 73.701394483 | 28.631426805 | -2.155248405 | C | 90.410251151 | 28.861635869 | 3.333496191  |
| H  | 72.627054101 | 28.733328633 | -2.361985264 | H | 91.323999000 | 28.427995000 | 2.916007000  |
| C  | 75.362106029 | 27.308323680 | -0.788257038 | N | 87.978669242 | 21.448714857 | 1.202069002  |
| C  | 76.248275510 | 28.164061862 | -0.021934035 | C | 88.398917656 | 21.038174624 | 2.419024725  |
| N  | 77.480716699 | 27.579050470 | 0.109048835  | N | 89.553292066 | 20.387539541 | 2.327341367  |
| C  | 77.392565307 | 26.366134985 | -0.523255656 | C | 89.879194594 | 20.394582197 | 0.982158860  |
| C  | 76.082320366 | 26.189298628 | -1.109504503 | C | 88.906699582 | 21.054100875 | 0.265959683  |
| Fe | 79.021999000 | 28.208999000 | 1.280001000  | C | 88.745466224 | 21.321461662 | -1.189811427 |
| N  | 79.817916808 | 29.071027186 | -0.416396534 | H | 88.624997000 | 22.392991000 | -1.404992000 |
| C  | 81.153814269 | 29.253204605 | -0.680967475 | O | 86.828114678 | 22.767442199 | 5.180841200  |
| C  | 81.299036811 | 29.864695671 | -1.893361164 | O | 84.662896227 | 24.376008362 | 4.589129003  |
| N  | 80.013105174 | 30.047156746 | -2.353119688 | O | 84.936595656 | 21.813680701 | -1.961526292 |
| C  | 79.152201308 | 29.559681720 | -1.445965048 | C | 84.743543382 | 20.503003196 | -1.836333872 |
| C  | 78.360578421 | 25.384674710 | -0.504994867 | O | 84.948201680 | 19.885347341 | -0.786545693 |
| C  | 79.562367176 | 25.451462716 | 0.173757697  | C | 84.229147771 | 19.842316846 | -3.080999458 |
| N  | 80.035897972 | 26.532249466 | 0.859359120  | H | 84.926998000 | 19.944991000 | -3.924992000 |
| C  | 81.247637645 | 26.168175542 | 1.394284675  | O | 84.003005024 | 20.641629001 | 1.752358440  |
| C  | 81.551844888 | 24.809647225 | 1.052974317  | O | 88.082498894 | 24.249825625 | 3.166995059  |
| C  | 80.497075485 | 24.356058039 | 0.283816538  | H | 78.153763110 | 24.443834838 | -1.004842110 |
| C  | 80.380893147 | 23.015975634 | -0.241293913 | H | 83.004897581 | 26.564601115 | 2.508629566  |
| O  | 79.484421980 | 22.588807200 | -0.977405010 | H | 79.641563154 | 31.713921824 | 4.018052032  |
| C  | 82.791696845 | 24.092292786 | 1.438241454  | H | 74.834897060 | 29.663614736 | 0.403929804  |
| C  | 83.894722693 | 24.251212051 | 0.376693694  | H | 74.653704349 | 24.632236360 | -1.461463122 |
| C  | 85.229464663 | 23.752752934 | 0.888757906  | H | 75.444900826 | 25.236256853 | -2.927650085 |
| O  | 85.875428546 | 22.907173523 | 0.181007088  | H | 76.327034511 | 24.168960816 | -1.822258682 |
| C  | 82.047252664 | 26.976602726 | 2.189298477  | H | 81.203640776 | 22.336703823 | 0.069048946  |
| C  | 81.713699975 | 28.223579000 | 2.664350590  | H | 73.509030716 | 26.608003887 | -1.498712577 |
| N  | 80.548399863 | 28.892458944 | 2.372091754  | H | 74.090967241 | 29.599952823 | -1.811169539 |
| C  | 80.540134335 | 30.006095658 | 3.170505430  | H | 74.216372649 | 28.359882250 | -3.087356719 |
| C  | 81.749591754 | 30.076104431 | 3.961890697  | H | 77.879127732 | 32.503919888 | 4.808231500  |
| C  | 82.489462591 | 28.966873439 | 3.632190498  | H | 75.602213090 | 34.013162260 | 3.386218428  |
| C  | 83.788267249 | 28.559337326 | 4.227738875  | H | 76.409319647 | 34.377709735 | 5.020931860  |
| C  | 83.634480269 | 27.891120426 | 5.612523741  | H | 81.468426010 | 30.926803127 | 5.901460214  |
| C  | 85.024192238 | 27.591741847 | 6.150311117  | H | 81.794503827 | 32.119146979 | 4.626981770  |
| O  | 85.456850134 | 26.387726676 | 6.071035896  | H | 83.113031961 | 31.101653784 | 5.252488443  |
| C  | 82.048360868 | 31.109965612 | 4.981118608  | H | 74.445419063 | 32.277869443 | 2.990083819  |
| C  | 79.501272669 | 30.904795205 | 3.302009174  | H | 74.020435517 | 30.861220118 | 2.010357940  |
| C  | 78.285406660 | 30.826329982 | 2.662194796  | H | 74.527169657 | 32.364904701 | 1.217135353  |
| N  | 77.960493000 | 29.906538888 | 1.702440565  | H | 81.932833491 | 28.953332543 | 0.016044796  |
| C  | 76.644662439 | 30.138079263 | 1.386229520  | H | 83.401463713 | 29.999012533 | -2.144632297 |
| C  | 76.121194932 | 31.255622021 | 2.138314788  | H | 82.476290070 | 30.084018489 | -3.670886368 |

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| H | 79.753886058 | 30.488011275 | -3.239395527 | H | 87.852759966 | 21.235014203 | 3.333389856  |
| H | 78.073307572 | 29.575836181 | -1.577235830 | H | 90.784927452 | 19.929409092 | 0.613363511  |
| H | 75.629451510 | 26.344332389 | 3.530567190  | H | 89.624550857 | 20.957447996 | -1.732311234 |
| H | 73.555335558 | 24.274232341 | 6.590602301  | H | 87.860876362 | 20.804272873 | -1.587100570 |
| H | 75.922108659 | 22.363858436 | 7.033610641  | H | 90.656601265 | 29.328560768 | 4.295437927  |
| H | 77.427000000 | 22.984000000 | 6.282000000  | H | 90.021630784 | 29.617288517 | 2.637363863  |
| H | 71.508019097 | 27.999274292 | 2.165307367  | H | 89.593920603 | 26.950642693 | 2.915140438  |
| H | 70.310453290 | 28.960678232 | 4.106996167  | H | 88.736236456 | 29.645497974 | 5.093769104  |
| H | 69.896196383 | 29.007123528 | 6.522917850  | H | 87.309946653 | 28.790817929 | 5.711860685  |
| H | 70.780719911 | 27.893813116 | 7.625088075  | H | 87.869240086 | 25.846193476 | 3.820712767  |
| H | 72.712116362 | 26.592412507 | 6.788103366  | H | 86.882979408 | 26.638123936 | 5.052102188  |
| H | 75.738948802 | 22.676504825 | 3.023677044  | H | 84.048613602 | 18.781369258 | -2.884511959 |
| H | 76.127533214 | 20.679652222 | 1.502868378  | H | 83.288956903 | 20.326868902 | -3.381381451 |
| H | 79.655741460 | 21.313483470 | 3.698070698  | H | 73.349259967 | 27.284172587 | 0.794281658  |
| H | 78.975305036 | 19.744239219 | 0.533149742  | H | 83.332085366 | 19.928675449 | 1.807854299  |
| H | 77.930019078 | 18.616794043 | 1.428486461  | H | 84.422298750 | 20.485501898 | 0.868006158  |
| H | 79.412888318 | 22.123867743 | 6.156461745  | H | 87.809994348 | 23.693920413 | 3.949194467  |
| H | 83.342046269 | 21.753620741 | 6.344016204  | H | 87.264907156 | 24.187835098 | 2.589940228  |
| H | 81.878255310 | 20.806350939 | 6.695422767  | H | 87.118540945 | 22.969031428 | 6.094780961  |
| H | 82.992599217 | 23.996253348 | 4.886707144  | H | 85.994271728 | 23.311679384 | 5.060245191  |
| H | 83.166901676 | 24.488474910 | 2.388659111  | H | 84.911664337 | 25.225797711 | 5.097152188  |
| H | 82.602916879 | 23.020664035 | 1.602887412  | H | 84.952129714 | 24.465130463 | 3.639822069  |
| H | 84.019406978 | 25.320277442 | 0.136087547  | H | 81.044818980 | 25.611964776 | 4.456833596  |
| H | 83.609963454 | 23.735030501 | -0.550177617 | O | 78.304551898 | 27.508432409 | 2.623387643  |
| H | 84.426488059 | 29.448313861 | 4.349432758  | O | 77.665392562 | 24.971828572 | 2.533773677  |
| H | 84.328136970 | 27.880329278 | 3.548974979  | H | 77.820293783 | 25.960755871 | 2.466085909  |
| H | 83.119737667 | 28.583049856 | 6.295257149  | H | 90.546822870 | 19.673135431 | 3.532223236  |
| H | 83.037676052 | 26.972366363 | 5.534681629  | O | 91.198915568 | 19.229359733 | 4.173208235  |
| H | 87.133409555 | 22.020471276 | 0.969448808  | H | 90.786872700 | 19.351042049 | 5.053117846  |

## Structure 8:

185

|    |              |              |             |    |              |              |              |
|----|--------------|--------------|-------------|----|--------------|--------------|--------------|
| C  | 80.956258523 | 24.630664662 | 4.919993304 | H  | 71.578000000 | 29.361003000 | 7.011997000  |
| N  | 79.814298642 | 24.067019322 | 5.315643107 | C  | 82.371224548 | 21.443900190 | 5.952924606  |
| C  | 80.159991661 | 22.816610736 | 5.797791150 | H  | 82.535000000 | 20.841000000 | 5.044000000  |
| C  | 81.512563194 | 22.624019834 | 5.672512216 | N  | 77.829068406 | 22.349681604 | 3.689907842  |
| N  | 81.994126060 | 23.791913704 | 5.116703777 | C  | 76.696474539 | 22.025387982 | 2.992911554  |
| Cu | 78.131000000 | 24.537000000 | 4.280000000 | N  | 76.825552160 | 20.997834210 | 2.126082387  |
| N  | 76.350811163 | 24.939550780 | 4.969443438 | C  | 78.139185974 | 20.648919763 | 2.242241321  |
| C  | 75.442231507 | 25.661474752 | 4.332239080 | C  | 78.750350492 | 21.502559946 | 3.204507520  |
| N  | 74.226505026 | 25.476568418 | 4.903025084 | C  | 78.757885734 | 19.538829796 | 1.479716093  |
| C  | 74.387294041 | 24.567904956 | 5.945635722 | H  | 79.537998000 | 19.027000000 | 2.065001000  |
| C  | 75.716857381 | 24.226615435 | 5.970163461 | O  | 73.144777058 | 27.939572223 | 0.127100820  |
| C  | 73.110181756 | 26.320829994 | 4.650982240 | C  | 73.885286175 | 27.557766353 | -1.044666303 |
| C  | 72.810169218 | 26.720350606 | 3.295158588 | C  | 73.664912692 | 28.638524532 | -2.095763714 |
| C  | 71.745605295 | 27.670095320 | 3.174329291 | H  | 72.590271375 | 28.737987666 | -2.302319087 |
| C  | 71.096673418 | 28.202017655 | 4.270095658 | C  | 75.335150971 | 27.311522869 | -0.745494490 |
| C  | 71.435312787 | 27.814596779 | 5.579360072 | C  | 76.227797256 | 28.164426658 | 0.010055473  |
| C  | 72.432828930 | 26.850755190 | 5.737739463 | N  | 77.461786029 | 27.579903510 | 0.130415329  |
| C  | 76.507599266 | 23.290051619 | 6.818879954 | C  | 77.367798149 | 26.371454962 | -0.507232666 |
| H  | 76.812821928 | 23.774663220 | 7.758105389 | C  | 76.049598595 | 26.194123457 | -1.079378732 |
| O  | 73.463015850 | 26.276394701 | 2.280939652 | Fe | 79.022001000 | 28.208998000 | 1.280000000  |
| C  | 70.890721352 | 28.530092123 | 6.773245255 | N  | 79.814481598 | 29.083143515 | -0.405271714 |

