

Supporting Information

Computational details

All density functional theory (DFT) calculations were conducted with the Gaussian 16 program. Geometry optimization was performed with B3LYP.^[1] LANL2DZ+f basis set with ECP was used for Pd, the 6-31+G (d) basis set was used for other atoms.^[2] Frequency analysis was conducted at the same level of theory to verify the stationary points to be energy minimum or a transition state and to obtain the thermal energy corrections. Single point energies were calculated with M06-L and a mixed basis set SDD for Pd and 6-311++G(d,p) for the other atoms.^[3] Solvent effect (Solvent=1,2-dichloroethane) was calculated by using SMD solvation model^[4]. The relative energies with ZPE corrections and free energies (at 298.15K) are in kcal/mol.

References:

- [1] Gaussian 16, Revision A.03, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.
- [2] (a) A. D. Becke, *J. Chem. Phys.* 1993, **98**, 5648-5652; (b) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B*, 1988, **37**, 785-789.
- [3] P. J. Hay, W. R. Wadt, *J. Chem. Phys.* 1985, **82**, 270-283.
- [4] Y. Zhao, D. G. Truhlar, *J. Chem. Phys.* 2006, **125**, 194101.
- [5] A. V. Marenich, C. J. Cramer, D. G. Truhlar, *J. Phys. Chem. B*. 2009, **113**, 6378-6396.

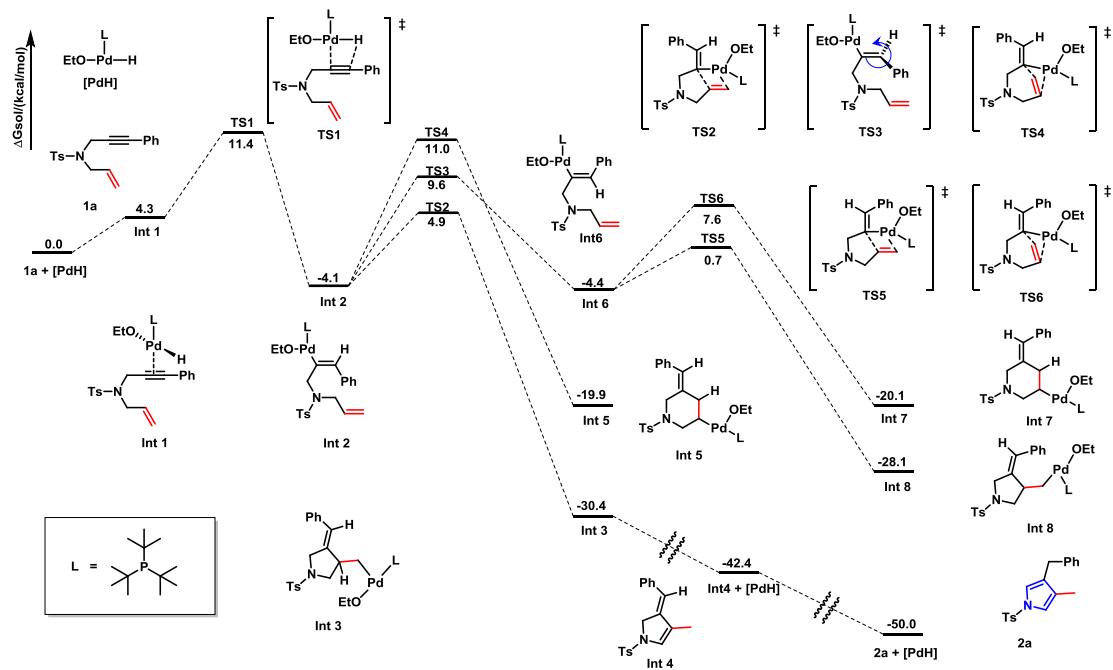


Figure S1. Gibbs energy profiles of cycloisomerization of 1a at the M06-L/6-311++G(d,p)/SDD/SMD(1,2-Dichloroethane)//B3LYP/6-31G+(d)/LANL2DZ+f level. (in kcal/mol)

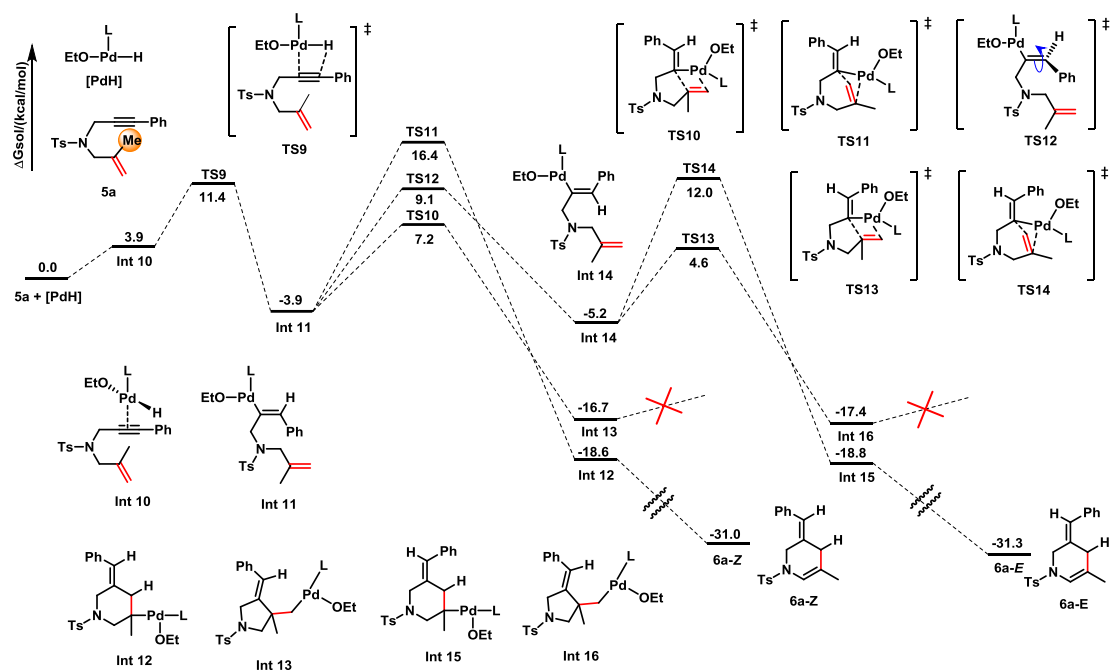


Figure S2. Gibbs energy profiles of cycloisomerization of 5a at the M06-L/6-311++G(d,p)/SDD/SMD(1,2-Dichloroethane)//B3LYP/6-31G+(d)/LANL2DZ+f level. (in kcal/mol)

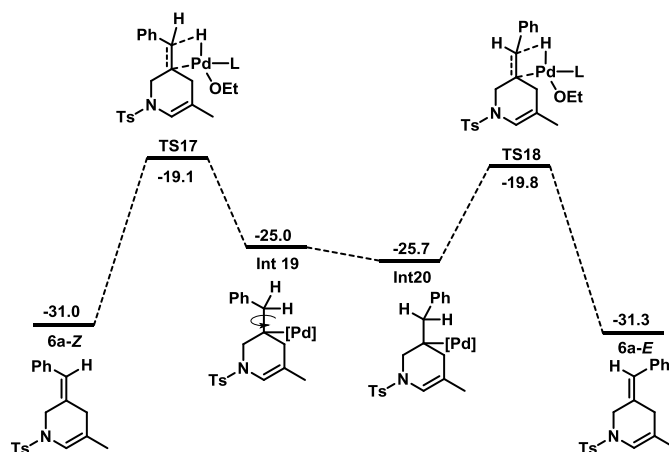


Figure S3. Gibbs energy profiles of isomerization process at the M06-L/6-311++G(d,p)/SDD/SMD(1,2-Dichloroethane)//B3LYP/6-31G+(d)/LANL2DZ+f level. (in kcal/mol). Palladium hydride coordinates with **6a-Z**, followed by alkene insertion via **TS17** to form **Int 19**. **Int 19** and **Int 20** can convert to each other via single bond rotation. With final β -H elimination via **TS18**, this pathway shows that **6a-Z** and **6a-E** can convert to each other.

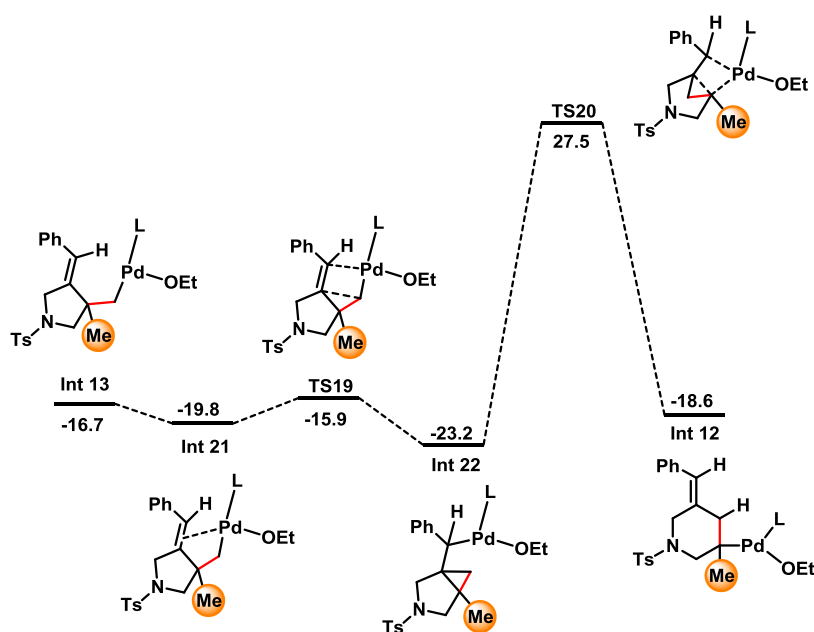


Figure S4. Gibbs energy profiles of an alternative process to form 6-membered rings at the M06-L/6-311++G(d,p)/SDD/SMD(1,2-Dichloroethane)//B3LYP/6-31G+(d)/LANL2DZ+f level. (in kcal/mol). The alkene moiety in **Int 13** complex to the palladium to give a cyclopropane intermediate **Int 22** via **TS19**. **Int 22** then undergoes a fragmentation via **TS20** which leads to **Int 12**. However, the barrier in this step is too high to achieve.

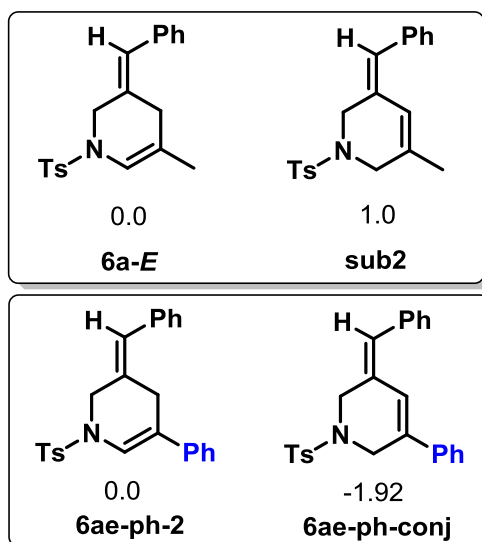


Figure S5. The relative free energies for R=Me and Ph. (kcal/mol)

Cartesian Coordinates

| | | | | | | | |
|----|-----------|-----------|-----------|----|-----------|-----------|-----------|
| | | | | H | -0.087777 | 0.355787 | -1.458992 |
| 1a | | | | H | -0.105511 | -1.249668 | -0.713422 |
| S | -1.559508 | -0.603974 | 1.381685 | C | 1.719063 | -0.248016 | -0.545657 |
| O | -1.843253 | 0.048439 | 2.663899 | C | 2.930729 | -0.312610 | -0.537038 |
| O | -1.105554 | -1.995939 | 1.299862 | C | 4.359218 | -0.379750 | -0.504484 |
| C | -3.043838 | -0.465081 | 0.369887 | C | 5.014485 | -1.149918 | 0.477503 |
| C | -3.938264 | 0.586183 | 0.593245 | C | 5.133706 | 0.321104 | -1.450648 |
| C | -5.071369 | 0.700811 | -0.212375 | C | 6.407125 | -1.212101 | 0.510435 |
| C | -5.330681 | -0.219065 | -1.240468 | H | 4.420993 | -1.692649 | 1.207392 |
| C | -4.424664 | -1.273199 | -1.432747 | C | 6.525971 | 0.251560 | -1.412613 |
| C | -3.285660 | -1.403906 | -0.637165 | H | 4.633104 | 0.915542 | -2.209506 |
| H | -3.764396 | 1.284467 | 1.405649 | C | 7.167434 | -0.513553 | -0.433143 |
| H | -5.772659 | 1.511868 | -0.029125 | H | 6.900129 | -1.808641 | 1.273754 |
| H | -4.618255 | -2.012210 | -2.206999 | H | 7.111773 | 0.796323 | -2.148689 |
| H | -2.608769 | -2.241395 | -0.772596 | H | 8.252786 | -0.565259 | -0.405491 |
| C | -6.548003 | -0.071374 | -2.122763 | H | -1.129931 | 2.143418 | -0.161996 |
| H | -6.875816 | -1.038235 | -2.518962 | H | -1.063030 | 2.015296 | 1.612696 |
| H | -7.386403 | 0.375504 | -1.577683 | H | 1.504809 | 2.189572 | 1.469055 |
| H | -6.332654 | 0.578920 | -2.981492 | H | 0.410401 | 3.880146 | -0.872569 |
| N | -0.351011 | 0.328370 | 0.643311 | H | 2.042568 | 4.069729 | -0.019013 |
| C | -0.521038 | 1.793977 | 0.688357 | | | | |
| C | 0.797947 | 2.520213 | 0.709744 | | | | |
| C | 1.098012 | 3.538647 | -0.100230 | 5a | | | |
| C | 0.254541 | -0.224508 | -0.588545 | S | -1.620309 | 0.037540 | 1.444453 |

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|---|-----------|-----------|-----------|----|-----------|-----------|-----------|
| O | -1.891517 | 1.224522 | 2.262022 | | | | |
| O | -1.163079 | -1.225175 | 2.034031 | | | | |
| C | -3.118102 | -0.321830 | 0.509476 | 3a | | | |
| C | -4.015140 | 0.709452 | 0.214511 | C | 0.969812 | -1.560793 | 1.019240 |
| C | -5.158433 | 0.426444 | -0.532836 | C | 1.268877 | -3.008312 | 0.712958 |
| C | -5.426147 | -0.872928 | -0.991732 | C | 1.835847 | -3.570833 | -0.360273 |
| C | -4.517853 | -1.892005 | -0.667446 | C | 0.181750 | -0.690110 | -1.286733 |
| C | -3.368335 | -1.627727 | 0.078479 | H | 0.356509 | -1.680495 | -1.718163 |
| H | -3.835050 | 1.711149 | 0.591219 | H | 0.435593 | 0.036057 | -2.065577 |
| H | -5.861231 | 1.227526 | -0.750967 | C | -1.225752 | -0.553924 | -0.912187 |
| H | -4.717542 | -2.911226 | -0.990524 | C | -2.389681 | -0.426427 | -0.589998 |
| H | -2.689674 | -2.429191 | 0.352243 | C | -3.759998 | -0.276473 | -0.205431 |
| C | -6.655063 | -1.162986 | -1.821043 | C | -4.093299 | 0.300748 | 1.036659 |
| H | -6.974346 | -2.205002 | -1.714018 | C | -4.797374 | -0.702591 | -1.058863 |
| H | -7.493257 | -0.518609 | -1.534586 | C | -5.429015 | 0.445267 | 1.410667 |
| H | -6.458112 | -0.987983 | -2.887457 | H | -3.297087 | 0.630015 | 1.698128 |
| N | -0.424350 | 0.498538 | 0.336601 | C | -6.130541 | -0.553624 | -0.677462 |
| C | -0.580392 | 1.813313 | -0.318629 | H | -4.546227 | -1.148661 | -2.016872 |
| C | 0.736467 | 2.540329 | -0.513826 | C | -6.452013 | 0.019903 | 0.556969 |
| C | 1.102100 | 2.951513 | -1.734653 | H | -5.671711 | 0.891327 | 2.371894 |
| C | 0.169670 | -0.578088 | -0.486063 | H | -6.920645 | -0.886854 | -1.345680 |
| H | -0.161339 | -0.462489 | -1.529397 | H | -7.492012 | 0.134081 | 0.851620 |
| H | -0.213871 | -1.535969 | -0.123292 | C | 1.158146 | -0.492157 | -0.084661 |
| C | 1.633610 | -0.615374 | -0.428253 | C | 0.888681 | 0.894318 | 0.546221 |
| C | 2.843174 | -0.702552 | -0.387928 | C | 2.601849 | -0.474497 | -0.621874 |
| C | 4.270003 | -0.788548 | -0.328546 | O | 1.116475 | 1.875623 | -0.347529 |
| C | 5.057229 | -0.438677 | -1.443932 | O | 2.920594 | -0.646220 | -1.779997 |
| C | 4.910525 | -1.225764 | 0.848382 | O | 0.511295 | 1.086786 | 1.681111 |
| C | 6.447601 | -0.524847 | -1.380355 | O | 3.478270 | -0.238187 | 0.370841 |
| H | 4.567588 | -0.101101 | -2.352801 | C | 0.868263 | 3.234775 | 0.099004 |
| C | 6.301456 | -1.307118 | 0.904776 | H | -0.175853 | 3.304949 | 0.418962 |
| H | 4.307252 | -1.497227 | 1.709761 | H | 1.504304 | 3.432976 | 0.967596 |
| C | 7.074399 | -0.958275 | -0.207518 | C | 1.175288 | 4.161249 | -1.062141 |
| H | 7.043447 | -0.252503 | -2.247838 | H | 0.532976 | 3.941371 | -1.921406 |
| H | 6.783175 | -1.644661 | 1.818877 | H | 0.999831 | 5.199813 | -0.758084 |
| H | 8.158351 | -1.023813 | -0.160651 | H | 2.219968 | 4.066626 | -1.377244 |
| H | -1.093524 | 1.695485 | -1.285558 | C | 4.883581 | -0.203087 | 0.006306 |
| H | -1.215420 | 2.416811 | 0.336843 | H | 5.144963 | -1.165573 | -0.444209 |
| H | 0.503194 | 2.734282 | -2.616883 | H | 5.023253 | 0.575529 | -0.750215 |
| H | 2.013797 | 3.522341 | -1.893946 | C | 5.676872 | 0.072869 | 1.269347 |
| C | 1.536313 | 2.824706 | 0.730685 | H | 5.516715 | -0.713625 | 2.014363 |
| H | 2.445064 | 3.388569 | 0.498381 | H | 6.746089 | 0.107844 | 1.029811 |
| H | 0.942306 | 3.401357 | 1.452837 | H | 5.391742 | 1.033016 | 1.712434 |
| H | 1.822876 | 1.892851 | 1.230592 | H | 1.987005 | -4.646915 | -0.397329 |