|   |              |              |              |   |              |              |              |
|---|--------------|--------------|--------------|---|--------------|--------------|--------------|
| C | 81.154475449 | 29.263234473 | -0.672822206 | O | 86.788013067 | 22.684622420 | 5.133166828  |
| C | 81.297484617 | 29.867865247 | -1.892885150 | O | 84.682706605 | 24.360701182 | 4.616179155  |
| N | 80.012959846 | 30.048969558 | -2.355563232 | O | 84.821963492 | 21.759325513 | -1.933995215 |
| C | 79.144717302 | 29.567685897 | -1.444013724 | C | 84.723555234 | 20.433542205 | -1.838100248 |
| C | 78.342635660 | 25.396623471 | -0.516461973 | O | 85.008181196 | 19.805252148 | -0.813751279 |
| C | 79.553596844 | 25.464600147 | 0.148757469  | C | 84.227925535 | 19.779764980 | -3.090568005 |
| N | 80.024495384 | 26.538590107 | 0.842882461  | H | 84.926997000 | 19.944989000 | -3.924992000 |
| C | 81.232781687 | 26.169036673 | 1.383453174  | O | 84.280873498 | 20.444662226 | 1.841015864  |
| C | 81.538388120 | 24.815290710 | 1.033344028  | O | 88.102868400 | 24.219777022 | 3.215235554  |
| C | 80.489416150 | 24.370676039 | 0.248271409  | H | 78.134391753 | 24.460820593 | -1.024718717 |
| C | 80.384248587 | 23.043880207 | -0.310327068 | H | 82.989311031 | 26.552127537 | 2.504628648  |
| O | 79.508517992 | 22.637086124 | -1.080771116 | H | 79.676228985 | 31.738740126 | 3.980304035  |
| C | 82.777035773 | 24.092351552 | 1.420118095  | H | 74.821910174 | 29.668323582 | 0.441223125  |
| C | 83.900384534 | 24.298281266 | 0.389945011  | H | 74.633162945 | 24.618962080 | -1.391725529 |
| C | 85.219542990 | 23.758604875 | 0.898944896  | H | 75.362381032 | 25.243834759 | -2.881568416 |
| O | 85.829578655 | 22.889310356 | 0.181527728  | H | 76.298827870 | 24.182720405 | -1.815491807 |
| C | 82.037719970 | 26.969431323 | 2.184314102  | H | 81.196259679 | 22.353730155 | 0.006174399  |
| C | 81.713276446 | 28.224028146 | 2.657407171  | H | 73.476204049 | 26.613925921 | -1.445095215 |
| N | 80.555690674 | 28.898097169 | 2.360208250  | H | 74.049621178 | 29.607871852 | -1.747962249 |
| C | 80.559611017 | 30.018301093 | 3.147442280  | H | 74.181368703 | 28.374996997 | -3.029717611 |
| C | 81.768611319 | 30.081508174 | 3.935106605  | H | 77.993786023 | 32.537530472 | 4.748861653  |
| C | 82.496146703 | 28.968221700 | 3.619444264  | H | 75.533749280 | 33.966959973 | 3.577425192  |
| C | 83.797474433 | 28.551796096 | 4.213103436  | H | 76.473893688 | 34.319593710 | 5.139860796  |
| C | 83.644686276 | 27.873278174 | 5.591977602  | H | 81.389470584 | 31.058745776 | 5.800856705  |
| C | 85.030428833 | 27.589158743 | 6.140929741  | H | 81.971123602 | 32.141482995 | 4.521389232  |
| O | 85.473707921 | 26.384256060 | 6.086150686  | H | 83.099124194 | 31.025057693 | 5.323614112  |
| C | 82.076594104 | 31.131822903 | 4.942956488  | H | 74.475183480 | 32.411400933 | 2.897330266  |
| C | 79.525594045 | 30.927964699 | 3.273546902  | H | 74.034715204 | 30.863748143 | 2.155183321  |
| C | 78.300363079 | 30.848356057 | 2.640606284  | H | 74.500149761 | 32.234638363 | 1.130257188  |
| N | 77.967261207 | 29.924246376 | 1.689701446  | H | 81.927600358 | 28.966202492 | 0.023343881  |
| C | 76.650030485 | 30.155845168 | 1.391661140  | H | 83.400065886 | 30.004092124 | -2.126106718 |
| C | 76.135131836 | 31.277368871 | 2.142279356  | H | 82.489532177 | 30.074359566 | -3.661213549 |
| C | 77.168328459 | 31.712664315 | 2.942983060  | H | 79.751305253 | 30.485621779 | -3.238823499 |
| C | 77.193337358 | 32.686229799 | 4.019680761  | H | 78.071827312 | 29.579782808 | -1.573768591 |
| C | 76.349347405 | 33.705696127 | 4.248357979  | H | 75.602793867 | 26.292606749 | 3.470766563  |
| C | 74.716951913 | 31.723325497 | 2.082208543  | H | 73.547142193 | 24.251146265 | 6.550144303  |
| C | 75.856662193 | 29.370293731 | 0.575819657  | H | 75.930066883 | 22.392163114 | 7.071569433  |
| C | 75.568354731 | 24.999320697 | -1.828473909 | H | 77.427000000 | 22.984000000 | 6.282000000  |
| C | 82.487852212 | 30.374635803 | -2.605427343 | H | 71.476897144 | 27.987799131 | 2.166510188  |
| H | 82.482006000 | 31.468995000 | -2.549000000 | H | 70.323261862 | 28.957568076 | 4.123213781  |
| O | 85.662610601 | 24.206371721 | 1.993389512  | H | 69.896796518 | 28.951762824 | 6.579303655  |
| O | 85.712656548 | 28.568663549 | 6.547601724  | H | 70.840152432 | 27.874380768 | 7.652094123  |
| H | 85.184223691 | 22.174080396 | -1.050786291 | H | 72.741231387 | 26.561330988 | 6.742937144  |
| N | 87.590479580 | 26.725827785 | 4.313218122  | H | 75.767334081 | 22.570635624 | 3.128486733  |
| C | 88.401138940 | 27.784078147 | 4.302759121  | H | 79.777050558 | 21.498267217 | 3.555361627  |
| N | 88.089422448 | 28.869465785 | 5.015206903  | H | 79.237672185 | 19.922015031 | 0.562320805  |
| N | 89.499871395 | 27.749742887 | 3.542608707  | H | 77.996302164 | 18.810129255 | 1.175739449  |
| C | 90.412633598 | 28.855377831 | 3.337747040  | H | 79.418432575 | 22.118992378 | 6.164781062  |
| H | 91.324001000 | 28.427993000 | 2.916005000  | H | 83.352831908 | 21.749134988 | 6.339600137  |
| N | 87.834224797 | 21.489874914 | 1.186788586  | H | 81.891494181 | 20.800644530 | 6.699472278  |
| C | 88.171524616 | 21.137085987 | 2.425437636  | H | 82.998470199 | 23.999344042 | 4.911415626  |
| N | 89.349186671 | 20.516750497 | 2.356896742  | H | 83.124786154 | 24.451634977 | 2.395982917  |
| C | 89.777927683 | 20.472638591 | 1.049874864  | H | 82.586772375 | 23.015479800 | 1.540145618  |
| C | 88.816437548 | 21.092114966 | 0.298954780  | H | 84.038395012 | 25.376928331 | 0.209140596  |
| C | 88.704518232 | 21.321843610 | -1.161966644 | H | 83.629691884 | 23.833275258 | -0.567286625 |
| H | 88.624999000 | 22.392989000 | -1.404994000 | H | 84.436179518 | 29.439361137 | 4.340284799  |

|   |              |              |              |   |              |              |              |
|---|--------------|--------------|--------------|---|--------------|--------------|--------------|
| H | 84.335444770 | 27.878127841 | 3.528187823  | H | 83.268191069 | 20.228117307 | -3.380410328 |
| H | 83.114334626 | 28.553573818 | 6.274971350  | H | 73.323313539 | 27.277095722 | 0.866679632  |
| H | 83.060143820 | 26.946930858 | 5.505568638  | H | 83.503943314 | 19.846246775 | 1.897320000  |
| H | 86.982412140 | 22.069701322 | 0.892061747  | H | 84.588984058 | 20.321859050 | 0.906945264  |
| H | 87.609031708 | 21.328377451 | 3.329700723  | H | 87.802288508 | 23.668737305 | 3.990532538  |
| H | 90.713654868 | 20.008769070 | 0.770228608  | H | 87.298456547 | 24.172918510 | 2.620977964  |
| H | 89.583407949 | 20.911213903 | -1.670046410 | H | 87.073751400 | 22.802873077 | 6.066471077  |
| H | 87.810670800 | 20.819189851 | -1.558241548 | H | 85.968693181 | 23.257420398 | 5.047476595  |
| H | 90.667926682 | 29.331285537 | 4.293008939  | H | 84.931119494 | 25.211642202 | 5.126596583  |
| H | 90.001295235 | 29.605819265 | 2.647876779  | H | 84.957996578 | 24.463999671 | 3.665960317  |
| H | 89.634548935 | 26.914612761 | 2.976664979  | H | 81.049454885 | 25.617630833 | 4.485113818  |
| H | 88.725826935 | 29.659407008 | 5.066215606  | O | 78.327146269 | 27.543065723 | 2.650879142  |
| H | 87.287596589 | 28.818644256 | 5.672612744  | O | 77.744552064 | 24.985664904 | 2.518374177  |
| H | 87.890179411 | 25.838760917 | 3.857394262  | H | 77.849257885 | 25.978429960 | 2.471816851  |
| H | 86.893109788 | 26.637031987 | 5.074355701  | H | 89.850748374 | 20.138211253 | 3.160569648  |
| H | 84.102102259 | 18.706057043 | -2.925043774 |   |              |              |              |