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|-----|-----------|-----------|-----------|-------|-----------|-----------|-----------|
| H | 2.170197 | -3.012468 | -1.229068 | H | -0.380663 | 2.514474 | 1.484149 |
| H | 0.974449 | -3.669580 | 1.530208 | H | -3.655241 | 1.147500 | 2.521459 |
| H | 1.569836 | -1.263444 | 1.887662 | H | -3.816847 | 0.973460 | 0.771727 |
| H | -0.070722 | -1.487811 | 1.359269 | H | -3.559544 | -0.451819 | 1.790616 |
| | | | | H | 1.263811 | -1.132458 | 1.198795 |
| | | | | O | 3.341570 | 0.342214 | 0.206019 |
| PdH | | | | C | 4.377720 | -0.591171 | 0.062530 |
| Pd | 1.393367 | 0.020874 | 0.200100 | H | 4.198799 | -1.281141 | -0.783247 |
| P | -0.911695 | -0.018775 | -0.001274 | H | 4.465685 | -1.216613 | 0.969460 |
| C | -1.304993 | 1.053900 | -1.578304 | C | 5.704211 | 0.140465 | -0.164068 |
| C | -0.340566 | 2.267644 | -1.570733 | H | 5.919306 | 0.808327 | 0.678487 |
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| H | 0.710796 | 1.951310 | -1.573924 | | | | |
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| H | -1.657148 | -0.557978 | -3.057219 | Pd | 1.333067 | 0.150701 | -0.064167 |
| H | -1.004969 | 0.940653 | -3.712584 | P | 3.067437 | -1.427064 | -0.250280 |
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| C | -1.615404 | -1.811015 | -0.252920 | H | 1.311214 | -3.055344 | 1.664107 |
| C | -3.039452 | -1.873188 | -0.846148 | H | 0.302577 | -2.375834 | 0.384735 |
| C | -0.646089 | -2.591023 | -1.175431 | H | 0.490067 | -4.136917 | 0.532294 |
| C | -1.617788 | -2.567748 | 1.094898 | H | 2.346207 | -3.524551 | -2.547602 |
| H | -3.777071 | -1.344894 | -0.236334 | H | 0.968693 | -4.273095 | -1.745944 |
| H | -3.089863 | -1.474994 | -1.862645 | H | 0.952682 | -2.532174 | -2.063096 |
| H | -3.352379 | -2.924980 | -0.899070 | H | 2.537046 | -5.296089 | -0.201535 |
| H | 0.374023 | -2.581095 | -0.780115 | H | 3.982153 | -4.431515 | -0.728902 |
| H | -0.983350 | -3.635216 | -1.228055 | H | 3.480982 | -4.378202 | 0.968736 |
| H | -0.616692 | -2.208605 | -2.195939 | C | 4.165575 | -1.154982 | -1.843771 |
| H | -1.857976 | -3.620436 | 0.895684 | C | 5.025217 | -2.382895 | -2.223569 |
| H | -0.637936 | -2.542146 | 1.581741 | C | 3.294828 | -0.782506 | -3.067367 |
| H | -2.369865 | -2.194960 | 1.793976 | C | 5.102619 | 0.054766 | -1.623216 |
| C | -1.755212 | 0.794425 | 1.550847 | H | 5.663860 | -2.732167 | -1.410150 |
| C | -1.087850 | 0.226647 | 2.828304 | H | 4.418856 | -3.224590 | -2.568302 |
| C | -1.453511 | 2.310883 | 1.565973 | H | 5.683230 | -2.101477 | -3.056959 |
| C | -3.282455 | 0.595747 | 1.647478 | H | 2.787111 | 0.173261 | -2.920826 |
| H | -1.256414 | -0.840844 | 2.971654 | H | 3.960981 | -0.684436 | -3.935590 |
| H | -0.007997 | 0.400576 | 2.822687 | H | 2.539968 | -1.528005 | -3.316684 |
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| H | -1.980485 | 2.863557 | 0.784929 | H | 4.552297 | 0.942699 | -1.295738 |
| H | -1.789784 | 2.717624 | 2.528827 | H | 5.903834 | -0.146377 | -0.909596 |

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| C | 4.232159 | -1.384150 | 1.311595 | H | 1.851356 | 2.871126 | 1.591651 |
| C | 4.555760 | 0.094357 | 1.644533 | C | 1.318176 | 5.543442 | -1.191333 |
| C | 3.459026 | -1.928660 | 2.534450 | H | -0.079701 | 4.131241 | -2.039020 |
| C | 5.551158 | -2.172983 | 1.168651 | C | 2.214067 | 5.800797 | -0.147503 |
| H | 5.125128 | 0.603315 | 0.866546 | H | 3.106607 | 5.044953 | 1.667636 |
| H | 3.637746 | 0.648738 | 1.856160 | H | 1.165524 | 6.281243 | -1.974845 |
| H | 5.173470 | 0.103042 | 2.554085 | H | 2.759724 | 6.740772 | -0.119759 |
| H | 3.277837 | -3.005347 | 2.486165 | O | 1.510611 | 0.640023 | 1.999381 |
| H | 4.074012 | -1.748083 | 3.426602 | C | 0.404645 | 0.421527 | 2.813191 |
| H | 2.519084 | -1.388186 | 2.668781 | H | 0.188987 | -0.663780 | 2.942331 |
| H | 6.071058 | -2.142513 | 2.136035 | H | -0.525980 | 0.858676 | 2.388451 |
| H | 5.400581 | -3.225683 | 0.915013 | C | 0.614488 | 1.031145 | 4.207098 |
| H | 6.229014 | -1.734435 | 0.431745 | H | 0.770357 | 2.114629 | 4.132295 |
| H | 1.168484 | -0.166067 | -1.581995 | H | -0.255544 | 0.849611 | 4.854866 |
| S | -4.348397 | 0.416092 | -1.525176 | H | 1.500384 | 0.596399 | 4.686245 |
| O | -3.683169 | -0.198082 | -2.680099 | H | -4.537891 | 1.548066 | 0.941026 |
| O | -5.348157 | 1.478831 | -1.675967 | H | -2.848988 | 1.652147 | 1.427260 |
| C | -5.123641 | -0.908035 | -0.582987 | H | -4.168313 | 3.656389 | -0.527996 |
| C | -4.552670 | -2.186595 | -0.589226 | H | -2.294548 | 3.980280 | 1.908836 |
| C | -5.138786 | -3.198668 | 0.168265 | H | -2.976429 | 5.325065 | 0.835736 |
| C | -6.293877 | -2.961220 | 0.933593 | | | | |
| C | -6.852240 | -1.675791 | 0.911592 | | | | |
| C | -6.278295 | -0.647856 | 0.158471 | TS1 | | | |
| H | -3.679019 | -2.390064 | -1.200398 | Pd | 1.166015 | -0.089802 | -0.499330 |
| H | -4.699125 | -4.193785 | 0.156373 | P | 3.376723 | -0.902125 | 0.140254 |
| H | -7.755172 | -1.473541 | 1.482857 | C | -0.681904 | 0.930155 | -0.642438 |
| H | -6.733569 | 0.336551 | 0.123657 | C | -2.040979 | 0.334630 | -0.613575 |
| C | -6.917790 | -4.072909 | 1.744680 | C | 0.100147 | 1.920192 | -0.653123 |
| H | -7.213307 | -4.913179 | 1.103913 | N | -2.570074 | 0.300444 | 0.766032 |
| H | -6.212331 | -4.465415 | 2.487827 | H | -2.701581 | 0.953041 | -1.227352 |
| H | -7.809373 | -3.728139 | 2.277856 | H | -2.005808 | -0.677854 | -1.020013 |
| N | -3.126642 | 1.070047 | -0.565383 | C | 0.322932 | 3.352456 | -0.696168 |
| C | -3.543532 | 1.875797 | 0.610490 | S | -4.098988 | 0.953071 | 1.017561 |
| C | -3.561639 | 3.355744 | 0.324259 | C | -2.125063 | -0.828175 | 1.609553 |
| C | -2.914773 | 4.263233 | 1.059990 | C | 1.563075 | 3.939386 | -0.993664 |
| C | -1.873089 | 0.303725 | -0.449503 | C | -0.791672 | 4.185907 | -0.457295 |
| H | -1.771434 | -0.308578 | -1.348856 | O | -4.152458 | 2.182502 | 0.211514 |
| H | -1.901709 | -0.370516 | 0.420485 | O | -4.312177 | 0.970667 | 2.466675 |
| C | -0.703160 | 1.193362 | -0.338255 | C | -5.302211 | -0.191764 | 0.320864 |
| C | 0.054978 | 2.159240 | -0.252906 | C | -1.312915 | -0.445608 | 2.822396 |
| C | 0.807914 | 3.379326 | -0.216903 | C | 1.692169 | 5.327626 | -1.054026 |
| C | 1.711309 | 3.639061 | 0.833374 | H | 2.422026 | 3.302887 | -1.183060 |
| C | 0.617451 | 4.338353 | -1.232404 | C | -0.653359 | 5.571647 | -0.516392 |
| C | 2.408283 | 4.846925 | 0.858280 | H | -1.754523 | 3.740811 | -0.221308 |

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| C | -5.650274 | -0.101927 | -1.031970 | H | 3.551228 | -1.336362 | 3.295106 |
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| C | -0.995964 | 0.785618 | 3.225234 | C | 4.625382 | -3.254423 | 1.444004 |
| C | 0.586403 | 6.148720 | -0.814977 | C | 3.391696 | -2.789428 | 0.640206 |
| H | 2.658239 | 5.767347 | -1.288384 | H | 4.538794 | -4.338284 | 1.602828 |
| H | -1.518024 | 6.201801 | -0.325373 | H | 5.569663 | -3.078701 | 0.920812 |
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| H | -5.237095 | 0.689410 | -1.649069 | C | 3.297928 | -3.674245 | -0.623162 |
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| H | 0.689061 | 7.229776 | -0.859518 | H | 2.083736 | -4.151657 | 1.685706 |
| C | -7.132572 | -2.021406 | -0.769889 | H | 4.207911 | -3.660386 | -1.228033 |
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| H | -7.223552 | -2.839187 | 1.223618 | H | 2.445892 | -3.405882 | -1.247117 |
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| H | 1.759806 | 1.384246 | -0.396823 | C | -0.887288 | -2.006490 | -3.024861 |
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| C | 3.890017 | -1.062605 | -2.636457 | H | -0.784738 | -2.524518 | -3.989494 |
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| H | 5.543373 | 1.279039 | -0.706135 | H | -1.333047 | 1.666240 | 2.687061 |
| H | 5.459497 | 1.019172 | -2.446871 | | | | |
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| H | 6.574730 | -1.112057 | -2.108428 | Int 2 | | | |
| H | 6.528547 | -1.102055 | -0.343935 | Pd | 1.154103 | 0.086361 | -0.389727 |
| H | 5.842563 | -2.461208 | -1.245735 | P | 3.546999 | -0.626227 | 0.089621 |
| H | 6.129458 | 0.487439 | 1.161110 | C | -0.552480 | 1.113179 | -0.507525 |
| C | 5.538813 | 0.000478 | 1.941820 | C | -1.937183 | 0.535793 | -0.398990 |
| C | 4.018950 | 0.115629 | 1.684972 | C | -0.179369 | 2.387349 | -0.732693 |
| H | 5.885765 | -1.029581 | 2.038478 | N | -2.369471 | 0.272687 | 1.003513 |
| H | 5.772810 | 0.513474 | 2.884874 | H | -2.660296 | 1.228842 | -0.836770 |
| C | 3.678459 | 1.617379 | 1.531484 | H | -1.953851 | -0.403019 | -0.965955 |
| C | 3.262172 | -0.340641 | 2.954272 | C | -0.926464 | 3.662278 | -0.733558 |
| H | 2.599312 | 1.785798 | 1.533821 | S | -4.037264 | 0.305420 | 1.276533 |
| H | 4.099006 | 2.150650 | 2.395025 | C | -1.619244 | -0.775107 | 1.730367 |
| H | 4.094290 | 2.075589 | 0.634037 | C | -0.348339 | 4.769901 | -1.387978 |
| H | 3.502477 | 0.359637 | 3.765681 | C | -2.172900 | 3.841293 | -0.102245 |
| H | 2.177032 | -0.316342 | 2.812133 | O | -4.538747 | 1.527761 | 0.632081 |

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| O | -4.228353 | 0.066934 | 2.710837 | C | 3.443848 | 1.881179 | 1.393940 |
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| C | -0.999596 | 6.002056 | -1.437310 | H | 3.656455 | 2.503321 | 2.274043 |
| H | 0.620335 | 4.654415 | -1.870799 | H | 3.841323 | 2.404050 | 0.523697 |
| C | -2.823850 | 5.075396 | -0.154261 | H | 3.546965 | 0.669594 | 3.702102 |
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| H | -3.786355 | 5.185381 | 0.338699 | H | 5.942565 | -2.580746 | 0.841569 |
| C | -5.641992 | -2.060792 | -1.624310 | C | 2.495686 | -2.901749 | 1.389169 |
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| C | -5.530453 | -3.378089 | 0.390144 | H | 2.417116 | -2.385628 | 2.346867 |
| H | -4.763362 | -2.363412 | 2.140356 | H | 1.581154 | -2.716588 | 0.816718 |
| H | -2.756476 | 7.118853 | -0.855241 | H | 2.554033 | -3.977997 | 1.604526 |
| C | -5.860600 | -3.284539 | -0.968977 | H | 4.629358 | -3.279223 | -1.303180 |
| H | -5.907714 | -1.960129 | -2.674612 | H | 3.681834 | -4.432716 | -0.369700 |
| H | -5.707921 | -4.309967 | 0.922111 | H | 2.851287 | -3.192788 | -1.309453 |
| C | -6.446122 | -4.460671 | -1.715719 | O | 0.168206 | -1.617058 | -0.938637 |
| H | -6.604460 | -5.317437 | -1.052897 | C | 0.331729 | -2.057398 | -2.259352 |
| H | -7.411203 | -4.203119 | -2.169536 | H | -0.124285 | -3.063990 | -2.299466 |
| H | -5.782728 | -4.783599 | -2.528297 | H | 1.397595 | -2.193525 | -2.518773 |
| H | 0.885840 | 2.537793 | -0.972404 | C | -0.322777 | -1.179709 | -3.331306 |
| C | 4.738154 | -0.219061 | -1.394036 | H | 0.100113 | -0.167008 | -3.314324 |
| C | 4.068647 | -0.739286 | -2.689762 | H | -0.157286 | -1.606218 | -4.330535 |
| C | 4.848342 | 1.312294 | -1.572801 | H | -1.404015 | -1.097585 | -3.170695 |
| C | 6.163752 | -0.799972 | -1.290986 | H | -2.313768 | -1.530756 | 2.119921 |
| H | 3.975199 | -1.824792 | -2.725115 | H | -0.983409 | -1.296577 | 1.004805 |
| H | 3.070321 | -0.308840 | -2.820822 | H | -0.200376 | -1.036690 | 3.372061 |
| H | 4.682038 | -0.435464 | -3.549226 | H | -0.123303 | 1.258582 | 4.189325 |
| H | 5.415085 | 1.800405 | -0.777035 | H | -1.331539 | 1.783926 | 2.881233 |
| H | 5.377120 | 1.513335 | -2.514065 | | | | |
| H | 3.864274 | 1.788164 | -1.647061 | | | | |
| H | 6.746350 | -0.472529 | -2.163654 | Ts4 | | | |
| H | 6.694399 | -0.459250 | -0.398131 | Pd | 0.996312 | -0.255520 | 1.241388 |
| H | 6.171561 | -1.892591 | -1.293771 | C | -0.278999 | 1.455904 | 0.955028 |
| H | 6.092294 | 1.127680 | 1.063135 | C | -1.660102 | 1.025675 | 0.466530 |
| C | 5.569433 | 0.615289 | 1.874652 | C | 0.245055 | 2.703299 | 0.799490 |
| C | 4.055569 | 0.474978 | 1.614040 | N | -2.417361 | 0.254142 | 1.486903 |
| H | 6.058340 | -0.348832 | 2.038255 | H | -2.284036 | 1.890726 | 0.235467 |
| H | 5.719841 | 1.216525 | 2.782311 | H | -1.543049 | 0.427483 | -0.453427 |

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| S | -4.077985 | 0.102796 | 1.209540 | P | 2.448800 | -0.485107 | -0.906054 |
| C | -1.759256 | -0.886430 | 2.151601 | C | 2.002511 | -2.167872 | -1.793207 |
| O | -4.536174 | 1.408486 | 0.721948 | C | 1.733266 | -3.252134 | -0.724475 |
| O | -4.639957 | -0.508068 | 2.419110 | C | 0.679214 | -2.008121 | -2.575891 |
| C | -0.454269 | -0.434908 | 2.776196 | C | 3.073492 | -2.699092 | -2.771431 |
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| H | 0.613723 | 1.323689 | 3.447750 | H | 0.952416 | -2.953217 | -0.021343 |
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| H | 1.892134 | -1.360251 | 4.018646 | H | -0.114679 | -1.568706 | -1.962444 |
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| H | -1.571992 | -1.717600 | 1.451728 | H | 3.998488 | 0.384423 | -3.568356 |
| H | 1.193317 | 2.872368 | 1.311941 | H | 2.861702 | 1.557915 | -4.237204 |
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| C | -1.206571 | 3.941802 | -0.911161 | C | 2.938194 | 2.222482 | -1.674528 |
| C | 0.262929 | 5.153465 | 0.571427 | H | 0.304475 | 1.464917 | -1.535510 |
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| H | -1.591191 | 3.018343 | -1.327606 | H | 0.272183 | 0.465137 | -2.995343 |
| C | -0.164422 | 6.360100 | 0.021736 | H | 2.691081 | 3.058348 | -2.342502 |
| H | 1.008837 | 5.159793 | 1.363499 | H | 2.541333 | 2.468113 | -0.686080 |
| C | -1.122073 | 6.365529 | -0.998206 | H | 4.026874 | 2.173150 | -1.611469 |
| H | -2.363251 | 5.140241 | -2.268761 | H | 5.353320 | 0.671809 | -1.856925 |
| H | 0.250332 | 7.296199 | 0.387155 | C | 5.375872 | -0.333993 | -1.430892 |
| H | -1.458036 | 7.303841 | -1.431477 | C | 4.314603 | -0.559815 | -0.333148 |
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| C | -4.354822 | -2.444216 | 0.148835 | H | 5.293359 | -1.055695 | -2.248381 |
| C | -4.348570 | -0.616772 | -1.453089 | C | 4.491289 | 0.511558 | 0.770957 |
| C | -4.482254 | -3.352228 | -0.901431 | C | 4.608102 | -1.922948 | 0.333530 |
| H | -4.335356 | -2.787312 | 1.178245 | H | 4.330021 | 1.531491 | 0.416751 |
| C | -4.477614 | -1.541468 | -2.492182 | H | 3.811186 | 0.326948 | 1.608304 |
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| H | -4.558101 | -3.446066 | -4.337863 | | | | |
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| C | 2.373717 | -1.864538 | -0.405029 | O | -1.869765 | 0.447728 | 2.132072 |
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| N | 2.622659 | 0.189904 | 0.901760 | H | -1.593656 | -1.030543 | 3.576755 |
| H | 4.203183 | -0.766047 | -0.068927 | C | -1.798196 | 0.933289 | 4.464149 |
| H | 3.055329 | 0.030079 | -1.177058 | H | -2.890554 | 0.897156 | 4.548814 |
| S | 3.622018 | 1.413222 | 1.504317 | H | -1.363531 | 0.625758 | 5.424631 |
| C | 1.170422 | 0.486461 | 0.821549 | H | -1.501689 | 1.969376 | 4.265113 |
| O | 4.981611 | 0.860671 | 1.537122 | P | -3.928136 | -0.286677 | -0.510548 |
| O | 2.965515 | 1.920178 | 2.713991 | C | -4.146447 | 1.479140 | -1.293430 |
| C | 0.402953 | -0.825439 | 0.782817 | C | -3.518585 | 2.506653 | -0.317572 |
| C | 0.859713 | -1.695993 | -0.388700 | C | -3.312994 | 1.573817 | -2.591953 |
| H | 0.564636 | -1.208071 | -1.338444 | C | -5.595274 | 1.901113 | -1.613787 |
| H | 0.381995 | -2.682683 | -0.367084 | H | -4.076159 | 2.617909 | 0.611609 |
| H | 0.890388 | 1.074430 | 1.695248 | H | -2.491495 | 2.237092 | -0.052300 |
| H | 0.962991 | 1.082829 | -0.084324 | H | -3.501444 | 3.488355 | -0.811198 |
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| C | 4.360224 | -3.457010 | -0.602203 | H | -3.307471 | 2.620845 | -2.923019 |
| C | 4.801022 | -4.612240 | 0.072390 | H | -2.269876 | 1.279698 | -2.430700 |
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| C | 6.136076 | -5.013217 | 0.020216 | H | -6.091266 | 1.218388 | -2.309505 |
| H | 4.086976 | -5.189384 | 0.656012 | H | -6.214016 | 1.981469 | -0.716621 |
| C | 6.636536 | -3.142746 | -1.422909 | H | -5.207441 | -0.488746 | -3.476594 |
| H | 4.977126 | -1.880221 | -1.945741 | C | -5.338657 | -1.392978 | -2.876934 |
| C | 7.062391 | -4.276139 | -0.725216 | C | -4.172372 | -1.629154 | -1.895618 |
| H | 6.454074 | -5.901057 | 0.561148 | H | -6.303560 | -1.324496 | -2.367191 |
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| C | 2.629646 | 3.737739 | 0.358288 | H | -2.001474 | -1.954188 | -2.029177 |
| C | 4.590444 | 2.778916 | -0.708437 | H | -2.919234 | -2.533846 | -3.422602 |
| C | 2.616799 | 4.752435 | -0.599044 | H | -2.600513 | -0.808337 | -3.240445 |
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| C | 4.562245 | 3.802580 | -1.658073 | H | -3.564107 | -3.248034 | -0.528075 |
| H | 5.370030 | 2.023970 | -0.727716 | H | -5.322136 | -3.138430 | -0.752838 |
| C | 3.579833 | 4.803439 | -1.620017 | H | -6.772713 | -1.778568 | -0.177967 |
| H | 1.850645 | 5.523040 | -0.545712 | C | -6.697007 | -0.833222 | 0.366190 |
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| H | 4.120259 | 5.654903 | -3.538289 | H | -7.085829 | -0.038858 | -0.277136 |
| H | 2.556285 | 6.210502 | -2.912235 | C | -4.791521 | -1.708176 | 1.774156 |
| H | 4.057929 | 6.826381 | -2.215271 | C | -5.305487 | 0.702921 | 1.782567 |
| H | 0.500869 | -1.357819 | 1.734318 | H | -4.766224 | -2.673822 | 1.267658 |
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| H | -5.491041 | -1.801753 | 2.616335 | H | 8.286128 | -0.180483 | -2.815311 |
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| H | -5.920494 | 0.462444 | 2.660691 | H | 0.583826 | 0.318555 | -1.594225 |
| H | -4.305232 | 0.969810 | 2.136218 | C | -4.234591 | 0.696634 | -1.784764 |
| | | | | C | -4.174004 | 2.135001 | -1.215190 |
| TS3 | | | | C | -3.337887 | 0.703447 | -3.043375 |
| Pd | -1.409638 | 0.519980 | 0.536713 | C | -5.681211 | 0.385003 | -2.224129 |
| P | -3.492785 | -0.512478 | -0.452150 | H | -4.778267 | 2.274958 | -0.320241 |
| C | 0.404110 | 0.074569 | 0.515497 | H | -3.149430 | 2.422675 | -0.962970 |
| C | 1.151864 | -0.733542 | 1.522190 | H | -4.545454 | 2.825206 | -1.985669 |
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| N | 2.211622 | -1.597724 | 0.957347 | H | -3.663078 | 1.528127 | -3.691734 |
| H | 1.636852 | -0.038880 | 2.217820 | H | -2.285928 | 0.877969 | -2.795406 |
| H | 0.458002 | -1.333287 | 2.126289 | H | -5.972208 | 1.099810 | -3.006955 |
| C | 1.166577 | 2.196738 | -0.692954 | H | -5.790484 | -0.618666 | -2.642964 |
| S | 3.728131 | -1.583742 | 1.740664 | H | -6.399872 | 0.493816 | -1.408989 |
| C | 1.783560 | -2.862241 | 0.335628 | H | -4.266357 | -2.120415 | -3.156320 |
| C | 1.518419 | 2.735588 | -1.946567 | C | -4.123767 | -2.758043 | -2.279974 |
| C | 1.391822 | 2.983528 | 0.455429 | C | -3.050092 | -2.201591 | -1.320064 |
| O | 4.114569 | -2.974397 | 2.020191 | H | -5.094463 | -2.899663 | -1.799908 |
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| C | 4.893815 | -0.943966 | 0.533751 | C | -1.729744 | -2.033802 | -2.108760 |
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| H | 1.094694 | 2.602710 | 1.428585 | H | -2.342049 | -4.157314 | -0.733671 |
| C | 5.788850 | -1.814184 | -0.086591 | H | -2.009334 | -2.915963 | 0.482746 |
| C | 4.902550 | 0.425162 | 0.246364 | H | -3.642923 | -3.586063 | 0.307948 |
| C | 2.524820 | -2.053471 | -1.964453 | H | -5.559634 | -2.872945 | 0.368325 |
| C | 2.316940 | 4.768970 | -0.901067 | C | -5.937308 | -1.860151 | 0.530696 |
| H | 2.347004 | 4.401761 | -3.029158 | C | -4.833453 | -0.853695 | 0.919139 |
| H | 2.132227 | 4.837174 | 1.250701 | H | -6.657493 | -1.917778 | 1.358782 |
| C | 6.702789 | -1.301891 | -1.011782 | H | -6.493007 | -1.554477 | -0.360619 |
| H | 5.774814 | -2.870768 | 0.158593 | C | -4.087196 | -1.360673 | 2.178637 |
| C | 5.816447 | 0.916058 | -0.682976 | C | -5.512937 | 0.470589 | 1.341976 |
| H | 4.212654 | 1.098529 | 0.745041 | H | -3.564012 | -2.306397 | 2.026507 |
| H | 2.755297 | 5.760488 | -0.979142 | H | -3.373368 | -0.609400 | 2.528338 |
| C | 6.731306 | 0.063398 | -1.326179 | H | -4.826013 | -1.523375 | 2.975921 |
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| C | 7.730114 | 0.618712 | -2.314738 | H | -4.766671 | 1.220381 | 1.618056 |
| H | 8.458773 | 1.269947 | -1.814674 | O | -2.625859 | 1.640720 | 1.776072 |
| | | | | C | -2.109343 | 2.801530 | 2.365151 |

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| H | -2.960390 | 3.445127 | 2.661433 | H | 6.413153 | 0.004013 | -1.270980 |
| H | -1.512573 | 3.395111 | 1.646853 | H | -4.047191 | 5.634701 | 0.149144 |
| C | -1.260472 | 2.521794 | 3.611166 | C | 5.746846 | -3.269310 | -0.516357 |
| H | -0.389427 | 1.904125 | 3.354282 | H | 4.347131 | -3.895521 | 1.005331 |
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| H | 2.622785 | -2.235714 | -3.031642 | H | 5.285470 | -5.310033 | -1.078146 |
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| H | 2.304061 | -3.697928 | 0.819895 | H | 1.309088 | 3.176196 | -0.250973 |
| H | 0.719041 | -2.995679 | 0.573078 | C | -4.724002 | -0.848706 | 0.602953 |
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| | | | | C | -5.185517 | 0.565166 | 0.182268 |
| | | | | C | -5.898327 | -1.825678 | 0.387344 |
| Int 6 | | | | H | -4.114275 | -1.698275 | 2.564137 |
| Pd | -1.059758 | 0.115147 | 0.319664 | H | -3.619842 | -0.020675 | 2.312230 |
| P | -3.066230 | -1.304963 | -0.306108 | H | -5.317228 | -0.410863 | 2.640749 |
| C | 0.565909 | 1.290656 | 0.264274 | H | -5.557754 | 0.610223 | -0.843586 |
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| N | 3.056369 | 1.350350 | -0.166470 | H | -6.785034 | -1.436146 | 0.907150 |
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| C | -0.823240 | 3.405567 | 0.076302 | H | -5.431140 | -0.672450 | -2.424174 |
| S | 4.506646 | 1.015926 | 0.654025 | C | -4.585947 | -1.211389 | -2.858776 |
| C | 3.163973 | 1.492118 | -1.634207 | C | -3.242021 | -0.856994 | -2.190715 |
| C | -0.946115 | 4.538331 | -0.752901 | H | -4.804568 | -2.281828 | -2.809057 |
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| O | 4.183398 | 1.015468 | 2.085309 | C | -2.989531 | 0.666912 | -2.310146 |
| O | 5.520537 | 1.917454 | 0.097562 | C | -2.110547 | -1.530034 | -3.001518 |
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| H | -3.843077 | 3.670424 | 1.667637 | C | -1.253265 | -3.478056 | -0.456593 |
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| H | 3.697966 | -1.600301 | 1.657363 | H | -0.996731 | -3.287018 | -1.499247 |
| C | 6.315648 | -2.156023 | -1.150414 | | | | |

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| H | -0.598136 | -2.880643 | 0.184833 | C | 0.067324 | 0.210918 | 2.784159 |
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| H | -3.972474 | -3.613334 | 1.670629 | H | 0.398751 | 6.602843 | -0.969999 |
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| H | -2.329163 | -3.018136 | 2.019737 | C | 6.229956 | -0.479615 | -1.908592 |
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| H | 1.310340 | 0.268290 | 3.581575 | C | 8.367883 | 0.873327 | -1.707215 |
| H | 3.933565 | 0.814274 | -2.038328 | H | 8.277787 | 0.959019 | -2.794860 |
| H | 2.213210 | 1.130463 | -2.045414 | H | 8.503558 | 1.881106 | -1.297180 |
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| H | 3.725252 | 3.983111 | -0.382427 | C | -4.027061 | 0.629638 | -1.211160 |
| | | | | C | -4.465494 | 1.066539 | 0.206098 |
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| TSS | | | | H | -4.916663 | 0.263426 | 0.785871 |
| Pd | -1.069984 | -0.019135 | 1.017706 | H | -3.627838 | 1.445788 | 0.795723 |
| P | -2.590829 | -0.680471 | -1.034088 | H | -5.208202 | 1.870204 | 0.100889 |
| C | 0.666571 | 0.789650 | 0.057288 | H | -3.312789 | 1.752826 | -2.979058 |
| C | 1.666372 | -0.277024 | -0.367236 | H | -4.250937 | 2.687753 | -1.819236 |
| C | 0.773475 | 2.024891 | -0.512030 | H | -2.576344 | 2.276829 | -1.446361 |
| N | 2.297459 | -0.762360 | 0.876929 | H | -5.990706 | 0.986875 | -2.034801 |
| H | 1.194785 | -1.126866 | -0.860496 | H | -5.059283 | -0.151217 | -3.009134 |
| H | 2.420503 | 0.151872 | -1.051461 | H | -5.789121 | -0.673122 | -1.484358 |
| C | 0.096158 | 3.279151 | -0.187095 | H | -3.256210 | -0.019217 | -4.174824 |
| S | 3.515957 | -1.917691 | 0.763093 | C | -2.738952 | -0.965700 | -3.997866 |
| C | 2.435787 | 0.330373 | 1.840934 | C | -1.760690 | -0.881019 | -2.804457 |
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| C | 0.012462 | 5.706599 | -0.491170 | H | -1.305610 | 1.277351 | -3.071748 |
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| H | -1.400145 | 2.490298 | 1.162700 | H | -1.431965 | -3.075071 | -2.839485 |
| C | 5.127648 | -1.132328 | -1.351304 | H | -3.320764 | -3.486235 | -2.559239 |
| C | 5.870050 | -0.455694 | 0.861807 | | | | |

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|-------|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | -4.031435 | -3.180751 | -1.789036 | C | -0.912996 | 1.259030 | -0.284317 |
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| H | -1.735697 | -1.080273 | 4.037321 | H | -5.896158 | 0.733953 | -0.135224 |
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| H | -4.765353 | -1.425389 | 3.679942 | H | 2.082269 | 6.999595 | 1.415527 |
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| H | 3.117360 | 1.115121 | 1.473484 | C | -7.088424 | -2.712146 | 2.815728 |
| H | 1.012083 | 2.007078 | 2.122749 | H | -8.170681 | -2.589102 | 2.683553 |
| H | 0.282982 | -0.814026 | 3.082275 | H | -6.887573 | -3.777441 | 2.968018 |
| H | -0.610014 | 0.766350 | 3.427474 | H | -6.813354 | -2.183027 | 3.736970 |
| | | | | H | -1.694511 | 4.209033 | -2.068380 |
| | | | | C | 3.519543 | -2.690195 | 1.122042 |
| Int 8 | | | | C | 3.468705 | -1.944751 | 2.481091 |
| Pd | 1.496609 | -0.106055 | 0.952604 | C | 2.429012 | -3.783242 | 1.208693 |
| P | 3.061151 | -1.396977 | -0.264332 | C | 4.890556 | -3.381167 | 0.977791 |
| C | -1.448076 | 2.337112 | -1.229863 | H | 4.201243 | -1.144123 | 2.575428 |
| C | -2.483231 | 1.697820 | -2.132187 | H | 2.472317 | -1.521337 | 2.682407 |
| C | -1.162009 | 3.652633 | -1.294713 | H | 3.662652 | -2.666108 | 3.286890 |
| N | -2.985498 | 0.602765 | -1.266672 | H | 2.448635 | -4.476739 | 0.365458 |
| H | -3.298479 | 2.366210 | -2.413028 | H | 2.608165 | -4.375881 | 2.115795 |
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| C | -0.250422 | 4.502285 | -0.507841 | H | 5.006515 | -4.110221 | 1.792001 |
| S | -4.052484 | -0.490128 | -1.995495 | H | 4.989510 | -3.927004 | 0.035850 |
| C | -1.806068 | 0.029471 | -0.581397 | H | 5.725952 | -2.681112 | 1.054968 |
| C | 0.015216 | 5.795232 | -1.008429 | H | 3.378321 | -4.361911 | -1.466579 |
| C | 0.343607 | 4.141866 | 0.721420 | C | 3.417629 | -3.572974 | -2.221235 |
| O | -3.332432 | -1.612367 | -2.627375 | C | 2.527558 | -2.362056 | -1.866027 |
| O | -4.973487 | 0.327356 | -2.798426 | H | 4.464626 | -3.299364 | -2.375265 |
| C | -4.922634 | -1.143510 | -0.567762 | H | 3.052347 | -4.010996 | -3.160301 |