### Structure 9:

187

|    |              |              |              |    |              |              |              |
|----|--------------|--------------|--------------|----|--------------|--------------|--------------|
| C  | 81.088728838 | 24.645640766 | 4.614830317  | H  | 72.582578348 | 28.781664014 | -2.261580475 |
| N  | 79.920550656 | 24.101664934 | 4.947340657  | C  | 75.328910287 | 27.315621003 | -0.735478605 |
| C  | 80.214116749 | 22.881963349 | 5.531408326  | C  | 76.205125496 | 28.149869651 | 0.056373709  |
| C  | 81.569532304 | 22.685399323 | 5.526379294  | N  | 77.448236995 | 27.579562354 | 0.142172826  |
| N  | 82.099304962 | 23.820332006 | 4.949387732  | C  | 77.387823435 | 26.420472207 | -0.584757855 |
| Cu | 78.131000000 | 24.537000000 | 4.280000000  | C  | 76.065982446 | 26.238741512 | -1.145295361 |
| N  | 76.271263790 | 24.819454421 | 4.866563530  | Fe | 79.021998000 | 28.209001000 | 1.280001000  |
| C  | 75.361775467 | 25.572504763 | 4.271349303  | N  | 79.797333557 | 29.107047086 | -0.384087337 |
| N  | 74.165491289 | 25.425836564 | 4.885135516  | C  | 81.135927531 | 29.278964608 | -0.665111505 |
| C  | 74.338382985 | 24.519628977 | 5.928474280  | C  | 81.267463543 | 29.886619202 | -1.885806319 |
| C  | 75.659663536 | 24.143920822 | 5.905778205  | N  | 79.979552627 | 30.075427995 | -2.332965288 |
| C  | 73.053522608 | 26.285652637 | 4.652848982  | C  | 79.117143965 | 29.597989177 | -1.415518204 |
| C  | 72.714282217 | 26.684659969 | 3.346044877  | C  | 78.394403550 | 25.477218799 | -0.673131469 |
| C  | 71.698631570 | 27.631347638 | 3.194012941  | C  | 79.594108749 | 25.517324385 | 0.019808968  |
| C  | 71.067902529 | 28.191839680 | 4.298505052  | N  | 80.040247288 | 26.554181378 | 0.791857837  |
| C  | 71.414511434 | 27.809238003 | 5.595939581  | C  | 81.246364117 | 26.172219609 | 1.323228621  |
| C  | 72.399612967 | 26.835578025 | 5.749606861  | C  | 81.561016072 | 24.833541379 | 0.925671510  |
| C  | 76.458202481 | 23.220980357 | 6.765772560  | C  | 80.530674835 | 24.419210033 | 0.099790377  |
| H  | 76.678428670 | 23.686051527 | 7.737740188  | C  | 80.425289944 | 23.105615829 | -0.498355654 |
| O  | 73.386168475 | 26.154931600 | 2.291548029  | O  | 79.524242724 | 22.718202592 | -1.245785346 |
| C  | 70.882915461 | 28.533333791 | 6.793535978  | C  | 82.790099989 | 24.097054389 | 1.314631640  |
| H  | 71.578000000 | 29.361000000 | 7.011998000  | C  | 83.924452503 | 24.332941684 | 0.303417207  |
| C  | 82.383803793 | 21.505133161 | 5.911142853  | C  | 85.236084952 | 23.791933547 | 0.829085351  |
| H  | 82.535000000 | 20.841000000 | 5.044000000  | O  | 85.841323885 | 22.907063206 | 0.126204109  |
| N  | 77.916927604 | 22.616051103 | 3.488642598  | C  | 82.044035858 | 26.954721112 | 2.149491667  |
| C  | 76.733528537 | 22.105786238 | 3.052680834  | C  | 81.707495499 | 28.190456569 | 2.660666614  |
| N  | 76.871064499 | 20.991323284 | 2.319575550  | N  | 80.536759798 | 28.858066309 | 2.399801250  |
| C  | 78.235669887 | 20.788729336 | 2.235891948  | C  | 80.559270778 | 29.980075849 | 3.181416469  |
| C  | 78.876699249 | 21.805848006 | 2.942613228  | C  | 81.784143366 | 30.044572118 | 3.943605705  |
| C  | 78.804732203 | 19.623656132 | 1.491316966  | C  | 82.505403668 | 28.931804066 | 3.613406760  |
| H  | 79.537999000 | 19.027000000 | 2.065001000  | C  | 83.812886636 | 28.513829388 | 4.189960055  |
| O  | 73.172796840 | 27.821700591 | 0.182737068  | C  | 83.665533902 | 27.839593528 | 5.571481722  |
| C  | 73.890303103 | 27.552373001 | -1.062701511 | C  | 85.053441315 | 27.565718385 | 6.119590026  |
| C  | 73.658192123 | 28.684115433 | -2.053604202 | O  | 85.507399957 | 26.364886636 | 6.058946819  |

|   |              |              |              |   |              |              |              |
|---|--------------|--------------|--------------|---|--------------|--------------|--------------|
| C | 82.113865517 | 31.102092769 | 4.936035034  | H | 74.494560709 | 32.375610315 | 3.005934608  |
| C | 79.534383542 | 30.896485961 | 3.316447567  | H | 74.029934816 | 30.876457927 | 2.180509705  |
| C | 78.303433532 | 30.815176619 | 2.697795104  | H | 74.534768325 | 32.289685815 | 1.231410806  |
| N | 77.955851733 | 29.880479638 | 1.764386180  | H | 81.917015661 | 28.975495045 | 0.019432779  |
| C | 76.636800070 | 30.116072590 | 1.472324094  | H | 83.366870698 | 29.974444306 | -2.161104018 |
| C | 76.137991877 | 31.253253064 | 2.211982238  | H | 82.426171437 | 30.087337083 | -3.675283524 |
| C | 77.181378328 | 31.691692875 | 2.995192321  | H | 79.710670964 | 30.508050136 | -3.216664207 |
| C | 77.220778810 | 32.695995964 | 4.041476838  | H | 78.043932266 | 29.619746108 | -1.533312319 |
| C | 76.416000803 | 33.758714762 | 4.194506873  | H | 75.510750053 | 26.200051105 | 3.407092118  |
| C | 74.729150007 | 31.724424363 | 2.157186900  | H | 73.513579204 | 24.231988411 | 6.567825248  |
| C | 75.834412465 | 29.337467382 | 0.660631563  | H | 75.924409159 | 22.281087667 | 6.953354115  |
| C | 75.602458786 | 25.078233428 | -1.954724426 | H | 77.427000000 | 22.984000000 | 6.282000000  |
| C | 82.454861803 | 30.374768055 | -2.615878065 | H | 71.410817201 | 27.941541836 | 2.190715510  |
| H | 82.482002000 | 31.469001000 | -2.548998000 | H | 70.308631230 | 28.959603770 | 4.145105062  |
| O | 85.672064450 | 24.247644950 | 1.920584789  | H | 69.888474919 | 28.955209930 | 6.605632353  |
| O | 85.726174867 | 28.549306615 | 6.529854431  | H | 70.838769519 | 27.883291882 | 7.675576545  |
| H | 85.163127304 | 22.202722718 | -1.090887605 | H | 72.719911551 | 26.543833469 | 6.749260660  |
| N | 87.567516991 | 26.719639092 | 4.217973476  | H | 75.780311087 | 22.571740479 | 3.278008063  |
| C | 88.378307269 | 27.780431951 | 4.225404628  | H | 79.931354824 | 21.953723224 | 3.141637767  |
| N | 88.064169354 | 28.855522030 | 4.951872916  | H | 79.314607512 | 19.954337684 | 0.571975731  |
| N | 89.474533098 | 27.760208508 | 3.464176872  | H | 77.988411429 | 18.951375818 | 1.196893726  |
| C | 90.396678911 | 28.862548476 | 3.293941905  | H | 79.441006272 | 22.207691290 | 5.875157666  |
| H | 91.323997000 | 28.428000000 | 2.916008000  | H | 83.367322162 | 21.800949858 | 6.297277211  |
| N | 87.817402168 | 21.458559401 | 1.146777112  | H | 81.865439773 | 20.928055819 | 6.685800334  |
| C | 88.146068556 | 21.083727679 | 2.382205100  | H | 83.121164972 | 24.015301272 | 4.804857050  |
| N | 89.305036177 | 20.429735723 | 2.303797787  | H | 83.127087718 | 24.431836408 | 2.302842004  |
| C | 89.731117986 | 20.389149384 | 0.996057330  | H | 82.599613209 | 23.017231786 | 1.405222803  |
| C | 88.787207413 | 21.044495680 | 0.254087982  | H | 84.054185467 | 25.415650661 | 0.144494640  |
| C | 88.685126168 | 21.313183464 | -1.200072262 | H | 83.668917263 | 23.882192006 | -0.664480155 |
| H | 88.625000000 | 22.392996000 | -1.404991000 | H | 84.453113357 | 29.401361853 | 4.309280112  |
| O | 86.849715462 | 22.655060381 | 5.057174495  | H | 84.344124751 | 27.839428555 | 3.500660804  |
| O | 84.763049403 | 24.365234391 | 4.556862595  | H | 83.134384549 | 28.521037729 | 6.252412981  |
| O | 84.777574874 | 21.787002804 | -1.963609203 | H | 83.083709429 | 26.911050605 | 5.490376822  |
| C | 84.700228509 | 20.459459106 | -1.858852127 | H | 86.980078031 | 22.056013354 | 0.856497317  |
| O | 85.007318595 | 19.842600326 | -0.835111274 | H | 87.592173581 | 21.283039174 | 3.290146400  |
| C | 84.208424685 | 19.793544669 | -3.105214423 | H | 90.654603952 | 19.905055783 | 0.710569151  |
| H | 84.927000000 | 19.944996000 | -3.924990000 | H | 89.559323816 | 20.904420182 | -1.717297526 |
| O | 84.189907054 | 20.495481083 | 1.777340887  | H | 87.784116324 | 20.839218343 | -1.614713575 |
| O | 88.120874691 | 24.207027998 | 3.116208485  | H | 90.614597504 | 29.341048584 | 4.256620668  |
| H | 78.214197694 | 24.581678946 | -1.260019444 | H | 90.017041839 | 29.610941858 | 2.584629828  |
| H | 83.006471108 | 26.544432621 | 2.444418656  | H | 89.611239931 | 26.936552976 | 2.881053456  |
| H | 79.697594894 | 31.715357993 | 4.010698264  | H | 88.702004876 | 29.643959246 | 5.012816792  |
| H | 74.804718261 | 29.654374254 | 0.531243629  | H | 87.279057099 | 28.791286334 | 5.628554009  |
| H | 74.677795666 | 24.658783952 | -1.532425128 | H | 87.886434090 | 25.834548778 | 3.771669998  |
| H | 75.386003514 | 25.376486712 | -2.990860631 | H | 86.893070064 | 26.615247218 | 4.997383733  |
| H | 76.346805266 | 24.275223716 | -1.988518129 | H | 84.072736272 | 18.722533674 | -2.929972424 |
| H | 81.251026861 | 22.413749762 | -0.227613060 | H | 83.258638131 | 20.246729259 | -3.418136606 |
| H | 73.487250790 | 26.622927268 | -1.490997795 | H | 73.256741060 | 26.738188973 | 1.473660485  |
| H | 74.036992405 | 29.639957458 | -1.664870569 | H | 83.484355006 | 19.819362976 | 1.846974977  |
| H | 74.173999489 | 28.461810971 | -2.999213229 | H | 84.539081108 | 20.361817261 | 0.859912865  |
| H | 77.989792058 | 32.538398946 | 4.802037246  | H | 87.833968345 | 23.651599573 | 3.894171320  |
| H | 75.643149576 | 34.024666920 | 3.476699479  | H | 87.304324747 | 24.178309092 | 2.539462846  |
| H | 76.532553637 | 34.406296637 | 5.063586357  | H | 87.159420351 | 22.778615052 | 5.981318276  |
| H | 81.433296484 | 31.047594948 | 5.800111638  | H | 86.038498089 | 23.239577971 | 4.983944326  |
| H | 82.016024358 | 32.106813733 | 4.500815422  | H | 84.995212927 | 25.212448755 | 5.083415729  |
| H | 83.138548022 | 30.988308349 | 5.307553902  | H | 85.025486750 | 24.485406892 | 3.604721056  |



|   |              |              |             |   |              |              |              |
|---|--------------|--------------|-------------|---|--------------|--------------|--------------|
| H | 81.217641914 | 25.614356817 | 4.152494922 | H | 89.798055945 | 20.030504615 | 3.102742732  |
| O | 78.349272299 | 27.464985227 | 2.628513889 | H | 77.964443367 | 24.658695159 | 1.633705110  |
| O | 77.433005739 | 25.143383557 | 2.297574742 | H | 72.228701862 | 27.938649929 | -0.070219841 |
| H | 77.784101891 | 26.100999668 | 2.286521348 |   |              |              |              |

Structure 10:

189

|    |              |              |              |   |              |              |              |
|----|--------------|--------------|--------------|---|--------------|--------------|--------------|
| C  | 81.081031688 | 24.632912955 | 4.582469251  | C | 79.606236969 | 25.509798043 | 0.006019557  |
| N  | 79.913921683 | 24.086118018 | 4.918053768  | N | 80.052469160 | 26.555446707 | 0.766871906  |
| C  | 80.208878591 | 22.872746235 | 5.511984929  | C | 81.258014435 | 26.170400971 | 1.303795325  |
| C  | 81.564593578 | 22.682906349 | 5.513680655  | C | 81.571187890 | 24.828702835 | 0.914547523  |
| N  | 82.092212944 | 23.816073974 | 4.930038168  | C | 80.539810646 | 24.411881686 | 0.091717650  |
| Cu | 78.131000000 | 24.537000000 | 4.280000000  | C | 80.432044814 | 23.094783300 | -0.495396750 |
| N  | 76.263386601 | 24.800240142 | 4.856635405  | O | 79.529204571 | 22.703710226 | -1.242160028 |
| C  | 75.354316702 | 25.555630676 | 4.263910626  | C | 82.799074130 | 24.094260042 | 1.304463475  |
| N  | 74.163816716 | 25.423003920 | 4.891751603  | C | 83.923140004 | 24.323996822 | 0.284826842  |
| C  | 74.339564343 | 24.522921460 | 5.939554680  | C | 85.247095554 | 23.800338849 | 0.805234227  |
| C  | 75.657933641 | 24.136333195 | 5.907026623  | O | 85.874787724 | 22.938243456 | 0.101694380  |
| C  | 73.048990322 | 26.279093749 | 4.658864916  | C | 82.056396164 | 26.949960287 | 2.130573671  |
| C  | 72.701491032 | 26.668313093 | 3.351154645  | C | 81.724214503 | 28.188816833 | 2.637041939  |
| C  | 71.678109339 | 27.607132561 | 3.198722340  | N | 80.558055207 | 28.862096789 | 2.363809675  |
| C  | 71.050348168 | 28.171671088 | 4.302924683  | C | 80.577416052 | 29.983660768 | 3.148024226  |
| C  | 71.408736845 | 27.802038307 | 5.601687012  | C | 81.796647369 | 30.045239798 | 3.917128982  |
| C  | 72.398599773 | 26.834192442 | 5.755827528  | C | 82.516936152 | 28.928548539 | 3.593789583  |
| C  | 76.455651177 | 23.212653957 | 6.764230916  | C | 83.819016123 | 28.509838924 | 4.181151274  |
| H  | 76.670397949 | 23.672698454 | 7.740064951  | C | 83.663695198 | 27.859047884 | 5.572114583  |
| O  | 73.372825343 | 26.138253007 | 2.297626541  | C | 85.048938658 | 27.576914849 | 6.121699196  |
| C  | 70.882107117 | 28.532323327 | 6.798257411  | O | 85.498409718 | 26.374045858 | 6.057990811  |
| H  | 71.578000000 | 29.361000000 | 7.011999000  | C | 82.126069068 | 31.100763055 | 4.911412600  |
| C  | 82.382776039 | 21.510048708 | 5.907886653  | C | 79.550150353 | 30.900909968 | 3.281487712  |
| H  | 82.535000000 | 20.841000000 | 5.044000000  | C | 78.316458626 | 30.821990614 | 2.661788930  |
| N  | 77.907587661 | 22.662578727 | 3.458752123  | N | 77.967383963 | 29.890266484 | 1.724505169  |
| C  | 76.722185849 | 22.120836328 | 3.100404436  | C | 76.643754807 | 30.115068478 | 1.439543433  |
| N  | 76.868230929 | 20.984043962 | 2.405702051  | C | 76.141762174 | 31.251609853 | 2.183199908  |
| C  | 78.236187581 | 20.790711264 | 2.286533232  | C | 77.191218722 | 31.694749160 | 2.964753208  |
| C  | 78.878026471 | 21.831346062 | 2.928207019  | C | 77.228850909 | 32.701528395 | 4.007229918  |
| C  | 78.781025395 | 19.621946441 | 1.522088765  | C | 76.422149564 | 33.764643622 | 4.155833452  |
| H  | 79.538000000 | 19.027000000 | 2.065001000  | C | 74.732897850 | 31.720209967 | 2.135478738  |
| O  | 73.173813997 | 27.794701062 | 0.189840592  | C | 75.838119878 | 29.327372874 | 0.634329132  |
| C  | 73.887414795 | 27.512985123 | -1.057579224 | C | 75.609440654 | 25.040098577 | -1.948158393 |
| C  | 73.643246689 | 28.634081327 | -2.058960939 | C | 82.453595080 | 30.374862280 | -2.621293577 |
| H  | 72.565406739 | 28.727332285 | -2.256719956 | H | 82.482001000 | 31.468999000 | -2.548999000 |
| C  | 75.328545237 | 27.284515883 | -0.736789332 | O | 85.670242015 | 24.267829453 | 1.902002583  |
| C  | 76.211868242 | 28.131587933 | 0.037651812  | O | 85.729261192 | 28.559017488 | 6.532597736  |
| N  | 77.460751580 | 27.568466060 | 0.112904642  | H | 85.217811962 | 22.246970964 | -1.102309123 |
| C  | 77.396614926 | 26.399209698 | -0.599369700 | N | 87.582312059 | 26.681218606 | 4.215958639  |
| C  | 76.070745852 | 26.206085089 | -1.145085492 | C | 88.377633017 | 27.752210878 | 4.211838400  |
| Fe | 79.021998000 | 28.209000000 | 1.280001000  | N | 88.043232852 | 28.840675804 | 4.915990746  |
| N  | 79.781406372 | 29.095473439 | -0.409809051 | N | 89.480626844 | 27.738314827 | 3.457901354  |
| C  | 81.122812044 | 29.269629005 | -0.684749426 | C | 90.392275722 | 28.850044942 | 3.297375004  |
| C  | 81.261017959 | 29.882730758 | -1.901304801 | H | 91.323997000 | 28.427997000 | 2.916007000  |
| N  | 79.974889345 | 30.076046309 | -2.355787523 | N | 87.899950660 | 21.387968436 | 1.162702654  |
| C  | 79.106395382 | 29.594753655 | -1.443126758 | C | 88.308361242 | 20.955998041 | 2.377407971  |
| C  | 78.404579408 | 25.458277766 | -0.682004789 | N | 89.459881331 | 20.302673356 | 2.283861384  |

|   |              |              |              |   |              |              |              |
|---|--------------|--------------|--------------|---|--------------|--------------|--------------|
| C | 89.795227632 | 20.326245031 | 0.943243273  | H | 79.933835440 | 22.030005436 | 3.067844792  |
| C | 88.833155267 | 21.002437764 | 0.228117187  | H | 79.242012791 | 19.944191113 | 0.575096499  |
| C | 88.684881180 | 21.308588437 | -1.219092856 | H | 77.951737125 | 18.946175528 | 1.270979376  |
| H | 88.624997000 | 22.392991000 | -1.404990000 | H | 79.437781769 | 22.197571384 | 5.859963288  |
| O | 86.861389461 | 22.659620435 | 5.071557457  | H | 83.366569051 | 21.813466024 | 6.288933509  |
| O | 84.749662123 | 24.366076072 | 4.548877221  | H | 81.868237664 | 20.936651588 | 6.688580027  |
| O | 84.835530247 | 21.823450448 | -1.982559842 | H | 83.115401094 | 24.014459968 | 4.787216488  |
| C | 84.707759836 | 20.503480577 | -1.856756529 | H | 83.142237788 | 24.437913443 | 2.287253569  |
| O | 84.969885742 | 19.894613936 | -0.811696131 | H | 82.613052954 | 23.013683021 | 1.405603347  |
| C | 84.212753279 | 19.822774935 | -3.095207582 | H | 84.047284560 | 25.406111953 | 0.111103799  |
| H | 84.926997000 | 19.944993000 | -3.924990000 | H | 83.664206018 | 23.860084758 | -0.677270768 |
| O | 84.058718612 | 20.631173195 | 1.753408600  | H | 84.466291265 | 29.394181688 | 4.288841294  |
| O | 88.110304390 | 24.194532504 | 3.086014839  | H | 84.348043320 | 27.821055893 | 3.504258140  |
| H | 78.229017496 | 24.554205665 | -1.258102299 | H | 83.141450229 | 28.555625187 | 6.245400925  |
| H | 83.014674639 | 26.533308445 | 2.431161020  | H | 83.072035665 | 26.934387325 | 5.506079354  |
| H | 79.712192983 | 31.717941707 | 3.978450168  | H | 87.067520127 | 21.974252660 | 0.930574651  |
| H | 74.806270650 | 29.637588629 | 0.508963083  | H | 87.757571169 | 21.146023380 | 3.291372681  |
| H | 74.670605746 | 24.637330701 | -1.542126791 | H | 90.700255510 | 19.857978018 | 0.573749364  |
| H | 75.420059106 | 25.327437676 | -2.993461072 | H | 89.540164509 | 20.908045957 | -1.775190738 |
| H | 76.343676400 | 24.226904187 | -1.955676890 | H | 87.770476605 | 20.852455186 | -1.624394385 |
| H | 81.254845264 | 22.402507200 | -0.217136096 | H | 90.605101488 | 29.322476355 | 4.264569814  |
| H | 73.484503042 | 26.577621215 | -1.472548722 | H | 90.007179590 | 29.602083066 | 2.594444682  |
| H | 74.024025002 | 29.593902582 | -1.683884776 | H | 89.639322711 | 26.907365800 | 2.890798965  |
| H | 74.149370291 | 28.403086665 | -3.007228716 | H | 88.698840585 | 29.612621239 | 5.003844452  |
| H | 77.998389911 | 32.545458227 | 4.767234664  | H | 87.268951322 | 28.771968588 | 5.604899056  |
| H | 75.649084925 | 34.024144517 | 3.436473822  | H | 87.887833625 | 25.794132518 | 3.754900180  |
| H | 76.537806795 | 34.417624679 | 5.019754714  | H | 86.894059252 | 26.586545970 | 4.984414748  |
| H | 81.454797692 | 31.036620788 | 5.782167692  | H | 84.061910285 | 18.756632591 | -2.897847220 |
| H | 82.017402561 | 32.107010882 | 4.483244079  | H | 83.265174664 | 20.281441178 | -3.410928960 |
| H | 83.156032891 | 30.992752947 | 5.273574167  | H | 73.248030259 | 26.720668047 | 1.478791616  |
| H | 74.499765970 | 32.358340845 | 2.993255635  | H | 83.361453148 | 19.941632087 | 1.811718836  |
| H | 74.035046568 | 30.872512635 | 2.147536320  | H | 84.448461100 | 20.476486957 | 0.854326101  |
| H | 74.536951435 | 32.297784301 | 1.219638500  | H | 87.835667225 | 23.619692842 | 3.855802871  |
| H | 81.900459076 | 28.961936627 | 0.001396109  | H | 87.286589171 | 24.164300661 | 2.513079338  |
| H | 83.362595504 | 29.972011648 | -2.162519382 | H | 87.178901298 | 22.804577249 | 5.990972722  |
| H | 82.432291241 | 30.092319040 | -3.682062733 | H | 86.052713076 | 23.245900877 | 4.996698198  |
| H | 79.713254138 | 30.513360980 | -3.238455352 | H | 84.983807804 | 25.211286270 | 5.078627779  |
| H | 78.034522905 | 29.617183982 | -1.566162998 | H | 85.031449316 | 24.484341607 | 3.599658530  |
| H | 75.501256828 | 26.177128687 | 3.395396271  | H | 81.205543033 | 25.599389987 | 4.111595652  |
| H | 73.518451304 | 24.243125839 | 6.586998991  | O | 78.333250093 | 27.464249896 | 2.617432394  |
| H | 75.925781849 | 22.268297096 | 6.943189400  | O | 77.413252124 | 25.155513482 | 2.291253458  |
| H | 77.427000000 | 22.984000000 | 6.282000000  | H | 77.791088072 | 26.101864162 | 2.271150031  |
| H | 71.383299351 | 27.908114072 | 2.194962514  | H | 77.944668291 | 24.633490425 | 1.655618201  |
| H | 70.284213018 | 28.932245183 | 4.148952955  | H | 72.229560880 | 27.910586231 | -0.061356097 |
| H | 69.887169893 | 28.953795754 | 6.612430898  | H | 90.379299596 | 19.611113814 | 3.568376314  |
| H | 70.840412616 | 27.885939410 | 7.683186108  | O | 90.914259688 | 19.222317362 | 4.339539407  |
| H | 72.725851016 | 26.550892884 | 6.755774647  | H | 91.723050679 | 18.875699569 | 3.910996703  |
| H | 75.767082597 | 22.568004884 | 3.354103097  |   |              |              |              |

### Structure 11:

183

|   |              |              |             |   |              |              |             |
|---|--------------|--------------|-------------|---|--------------|--------------|-------------|
| O | 85.019470352 | 24.345785380 | 4.240564761 | O | 84.422948109 | 20.241426981 | 1.672397631 |
| O | 88.468956894 | 24.590811509 | 1.776477073 | O | 86.430772358 | 22.073388896 | 4.883766797 |

|    |              |              |              |   |              |              |              |
|----|--------------|--------------|--------------|---|--------------|--------------|--------------|
| Fe | 79.100034000 | 28.054773000 | 1.364498000  | C | 73.066937135 | 27.890275059 | 5.688553379  |
| C  | 82.221286453 | 26.882216652 | 1.984222763  | C | 73.513195951 | 27.187964731 | 4.576018201  |
| C  | 78.281176290 | 25.133587367 | -0.199762185 | C | 72.957384817 | 27.394195313 | 3.267368857  |
| C  | 75.984252698 | 29.285735344 | 0.629258864  | O | 73.390723142 | 26.746720988 | 2.243497748  |
| C  | 79.735029553 | 30.819066625 | 3.244803576  | C | 78.678452407 | 19.639840964 | 1.799107076  |
| N  | 80.690779522 | 28.751567440 | 2.352448828  | C | 78.216781209 | 20.897005392 | 2.478591367  |
| C  | 81.893223298 | 28.112038416 | 2.523292005  | C | 78.924577540 | 22.004127912 | 2.902853589  |
| C  | 82.745729740 | 28.878839905 | 3.409579232  | N | 76.863427311 | 21.158585142 | 2.639801906  |
| C  | 82.020085301 | 29.972684598 | 3.796768255  | C | 76.807551662 | 22.399728126 | 3.147580101  |
| C  | 80.746759355 | 29.883311923 | 3.118993858  | N | 78.025431693 | 22.964216933 | 3.323814843  |
| C  | 82.407353713 | 31.037226926 | 4.762612472  | C | 82.494298073 | 21.494257343 | 5.692759339  |
| O  | 79.336035000 | 22.138773000 | -0.333505000 | C | 81.753097129 | 22.737510510 | 5.358353615  |
| C  | 84.124672970 | 28.519435597 | 3.851266312  | C | 80.411487137 | 23.010828512 | 5.384992542  |
| C  | 84.178096617 | 27.912461670 | 5.271605108  | N | 82.343361083 | 23.870194157 | 4.829870579  |
| C  | 85.622691860 | 27.603120369 | 5.631040384  | C | 81.376256887 | 24.764609732 | 4.545957309  |
| O  | 86.374001525 | 28.571568073 | 5.929094468  | N | 80.181250707 | 24.271158678 | 4.861531720  |
| O  | 86.017983277 | 26.381792928 | 5.561909533  | C | 82.520411879 | 30.395144065 | -2.539921364 |
| N  | 77.511073778 | 27.410647821 | 0.287703678  | C | 81.332543115 | 29.888584258 | -1.811594923 |
| C  | 77.360445914 | 26.160921189 | -0.254763415 | C | 81.209300338 | 29.273772377 | -0.593973872 |
| C  | 76.048388101 | 26.019596580 | -0.851300979 | N | 80.046934536 | 29.960871805 | -2.302916746 |
| C  | 75.390729668 | 27.198125329 | -0.626232732 | C | 79.202062301 | 29.405985869 | -1.410136934 |
| C  | 76.309704132 | 28.045948390 | 0.109629405  | N | 79.880125648 | 28.975822100 | -0.352895020 |
| C  | 75.581540241 | 24.799668066 | -1.566099908 | C | 91.068980905 | 28.492728856 | 2.839990204  |
| N  | 78.094925835 | 29.761147866 | 1.779632205  | N | 90.138143818 | 27.403076787 | 3.060931993  |
| C  | 76.803137712 | 30.063428269 | 1.427425342  | C | 89.115916500 | 27.428018102 | 3.924337702  |
| C  | 76.374782112 | 31.290755100 | 2.054639924  | N | 88.287804364 | 26.386433038 | 3.972316187  |
| C  | 77.437670491 | 31.728466236 | 2.814331163  | N | 88.930962708 | 28.469063745 | 4.738671190  |
| C  | 78.502483899 | 30.757913802 | 2.621033600  | H | 77.183435000 | 24.806884000 | 7.570902000  |
| C  | 75.040652573 | 31.920704108 | 1.878171173  | H | 72.452456000 | 30.244969000 | 7.189248000  |
| C  | 77.558158096 | 32.909489305 | 3.644479567  | H | 79.552516000 | 19.139805000 | 2.252830000  |
| C  | 76.551093863 | 33.597127234 | 4.209225726  | H | 82.592179000 | 20.840344000 | 4.808238000  |
| N  | 80.090681740 | 26.351727219 | 0.885965897  | H | 82.462948946 | 31.482472813 | -2.691676625 |
| C  | 79.543998120 | 25.217610623 | 0.359366005  | H | 81.992296971 | 29.037698830 | 0.114450633  |
| C  | 80.497256189 | 24.128842901 | 0.429416696  | H | 79.920283615 | 31.658620205 | 3.908696974  |
| C  | 81.649409905 | 24.659010721 | 0.991778594  | H | 78.577262639 | 33.262472520 | 3.824073805  |
| C  | 81.365579823 | 26.036909064 | 1.283698876  | H | 78.134577803 | 29.336973542 | -1.565097287 |
| C  | 80.343181463 | 22.722880249 | 0.078851457  | H | 90.234252727 | 26.564127594 | 2.492646373  |
| C  | 82.940096546 | 23.981459599 | 1.289242693  | H | 75.851156532 | 26.643437982 | 3.059859771  |
| C  | 83.955715689 | 24.113556895 | 0.142976020  | H | 73.548955405 | 27.716472786 | 6.650797315  |
| C  | 85.316525763 | 23.589251269 | 0.549054923  | H | 70.660919835 | 29.773083174 | 4.226331742  |
| O  | 85.879323980 | 22.722531275 | -0.208238557 | H | 75.509831635 | 33.293607511 | 4.118754647  |
| O  | 85.849363346 | 24.045609335 | 1.601144110  | H | 76.760859098 | 34.484057746 | 4.807140474  |
| C  | 73.994022824 | 27.552316001 | -1.054728612 | H | 72.930700733 | 28.730349116 | -2.509617152 |
| O  | 73.216957855 | 28.133103852 | -0.000115061 | H | 74.438014480 | 29.489763288 | -1.921600406 |
| C  | 73.972695604 | 28.537624888 | -2.216463269 | H | 74.517808591 | 28.132291442 | -3.080486503 |
| Cu | 78.405034000 | 24.763772000 | 4.178497000  | H | 73.287900039 | 27.551657767 | 0.829139466  |
| C  | 76.683998852 | 24.135939154 | 6.852316002  | H | 71.432031316 | 28.526766810 | 2.240155810  |
| C  | 75.987120360 | 24.951413364 | 5.826761993  | H | 70.772020988 | 30.267138443 | 6.580830736  |
| C  | 74.739156884 | 25.497124864 | 5.894803107  | H | 71.336149786 | 28.937677688 | 7.624619762  |
| N  | 76.585200098 | 25.377488321 | 4.642594288  | H | 73.959875191 | 25.410394746 | 6.639869612  |
| C  | 75.706497463 | 26.149649489 | 4.010674599  | H | 81.557586766 | 25.745832705 | 4.131197652  |
| N  | 74.569226789 | 26.259627657 | 4.751420193  | H | 79.601183942 | 22.366579060 | 5.701283428  |
| C  | 71.624180710 | 29.614718661 | 6.806928253  | H | 83.363048832 | 24.021131707 | 4.651379529  |
| C  | 72.046783142 | 28.838704504 | 5.594688921  | H | 83.495661657 | 21.713560417 | 6.083129656  |
| C  | 71.468788870 | 29.046439569 | 4.327111056  | H | 81.946421320 | 20.928656046 | 6.456293051  |
| C  | 71.901249322 | 28.355386235 | 3.209967310  | H | 79.767820405 | 30.366793709 | -3.195503410 |

|   |              |              |              |   |              |              |              |
|---|--------------|--------------|--------------|---|--------------|--------------|--------------|
| H | 79.991766535 | 22.187760967 | 2.922685640  | H | 85.360113929 | 25.185888323 | 4.709932759  |
| H | 75.884683903 | 22.906831223 | 3.410402092  | H | 91.665387055 | 28.699147410 | 3.739373137  |
| H | 78.944499198 | 19.852088560 | 0.751174276  | H | 90.547643405 | 29.406109065 | 2.521279592  |
| H | 77.854588116 | 18.912783249 | 1.788037349  | C | 84.159649416 | 19.308306947 | -3.117490559 |
| H | 75.968075250 | 23.517126078 | 7.407886648  | C | 84.749439195 | 20.084691115 | -1.981591743 |
| H | 77.434062437 | 23.474641721 | 6.402341141  | O | 85.194621091 | 19.555127486 | -0.959634608 |
| H | 83.424169424 | 30.173531244 | -1.961190549 | O | 84.728660488 | 21.406873133 | -2.167888637 |
| H | 82.613872808 | 29.916095832 | -3.524861813 | C | 88.810160597 | 20.774731625 | -1.314952374 |
| H | 75.121226122 | 33.015143112 | 1.926982245  | C | 88.811680067 | 20.733946748 | 0.168936647  |
| H | 74.589830547 | 31.652271848 | 0.915121306  | C | 89.648297647 | 20.108932568 | 1.053041023  |
| H | 74.344832062 | 31.607816520 | 2.673148634  | N | 87.831759106 | 21.339921334 | 0.934561252  |
| H | 82.042476299 | 32.024127711 | 4.448769371  | C | 88.045833082 | 21.097580691 | 2.229099972  |
| H | 81.984088528 | 30.829566976 | 5.758600975  | N | 89.150540196 | 20.353458320 | 2.312221438  |
| H | 83.498656824 | 31.094112567 | 4.868173296  | H | 84.681485000 | 19.503926000 | -4.065239000 |
| H | 74.965086592 | 29.620179316 | 0.463937235  | H | 88.765971000 | 21.799802000 | -1.706250000 |
| H | 83.220234586 | 26.508882065 | 2.195047474  | H | 89.717607210 | 20.294614090 | -1.696998592 |
| H | 77.998414135 | 24.167242625 | -0.609768886 | H | 87.940365168 | 20.228784762 | -1.706872848 |
| H | 74.524665265 | 24.880642893 | -1.845370427 | H | 84.197882482 | 18.239204056 | -2.890465052 |
| H | 76.162207976 | 24.638828341 | -2.487013591 | H | 83.114686952 | 19.618579550 | -3.255673847 |
| H | 75.701239640 | 23.901632432 | -0.942678488 | H | 90.538875933 | 19.515862115 | 0.895473774  |
| H | 81.276136936 | 22.139485260 | 0.236615206  | H | 87.443812490 | 21.442756249 | 3.068872130  |
| H | 83.592537101 | 23.597881199 | -0.755513658 | H | 87.029103220 | 21.924872282 | 0.528647126  |
| H | 84.084331035 | 25.178530102 | -0.112760572 | H | 84.740769224 | 20.105239342 | 0.744294899  |
| H | 83.382065901 | 24.419099294 | 2.191984686  | H | 83.589025000 | 19.723529000 | 1.696373000  |
| H | 82.785853569 | 22.915481640 | 1.510935272  | H | 87.517364849 | 24.275894600 | 1.680391527  |
| H | 83.778556022 | 28.641401659 | 5.992375607  | H | 89.012648516 | 23.773220024 | 1.800225182  |
| H | 83.564480187 | 27.002428229 | 5.325455281  | H | 85.147820556 | 21.895881435 | -1.357052110 |
| H | 84.585686299 | 27.820413008 | 3.136339865  | H | 91.740917000 | 28.167083000 | 2.038154000  |
| H | 84.750976415 | 29.426064392 | 3.845475235  | H | 73.515257154 | 26.617282720 | -1.394659416 |
| H | 88.373490158 | 25.646349481 | 3.254966703  | H | 89.557863023 | 20.014009548 | 3.184182799  |
| H | 87.507683348 | 26.372236327 | 4.660045464  | O | 78.528061020 | 27.286901255 | 2.739170315  |
| H | 89.549800690 | 29.273843055 | 4.702909974  | H | 85.742666332 | 21.388403175 | 5.015106143  |
| H | 88.045453269 | 28.530263419 | 5.285481281  | H | 85.910680092 | 22.904379655 | 4.679781212  |
| H | 85.278770312 | 24.383531607 | 3.280747936  |   |              |              |              |