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| C | 1.070695 | -2.846133 | -1.674409 | O | 3.770161 | -3.159796 | -1.003497 |
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| H | 0.401837 | -2.020511 | -1.420733 | C | 0.463179 | -1.442793 | 2.216825 |
| H | 0.718066 | -3.284795 | -2.617074 | C | -0.230367 | -2.500334 | 1.566018 |
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| C | 5.719785 | -1.018890 | -1.503452 | H | -2.894400 | 0.564501 | 3.489981 |
| C | 4.628945 | -0.318416 | -0.666294 | C | -1.574835 | 1.373729 | 4.996016 |
| H | 6.574918 | -0.336887 | -1.607577 | H | -1.836520 | 2.424867 | 4.824336 |
| H | 6.090007 | -1.935559 | -1.036950 | H | -2.184551 | 0.996166 | 5.829243 |
| C | 4.158708 | 0.957106 | -1.407887 | H | -0.518308 | 1.334574 | 5.288472 |
| C | 5.267925 | 0.180546 | 0.650299 | H | 2.572941 | -1.702975 | 2.583586 |
| H | 3.691635 | 0.758072 | -2.372727 | H | 2.158034 | -0.184891 | 1.760353 |
| H | 3.455538 | 1.531967 | -0.799319 | H | -0.391163 | -2.964611 | -2.040125 |
| H | 5.035204 | 1.592086 | -1.594978 | C | -2.301703 | -3.022258 | -1.066310 |
| H | 5.763348 | -0.612005 | 1.215800 | C | -3.233018 | -2.529158 | -0.126974 |
| H | 6.036544 | 0.923039 | 0.398228 | C | -2.741685 | -4.020727 | -1.962784 |
| H | 4.536371 | 0.676152 | 1.297106 | C | -4.532209 | -3.031020 | -0.073536 |
| O | 0.537641 | 0.967960 | 2.372140 | H | -2.935481 | -1.731980 | 0.548361 |
| C | -0.452223 | 0.342091 | 3.141940 | C | -4.043083 | -4.519529 | -1.912594 |
| H | -0.134231 | -0.655903 | 3.505524 | H | -2.044013 | -4.412676 | -2.700014 |
| H | -1.380006 | 0.175777 | 2.556680 | C | -4.945799 | -4.029780 | -0.963343 |
| C | -0.795574 | 1.213388 | 4.355766 | H | -5.229850 | -2.633139 | 0.659439 |
| H | -1.158165 | 2.195683 | 4.030508 | H | -4.352228 | -5.291139 | -2.613222 |
| H | -1.573822 | 0.739570 | 4.970281 | H | -5.961168 | -4.415145 | -0.921152 |
| H | 0.094617 | 1.369101 | 4.976805 | C | 4.603457 | -0.774235 | -0.238276 |
| H | -2.114449 | -0.499850 | 0.323919 | C | 5.173273 | 0.016176 | 0.766263 |
| H | -1.287640 | -0.679732 | -1.240304 | C | 4.643379 | -0.367997 | -1.574363 |
| H | -1.058645 | 1.575052 | 0.750179 | C | 5.775339 | 1.225693 | 0.421957 |
| | | | | H | 5.164600 | -0.325133 | 1.796441 |
| | | | | C | 5.251891 | 0.846395 | -1.900090 |
| TS6 | | | | H | 4.226281 | -1.004894 | -2.347819 |
| Pd | -0.763871 | -0.207206 | 0.997715 | C | 5.824998 | 1.661322 | -0.912924 |
| C | -0.174451 | -1.826354 | -0.293655 | H | 6.222904 | 1.837115 | 1.202555 |
| C | 1.311026 | -1.601501 | -0.599323 | H | 5.289615 | 1.158719 | -2.941197 |
| C | -0.911749 | -2.574948 | -1.159215 | C | 6.503939 | 2.962862 | -1.270989 |
| N | 2.179396 | -1.956768 | 0.550553 | H | 6.306830 | 3.245635 | -2.310027 |
| H | 1.627063 | -2.223520 | -1.441920 | H | 6.163144 | 3.781460 | -0.625943 |
| H | 1.471987 | -0.546143 | -0.872526 | H | 7.592159 | 2.885503 | -1.147895 |
| S | 3.791412 | -2.319453 | 0.199148 | P | -1.584720 | 1.734823 | -0.550200 |
| C | 1.917894 | -1.258708 | 1.825738 | C | -0.251605 | 3.160650 | -0.435733 |

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| C | 0.286918 | 3.232487 | 1.011993 | C | -2.559150 | 3.673223 | -0.388971 |
| C | 0.966825 | 2.819448 | -1.323231 | N | -3.082726 | 0.397868 | 0.830430 |
| C | -0.753263 | 4.563880 | -0.843612 | H | -4.291148 | 1.778539 | -0.182952 |
| H | -0.470068 | 3.494751 | 1.747808 | H | -3.310584 | 0.744518 | -1.253754 |
| H | 0.717448 | 2.281607 | 1.336004 | S | -4.400490 | -0.545632 | 1.311012 |
| H | 1.074731 | 3.998794 | 1.043490 | C | -1.757488 | -0.270302 | 0.775803 |
| H | 0.761864 | 2.920752 | -2.391480 | O | -5.566573 | 0.347438 | 1.312858 |
| H | 1.773213 | 3.525155 | -1.083062 | O | -3.974426 | -1.260298 | 2.518813 |
| H | 1.352155 | 1.812707 | -1.131371 | C | -0.668799 | 0.790471 | 0.809995 |
| H | 0.092731 | 5.263767 | -0.788486 | C | -0.811505 | 1.807360 | -0.329214 |
| H | -1.140091 | 4.602679 | -1.864246 | H | -0.608944 | 1.307693 | -1.296430 |
| H | -1.524302 | 4.945148 | -0.171380 | H | -0.084261 | 2.616138 | -0.215994 |
| H | -1.093381 | 3.160429 | -3.456584 | H | -1.671454 | -0.939495 | 1.631586 |
| C | -2.019947 | 2.586078 | -3.375773 | H | -1.684210 | -0.870653 | -0.148031 |
| C | -1.870486 | 1.358089 | -2.451136 | H | -3.618667 | 3.912211 | -0.282980 |
| H | -2.817700 | 3.265377 | -3.070847 | C | -1.678071 | 4.853260 | -0.514856 |
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| C | -0.692638 | 0.510359 | -2.987519 | C | -1.963046 | 6.003223 | 0.246788 |
| C | -3.129615 | 0.474304 | -2.605939 | C | 0.202298 | 6.051593 | -1.506926 |
| H | -0.569247 | -0.406897 | -2.412970 | H | -0.383490 | 4.053758 | -2.048206 |
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| H | -3.179111 | 0.119970 | -3.644576 | C | -0.078837 | 7.175062 | -0.723978 |
| H | -3.096622 | -0.409435 | -1.963600 | H | 1.033254 | 6.070930 | -2.208175 |
| H | -4.058294 | 1.013401 | -2.408866 | H | -1.404440 | 8.018158 | 0.758185 |
| H | -4.450640 | 2.844754 | -1.661759 | H | 0.537195 | 8.067036 | -0.803897 |
| C | -4.079418 | 3.346303 | -0.765081 | C | -4.675602 | -1.781511 | 0.028369 |
| C | -3.270814 | 2.418414 | 0.166583 | C | -3.996929 | -3.003260 | 0.088883 |
| H | -4.959130 | 3.703308 | -0.211322 | C | -5.545844 | -1.501832 | -1.028912 |
| H | -3.513024 | 4.229026 | -1.073580 | C | -4.191705 | -3.942679 | -0.923927 |
| C | -4.139144 | 1.190911 | 0.532450 | H | -3.343621 | -3.219073 | 0.928206 |
| C | -3.020356 | 3.177607 | 1.489639 | C | -5.728843 | -2.454447 | -2.033584 |
| H | -4.383363 | 0.556906 | -0.321405 | H | -6.088664 | -0.562193 | -1.049103 |
| H | -3.642423 | 0.575561 | 1.288222 | C | -5.058705 | -3.686562 | -1.998669 |
| H | -5.086347 | 1.546580 | 0.961287 | H | -3.667794 | -4.894812 | -0.872798 |
| H | -2.581318 | 4.165947 | 1.330634 | H | -6.411786 | -2.238620 | -2.852297 |
| H | -3.992067 | 3.336544 | 1.978075 | C | -5.289226 | -4.728234 | -3.069051 |
| H | -2.377760 | 2.601229 | 2.160467 | H | -5.673319 | -4.278590 | -3.990804 |
| H | 0.165569 | -1.078354 | 3.193514 | H | -4.365341 | -5.265632 | -3.311286 |
| | | | | H | -6.022497 | -5.475635 | -2.737088 |
| | | | | H | -0.654221 | 1.294599 | 1.781506 |
| Int 7 | | | | Pd | 1.175996 | -0.019645 | 0.450145 |
| C | -2.224918 | 2.368441 | -0.360045 | O | 1.093081 | -1.129147 | 2.142239 |
| C | -3.311570 | 1.314889 | -0.304165 | C | 0.662603 | -0.594295 | 3.368543 |

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|---|-----------|-----------|-----------|-----|-----------|-----------|-----------|
| H | -0.389031 | -0.264854 | 3.336959 | H | 4.972337 | -2.234428 | 2.824321 |
| H | 1.265940 | 0.283001 | 3.667248 | H | 3.305151 | -2.257971 | 2.221314 |
| C | 0.792430 | -1.682818 | 4.440822 | | | | |
| H | 1.833685 | -2.010289 | 4.542065 | | | | |
| H | 0.451620 | -1.299282 | 5.411791 | TS2 | | | |
| H | 0.181099 | -2.553441 | 4.177718 | Pd | 1.347651 | -0.734819 | -0.990321 |
| P | 3.405904 | -0.855786 | -0.373913 | P | 2.869109 | 0.464402 | 0.796309 |
| C | 3.165440 | -2.585100 | -1.229338 | C | -0.514224 | 0.373873 | -0.872129 |
| C | 2.236205 | -3.433335 | -0.324282 | C | -1.512814 | -0.055662 | 0.182964 |
| C | 2.398224 | -2.400771 | -2.558637 | C | -0.529577 | 1.570511 | -1.521769 |
| C | 4.456494 | -3.378229 | -1.518552 | N | -1.861370 | -1.452071 | -0.142900 |
| H | 2.697869 | -3.724369 | 0.618412 | H | -1.097879 | -0.028072 | 1.192244 |
| H | 1.309939 | -2.902261 | -0.083888 | H | -2.420301 | 0.570218 | 0.152005 |
| H | 1.976048 | -4.355457 | -0.862548 | C | -1.306319 | 2.803230 | -1.327337 |
| H | 2.991936 | -1.915698 | -3.337128 | S | -2.887839 | -2.284605 | 0.905966 |
| H | 2.122030 | -3.393511 | -2.938206 | C | -2.090796 | -1.559359 | -1.586139 |
| H | 1.468848 | -1.837289 | -2.419591 | C | -1.341535 | 3.716294 | -2.406653 |
| H | 4.192622 | -4.313531 | -2.032353 | C | -2.010141 | 3.157736 | -0.155236 |
| H | 5.151290 | -2.835194 | -2.165437 | O | -2.369317 | -2.023146 | 2.252744 |
| H | 4.988138 | -3.655193 | -0.604953 | O | -3.001061 | -3.641564 | 0.360841 |
| H | 4.819926 | -0.911678 | -3.284960 | C | -4.513592 | -1.520187 | 0.793425 |
| C | 5.167817 | -0.100294 | -2.640648 | C | -0.811006 | -1.117502 | -2.288242 |
| C | 4.069716 | 0.414786 | -1.687806 | C | -2.068849 | 4.902557 | -2.337689 |
| H | 6.053631 | -0.450186 | -2.103488 | H | -0.789929 | 3.478294 | -3.313691 |
| H | 5.486347 | 0.719848 | -3.299760 | C | -2.736353 | 4.347304 | -0.085225 |
| C | 2.854136 | 0.893334 | -2.520217 | H | -1.967680 | 2.524439 | 0.722340 |
| C | 4.601422 | 1.678814 | -0.973545 | C | -4.853855 | -0.485303 | 1.667743 |
| H | 2.081966 | 1.334659 | -1.875283 | C | -5.419018 | -1.960179 | -0.179269 |
| H | 3.181512 | 1.679600 | -3.214422 | C | 0.309068 | -1.976352 | -2.337901 |
| H | 2.389919 | 0.105854 | -3.114135 | C | -2.776866 | 5.222976 | -1.174533 |
| H | 4.799223 | 2.448287 | -1.732142 | H | -2.079744 | 5.579091 | -3.188499 |
| H | 3.870503 | 2.092451 | -0.270676 | H | -3.264051 | 4.596621 | 0.832074 |
| H | 5.538242 | 1.506341 | -0.439903 | C | -6.108879 | 0.118094 | 1.555581 |
| H | 6.534564 | -0.219591 | 0.120089 | H | -4.156541 | -0.178575 | 2.440803 |
| C | 6.177454 | -1.125529 | 0.617390 | C | -6.666313 | -1.345301 | -0.276850 |
| C | 4.703128 | -1.025286 | 1.059597 | H | -5.157521 | -2.790333 | -0.827797 |
| H | 6.803655 | -1.269152 | 1.509173 | H | -3.341368 | 6.149597 | -1.112731 |
| H | 6.360806 | -1.973431 | -0.048515 | C | -7.031185 | -0.295950 | 0.583921 |
| C | 4.525972 | 0.193307 | 1.999417 | H | -6.377315 | 0.916830 | 2.243081 |
| C | 4.355593 | -2.265226 | 1.915569 | H | -7.373468 | -1.694193 | -1.026404 |
| H | 4.789786 | 1.144990 | 1.536433 | C | -8.388134 | 0.357631 | 0.463589 |
| H | 3.496804 | 0.257899 | 2.364530 | H | -8.541198 | 1.110523 | 1.243240 |
| H | 5.185900 | 0.060808 | 2.867878 | H | -8.503418 | 0.853418 | -0.508747 |
| H | 4.583583 | -3.207156 | 1.410380 | H | -9.193789 | -0.382190 | 0.546603 |

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| H | 0.141040 | 1.636728 | -2.381034 | C | 4.416403 | -3.465593 | -2.615355 |
| C | 4.036229 | 1.706935 | -0.147410 | H | 5.318809 | -3.148493 | -2.079270 |
| C | 4.445412 | 1.059234 | -1.491047 | H | 4.491838 | -4.545457 | -2.807678 |
| C | 3.245855 | 2.985286 | -0.508574 | H | 4.394511 | -2.939668 | -3.577863 |
| C | 5.312146 | 2.136370 | 0.609042 | H | -2.316520 | -2.598826 | -1.835213 |
| H | 5.042538 | 0.156817 | -1.373597 | H | -2.929281 | -0.918304 | -1.905208 |
| H | 3.573659 | 0.782674 | -2.090756 | H | -0.958886 | -0.453629 | -3.134390 |
| H | 5.039769 | 1.790818 | -2.057068 | H | 0.267308 | -2.915388 | -1.787315 |
| H | 3.076144 | 3.636326 | 0.352723 | H | 0.940335 | -1.965947 | -3.222622 |
| H | 3.835498 | 3.562085 | -1.233957 | | | | |
| H | 2.281343 | 2.759679 | -0.974822 | | | | |
| H | 5.856661 | 2.863559 | -0.010378 | Int 3 | | | |
| H | 5.099112 | 2.620110 | 1.565078 | Pd | -1.862522 | -0.603616 | 1.155770 |
| H | 5.992536 | 1.302909 | 0.793999 | P | -3.501828 | -0.898986 | -0.520233 |
| H | 3.286340 | 3.211541 | 2.532015 | C | 1.072178 | 1.189965 | 0.088009 |
| C | 2.908331 | 2.361154 | 3.106188 | C | 2.146978 | 1.428636 | -0.946683 |
| C | 2.001474 | 1.447147 | 2.252910 | C | 0.290702 | 2.107790 | 0.686215 |
| H | 3.758899 | 1.845644 | 3.552808 | N | 3.103518 | 0.332917 | -0.645864 |
| H | 2.307049 | 2.775156 | 3.928721 | H | 2.646335 | 2.394055 | -0.849768 |
| C | 0.881081 | 2.338096 | 1.675739 | H | 1.754111 | 1.346270 | -1.975618 |
| C | 1.293329 | 0.433629 | 3.183665 | C | 0.191572 | 3.552784 | 0.428594 |
| H | 0.204261 | 1.766385 | 1.047032 | S | 4.347117 | 0.113229 | -1.773608 |
| H | 0.302625 | 2.757940 | 2.510607 | C | 2.318003 | -0.862639 | -0.275272 |
| H | 1.249128 | 3.177559 | 1.086873 | C | 0.510072 | 4.163489 | -0.801754 |
| H | 0.648214 | 0.988721 | 3.878289 | C | -0.279580 | 4.382527 | 1.468314 |
| H | 0.655621 | -0.263989 | 2.631191 | O | 3.955687 | -0.837262 | -2.831606 |
| H | 1.985178 | -0.151265 | 3.791237 | O | 4.797239 | 1.464122 | -2.138749 |
| H | 3.963149 | -0.290022 | 3.786363 | C | 5.604979 | -0.684339 | -0.771434 |
| C | 4.661671 | -0.500419 | 2.973989 | C | 1.094988 | -0.286249 | 0.494426 |
| C | 3.976217 | -0.908701 | 1.651602 | C | 0.394286 | 5.545073 | -0.970965 |
| H | 5.285999 | -1.342871 | 3.302900 | H | 0.824454 | 3.556860 | -1.644913 |
| H | 5.323853 | 0.362136 | 2.854134 | C | -0.392258 | 5.762478 | 1.301184 |
| C | 3.058819 | -2.128746 | 1.909153 | H | -0.547121 | 3.928928 | 2.420139 |
| C | 5.091547 | -1.391454 | 0.696889 | C | 5.960052 | -2.006444 | -1.033788 |
| H | 2.242445 | -1.922952 | 2.603685 | C | 6.240686 | 0.046401 | 0.238570 |
| H | 2.628820 | -2.495753 | 0.974035 | C | -0.152242 | -1.109284 | 0.148257 |
| H | 3.663028 | -2.936714 | 2.344836 | C | -0.050956 | 6.353114 | 0.079477 |
| H | 5.894051 | -0.658316 | 0.580670 | H | 0.647091 | 5.989608 | -1.930618 |
| H | 5.544574 | -2.291094 | 1.137005 | H | -0.748073 | 6.377886 | 2.124099 |
| H | 4.681099 | -1.647169 | -0.280883 | C | 6.961976 | -2.606529 | -0.264297 |
| O | 3.066962 | -1.771083 | -1.574273 | H | 5.463960 | -2.549494 | -1.831719 |
| C | 3.151127 | -3.144656 | -1.805926 | C | 7.234401 | -0.567948 | 0.995579 |
| H | 2.289716 | -3.547802 | -2.371762 | H | 5.959514 | 1.078451 | 0.423083 |
| H | 3.181995 | -3.724813 | -0.859101 | H | -0.007685 | -2.157761 | 0.442445 |

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| H | -0.355677 | -1.059765 | -0.923567 | H | -1.455219 | 1.042520 | -1.541099 |
| H | -0.139162 | 7.428225 | -0.054786 | H | -2.208726 | 1.701796 | -3.000116 |
| C | 7.611712 | -1.902465 | 0.757767 | H | -4.990904 | 1.904453 | -0.664444 |
| H | 7.241936 | -3.637502 | -0.467807 | H | -3.818898 | 2.731698 | -1.685486 |
| H | 7.730089 | -0.002991 | 1.782135 | H | -3.292750 | 2.049126 | -0.146470 |
| C | 8.697650 | -2.548763 | 1.586230 | O | -0.891754 | -0.185559 | 2.863529 |
| H | 9.653109 | -2.022523 | 1.465683 | C | -0.363991 | -1.200792 | 3.671364 |
| H | 8.852420 | -3.593850 | 1.299536 | H | -1.114733 | -1.980531 | 3.904060 |
| H | 8.448921 | -2.525502 | 2.654622 | H | 0.475813 | -1.721339 | 3.165891 |
| H | -0.327268 | 1.741889 | 1.506125 | C | 0.154633 | -0.605112 | 4.984605 |
| C | -5.096753 | -0.880284 | 0.605082 | H | 0.933045 | 0.140971 | 4.785048 |
| C | -4.871449 | 0.182793 | 1.711897 | H | 0.576447 | -1.388079 | 5.630170 |
| C | -5.237038 | -2.228696 | 1.349831 | H | -0.659612 | -0.108587 | 5.525892 |
| C | -6.427387 | -0.580021 | -0.114320 | H | 2.923212 | -1.534045 | 0.341137 |
| H | -4.769128 | 1.199028 | 1.333047 | H | 1.994948 | -1.411816 | -1.172105 |
| H | -3.987794 | -0.039619 | 2.328190 | H | 1.274837 | -0.349850 | 1.570697 |
| H | -5.734282 | 0.169298 | 2.392005 | | | | |
| H | -5.534420 | -3.052447 | 0.697562 | | | | |
| H | -6.023361 | -2.120807 | 2.108830 | Int 4 | | | |
| H | -4.315929 | -2.507975 | 1.871821 | C | -1.440586 | -1.148351 | 0.598013 |
| H | -7.246358 | -0.646569 | 0.615533 | C | -0.661204 | -0.824844 | -0.668263 |
| H | -6.645232 | -1.292987 | -0.913784 | C | -2.668455 | -0.702879 | 0.969179 |
| H | -6.458646 | 0.426842 | -0.537662 | N | 0.519683 | -1.717927 | -0.586328 |
| H | -5.567723 | -3.222764 | -1.335311 | H | -1.215398 | -1.038444 | -1.587597 |
| C | -4.824943 | -3.003717 | -2.105502 | H | -0.345500 | 0.226823 | -0.696135 |
| C | -3.464166 | -2.568609 | -1.519207 | C | -3.591611 | 0.219946 | 0.310340 |
| H | -5.248396 | -2.260599 | -2.786343 | S | 1.975633 | -1.286784 | -1.340930 |
| H | -4.678899 | -3.928227 | -2.681104 | C | 0.501672 | -2.361887 | 0.663276 |
| C | -2.937114 | -3.680621 | -0.579971 | C | -4.857578 | 0.419662 | 0.907766 |
| C | -2.455183 | -2.481926 | -2.688472 | C | -3.319767 | 0.936075 | -0.877019 |
| H | -1.958452 | -3.424460 | -0.164834 | O | 1.597056 | -0.864007 | -2.690957 |
| H | -2.827243 | -4.605902 | -1.161841 | O | 2.884190 | -2.407833 | -1.086820 |
| H | -3.607150 | -3.898061 | 0.252090 | C | 2.608684 | 0.154173 | -0.476249 |
| H | -2.364174 | -3.481468 | -3.133820 | C | -0.622610 | -2.087882 | 1.365699 |
| H | -1.456494 | -2.184471 | -2.358711 | C | -5.803219 | 1.277451 | 0.352029 |
| H | -2.777000 | -1.806644 | -3.483932 | H | -5.094660 | -0.115871 | 1.824693 |
| H | -4.302022 | -0.397227 | -3.611677 | C | -4.268036 | 1.795834 | -1.433411 |
| C | -4.584526 | 0.413790 | -2.935710 | H | -2.364052 | 0.836480 | -1.376398 |
| C | -3.590808 | 0.587612 | -1.767980 | C | 2.344680 | 1.430908 | -0.976905 |
| H | -4.591649 | 1.337410 | -3.530697 | C | 3.333109 | -0.015493 | 0.709503 |
| H | -5.609085 | 0.235737 | -2.599051 | C | -1.009266 | -2.685241 | 2.684111 |
| C | -2.171300 | 0.825999 | -2.338353 | C | -5.514536 | 1.972690 | -0.827103 |
| C | -3.952625 | 1.881869 | -1.003629 | H | -6.767236 | 1.403973 | 0.838682 |
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| C | 2.809243 | 2.546292 | -0.275690 | C | 0.899477 | -1.074975 | 3.208761 |
| H | 1.807880 | 1.545298 | -1.913150 | H | 1.364723 | -1.877127 | 3.790997 |
| C | 3.786823 | 1.109136 | 1.394366 | H | 1.123203 | -0.126592 | 3.717533 |
| H | 3.556839 | -1.012967 | 1.073833 | H | -0.188454 | -1.214392 | 3.249011 |
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| C | 3.531453 | 2.406533 | 0.917236 | C | 0.806768 | 2.359210 | 0.168293 |
| H | 2.611451 | 3.540307 | -0.669700 | C | 1.305223 | 3.521467 | 0.781973 |
| H | 4.357178 | 0.978106 | 2.311449 | C | 0.638750 | 2.361381 | -1.227467 |
| C | 4.038988 | 3.613173 | 1.671051 | C | 1.644090 | 4.645614 | 0.025437 |
| H | 5.134494 | 3.608288 | 1.733498 | H | 1.434712 | 3.542350 | 1.862183 |
| H | 3.735238 | 4.546014 | 1.185893 | C | 0.978914 | 3.484034 | -1.984785 |
| H | 3.656598 | 3.628021 | 2.699213 | H | 0.219323 | 1.487629 | -1.718769 |
| H | -3.045739 | -1.098906 | 1.910980 | C | 1.484337 | 4.630576 | -1.363167 |
| H | 1.310299 | -3.037749 | 0.909752 | H | 2.030280 | 5.532274 | 0.522014 |
| H | -1.939648 | -3.263840 | 2.605102 | H | 0.840718 | 3.464116 | -3.062905 |
| | | | | H | 1.744072 | 5.504840 | -1.954351 |
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| TS7 | | | | P | -3.596760 | 0.142520 | 0.022126 |
| S | 4.022808 | -2.106201 | -0.793944 | C | -4.210915 | -0.695397 | -1.626230 |
| O | 3.809950 | -2.006667 | -2.239093 | C | -3.162063 | -0.390873 | -2.725908 |
| O | 4.470240 | -3.341918 | -0.143822 | C | -4.208849 | -2.232692 | -1.465472 |
| C | 5.155670 | -0.792531 | -0.323190 | C | -5.611578 | -0.265120 | -2.111615 |
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| C | 5.807619 | -0.853026 | 0.913780 | H | -4.406340 | -2.671820 | -2.453111 |
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| H | 6.355831 | 2.170877 | -1.457932 | H | -5.860156 | -0.857222 | -3.003176 |
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| H | 5.669155 | -1.713733 | 1.560176 | H | -5.661811 | 0.785962 | -2.406340 |
| C | 7.812340 | 2.400266 | 0.852487 | H | -6.207740 | -1.669210 | 0.552749 |
| H | 7.680229 | 2.673102 | 1.905945 | C | -6.004004 | -0.955783 | 1.354255 |
| H | 8.857910 | 2.088575 | 0.726797 | C | -4.495464 | -0.684337 | 1.537482 |
| H | 7.661135 | 3.299810 | 0.246902 | H | -6.577639 | -0.047186 | 1.155684 |
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| C | 1.754949 | -0.553772 | -0.529493 | C | -3.775366 | -2.021224 | 1.836345 |
| H | 2.424130 | 0.244495 | -0.874435 | C | -4.311339 | 0.187788 | 2.799964 |
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| H | -3.260129 | 0.442130 | 2.971161 | N | -2.088820 | -1.551704 | -0.100846 |
| H | -4.897499 | 1.109564 | 2.773980 | C | -1.330435 | -0.568245 | 0.703208 |
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| C | -4.106307 | 2.030625 | -0.039272 | H | -2.294068 | -1.966829 | -2.188914 |
| H | -5.809032 | 3.365298 | 0.005422 | C | -0.769865 | -0.480585 | -1.624720 |
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| H | -3.819164 | 3.725695 | -1.345814 | C | -1.337745 | 2.428635 | -0.143073 |
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| C | -0.798036 | -3.194049 | -0.265012 | C | -2.804215 | 3.960017 | 1.067912 |
| H | -1.703119 | -3.645096 | 0.198661 | H | -1.087795 | 2.983208 | 1.925863 |
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| H | 0.645400 | -3.778422 | -1.784658 | C | -3.584629 | 4.140829 | -0.076282 |
| H | -0.088244 | -5.151298 | -0.920284 | H | -3.055050 | 4.480625 | 1.989132 |
| H | -1.024097 | -4.260733 | -2.147598 | H | -3.845328 | 3.597802 | -2.149442 |
| H | -1.089579 | 1.210555 | 1.093151 | H | -4.446875 | 4.802556 | -0.053665 |
| | | | | H | 0.549782 | 1.869058 | -0.990094 |
| | | | | H | -0.870528 | -1.076482 | 1.549966 |
| Int 9 | | | | Pd | 1.578399 | -0.927253 | 0.034849 |
| S | -3.527497 | -2.245474 | 0.428788 | P | 3.572155 | 0.481035 | 0.100119 |
| O | -3.324874 | -2.550527 | 1.846094 | C | 4.881098 | -0.868120 | -0.456155 |
| O | -3.854398 | -3.273917 | -0.564850 | C | 4.411401 | -2.250824 | 0.063286 |
| C | -4.800165 | -0.979029 | 0.330102 | C | 4.876362 | -0.985052 | -1.997918 |
| C | -5.078411 | -0.190804 | 1.448793 | C | 6.332802 | -0.641068 | 0.014975 |
| C | -6.063588 | 0.795190 | 1.358583 | H | 4.379257 | -2.328450 | 1.149213 |
| C | -6.778022 | 1.003334 | 0.170659 | H | 3.420391 | -2.522156 | -0.323846 |
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| H | -6.283348 | 1.406705 | 2.230625 | H | 3.863234 | -1.112396 | -2.393700 |
| H | -7.028603 | 0.332109 | -1.867000 | H | 6.967988 | -1.428120 | -0.415383 |
| H | -5.293157 | -1.433792 | -1.720666 | H | 6.743647 | 0.318891 | -0.305282 |
| C | -7.863591 | 2.051013 | 0.085464 | H | 6.434606 | -0.710269 | 1.100889 |
| H | -7.838526 | 2.725078 | 0.947813 | H | 5.922624 | 1.708984 | -1.773507 |
| H | -7.763318 | 2.657567 | -0.822537 | C | 5.383091 | 2.456425 | -1.187825 |
| H | -8.858137 | 1.586400 | 0.055969 | C | 3.899643 | 2.087870 | -0.968239 |

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| H | 5.923776 | 2.613253 | -0.251251 | H | 5.733026 | -2.370293 | -2.476366 |
| H | 5.429224 | 3.398181 | -1.752875 | H | 6.983517 | -1.542073 | 1.556244 |
| C | 3.234771 | 1.885471 | -2.350745 | H | 4.655359 | -1.858642 | 2.346713 |
| C | 3.209196 | 3.314064 | -0.325932 | C | 7.955675 | -1.776674 | -0.988048 |
| H | 2.177551 | 1.626517 | -2.258940 | H | 8.528696 | -2.693472 | -0.794781 |
| H | 3.303621 | 2.824659 | -2.916741 | H | 8.006478 | -1.577089 | -2.063283 |
| H | 3.714533 | 1.110279 | -2.948904 | H | 8.464535 | -0.959599 | -0.464560 |
| H | 3.275683 | 4.153596 | -1.030991 | N | 1.552653 | -0.893267 | 0.969225 |
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| H | 3.690878 | 3.637275 | 0.599289 | H | 1.298421 | -0.573747 | -1.135876 |
| H | 5.077414 | 2.794422 | 1.829108 | C | 1.693433 | 0.019953 | 2.029140 |
| C | 5.163250 | 1.788735 | 2.247702 | H | 1.981759 | -0.337418 | 3.007520 |
| C | 3.920307 | 0.916679 | 1.971408 | C | 1.321145 | 1.263758 | 1.612014 |
| H | 5.276841 | 1.904571 | 3.334730 | C | 1.363313 | 2.523032 | 2.424222 |
| H | 6.086495 | 1.341298 | 1.871617 | H | 1.577295 | 2.307358 | 3.476574 |
| C | 2.668025 | 1.631388 | 2.533866 | H | 2.144746 | 3.197523 | 2.050989 |
| C | 4.053348 | -0.387351 | 2.791739 | H | 0.412904 | 3.060092 | 2.364860 |
| H | 2.451018 | 2.582825 | 2.045814 | C | 0.899505 | 1.171307 | 0.216312 |
| H | 1.785349 | 0.988905 | 2.453437 | C | 0.924235 | 2.327539 | -0.763714 |
| H | 2.832301 | 1.841154 | 3.599775 | H | 0.577585 | 1.967442 | -1.742919 |
| H | 4.988908 | -0.918196 | 2.601689 | C | 2.282815 | 2.999060 | -0.942098 |
| H | 4.044991 | -0.125258 | 3.858342 | C | 3.477775 | 2.266702 | -1.002421 |
| H | 3.215446 | -1.070341 | 2.615937 | C | 2.351260 | 4.392294 | -1.093662 |
| O | 0.659007 | -2.678967 | 0.446046 | C | 4.703344 | 2.905112 | -1.213421 |
| C | 0.504450 | -3.661460 | -0.530094 | H | 3.456060 | 1.186622 | -0.876225 |
| H | 1.472073 | -3.942922 | -0.996655 | C | 3.573727 | 5.035935 | -1.307632 |
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| C | -0.131522 | -4.915462 | 0.082348 | C | 4.756700 | 4.293616 | -1.368589 |
| H | -1.110409 | -4.679061 | 0.511871 | H | 5.616900 | 2.316428 | -1.254438 |
| H | -0.263273 | -5.694635 | -0.681399 | H | 3.601244 | 6.117122 | -1.420807 |
| H | 0.506353 | -5.313473 | 0.880749 | H | 5.709432 | 4.791486 | -1.530854 |
| | | | | H | 0.180211 | 3.065419 | -0.438972 |
| | | | | Pd | -1.281036 | 0.551499 | 0.112135 |
| TS8 | | | | P | -3.293229 | -0.653288 | -0.410704 |
| S | 2.203176 | -2.460432 | 0.934070 | C | -4.728378 | 0.482270 | -1.087196 |
| O | 1.452898 | -3.166694 | -0.107175 | C | -4.802534 | 1.760584 | -0.220661 |
| O | 2.235174 | -2.903944 | 2.327735 | C | -4.360564 | 0.964232 | -2.509424 |
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| C | 4.184757 | -2.418167 | -0.989225 | H | -5.174216 | 1.568471 | 0.786536 |
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| C | 4.894096 | -1.952139 | 1.292317 | H | -5.075708 | 1.744739 | -2.800869 |
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| H | -6.829108 | 0.548131 | -1.575766 | C | 2.458708 | 0.089528 | -0.591944 |
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| H | -1.724810 | -2.128320 | -3.593293 | H | 5.572594 | 3.360873 | 1.025345 |
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| C | -4.891954 | -2.742529 | 0.951549 | C | 0.290527 | -2.489657 | 0.538359 |
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| H | -5.206712 | -3.137892 | 1.927485 | C | -0.837690 | -2.363294 | 1.308414 |
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| H | -2.101048 | -2.857505 | 1.384316 | H | -2.145880 | -3.753468 | 2.326677 |
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| H | -4.736725 | -1.058451 | 3.111076 | C | -3.544204 | 0.377744 | 0.559143 |
| H | -3.960764 | 0.316627 | 2.314525 | C | -4.337236 | 0.226015 | -0.587422 |
| O | -1.854084 | 2.525608 | 0.616872 | C | -3.284928 | 1.675095 | 1.024023 |
| C | -2.302834 | 2.829921 | 1.899188 | C | -4.855378 | 1.339467 | -1.254632 |
| H | -1.660126 | 2.392609 | 2.692086 | H | -4.549755 | -0.773631 | -0.961332 |
| H | -3.319894 | 2.428937 | 2.095450 | C | -3.801843 | 2.792151 | 0.361992 |
| C | -2.359035 | 4.351249 | 2.103778 | H | -2.673471 | 1.810622 | 1.914173 |
| H | -3.025749 | 4.807911 | 1.362026 | C | -4.589110 | 2.627469 | -0.781334 |
| H | -2.728702 | 4.603414 | 3.108343 | H | -3.593465 | 3.789558 | 0.741783 |
| H | -1.364361 | 4.797865 | 1.977326 | H | -4.994651 | 3.494582 | -1.296495 |
| H | -0.407282 | -0.766034 | -0.277429 | H | -2.876434 | -0.609466 | 2.343079 |
| | | | | H | -5.469030 | 1.200055 | -2.141260 |