## Structure 12:

185

|    |              |              |              |   |              |              |              |
|----|--------------|--------------|--------------|---|--------------|--------------|--------------|
| O  | 85.024041132 | 24.345008614 | 4.226767784  | C | 84.123331598 | 28.525353171 | 3.829527152  |
| O  | 88.484737059 | 24.596314674 | 1.722101729  | C | 84.175329439 | 27.931744691 | 5.254923910  |
| O  | 84.421429651 | 20.243348982 | 1.677729909  | C | 85.619618555 | 27.618717770 | 5.608026910  |
| O  | 86.438443907 | 22.093893213 | 4.918382550  | O | 86.375349322 | 28.583212066 | 5.903411522  |
| Fe | 79.100034000 | 28.054771000 | 1.364498000  | O | 86.010311401 | 26.397972358 | 5.527258464  |
| C  | 82.215976389 | 26.870265597 | 1.987365455  | N | 77.506765527 | 27.405988484 | 0.270975940  |
| C  | 78.286819083 | 25.128660317 | -0.218404076 | C | 77.364189598 | 26.157726334 | -0.277223866 |
| C  | 75.982466142 | 29.277916390 | 0.609542821  | C | 76.056724154 | 26.010914324 | -0.883701990 |
| C  | 79.732849669 | 30.817704685 | 3.219138714  | C | 75.396673052 | 27.189590489 | -0.659937885 |
| N  | 80.683929904 | 28.741067220 | 2.348111995  | C | 76.307955726 | 28.040381971 | 0.083750389  |
| C  | 81.888251017 | 28.105106225 | 2.517242232  | C | 75.600644326 | 24.792884238 | -1.603394385 |
| C  | 82.746187955 | 28.881652528 | 3.389605199  | N | 78.087070789 | 29.749941057 | 1.771961041  |
| C  | 82.021232824 | 29.978703338 | 3.770066638  | C | 76.796791675 | 30.049469227 | 1.415345768  |
| C  | 80.743144360 | 29.881841607 | 3.100243990  | C | 76.367932936 | 31.281920741 | 2.039341752  |
| C  | 82.412455588 | 31.050096369 | 4.724219201  | C | 77.431889626 | 31.724828254 | 2.794195362  |
| O  | 79.336034000 | 22.138771000 | -0.333503000 | C | 78.498786672 | 30.750396786 | 2.605148959  |

|    |              |              |              |   |              |              |              |
|----|--------------|--------------|--------------|---|--------------|--------------|--------------|
| C  | 75.033154828 | 31.910014287 | 1.863962770  | H | 72.452456000 | 30.244969000 | 7.182489000  |
| C  | 77.556487422 | 32.909413332 | 3.615877028  | H | 79.552516000 | 19.139805000 | 2.228305000  |
| C  | 76.555235361 | 33.595255109 | 4.187124956  | H | 82.592179000 | 20.840344000 | 4.808238000  |
| N  | 80.081619395 | 26.340214602 | 0.903594833  | H | 82.481694405 | 31.475548247 | -2.702456625 |
| C  | 79.540979294 | 25.209914661 | 0.359728235  | H | 82.003340505 | 29.043875534 | 0.110239246  |
| C  | 80.500443990 | 24.124725684 | 0.417540659  | H | 79.924265404 | 31.667183241 | 3.871308401  |
| C  | 81.649110634 | 24.653080021 | 0.986880159  | H | 78.577696021 | 33.266288540 | 3.783044524  |
| C  | 81.358315356 | 26.024599114 | 1.294039757  | H | 78.157303110 | 29.317123341 | -1.594858756 |
| C  | 80.354040464 | 22.725320053 | 0.049950561  | H | 90.184737288 | 26.591525521 | 2.420964456  |
| C  | 82.941842926 | 23.976191001 | 1.279507651  | H | 75.955053830 | 26.784818447 | 3.164894817  |
| C  | 83.958760006 | 24.116901426 | 0.134429777  | H | 73.554455073 | 27.762778310 | 6.646795074  |
| C  | 85.315984842 | 23.589186220 | 0.540284987  | H | 70.676672575 | 29.784898247 | 4.184120025  |
| O  | 85.869781700 | 22.706393377 | -0.210199748 | H | 75.513347142 | 33.286815203 | 4.109972370  |
| O  | 85.862428551 | 24.049113439 | 1.586932471  | H | 76.767457529 | 34.484960595 | 4.780851269  |
| C  | 74.019268334 | 27.529577612 | -1.135849221 | H | 72.942612739 | 28.764142090 | -2.536684635 |
| O  | 73.216110048 | 27.974985160 | 0.005061647  | H | 74.403137384 | 29.544024116 | -1.856930557 |
| C  | 73.981999069 | 28.595366133 | -2.220008045 | H | 74.562082288 | 28.263698084 | -3.093191925 |
| Cu | 78.405034000 | 24.763772000 | 4.178499000  | H | 73.265044477 | 27.132002390 | 1.398440243  |
| C  | 76.670686934 | 24.138084092 | 6.861951174  | H | 71.455348162 | 28.495379275 | 2.230067707  |
| C  | 75.988643628 | 24.965171394 | 5.839033117  | H | 70.784890982 | 30.323710069 | 6.543675639  |
| C  | 74.720896269 | 25.481952063 | 5.878362340  | H | 71.286771283 | 28.969320433 | 7.587162324  |
| N  | 76.631247013 | 25.447050316 | 4.706268357  | H | 73.915664469 | 25.353658451 | 6.587349056  |
| C  | 75.765125220 | 26.244917388 | 4.080406900  | H | 81.565688218 | 25.761506997 | 4.185596248  |
| N  | 74.594222462 | 26.291146080 | 4.769137756  | H | 79.591288906 | 22.378025485 | 5.716205048  |
| C  | 71.612713560 | 29.646023276 | 6.784399309  | H | 83.357798498 | 24.010347211 | 4.662358807  |
| C  | 72.044552430 | 28.867958568 | 5.572567331  | H | 83.474038640 | 21.700071816 | 6.103617481  |
| C  | 71.482810103 | 29.061166728 | 4.312670675  | H | 81.917920047 | 20.914743991 | 6.444951654  |
| C  | 71.927111455 | 28.342738776 | 3.198172190  | H | 79.797616383 | 30.343961711 | -3.216210550 |
| C  | 73.071262059 | 27.928133215 | 5.686745663  | H | 79.928801800 | 22.060342039 | 2.939200266  |
| C  | 73.521308188 | 27.213829646 | 4.578471433  | H | 75.815436645 | 22.879900231 | 3.214171228  |
| C  | 72.957511117 | 27.407271598 | 3.318068402  | H | 76.069541488 | 20.547059004 | 2.237266962  |
| O  | 73.423994145 | 26.659984302 | 2.282489149  | H | 78.869205303 | 19.696844394 | 0.686444938  |
| C  | 78.645539419 | 19.536610298 | 1.752327370  | H | 77.866099109 | 18.767141424 | 1.825352010  |
| C  | 78.190407475 | 20.807685636 | 2.378504448  | H | 75.950666638 | 23.530790530 | 7.424505359  |
| C  | 78.859882401 | 21.908277065 | 2.853239866  | H | 77.414122534 | 23.472026602 | 6.407860675  |
| N  | 76.856545559 | 21.145812396 | 2.486549888  | H | 83.444462156 | 30.173271967 | -1.968413072 |
| C  | 76.760547938 | 22.393141866 | 3.005016635  | H | 82.639812700 | 29.911176150 | -3.530626451 |
| N  | 77.968013685 | 22.888610228 | 3.236125569  | H | 75.109506401 | 33.004228737 | 1.922865178  |
| C  | 82.478400710 | 21.486290221 | 5.695138254  | H | 74.585467053 | 31.651027166 | 0.896520255  |
| C  | 81.744434151 | 22.734077429 | 5.361651344  | H | 74.335709367 | 31.587617734 | 2.653926300  |
| C  | 80.403399614 | 23.019787781 | 5.396131613  | H | 82.040174890 | 32.033372530 | 4.409001354  |
| N  | 82.341028174 | 23.866677131 | 4.848049098  | H | 81.999628646 | 30.845103561 | 5.725383139  |
| C  | 81.375102852 | 24.775157796 | 4.583459764  | H | 83.504736630 | 31.111655636 | 4.819060529  |
| N  | 80.175214483 | 24.289570660 | 4.891473994  | H | 74.972203502 | 29.636757952 | 0.430814820  |
| C  | 82.546777459 | 30.392041292 | -2.551522163 | H | 83.216397031 | 26.498894874 | 2.195654721  |
| C  | 81.350593830 | 29.880794140 | -1.821487928 | H | 78.010820411 | 24.168627964 | -0.643886084 |
| C  | 81.224607030 | 29.271371213 | -0.596650529 | H | 74.551582849 | 24.875107251 | -1.911053247 |
| N  | 80.066808989 | 29.947609524 | -2.325563443 | H | 76.204559491 | 24.623449612 | -2.507854691 |
| C  | 79.224187052 | 29.393982928 | -1.432470745 | H | 75.699814686 | 23.897901274 | -0.971718087 |
| N  | 79.897781732 | 28.970793980 | -0.366512079 | H | 81.297283083 | 22.149320142 | 0.166155516  |
| C  | 91.075223386 | 28.481809462 | 2.846763310  | H | 83.595189581 | 23.604749327 | -0.767050388 |
| N  | 90.111670462 | 27.413111113 | 3.021996629  | H | 84.083694394 | 25.183705549 | -0.117946113 |
| C  | 89.097521526 | 27.429498731 | 3.891066910  | H | 83.381429731 | 24.408824522 | 2.185618150  |
| N  | 88.245868972 | 26.407247550 | 3.907039605  | H | 82.789219136 | 22.908513620 | 1.494137308  |
| N  | 88.946289159 | 28.444596724 | 4.745040980  | H | 83.780006658 | 28.668446393 | 5.969732759  |
| H  | 77.183435000 | 24.806884000 | 7.570902000  | H | 83.560035794 | 27.023744995 | 5.317705825  |