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|---|----------|-----------|-----------|--------|-----------|-----------|-----------|
| S | 1.521280 | -1.129241 | -1.513419 | Int 10 | | | |
| O | 0.914256 | -0.467307 | -2.667364 | Pd | -1.345212 | 0.096031 | -0.134759 |
| O | 2.330824 | -2.342034 | -1.631281 | P | -3.513272 | -0.548225 | 0.508168 |

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| C | -3.033924 | -2.581534 | -1.409739 | C | 6.237528 | -0.093169 | 1.716914 |
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| C | -5.161266 | -2.919102 | -0.106152 | C | 4.243673 | -0.428473 | 3.029391 |
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| H | -3.097853 | -3.639328 | -1.699890 | H | 7.230370 | 0.335091 | 1.597701 |
| H | -3.394693 | -3.406591 | 1.927801 | H | 3.672792 | -0.267214 | 3.941079 |
| H | -2.908710 | -4.339498 | 0.515454 | H | 2.717763 | -1.668642 | 2.133446 |
| H | -1.889593 | -3.004795 | 1.068929 | C | 6.124891 | 0.956342 | 4.020343 |
| H | -5.142813 | -3.985509 | -0.369814 | H | 6.846802 | 0.359147 | 4.593511 |
| H | -5.695459 | -2.828874 | 0.843034 | H | 6.661653 | 1.830495 | 3.634375 |
| H | -5.743539 | -2.409161 | -0.876735 | H | 5.359811 | 1.307904 | 4.720383 |
| C | -3.804285 | -0.406911 | 2.435637 | N | 2.797304 | -1.418239 | -1.436584 |
| C | -5.035246 | -1.196298 | 2.938291 | C | 3.296130 | -1.003297 | -2.755380 |
| C | -2.567618 | -0.895424 | 3.227094 | C | 3.873991 | 0.395363 | -2.875953 |
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| H | -5.184371 | -0.966642 | 4.002190 | C | 4.270547 | 0.756833 | -4.287304 |
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| C | -6.297108 | 0.386768 | 0.159953 | C | -0.030834 | 3.464572 | -0.299631 |
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| H | -5.183231 | 2.605089 | -0.874690 | H | -0.760105 | 3.142753 | -1.040487 |
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| H | -6.402687 | 0.786288 | 1.171983 | H | 1.041806 | 6.184930 | 1.455460 |
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| S | 3.737868 | -2.438498 | -0.467583 | C | -1.282884 | 0.890089 | -3.062536 |
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| O | 2.821411 | -3.389112 | 0.178686 | H | -0.186781 | 0.716354 | -3.007040 |
| C | 4.431278 | -1.424160 | 0.845124 | C | -1.534148 | 1.957484 | -4.137643 |

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| H | -1.065440 | 2.907312 | -3.851545 | H | -4.565251 | 1.995817 | -3.611345 |
| H | -1.121925 | 1.646638 | -5.108646 | H | -4.956931 | 0.338892 | -3.167854 |
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| H | 2.457867 | -1.105533 | -3.460200 | H | -3.912108 | 3.327192 | -1.075767 |
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| C | 0.236229 | 3.729047 | 0.804876 | H | -6.380325 | 2.398609 | 1.383045 |
| C | 0.751472 | 5.024524 | 0.750913 | H | -5.643574 | 2.723402 | -0.183239 |
| C | 2.108032 | 5.233070 | 0.483868 | H | -6.550752 | 1.226340 | 0.074985 |
| C | 2.947985 | 4.134291 | 0.273243 | C | -4.980528 | 0.300958 | 2.223715 |
| C | 2.440227 | 2.836670 | 0.328788 | H | -5.369429 | 0.911220 | 3.049938 |
| C | 1.072751 | 2.619841 | 0.596229 | H | -5.771388 | -0.397196 | 1.941150 |
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| H | 4.003135 | 4.285830 | 0.061477 | H | -2.778482 | 1.865475 | 2.163450 |
| H | 3.094395 | 1.986592 | 0.159351 | H | -3.325494 | 3.076431 | 0.993428 |
| C | 0.607062 | 1.247952 | 0.698283 | C | 1.734003 | -1.075480 | 1.348237 |
| C | 0.824602 | 0.025782 | 0.936766 | N | 2.334382 | -1.747715 | 0.174580 |
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| P | -3.547021 | 0.255799 | -0.252286 | S | 3.927578 | -2.291363 | 0.414161 |
| C | -3.444300 | 1.320433 | -1.891885 | C | 1.436102 | -2.637208 | -0.599575 |
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| C | -4.280733 | -2.412440 | 0.473703 | C | 1.665967 | -1.105273 | -2.589385 |
| H | -3.213537 | -2.564605 | 0.661213 | C | 0.546076 | -3.322991 | -2.861901 |
| H | -4.771095 | -2.122643 | 1.403400 | C | 5.976075 | 0.588246 | -1.590823 |
| H | -4.725600 | -3.368317 | 0.162436 | H | 4.715627 | -1.092007 | -2.096821 |
| C | -3.839825 | -2.037442 | -1.919169 | C | 6.334437 | 0.972344 | 0.762272 |
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| C | -2.267905 | 0.783611 | -2.744623 | H | 0.368078 | -2.996219 | -3.891565 |
| H | -2.155813 | 1.428146 | -3.627489 | H | 1.135204 | -4.250267 | -2.892755 |
| H | -1.324999 | 0.804232 | -2.190583 | H | -0.421694 | -3.579139 | -2.408553 |
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| C | -4.723617 | 1.323260 | -2.757059 | H | 6.155630 | 0.855965 | -2.629955 |

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| H | 6.793632 | 1.537462 | 1.570230 | H | -0.410192 | 6.922883 | -1.694559 |
| C | 7.482610 | 2.505834 | -0.901942 | H | -3.735600 | 5.218135 | 0.450020 |
| H | 7.685488 | 3.123964 | -0.021239 | C | -5.673246 | -1.841521 | -1.864291 |
| H | 8.448065 | 2.151073 | -1.286464 | H | -4.928134 | 0.164646 | -1.584307 |
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| H | -0.704521 | -1.704323 | 3.073586 | H | 0.179197 | -2.308121 | 3.065757 |
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| H | -0.244262 | -4.117345 | 2.508109 | H | -1.296674 | -2.287570 | 4.030021 |
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| Int 11 | | | | H | -5.864357 | -4.543251 | -2.874440 |
| Pd | 1.173229 | 0.104588 | -0.436971 | H | -6.804213 | -5.068757 | -1.468658 |
| P | 3.583367 | -0.598363 | -0.019132 | H | 0.929610 | 2.567370 | -0.873263 |
| C | -0.531323 | 1.138917 | -0.507273 | C | 4.750863 | 0.013652 | -1.449776 |
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| N | -2.380748 | 0.248898 | 0.932701 | C | 6.200713 | -0.512887 | -1.408717 |
| H | -2.630380 | 1.283442 | -0.870433 | H | 4.052959 | -1.472500 | -2.945512 |
| H | -1.934308 | -0.346867 | -1.057058 | H | 3.079777 | 0.001980 | -2.875984 |
| C | -0.872832 | 3.702717 | -0.623902 | H | 4.691147 | 0.027997 | -3.616183 |
| S | -4.051959 | 0.318988 | 1.185234 | H | 5.348448 | 1.981333 | -0.621335 |
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| C | -2.130893 | 3.871480 | -0.013680 | H | 6.766100 | -0.065581 | -2.238433 |
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| H | 0.713076 | 4.721092 | -1.681582 | H | 6.082226 | -0.434127 | 1.958045 |
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| C | -5.109455 | -0.802270 | -1.126227 | C | 3.397565 | -0.346157 | 2.831825 |
| C | -5.087968 | -2.229442 | 0.838834 | H | 2.294265 | 1.668942 | 1.436126 |
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| C | -2.156050 | 6.220102 | -0.631755 | H | 3.525303 | 0.302683 | 3.708776 |

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| H | 2.322379 | -0.493443 | 2.692179 | C | 1.247047 | -1.167753 | -1.472792 |
| H | 3.858003 | -1.306045 | 3.074198 | C | 0.686041 | 5.218313 | -1.917329 |
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| H | -0.972994 | -1.292988 | 0.908733 | H | -0.101611 | -2.187599 | -2.820242 |
| O | 0.190048 | -1.568208 | -1.071211 | H | 0.140302 | -3.005507 | -1.194322 |
| C | 0.369811 | -1.938518 | -2.411077 | H | 2.604205 | -1.266536 | -3.112948 |
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| H | 1.273314 | 1.297958 | 1.310332 | H | -2.389667 | -2.623684 | 1.324095 |
| H | 0.549924 | -0.303392 | 1.524589 | H | -3.544340 | -3.054358 | 2.605720 |
| C | 0.841278 | 2.893952 | -1.159751 | H | -2.635626 | 0.282627 | 3.703229 |
| S | 3.481459 | -0.445402 | 1.796217 | H | -2.581405 | -1.456925 | 3.970173 |
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| C | 1.899657 | 3.279301 | -0.307105 | H | -5.146826 | 0.244384 | 3.109504 |
| O | 3.177911 | -1.649986 | 2.587943 | H | -5.775182 | -1.074909 | 2.113784 |
| O | 3.501651 | 0.873985 | 2.444557 | H | -3.905996 | 1.998421 | 3.194728 |
| C | 5.044085 | -0.721525 | 0.958204 | | | | |

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|------|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | -4.040866 | 2.495136 | 2.229954 | H | -1.552331 | -0.553706 | 0.464829 |
| C | -3.018305 | 2.005507 | 1.180432 | S | -4.009873 | -0.156772 | -1.273309 |
| H | -5.080232 | 2.371057 | 1.924330 | C | -1.647737 | 0.803010 | -2.140658 |
| H | -3.874855 | 3.568650 | 2.400430 | O | -4.495335 | -1.462259 | -0.812301 |
| C | -1.611942 | 2.189538 | 1.794873 | O | -4.529204 | 0.471332 | -2.493287 |
| C | -3.054745 | 2.958272 | -0.038182 | C | -0.373677 | 0.341344 | -2.849650 |
| H | -0.837323 | 2.010475 | 1.053489 | C | -0.185744 | -1.072509 | -2.870364 |
| H | -1.512793 | 3.232028 | 2.127519 | C | 0.082026 | 1.245890 | -3.967618 |
| H | -1.420940 | 1.555519 | 2.659823 | H | 0.658676 | -1.470231 | -3.432262 |
| H | -2.740694 | 3.957817 | 0.291454 | H | -1.062726 | -1.713311 | -2.906172 |
| H | -2.357780 | 2.640540 | -0.818925 | H | 0.311747 | 2.251486 | -3.605395 |
| H | -4.046253 | 3.061170 | -0.481430 | H | 0.968940 | 0.857577 | -4.470427 |
| H | -5.732116 | 2.141019 | -0.142717 | H | -0.724980 | 1.310547 | -4.714430 |
| C | -5.988870 | 1.080271 | -0.125814 | O | 2.270975 | 1.701385 | -2.045039 |
| C | -4.841852 | 0.148644 | -0.575147 | C | 3.195395 | 1.363085 | -3.034917 |
| H | -6.826578 | 0.944399 | -0.824117 | H | 2.809994 | 0.606492 | -3.749766 |
| H | -6.360726 | 0.831656 | 0.872693 | H | 4.115080 | 0.907771 | -2.612005 |
| C | -4.381652 | 0.538789 | -2.001697 | C | 3.614634 | 2.606313 | -3.832698 |
| C | -5.439441 | -1.271950 | -0.695223 | H | 4.043613 | 3.361403 | -3.162486 |
| H | -3.933157 | 1.533335 | -2.057624 | H | 4.365951 | 2.351999 | -4.594227 |
| H | -3.666341 | -0.195051 | -2.384541 | H | 2.748860 | 3.057437 | -4.332401 |
| H | -5.257749 | 0.537116 | -2.665841 | H | -2.336001 | 1.227824 | -2.878696 |
| H | -5.917781 | -1.612125 | 0.226835 | H | -1.406539 | 1.598623 | -1.415160 |
| H | -6.223487 | -1.238842 | -1.465440 | H | 1.315265 | -2.883504 | -1.186279 |
| H | -4.677613 | -1.986184 | -1.009853 | C | -0.123645 | -3.952840 | -0.023068 |
| O | -2.694078 | -2.345829 | -1.414072 | C | -1.152223 | -4.014114 | 0.943685 |
| C | -2.391887 | -3.681746 | -1.667318 | C | 0.528226 | -5.165667 | -0.349235 |
| H | -1.945436 | -4.185751 | -0.782784 | C | -1.528777 | -5.228496 | 1.519419 |
| H | -1.658048 | -3.805378 | -2.489685 | H | -1.646647 | -3.111053 | 1.279905 |
| C | -3.656517 | -4.455043 | -2.067310 | C | 0.151892 | -6.377514 | 0.224955 |
| H | -4.117992 | -3.999970 | -2.952306 | H | 1.336593 | -5.146831 | -1.077200 |
| H | -3.412210 | -5.500808 | -2.301654 | C | -0.886579 | -6.417322 | 1.161758 |
| H | -4.396247 | -4.450010 | -1.257765 | H | -2.325909 | -5.242196 | 2.258576 |
| H | 3.075272 | -1.931366 | -0.639113 | H | 0.668991 | -7.291236 | -0.057284 |
| H | 1.635197 | -2.254838 | 0.360238 | H | -1.184230 | -7.359826 | 1.613545 |
| | | | | C | -4.247582 | 1.011100 | 0.075426 |
| | | | | C | -4.299620 | 2.382417 | -0.197851 |
| | | | | C | -4.362878 | 0.540467 | 1.386043 |
| | | | | C | -4.457737 | 3.281829 | 0.856014 |
| | | | | H | -4.241428 | 2.734983 | -1.222611 |
| | | | | C | -4.521719 | 1.456297 | 2.428488 |
| | | | | H | -4.354102 | -0.527084 | 1.581052 |
| | | | | C | -4.571969 | 2.836556 | 2.183502 |
| | | | | H | -4.503532 | 4.347460 | 0.642109 |
| TS11 | | | | | | | |
| Pd | 1.079737 | 0.144434 | -1.257084 | | | | |
| C | -0.226015 | -1.521166 | -0.925057 | | | | |
| C | -1.626755 | -1.123046 | -0.476236 | | | | |
| C | 0.343897 | -2.741464 | -0.710044 | | | | |
| N | -2.344333 | -0.324977 | -1.501023 | | | | |
| H | -2.251623 | -1.999937 | -0.297503 | | | | |

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| H | -4.618870 | 1.088999 | 3.447642 | H | 3.912549 | 2.121325 | -0.741640 |
| C | -4.778499 | 3.821585 | 3.310472 | | | | |
| H | -4.561404 | 3.369456 | 4.283700 | | | | |
| H | -4.138010 | 4.703327 | 3.194041 | TS12 | | | |
| H | -5.817553 | 4.176293 | 3.334996 | Pd | -1.225831 | 0.657618 | 0.408687 |
| P | 2.250262 | 0.576871 | 1.116919 | P | -3.563314 | -0.198964 | 0.012387 |
| C | 1.627187 | 2.325068 | 1.730848 | C | 0.485262 | -0.004831 | 0.050116 |
| C | 1.520677 | 3.273320 | 0.513741 | C | 1.360768 | -0.794778 | 0.961761 |
| C | 0.194467 | 2.200462 | 2.296470 | C | 0.520322 | 0.595349 | -1.199291 |
| C | 2.504348 | 3.001937 | 2.806987 | N | 2.159814 | -1.833890 | 0.266154 |
| H | 2.477199 | 3.484852 | 0.040475 | H | 2.072406 | -0.087325 | 1.410315 |
| H | 0.871747 | 2.866387 | -0.266080 | H | 0.784888 | -1.220987 | 1.793479 |
| H | 1.093444 | 4.225487 | 0.859878 | C | 1.159629 | 1.874747 | -1.552952 |
| H | 0.158972 | 1.699926 | 3.266992 | S | 3.553428 | -2.301449 | 1.149089 |
| H | -0.206472 | 3.212422 | 2.442564 | C | 1.402926 | -2.967696 | -0.307206 |
| H | -0.479774 | 1.681954 | 1.606627 | C | 1.286065 | 2.221542 | -2.912911 |
| H | 2.025842 | 3.946587 | 3.102864 | C | 1.690373 | 2.756287 | -0.589662 |
| H | 2.617499 | 2.398212 | 3.710098 | O | 4.061996 | -3.508892 | 0.486689 |
| H | 3.500513 | 3.253281 | 2.437433 | O | 3.261924 | -2.319005 | 2.592989 |
| H | 1.655301 | 0.576768 | 4.341957 | C | 4.686729 | -0.943972 | 0.846767 |
| C | 2.294069 | -0.237193 | 3.988700 | C | 1.623625 | -3.210404 | -1.789689 |
| C | 1.918269 | -0.698667 | 2.564001 | C | 1.930767 | 3.397581 | -3.298565 |
| H | 3.334022 | 0.079710 | 4.082814 | H | 0.878581 | 1.555074 | -3.670437 |
| H | 2.144844 | -1.080951 | 4.677920 | C | 2.338931 | 3.927186 | -0.975668 |
| C | 0.420069 | -1.076520 | 2.571956 | H | 1.571660 | 2.525304 | 0.465114 |
| C | 2.670875 | -2.015488 | 2.258451 | C | 5.292007 | -0.824186 | -0.409024 |
| H | 0.126592 | -1.503150 | 1.614890 | C | 4.983120 | -0.051902 | 1.876853 |
| H | 0.257866 | -1.844263 | 3.340971 | C | 2.265689 | -2.353065 | -2.590163 |
| H | -0.241501 | -0.242047 | 2.802791 | C | 1.043018 | -4.513173 | -2.282295 |
| H | 2.320161 | -2.787011 | 2.956967 | C | 2.462876 | 4.256253 | -2.331694 |
| H | 2.466259 | -2.377604 | 1.246545 | H | 2.015627 | 3.644550 | -4.354070 |
| H | 3.751348 | -1.932756 | 2.389102 | H | 2.739480 | 4.593845 | -0.215817 |
| H | 4.970592 | -0.345444 | 2.689542 | C | 6.189912 | 0.216247 | -0.629656 |
| C | 5.045564 | 0.605619 | 2.157299 | H | 5.067604 | -1.541075 | -1.192475 |
| C | 4.186207 | 0.662812 | 0.876069 | C | 5.887333 | 0.986927 | 1.635656 |
| H | 6.098866 | 0.726588 | 1.866943 | H | 4.524264 | -0.179848 | 2.852064 |
| H | 4.810189 | 1.411897 | 2.857499 | H | 2.394975 | -2.562202 | -3.649578 |
| C | 4.577380 | -0.522563 | -0.040391 | H | 2.685562 | -1.428852 | -2.206497 |
| C | 4.562379 | 1.958028 | 0.120715 | H | -0.028227 | -4.590353 | -2.047583 |
| H | 4.428843 | -1.496757 | 0.428763 | H | 1.161509 | -4.622033 | -3.364840 |
| H | 4.013689 | -0.504196 | -0.976951 | H | 1.536084 | -5.366446 | -1.795944 |
| H | 5.644132 | -0.438918 | -0.289989 | H | 2.960363 | 5.175795 | -2.629011 |
| H | 4.525967 | 2.839308 | 0.766817 | C | 6.499557 | 1.140409 | 0.384942 |
| H | 5.600044 | 1.862741 | -0.227950 | H | 6.663133 | 0.312641 | -1.604402 |

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| H | 6.121236 | 1.683221 | 2.437485 |
| C | 7.472629 | 2.265698 | 0.122225 |
| H | 8.437592 | 1.881616 | -0.231022 |
| H | 7.091040 | 2.943499 | -0.651996 |
| H | 7.655442 | 2.856927 | 1.025114 |
| H | 0.203932 | 0.004840 | -2.062301 |
| C | -4.492882 | 0.984582 | -1.221602 |
| C | -4.178521 | 2.446035 | -0.819330 |
| C | -3.924358 | 0.807977 | -2.647813 |
| C | -6.023662 | 0.794176 | -1.284849 |
| H | -4.534657 | 2.710276 | 0.174987 |
| H | -3.103590 | 2.645094 | -0.841382 |
| H | -4.667637 | 3.112974 | -1.543147 |
| H | -4.221034 | -0.134951 | -3.113775 |
| H | -4.321501 | 1.615523 | -3.277298 |
| H | -2.832480 | 0.886370 | -2.666919 |
| H | -6.431201 | 1.479893 | -2.041183 |
| H | -6.314291 | -0.219004 | -1.574245 |
| H | -6.515400 | 1.032599 | -0.339283 |
| H | -5.094653 | -1.907082 | -2.278179 |
| C | -4.801501 | -2.491085 | -1.401787 |
| C | -3.486649 | -1.982119 | -0.772327 |
| H | -5.638146 | -2.495894 | -0.699802 |
| H | -4.652592 | -3.525634 | -1.742131 |
| C | -2.385702 | -2.008418 | -1.858991 |
| C | -3.031974 | -2.992160 | 0.306249 |
| H | -1.421336 | -1.689182 | -1.455562 |
| H | -2.277980 | -3.040034 | -2.221049 |
| H | -2.612470 | -1.385719 | -2.724250 |
| H | -2.827645 | -3.954475 | -0.182262 |
| H | -2.109293 | -2.671125 | 0.801260 |
| H | -3.788027 | -3.175692 | 1.071832 |
| H | -5.562286 | -2.266232 | 1.500900 |
| C | -5.805328 | -1.211850 | 1.654398 |
| C | -4.561460 | -0.298699 | 1.682296 |
| H | -6.308185 | -1.138896 | 2.628782 |
| H | -6.531018 | -0.912813 | 0.892438 |
| C | -3.580734 | -0.787621 | 2.777398 |
| C | -5.008515 | 1.115454 | 2.123010 |
| H | -3.187852 | -1.789997 | 2.598441 |
| H | -2.744194 | -0.090621 | 2.881199 |
| H | -4.118442 | -0.816044 | 3.735469 |
| H | -5.806048 | 1.524983 | 1.497796 |
| H | -5.413426 | 1.034176 | 3.141512 |

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| H | -4.159086 | 1.803337 | 2.147048 |
| H | 1.621557 | -3.895124 | 0.237353 |
| H | 0.338085 | -2.762956 | -0.134170 |
| O | -2.027591 | 2.036847 | 1.722359 |
| C | -1.290850 | 3.187735 | 2.027228 |
| H | -1.991791 | 3.953584 | 2.412495 |
| H | -0.823903 | 3.626884 | 1.125274 |
| C | -0.207707 | 2.950874 | 3.087000 |
| H | 0.524585 | 2.213271 | 2.731870 |
| H | 0.326521 | 3.881857 | 3.325959 |
| H | -0.654145 | 2.560697 | 4.009670 |

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|---|-----------|-----------|-----------|
| C | 1.604917 | -1.778105 | 0.837141 |
| C | 2.546549 | -0.704041 | 0.338061 |
| C | 1.845843 | -3.101899 | 0.743555 |
| N | 2.593670 | 0.390296 | 1.322127 |
| H | 3.551735 | -1.110610 | 0.227377 |
| H | 2.216432 | -0.313934 | -0.643908 |
| S | 3.976616 | 1.369471 | 1.294525 |
| C | 1.288296 | 1.067879 | 1.463992 |
| O | 5.122212 | 0.456313 | 1.210484 |
| O | 3.820125 | 2.315357 | 2.404198 |
| C | 0.272325 | 0.095973 | 2.070944 |
| C | 0.342543 | -1.309454 | 1.543330 |
| H | -0.507395 | -1.442408 | 0.734951 |
| H | 0.048742 | -2.035120 | 2.307522 |
| H | 1.415157 | 1.927542 | 2.122327 |
| H | 0.953391 | 1.431655 | 0.479388 |
| H | 1.124312 | -3.763494 | 1.227020 |
| C | 2.972054 | -3.806693 | 0.103420 |
| C | 3.447747 | -4.995429 | 0.691985 |
| C | 3.569636 | -3.380131 | -1.097943 |
| C | 4.506552 | -5.706524 | 0.128196 |
| H | 2.987752 | -5.352093 | 1.611050 |
| C | 4.626418 | -4.094588 | -1.666675 |
| H | 3.185763 | -2.502577 | -1.609661 |
| C | 5.104535 | -5.255830 | -1.053532 |
| H | 4.864313 | -6.613291 | 0.609280 |
| H | 5.070398 | -3.747407 | -2.596347 |
| H | 5.927877 | -5.809799 | -1.496675 |
| C | 3.929939 | 2.316687 | -0.235988 |
| C | 3.235318 | 3.531107 | -0.278257 |

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|----|-----------|-----------|-----------|--------|-----------|-----------|-----------|
| C | 4.570289 | 1.821720 | -1.374631 | H | -1.962337 | -3.125924 | -1.003126 |
| C | 3.178753 | 4.242229 | -1.475944 | H | -4.942364 | -3.561218 | 1.023162 |
| H | 2.766909 | 3.920917 | 0.619683 | H | -4.318411 | -2.065089 | 1.730542 |
| C | 4.504243 | 2.549383 | -2.565532 | H | -5.804610 | -2.047840 | 0.759465 |
| H | 5.133498 | 0.895535 | -1.319331 | H | -6.631006 | -0.751302 | -0.611126 |
| C | 3.809139 | 3.765147 | -2.637675 | C | -6.263551 | 0.199116 | -1.006970 |
| H | 2.642809 | 5.188463 | -1.506469 | C | -4.968805 | 0.679018 | -0.318015 |
| H | 5.011336 | 2.168762 | -3.449244 | H | -7.049143 | 0.945470 | -0.823169 |
| C | 3.751978 | 4.559073 | -3.922160 | H | -6.158285 | 0.100024 | -2.091002 |
| H | 4.204200 | 4.009418 | -4.753926 | C | -5.208488 | 0.790077 | 1.208696 |
| H | 2.717253 | 4.797663 | -4.196976 | C | -4.661510 | 2.116009 | -0.800913 |
| H | 4.287248 | 5.512000 | -3.821116 | H | -5.494435 | -0.153888 | 1.674862 |
| Pd | -1.502638 | 0.121238 | 0.972262 | H | -4.317073 | 1.184709 | 1.704185 |
| O | -2.198419 | 2.022386 | 1.276858 | H | -6.034922 | 1.495618 | 1.374925 |
| C | -1.773875 | 2.849739 | 2.320282 | H | -4.606850 | 2.195810 | -1.889756 |
| H | -0.679768 | 3.016579 | 2.304347 | H | -5.487806 | 2.763727 | -0.476347 |
| H | -2.011496 | 2.419287 | 3.312392 | H | -3.741978 | 2.495812 | -0.347665 |
| C | -2.466469 | 4.213711 | 2.206500 | C | 0.139947 | 0.211520 | 3.579578 |
| H | -3.555505 | 4.101112 | 2.266096 | H | -0.167939 | 1.217533 | 3.878650 |
| H | -2.142137 | 4.882148 | 3.016295 | H | -0.594010 | -0.499885 | 3.975665 |
| H | -2.224949 | 4.687498 | 1.247186 | H | 1.107319 | 0.006031 | 4.065955 |
| P | -3.400413 | -0.439127 | -0.591670 | | | | |
| C | -2.730164 | -0.153524 | -2.398921 | | | | |
| C | -1.910974 | 1.161349 | -2.391941 | Int 13 | | | |
| C | -1.727265 | -1.270493 | -2.767602 | Pd | 1.108280 | -0.574651 | 1.094453 |
| C | -3.794714 | -0.075972 | -3.513519 | P | 2.753702 | -0.919931 | -0.881362 |
| H | -2.513347 | 2.047099 | -2.193252 | C | -0.819353 | 1.613213 | 1.100682 |
| H | -1.116565 | 1.131730 | -1.638886 | C | -1.718413 | 1.896709 | -0.082749 |
| H | -1.444891 | 1.288106 | -3.379315 | C | 0.301591 | 2.276539 | 1.480861 |
| H | -2.202783 | -2.240166 | -2.932597 | N | -2.789991 | 0.871572 | 0.033130 |
| H | -1.230061 | -0.992881 | -3.706863 | H | -2.170330 | 2.894331 | -0.045733 |
| H | -0.945429 | -1.387731 | -2.009398 | H | -1.172241 | 1.817580 | -1.031953 |
| H | -3.286988 | 0.046260 | -4.480955 | C | 0.943998 | 3.485442 | 0.941248 |
| H | -4.406460 | -0.979478 | -3.578927 | S | -3.543945 | 0.470865 | -1.427088 |
| H | -4.463109 | 0.779765 | -3.393479 | C | -2.303116 | -0.240399 | 0.879263 |
| H | -4.129961 | -2.940037 | -2.534944 | C | 0.504905 | 4.207384 | -0.188333 |
| C | -4.738646 | -2.873610 | -1.629400 | C | 2.069565 | 3.980790 | 1.634636 |
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| H | -5.632797 | -2.291403 | -1.863216 | O | -3.773202 | 1.752657 | -2.110444 |
| H | -5.065880 | -3.894948 | -1.388234 | C | -5.108949 | -0.201395 | -0.866042 |
| C | -2.698145 | -3.184030 | -0.200576 | C | -1.437002 | 0.478378 | 1.936425 |
| C | -4.808291 | -2.485278 | 0.845871 | C | 1.163691 | 5.367776 | -0.598150 |
| H | -2.202108 | -2.923020 | 0.739358 | H | -0.352805 | 3.874861 | -0.759449 |
| H | -3.015667 | -4.233069 | -0.123214 | C | 2.728018 | 5.139013 | 1.225357 |

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|---|-----------|-----------|-----------|--------|-----------|-----------|-----------|
| H | 2.426379 | 3.443084 | 2.510439 | C | 1.500589 | 1.225394 | -2.228223 |
| C | -5.356649 | -1.567635 | -0.992545 | C | 3.732411 | 1.735453 | -1.319439 |
| C | -6.075419 | 0.661954 | -0.338251 | H | 1.048841 | 1.460941 | -1.260888 |
| C | -0.360030 | -0.434828 | 2.511657 | H | 1.578030 | 2.164140 | -2.793350 |
| C | -2.338647 | 1.077254 | 3.046485 | H | 0.821391 | 0.570224 | -2.772978 |
| C | 2.276944 | 5.840613 | 0.102888 | H | 3.649557 | 2.664515 | -1.899011 |
| H | 0.801428 | 5.905286 | -1.470906 | H | 3.345627 | 1.945861 | -0.317880 |
| H | 3.591111 | 5.494320 | 1.782618 | H | 4.795749 | 1.499364 | -1.241327 |
| C | -6.589760 | -2.075492 | -0.572392 | H | 5.852653 | -0.206616 | -1.545673 |
| H | -4.599115 | -2.216454 | -1.420138 | C | 5.688117 | -1.230083 | -1.199649 |
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| H | -5.871821 | 1.725428 | -0.261799 | H | 6.614051 | -1.553060 | -0.702555 |
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| H | -1.743686 | 1.689279 | 3.732826 | H | 4.849712 | 0.641720 | 0.736959 |
| H | -3.134955 | 1.703426 | 2.625820 | H | 4.013739 | -0.526171 | 1.773600 |
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| C | -7.574931 | -1.237111 | -0.034065 | H | 4.513019 | -3.550720 | -0.401285 |
| H | -6.786035 | -3.140514 | -0.670395 | H | 5.458495 | -2.925113 | 0.945848 |
| H | -8.051933 | 0.806025 | 0.484555 | H | 3.683048 | -2.944380 | 1.055081 |
| C | -8.910925 | -1.784735 | 0.410986 | O | 1.671539 | -2.336535 | 1.935765 |
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| H | -8.949226 | -2.874565 | 0.316730 | H | 1.083604 | -2.040275 | 3.919798 |
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| H | 0.767659 | 1.921078 | 2.398669 | C | 2.176925 | -3.877490 | 3.690389 |
| C | 2.122517 | -2.413668 | -1.963499 | H | 3.036258 | -4.283092 | 3.143976 |
| C | 1.605268 | -3.521852 | -1.014157 | H | 2.378855 | -3.966148 | 4.766904 |
| C | 0.898603 | -1.971667 | -2.798337 | H | 1.299851 | -4.488623 | 3.447128 |
| C | 3.164854 | -3.028018 | -2.922411 | H | -3.151518 | -0.771646 | 1.321574 |
| H | 2.389878 | -3.980104 | -0.413770 | H | -1.694484 | -0.951926 | 0.304196 |
| H | 0.849609 | -3.145782 | -0.319949 | | | | |
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| H | 1.156838 | -1.295575 | -3.616846 | Int 14 | | | |
| H | 0.453877 | -2.866310 | -3.254074 | Pd | 1.054425 | 0.099252 | -0.522171 |
| H | 0.119070 | -1.504154 | -2.188354 | P | 3.238772 | -1.097882 | 0.039108 |
| H | 2.678720 | -3.823089 | -3.505619 | C | -0.661970 | 1.132049 | -0.497990 |
| H | 3.569998 | -2.304569 | -3.634342 | C | -1.990938 | 0.392977 | -0.494602 |
| H | 4.001469 | -3.489032 | -2.391723 | C | -0.610967 | 2.466008 | -0.308634 |
| H | 2.932848 | -0.250171 | -4.059068 | N | -2.638449 | 0.312893 | 0.841113 |
| C | 3.544996 | 0.399708 | -3.428907 | H | -2.676658 | 0.912110 | -1.170018 |
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| H | 4.549996 | -0.026337 | -3.374353 | C | 0.563429 | 3.357816 | -0.368894 |
| H | 3.626058 | 1.365291 | -3.948494 | S | -4.138451 | 1.044573 | 1.027543 |