|   |              |              |              |   |              |              |              |
|---|--------------|--------------|--------------|---|--------------|--------------|--------------|
| H | 84.580896586 | 27.818333719 | 3.119942581  | H | 88.765971000 | 21.799802000 | -1.706250000 |
| H | 84.751797457 | 29.430294466 | 3.814302625  | H | 89.710921354 | 20.290461275 | -1.708553188 |
| H | 88.340967492 | 25.664294047 | 3.196781956  | H | 87.932888120 | 20.232499073 | -1.714746729 |
| H | 87.475079091 | 26.385292903 | 4.607411861  | H | 84.205163485 | 18.234323069 | -2.893627701 |
| H | 89.539613214 | 29.263801796 | 4.680973595  | H | 83.114656169 | 19.608400512 | -3.257710168 |
| H | 88.045609851 | 28.518659823 | 5.273174227  | H | 90.545634245 | 19.516767648 | 0.882857133  |
| H | 85.287194995 | 24.381427623 | 3.269585624  | H | 87.452285147 | 21.432488675 | 3.066856684  |
| H | 85.355871620 | 25.191916144 | 4.690973334  | H | 87.029109590 | 21.916162789 | 0.527484832  |
| H | 91.670248923 | 28.638358624 | 3.757513973  | H | 84.743227399 | 20.117011647 | 0.750887447  |
| H | 90.583382165 | 29.421824639 | 2.558577896  | H | 83.589025000 | 19.723529000 | 1.696373000  |
| C | 84.161207114 | 19.303875861 | -3.118082373 | H | 87.531876636 | 24.283252506 | 1.634187429  |
| C | 84.746119824 | 20.081696518 | -1.981599728 | H | 89.016029379 | 23.771344044 | 1.831883587  |
| O | 85.190036728 | 19.554991644 | -0.957165285 | H | 85.141008526 | 21.895890474 | -1.358558843 |
| O | 84.723699365 | 21.404649573 | -2.169884382 | H | 91.740917000 | 28.167083000 | 2.038155000  |
| C | 88.806734101 | 20.772498374 | -1.321604002 | H | 73.564025874 | 26.609116826 | -1.526917921 |
| C | 88.811866196 | 20.727938867 | 0.161995618  | H | 89.572076560 | 20.011119326 | 3.173910364  |
| C | 89.653714177 | 20.107869561 | 1.043414732  | O | 78.492289128 | 27.300061512 | 2.735150100  |
| N | 87.833449706 | 21.332366554 | 0.931169693  | H | 85.750958473 | 21.411214373 | 5.062704898  |
| C | 88.052067919 | 21.089847510 | 2.225106067  | H | 85.920390453 | 22.919287821 | 4.685603392  |
| N | 89.160015866 | 20.349748295 | 2.304297139  | H | 72.293454962 | 28.060020645 | -0.326451111 |
| H | 84.681485000 | 19.503926000 | -4.065239000 |   |              |              |              |

### Structure 13:

185

|    |              |              |              |    |              |              |              |
|----|--------------|--------------|--------------|----|--------------|--------------|--------------|
| O  | 85.015484198 | 24.342076487 | 4.234276926  | N  | 78.063625070 | 29.697266894 | 1.851776026  |
| O  | 88.479925415 | 24.573847649 | 1.755516325  | C  | 76.784229832 | 30.026563863 | 1.479960178  |
| O  | 84.423677124 | 20.240138825 | 1.671833041  | C  | 76.370400766 | 31.267075761 | 2.091447716  |
| O  | 86.443196047 | 22.077179697 | 4.880263716  | C  | 77.432389705 | 31.697707357 | 2.852873786  |
| Fe | 79.100034000 | 28.054773000 | 1.364498000  | C  | 78.483276944 | 30.707557518 | 2.679266822  |
| C  | 82.226513319 | 26.859580510 | 1.990022549  | C  | 75.047381980 | 31.921192100 | 1.893399527  |
| C  | 78.277181859 | 25.123414545 | -0.181984400 | C  | 77.569952756 | 32.890871123 | 3.658545049  |
| C  | 75.971475151 | 29.269266694 | 0.660476815  | C  | 76.577242963 | 33.602055421 | 4.216384288  |
| C  | 79.723399285 | 30.775172552 | 3.282476555  | N  | 80.074028648 | 26.338138847 | 0.940987145  |
| N  | 80.682182812 | 28.715421270 | 2.373689245  | C  | 79.535269763 | 25.205881350 | 0.389696507  |
| C  | 81.898250999 | 28.087635125 | 2.531392879  | C  | 80.499052759 | 24.122626183 | 0.425317618  |
| C  | 82.752943211 | 28.862617888 | 3.403198610  | C  | 81.652846298 | 24.652787090 | 0.984623954  |
| C  | 82.020101573 | 29.952026475 | 3.795658309  | C  | 81.359050424 | 26.020811048 | 1.304835860  |
| C  | 80.740557806 | 29.847719040 | 3.137507558  | C  | 80.352014213 | 22.729853758 | 0.045259895  |
| C  | 82.414349619 | 31.023295065 | 4.752483633  | C  | 82.946166322 | 23.971117605 | 1.270740851  |
| O  | 79.336035000 | 22.138773000 | -0.333504000 | C  | 83.967832181 | 24.116699962 | 0.132068649  |
| C  | 84.133550210 | 28.510044252 | 3.836979727  | C  | 85.325377671 | 23.584055246 | 0.541799840  |
| C  | 84.190924854 | 27.907956658 | 5.260703219  | O  | 85.889903077 | 22.720603105 | -0.217891266 |
| C  | 85.635197672 | 27.596900158 | 5.619737361  | O  | 85.854508471 | 24.031504081 | 1.599301055  |
| O  | 86.386422500 | 28.565234440 | 5.915541861  | C  | 74.001913879 | 27.551867911 | -1.057421468 |
| O  | 86.029766010 | 26.374760720 | 5.554253902  | O  | 73.214391264 | 28.123533165 | -0.013129118 |
| N  | 77.506791173 | 27.395816016 | 0.321800341  | C  | 73.992980655 | 28.546392720 | -2.217382119 |
| C  | 77.359358295 | 26.151445071 | -0.235647467 | Cu | 78.405034000 | 24.763772000 | 4.178497000  |
| C  | 76.057803502 | 26.016646022 | -0.846840755 | C  | 76.685503291 | 24.129629605 | 6.861074847  |
| C  | 75.394364127 | 27.194967291 | -0.621477135 | C  | 75.976335524 | 24.939506475 | 5.840255694  |
| C  | 76.303741254 | 28.033660787 | 0.131018400  | C  | 74.733194358 | 25.496437757 | 5.924458570  |
| C  | 75.592904683 | 24.803145115 | -1.575536674 | N  | 76.557982584 | 25.340925039 | 4.639987714  |

|   |              |              |              |   |              |              |              |
|---|--------------|--------------|--------------|---|--------------|--------------|--------------|
| C | 75.668974862 | 26.103913008 | 4.011642261  | H | 81.554093874 | 25.753135664 | 4.154483851  |
| N | 74.546171228 | 26.238622457 | 4.771701733  | H | 79.602985893 | 22.362853334 | 5.706997729  |
| C | 71.622688370 | 29.619935029 | 6.807121814  | H | 83.362177987 | 24.022285987 | 4.656082116  |
| C | 72.047769623 | 28.845754353 | 5.596387052  | H | 83.500023187 | 21.716778747 | 6.076683638  |
| C | 71.484390941 | 29.066354451 | 4.324152675  | H | 81.953346872 | 20.929971672 | 6.458463658  |
| C | 71.920272227 | 28.374980311 | 3.208950232  | H | 79.732781424 | 30.326212485 | -3.139266838 |
| C | 73.059130248 | 27.886989384 | 5.698462572  | H | 79.978091457 | 22.144966190 | 2.920490853  |
| C | 73.502681963 | 27.179101643 | 4.591956340  | H | 75.857231553 | 22.889370940 | 3.343853211  |
| C | 72.957848146 | 27.393459830 | 3.276289678  | H | 78.970386731 | 19.812943319 | 0.715082402  |
| O | 73.384626587 | 26.736033822 | 2.257877420  | H | 77.872932843 | 18.870637287 | 1.749897442  |
| C | 78.687642687 | 19.605767148 | 1.758136435  | H | 75.981055894 | 23.504687677 | 7.424335336  |
| C | 78.240454179 | 20.863855093 | 2.418110260  | H | 77.439938664 | 23.476464762 | 6.406117521  |
| C | 78.910666143 | 21.971747095 | 2.874645419  | H | 83.392536837 | 30.119863916 | -1.916989863 |
| N | 76.906213981 | 21.179996449 | 2.574823175  | H | 82.573615685 | 29.864300525 | -3.476441643 |
| C | 76.800706282 | 22.417742161 | 3.102440000  | H | 75.148695145 | 33.013240272 | 1.937415884  |
| N | 78.010828500 | 22.931411284 | 3.295159229  | H | 74.605468900 | 31.654958878 | 0.926262409  |
| C | 82.497336906 | 21.494760049 | 5.691456210  | H | 74.337344013 | 31.624662344 | 2.681073874  |
| C | 81.753859272 | 22.735650730 | 5.356280321  | H | 82.046004916 | 32.007364168 | 4.434153535  |
| C | 80.411237544 | 23.007629201 | 5.385390137  | H | 81.998852956 | 30.821609267 | 5.752387349  |
| N | 82.342435928 | 23.872381906 | 4.838790042  | H | 83.505797238 | 31.080997735 | 4.847820906  |
| C | 81.373965815 | 24.768900485 | 4.563496568  | H | 74.958484509 | 29.612216056 | 0.476864392  |
| N | 80.178809353 | 24.272263989 | 4.873618430  | H | 83.232896260 | 26.492654980 | 2.181640364  |
| C | 82.487350484 | 30.345410751 | -2.491831239 | H | 78.004397447 | 24.163076995 | -0.610656807 |
| C | 81.299054481 | 29.849614016 | -1.757580523 | H | 74.540214927 | 24.890146351 | -1.865087459 |
| C | 81.179651665 | 29.245001424 | -0.534360105 | H | 76.183025080 | 24.647380770 | -2.491098646 |
| N | 80.011575557 | 29.930259416 | -2.241989135 | H | 75.703194089 | 23.900989009 | -0.956201047 |
| C | 79.164239718 | 29.395170365 | -1.340630920 | H | 81.302169803 | 22.155592450 | 0.147707026  |
| N | 79.847127805 | 28.966843120 | -0.284093973 | H | 83.610959149 | 23.611673539 | -0.775236988 |
| C | 91.074633631 | 28.484701292 | 2.845518396  | H | 84.100652476 | 25.183949326 | -0.110770233 |
| N | 90.146404906 | 27.392274191 | 3.059051418  | H | 83.384600562 | 24.396279227 | 2.181945323  |
| C | 89.125157514 | 27.412233541 | 3.922836825  | H | 82.792484355 | 22.903055814 | 1.479214616  |
| N | 88.299085295 | 26.368939013 | 3.967228618  | H | 83.794948356 | 28.641074151 | 5.978942644  |
| N | 88.943929852 | 28.447286109 | 4.745358095  | H | 83.574412926 | 27.000257749 | 5.319343693  |
| H | 77.183435000 | 24.806884000 | 7.570902000  | H | 84.595082667 | 27.809777423 | 3.123637047  |
| H | 72.452456000 | 30.244969000 | 7.189248000  | H | 84.757620343 | 29.418984157 | 3.826508391  |
| H | 79.552516000 | 19.139805000 | 2.252830000  | H | 88.380368886 | 25.636910357 | 3.241252142  |
| H | 82.592179000 | 20.840344000 | 4.808238000  | H | 87.513433178 | 26.356165539 | 4.648343855  |
| H | 82.435604343 | 31.432918373 | -2.644990301 | H | 89.560718410 | 29.253905974 | 4.707086909  |
| H | 81.965384967 | 29.008610504 | 0.169554079  | H | 88.054403696 | 28.512279689 | 5.285329386  |
| H | 79.916386103 | 31.622784541 | 3.934866156  | H | 85.276542997 | 24.377055645 | 3.274619423  |
| H | 78.595892656 | 33.236415254 | 3.826222521  | H | 85.360919419 | 25.180907099 | 4.703329096  |
| H | 78.096335093 | 29.329177241 | -1.492452964 | H | 91.674970160 | 28.682702558 | 3.744099252  |
| H | 90.240912646 | 26.558318004 | 2.482804864  | H | 90.551454051 | 29.400493255 | 2.537480867  |
| H | 75.777238651 | 26.561912788 | 3.038709484  | C | 84.163268815 | 19.304282096 | -3.116924668 |
| H | 73.531857955 | 27.710215073 | 6.664587176  | C | 84.756157568 | 20.080057876 | -1.982605026 |
| H | 70.688879827 | 29.805603032 | 4.218655140  | O | 85.193807987 | 19.549719463 | -0.957780873 |
| H | 75.530392260 | 33.307889306 | 4.138960307  | O | 84.746580696 | 21.401555285 | -2.174893970 |
| H | 76.800363200 | 34.496406108 | 4.795846360  | C | 88.812361477 | 20.770259167 | -1.326943032 |
| H | 72.953774781 | 28.741973795 | -2.516118605 | C | 88.814176654 | 20.717461338 | 0.156349905  |
| H | 74.457142084 | 29.494822698 | -1.910447863 | C | 89.651295941 | 20.087144608 | 1.036333180  |
| H | 74.544060490 | 28.146097305 | -3.077679492 | N | 87.835487333 | 21.320088094 | 0.926140941  |
| H | 73.283376890 | 27.543849067 | 0.816958444  | C | 88.051020118 | 21.071241833 | 2.219099981  |
| H | 71.468387234 | 28.559626737 | 2.234206111  | N | 89.155022810 | 20.325561356 | 2.297322316  |
| H | 70.771898110 | 30.273479831 | 6.581537446  | H | 84.681485000 | 19.503926000 | -4.065239000 |
| H | 71.334182258 | 28.942174898 | 7.623859658  | H | 88.765971000 | 21.799802000 | -1.706250000 |
| H | 73.969328496 | 25.429461057 | 6.687503431  | H | 89.720797334 | 20.295949730 | -1.713652321 |

|   |              |              |              |   |              |              |              |
|---|--------------|--------------|--------------|---|--------------|--------------|--------------|
| H | 87.943737368 | 20.226335855 | -1.723918108 | H | 85.164752342 | 21.892732075 | -1.364654800 |
| H | 84.204161168 | 18.234902707 | -2.891813643 | H | 91.740917000 | 28.167083000 | 2.038155000  |
| H | 83.117191855 | 19.612669937 | -3.250727522 | H | 73.527520349 | 26.618528037 | -1.413577152 |
| H | 90.541883406 | 19.495300440 | 0.874432545  | H | 89.564659058 | 19.982145008 | 3.166748808  |
| H | 87.450953028 | 21.414835490 | 3.060766348  | O | 78.496452019 | 27.177801260 | 2.885740033  |
| H | 87.035265888 | 21.909248839 | 0.523874392  | H | 85.756235668 | 21.393727624 | 5.024176403  |
| H | 84.744653462 | 20.095602565 | 0.745928974  | H | 85.921380459 | 22.904946319 | 4.669476600  |
| H | 83.589025000 | 19.723529000 | 1.696373000  | H | 77.762837496 | 27.722679721 | 3.249235909  |
| H | 87.527993296 | 24.257142398 | 1.668430362  | H | 76.124266345 | 20.568652581 | 2.349365530  |
| H | 89.023160244 | 23.754394048 | 1.792058382  |   |              |              |              |

#### Structure 14:

187

|    |              |              |              |    |              |              |              |
|----|--------------|--------------|--------------|----|--------------|--------------|--------------|
| O  | 84.950566358 | 24.376624840 | 4.188981923  | C  | 81.652226817 | 24.678455257 | 0.974699307  |
| O  | 88.427747519 | 24.561546963 | 1.779145487  | C  | 81.353162632 | 26.041849236 | 1.300523715  |
| O  | 84.243299062 | 20.450300181 | 1.627858008  | C  | 80.396586218 | 22.812843583 | -0.116343200 |
| O  | 86.170528455 | 22.185373571 | 5.322984743  | C  | 82.942511051 | 23.996521775 | 1.241752769  |
| Fe | 79.100034000 | 28.054771000 | 1.364498000  | C  | 83.911641637 | 24.095463905 | 0.055734042  |
| C  | 82.228442747 | 26.890581128 | 1.966938889  | C  | 85.294702531 | 23.626114045 | 0.448040810  |
| C  | 78.289671535 | 25.132603389 | -0.212546583 | O  | 85.872667703 | 22.755743062 | -0.282955282 |
| C  | 75.957739941 | 29.253979746 | 0.666417155  | O  | 85.810553087 | 24.139491488 | 1.484385462  |
| C  | 79.736591670 | 30.826682067 | 3.220300689  | C  | 73.983879958 | 27.511724172 | -1.058105928 |
| N  | 80.691411878 | 28.753780125 | 2.327141859  | O  | 73.193520580 | 28.128386407 | -0.032711597 |
| C  | 81.911416273 | 28.134209526 | 2.473746650  | C  | 73.971547024 | 28.450696710 | -2.257498812 |
| C  | 82.784379125 | 28.934372745 | 3.301067058  | Cu | 78.344796000 | 24.708341000 | 4.135975000  |
| C  | 82.060206651 | 30.032585047 | 3.685555534  | C  | 76.657296219 | 24.151847101 | 6.862196743  |
| C  | 80.763817396 | 29.906871252 | 3.063997721  | C  | 75.965583502 | 24.983022593 | 5.846141079  |
| C  | 82.470970797 | 31.126221424 | 4.607970763  | C  | 74.747902126 | 25.591302236 | 5.939600289  |
| O  | 79.438901018 | 22.335670005 | -0.736523715 | N  | 76.541637657 | 25.342472049 | 4.630330199  |
| C  | 84.168195858 | 28.576825909 | 3.725104531  | C  | 75.678967288 | 26.131395152 | 4.000106479  |
| C  | 84.202972203 | 27.914369145 | 5.118987443  | N  | 74.572939751 | 26.320091501 | 4.774619796  |
| C  | 85.637971032 | 27.601291484 | 5.500241836  | C  | 71.606679292 | 29.703969046 | 6.738202035  |
| O  | 86.393768075 | 28.564960340 | 5.797764637  | C  | 72.060932805 | 28.929053514 | 5.541869921  |
| O  | 86.017677451 | 26.375763737 | 5.451493046  | C  | 71.509135351 | 29.137585866 | 4.260527688  |
| N  | 77.492789513 | 27.383891041 | 0.324406401  | C  | 71.959954599 | 28.439250312 | 3.160088663  |
| C  | 77.348575864 | 26.141547242 | -0.237054214 | C  | 73.080703822 | 27.982461944 | 5.669273956  |
| C  | 76.040967523 | 25.993088245 | -0.830176948 | C  | 73.539868316 | 27.262722060 | 4.577717137  |
| C  | 75.377326147 | 27.171275972 | -0.606944523 | C  | 72.999314234 | 27.459133797 | 3.255203920  |
| C  | 76.287817711 | 28.015939638 | 0.139601605  | O  | 73.428910721 | 26.786966755 | 2.252204234  |
| C  | 75.573956611 | 24.763954167 | -1.530040582 | C  | 78.668860405 | 19.546474565 | 1.739579319  |
| N  | 78.060377032 | 29.704282851 | 1.843294481  | C  | 78.215110835 | 20.838832409 | 2.323854124  |
| C  | 76.773675361 | 30.023525901 | 1.475413173  | C  | 78.883753452 | 21.935809442 | 2.808495620  |
| C  | 76.359216918 | 31.275841513 | 2.070413492  | N  | 76.880231357 | 21.179059845 | 2.414419374  |
| C  | 77.424979159 | 31.720999492 | 2.818091975  | C  | 76.770070667 | 22.418098796 | 2.936427096  |
| C  | 78.482241623 | 30.734054796 | 2.647267208  | N  | 77.978556031 | 22.910657843 | 3.187141646  |
| C  | 75.035532196 | 31.924335785 | 1.865366543  | C  | 82.519889695 | 21.519169963 | 5.672860166  |
| C  | 77.559825111 | 32.926526850 | 3.613141684  | C  | 81.742340564 | 22.734715886 | 5.323414245  |
| C  | 76.563236773 | 33.646525272 | 4.157902250  | C  | 80.392815636 | 22.973620654 | 5.349601147  |
| N  | 80.067588047 | 26.358323232 | 0.928232938  | N  | 82.301617835 | 23.878407214 | 4.788698411  |
| C  | 79.548476409 | 25.235702592 | 0.344766989  | C  | 81.313088639 | 24.746158591 | 4.500898353  |
| C  | 80.521058694 | 24.165183783 | 0.370041753  | N  | 80.130956827 | 24.225455381 | 4.821882257  |



|   |              |              |              |   |              |              |              |
|---|--------------|--------------|--------------|---|--------------|--------------|--------------|
| C | 82.368422517 | 30.372045438 | -2.616610882 | H | 78.036100005 | 24.174734597 | -0.656662749 |
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| N | 79.811648128 | 28.937476078 | -0.340104487 | H | 83.529436986 | 23.526700102 | -0.801719683 |
| C | 91.042083956 | 28.505603064 | 2.799275079  | H | 83.998184410 | 25.148542773 | -0.260200614 |
| N | 90.112168241 | 27.416540384 | 2.997489893  | H | 83.421865782 | 24.450161668 | 2.114862929  |
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| H | 79.552517000 | 19.139803000 | 2.252830000  | H | 88.366108691 | 25.659650714 | 3.218029567  |
| H | 82.592179000 | 20.840344000 | 4.808238000  | H | 87.554921586 | 26.343707315 | 4.657242836  |
| H | 82.264671057 | 31.452708729 | -2.791524512 | H | 89.554086153 | 29.256972623 | 4.637100466  |
| H | 81.935740215 | 29.034133126 | 0.068564324  | H | 88.109115184 | 28.487916323 | 5.288952096  |
| H | 79.939992829 | 31.686675384 | 3.853327013  | H | 85.229779291 | 24.390209171 | 3.237546942  |
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| H | 78.030966452 | 29.245151727 | -1.520035901 | H | 91.602398073 | 28.728718182 | 3.717098470  |
| H | 90.219154117 | 26.580983354 | 2.427718175  | H | 90.531893643 | 29.412187937 | 2.445433271  |
| H | 75.811191536 | 26.587088897 | 3.029160373  | C | 84.089962391 | 19.362658745 | -3.149595065 |
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| H | 72.931924521 | 28.638760296 | -2.561198830 | C | 88.859668672 | 20.704432235 | 0.104952902  |
| H | 74.443915625 | 29.409965744 | -1.999891329 | C | 89.770141585 | 20.147053993 | 0.965274453  |
| H | 74.515810869 | 28.006191042 | -3.102243273 | N | 87.925840308 | 21.303610436 | 0.912899603  |
| H | 73.273266551 | 27.574444718 | 0.808115255  | C | 88.285105053 | 21.097088863 | 2.200457671  |
| H | 71.521492365 | 28.611807708 | 2.176899653  | N | 89.408261161 | 20.395961937 | 2.271504835  |
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| H | 81.470055157 | 25.727275858 | 4.076166860  | H | 87.899508397 | 20.259353878 | -1.761492226 |
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| H | 74.588616694 | 31.637101772 | 0.904703063  | H | 85.731039234 | 22.975221708 | 4.897038013  |
| H | 74.325889896 | 31.645648237 | 2.660793925  | H | 77.964629526 | 27.812551423 | 3.388252500  |
| H | 82.184548248 | 32.113658673 | 4.220313993  | H | 76.096273905 | 20.584155698 | 2.145993250  |
| H | 81.991342215 | 31.005889423 | 5.592549841  | H | 90.558173580 | 19.595851958 | 3.324512659  |
| H | 83.556912922 | 31.122994517 | 4.761797775  | O | 91.297808016 | 19.058570700 | 3.746746428  |
| H | 74.944478185 | 29.599077559 | 0.481432580  | H | 91.142248346 | 19.162498269 | 4.708880999  |
| H | 83.233270979 | 26.520400302 | 2.157067781  |   |              |              |              |