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|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | -2.341536 | -0.853959 | 1.683721 | H | 5.862559 | 1.166834 | -1.605484 |
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| C | 1.656241 | 3.124556 | -1.228178 | H | 6.778033 | -1.079187 | -1.637546 |
| O | -4.056347 | 2.344372 | 0.346601 | H | 6.395596 | -1.516149 | 0.030642 |
| O | -4.480181 | 0.937726 | 2.450612 | H | 5.815722 | -2.517692 | -1.308862 |
| C | -5.350639 | 0.061068 | 0.125350 | H | 5.808800 | -0.181184 | 1.777534 |
| C | -1.512659 | -0.590069 | 2.928476 | C | 5.066740 | -0.741340 | 2.351231 |
| C | 1.669393 | 5.404372 | 0.379925 | C | 3.624627 | -0.514320 | 1.853261 |
| H | -0.256483 | 4.735808 | 1.074804 | H | 5.351444 | -1.797158 | 2.335131 |
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| H | 1.627724 | 2.265882 | -1.896792 | C | 3.283934 | 0.995244 | 1.922529 |
| C | -5.601821 | 0.328576 | -1.225231 | C | 2.661140 | -1.202523 | 2.846862 |
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| C | -1.033702 | 0.613374 | 3.256867 | H | 3.404616 | 1.341822 | 2.958039 |
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| C | 2.754707 | 5.148844 | -0.465730 | H | 2.784274 | -0.725138 | 3.828459 |
| H | 1.662843 | 6.295337 | 1.003311 | H | 1.613113 | -1.079938 | 2.557648 |
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| H | -1.224984 | 1.484596 | 2.639622 | C | 1.627407 | -3.371414 | 0.549858 |
| H | -0.813173 | -2.625337 | 3.205634 | C | 3.074087 | -3.539615 | -1.437424 |
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| C | 4.735451 | -0.603473 | -1.102893 | H | 1.358522 | -1.105623 | -3.358278 |
| C | 4.232737 | -0.624708 | -2.567266 | C | -0.542484 | -0.148175 | -3.740267 |
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| H | 5.041801 | -0.274394 | -3.223051 | | | | |
| H | 5.646118 | 0.996664 | 0.132963 | | | | |

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|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Pd | -1.022649 | 0.103726 | -0.943051 | H | 9.045045 | 1.621815 | -0.967961 |
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| C | 0.477562 | 0.653394 | 0.512199 | C | -2.914100 | -2.848449 | 0.371694 |
| C | 1.292616 | -0.484326 | 1.108803 | C | -2.547230 | -3.181504 | -1.093249 |
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| C | 1.443495 | 0.837760 | -1.287297 | C | -3.900489 | -1.347790 | 3.358900 |
| C | -0.392896 | 5.458768 | 1.569092 | C | -2.933452 | -0.510682 | 2.492047 |
| H | 0.774710 | 4.009081 | 2.645801 | H | -4.936725 | -1.313629 | 3.021794 |
| C | -1.606528 | 4.622885 | -0.347277 | H | -3.876329 | -0.951997 | 4.384445 |
| H | -1.433662 | 2.510009 | -0.732028 | C | -1.515406 | -0.713309 | 3.072899 |
| C | 5.926517 | -1.599106 | -0.730225 | C | -3.248065 | 0.990618 | 2.694111 |
| C | 5.803413 | 0.019676 | 1.080783 | H | -0.799343 | -0.048250 | 2.596027 |
| C | 0.454558 | 0.704746 | -2.310562 | H | -1.541715 | -0.459848 | 4.142054 |
| C | 2.148658 | 2.175897 | -1.157829 | H | -1.147462 | -1.735480 | 2.994395 |
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| H | -0.115840 | 6.276642 | 2.229406 | H | -2.601839 | 1.628825 | 2.083921 |
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| C | 7.171738 | -1.078119 | -1.095603 | H | -5.795706 | 0.195034 | 1.724506 |
| H | 5.488809 | -2.434636 | -1.267108 | C | -5.867121 | -0.390231 | 0.805391 |
| C | 7.043794 | 0.525632 | 0.701780 | C | -4.644428 | -0.238695 | -0.125562 |
| H | 5.271775 | 0.430854 | 1.933141 | H | -6.750944 | -0.025531 | 0.263383 |
| H | 0.136528 | 1.613899 | -2.817777 | H | -6.062970 | -1.432309 | 1.073335 |
| H | 0.460484 | -0.189564 | -2.933073 | C | -4.439743 | 1.259222 | -0.456094 |
| H | 2.806691 | 2.288835 | -2.032046 | C | -5.001086 | -0.926339 | -1.463224 |
| H | 1.443956 | 3.010068 | -1.165957 | H | -4.163632 | 1.866156 | 0.408083 |
| H | 2.757512 | 2.230424 | -0.252260 | H | -3.670336 | 1.378712 | -1.223605 |
| H | -1.643857 | 6.684200 | 0.301767 | H | -5.380687 | 1.663178 | -0.855458 |
| C | 7.747985 | -0.012921 | -0.391045 | H | -5.338203 | -1.957727 | -1.333546 |
| H | 7.702618 | -1.513943 | -1.938591 | H | -5.838406 | -0.372979 | -1.912204 |
| H | 7.478566 | 1.347714 | 1.266303 | H | -4.153902 | -0.899496 | -2.151126 |
| C | 9.098511 | 0.542558 | -0.778687 | O | -2.169510 | -0.467141 | -2.595750 |
| H | 9.832096 | 0.391295 | 0.023472 | C | -2.342375 | 0.347598 | -3.714778 |
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| H | -2.982402 | 1.230418 | -3.494533 | H | -2.979842 | -1.694315 | 0.286214 |
| C | -2.990608 | -0.448392 | -4.857080 | C | -4.140846 | -4.057313 | -2.563913 |
| H | -3.975232 | -0.830902 | -4.563481 | H | -2.123419 | -3.922746 | -3.297352 |
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| H | -2.361422 | -1.306108 | -5.124670 | H | -5.308416 | -2.504934 | 0.230370 |
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| | | | | C | 4.579854 | -0.763203 | -0.297961 |
| | | | | C | 5.133148 | -0.084589 | 0.793421 |
| TS14 | | | | C | 4.655748 | -0.225497 | -1.585435 |
| Pd | -0.852186 | -0.368361 | 0.947444 | C | 5.755766 | 1.145899 | 0.586132 |
| C | -0.205304 | -1.765510 | -0.530693 | H | 5.096456 | -0.526979 | 1.783767 |
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| C | -0.954986 | -2.362415 | -1.499079 | H | 4.250168 | -0.776261 | -2.428045 |
| N | 2.129678 | -1.999774 | 0.318023 | C | 5.843123 | 1.711574 | -0.696726 |
| H | 1.603238 | -2.064296 | -1.698227 | H | 6.190316 | 1.670559 | 1.434252 |
| H | 1.454504 | -0.452036 | -0.964867 | H | 5.349677 | 1.422087 | -2.776908 |
| S | 3.745988 | -2.336529 | -0.037549 | C | 6.552322 | 3.028584 | -0.910205 |
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| O | 3.742392 | -3.047983 | -1.320733 | H | 6.296863 | 3.752425 | -0.127813 |
| O | 4.311579 | -2.937937 | 1.175478 | H | 7.642082 | 2.895025 | -0.885244 |
| C | 0.397426 | -1.745055 | 2.071605 | P | -1.434288 | 1.850936 | -0.496091 |
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| C | 0.153404 | -1.678882 | 3.558206 | C | 0.304847 | 3.008327 | 1.451294 |
| H | -1.258932 | -3.027665 | 1.521730 | C | 1.246389 | 2.852424 | -0.823845 |
| H | 0.322566 | -3.430063 | 0.722766 | C | -0.421620 | 4.635670 | -0.317880 |
| H | 0.342275 | -0.676667 | 3.952190 | H | -0.521500 | 3.229069 | 2.123609 |
| H | -0.870995 | -1.955510 | 3.814018 | H | 0.635781 | 1.993699 | 1.688774 |
| H | 0.827059 | -2.392982 | 4.057571 | H | 1.126410 | 3.702584 | 1.679176 |
| O | -1.378023 | 0.698993 | 2.688466 | H | 1.177122 | 3.092145 | -1.887395 |
| C | -2.476217 | 0.242562 | 3.419912 | H | 2.051235 | 3.472394 | -0.406850 |
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| H | -3.440999 | 0.536929 | 2.956387 | H | 0.447865 | 5.262098 | -0.072161 |
| C | -2.450269 | 0.811957 | 4.845645 | H | -0.675098 | 4.827987 | -1.362763 |
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| H | 0.657507 | 1.310881 | -2.759788 | C | 1.385450 | 6.993765 | -0.408704 |
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| C | -4.140000 | 1.375415 | 0.166005 | C | -5.158009 | -2.003242 | -2.458353 |
| C | -3.032594 | 3.137092 | 1.516420 | H | -5.317003 | 0.109535 | -2.020753 |
| H | -4.331825 | 0.901884 | -0.797793 | C | -4.880415 | -3.285869 | -1.963933 |
| H | -3.774594 | 0.610604 | 0.855203 | H | -4.304776 | -4.401458 | -0.206200 |
| H | -5.102448 | 1.739207 | 0.551831 | H | -5.455214 | -1.882011 | -3.497521 |
| H | -2.536344 | 4.110938 | 1.536209 | C | -4.990057 | -4.506138 | -2.848496 |
| H | -4.045934 | 3.289242 | 1.913373 | H | -5.178064 | -4.230264 | -3.891101 |
| H | -2.495595 | 2.449581 | 2.173865 | H | -4.071505 | -5.104735 | -2.816997 |
| | | | | H | -5.811257 | -5.157249 | -2.522058 |
| | | | | Pd | 1.000090 | -0.211701 | 0.873859 |
| Int 15 | | | | O | 0.928647 | -1.877089 | 2.061579 |
| C | -1.341222 | 2.454677 | -0.339768 | C | 0.307123 | -1.931586 | 3.312877 |
| C | -2.514479 | 1.537366 | -0.600478 | H | -0.774470 | -1.707179 | 3.254025 |
| C | -1.393073 | 3.731033 | -0.773936 | H | 0.742001 | -1.202682 | 4.023202 |
| N | -2.951850 | 0.946598 | 0.676353 | C | 0.469499 | -3.339779 | 3.899538 |
| H | -3.342954 | 2.098727 | -1.033333 | H | 1.529834 | -3.589105 | 4.023872 |
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| S | -4.557765 | 0.415657 | 0.760966 | H | 0.019344 | -4.086375 | 3.234089 |
| C | -1.915102 | 0.056339 | 1.241571 | P | 2.954662 | -1.125097 | -0.461521 |
| O | -5.369344 | 1.482473 | 0.161492 | C | 2.198167 | -1.874019 | -2.094828 |
| O | -4.762521 | -0.028452 | 2.143489 | C | 0.915656 | -2.650168 | -1.703358 |
| C | -0.646952 | 0.856335 | 1.563944 | C | 1.728303 | -0.733205 | -3.025969 |
| C | -0.232993 | 1.875021 | 0.518774 | C | 3.120984 | -2.807840 | -2.905836 |
| H | 0.517400 | 1.365528 | -0.206712 | H | 1.109138 | -3.522464 | -1.079866 |
| H | 0.346736 | 2.678600 | 0.978372 | H | 0.212389 | -2.009748 | -1.160714 |
| H | -2.307501 | -0.394525 | 2.153402 | H | 0.423205 | -2.998459 | -2.622178 |
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| H | -2.324394 | 4.037189 | -1.252312 | H | 1.148240 | -1.173647 | -3.848090 |
| C | -0.404503 | 4.818530 | -0.646914 | H | 1.070481 | -0.026072 | -2.509169 |
| C | 0.986276 | 4.625356 | -0.739459 | H | 2.591995 | -3.127300 | -3.815094 |
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| C | 0.004676 | 7.206831 | -0.335982 | C | 5.142653 | -0.041277 | -2.148708 |
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| H | 5.734023 | -0.946724 | -1.993454 | O | -3.540778 | -2.006030 | -2.069648 |
| H | 5.847480 | 0.791388 | -2.284196 | C | -5.321479 | -1.105253 | -0.292126 |
| C | 3.416256 | 1.561815 | -1.273323 | C | -1.544513 | 1.339085 | 0.825975 |
| C | 5.098488 | 0.641841 | 0.261109 | C | 1.699364 | 5.010063 | 0.138469 |
| H | 2.854710 | 1.892785 | -0.393791 | H | 1.728121 | 3.034630 | 0.996123 |
| H | 4.121482 | 2.362377 | -1.536349 | C | 0.607763 | 5.219445 | -2.002335 |
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| H | 5.656960 | 1.557083 | 0.021245 | C | -5.970042 | -1.514069 | 0.872530 |
| H | 4.499532 | 0.847175 | 1.154508 | C | -5.955538 | -0.266273 | -1.215145 |
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| C | -0.601908 | 1.380642 | 2.988617 | H | 1.541475 | 6.865030 | -0.956938 |
| H | -0.692938 | 0.571997 | 3.718763 | C | -7.928552 | -0.216469 | 0.217629 |
| H | 0.331304 | 1.919058 | 3.190167 | H | -7.779129 | -1.381405 | 2.026178 |
| H | -1.437447 | 2.077158 | 3.165469 | H | -7.747455 | 0.823956 | -1.667930 |
| | | | | C | -9.337331 | 0.262633 | 0.479653 |
| | | | | H | -10.029609 | -0.109476 | -0.286368 |
| Int 16 | | | | H | -9.702116 | -0.077862 | 1.453870 |
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| P | 2.996758 | -1.115835 | -0.486318 | H | 0.677068 | 1.165167 | -1.921138 |
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| S | -3.664727 | -1.700326 | -0.636962 | H | 1.984396 | -3.854258 | -1.830515 |
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| O | -3.343135 | -2.732084 | 0.363797 | H | 4.487328 | -3.851677 | -1.190146 |

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| H | 5.032428 | -1.989517 | -2.810894 | C | 1.543343 | -2.268389 | 0.788356 |
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| C | 4.710929 | -0.439111 | 0.168735 | C | 2.137907 | 1.271128 | 1.247039 |
| H | 6.848298 | -0.444683 | -0.122630 | C | 0.243197 | -3.338904 | 2.616304 |
| H | 6.084497 | -1.915784 | -0.728497 | C | -5.492682 | 0.658652 | 0.128153 |
| C | 4.602225 | 1.104601 | 0.216280 | H | -5.791102 | -1.368058 | 0.806737 |
| C | 4.935549 | -0.891028 | 1.630072 | H | -4.907481 | 2.570194 | -0.689873 |
| H | 4.430687 | 1.564599 | -0.758548 | C | 1.040249 | 3.127530 | -0.528917 |
| H | 3.796442 | 1.416041 | 0.887681 | H | 1.637799 | 1.753592 | -2.091963 |
| H | 5.543935 | 1.511899 | 0.610302 | C | 1.569045 | 2.450607 | 1.723127 |
| H | 5.196644 | -1.949215 | 1.710075 | H | 2.590303 | 0.560789 | 1.931236 |
| H | 5.784667 | -0.321683 | 2.034213 | H | 1.223591 | -3.465873 | 3.087829 |
| H | 4.055197 | -0.688336 | 2.244123 | H | -0.399725 | -2.780349 | 3.311471 |
| O | 1.964143 | -0.191386 | 2.533790 | H | -0.205752 | -4.336808 | 2.504173 |
| C | 2.086065 | 0.645417 | 3.651575 | H | -6.469719 | 1.002387 | 0.457677 |
| H | 1.156839 | 1.197038 | 3.877108 | C | 1.008571 | 3.395810 | 0.846756 |
| H | 2.869412 | 1.415634 | 3.493534 | H | 0.629648 | 3.854188 | -1.226336 |
| C | 2.454103 | -0.185152 | 4.887196 | H | 1.568729 | 2.645933 | 2.793362 |
| H | 3.400328 | -0.717689 | 4.734474 | C | 0.393005 | 4.667432 | 1.382494 |
| H | 2.560725 | 0.459703 | 5.770924 | H | 0.114252 | 5.349874 | 0.573168 |
| H | 1.675770 | -0.930476 | 5.090391 | H | -0.512160 | 4.452394 | 1.965175 |
| H | -3.472433 | 0.447188 | 1.445397 | H | 1.087002 | 5.196828 | 2.046598 |
| H | -2.073044 | -0.650244 | 1.600221 | H | -1.283811 | -0.103919 | -2.096454 |
| | | | | C | -0.949992 | -2.366972 | 0.557069 |
| | | | | H | -1.434644 | -3.333078 | 0.327272 |
| 6a-E | | | | H | -1.639075 | -1.850972 | 1.238218 |
| C | -0.761877 | -1.558983 | -0.706654 | H | 2.472534 | -2.419316 | 1.327657 |
| C | 0.541622 | -1.851694 | -1.415667 | | | | |
| C | -1.617292 | -0.647692 | -1.211225 | 6a-Z | | | |
| N | 1.703298 | -1.739273 | -0.511504 | C | 0.095216 | -2.023159 | -0.86524200 |

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| C | -0.299899 | -2.012573 | 0.59479600 | | | | |
| C | 1.294405 | -1.650856 | -1.35451600 | 4a | | | |
| N | -1.583769 | -1.307987 | 0.80043600 | C | 1.267793 | -1.066291 | -0.419811 |
| H | -0.446180 | -3.041342 | 0.95727200 | C | 0.385791 | 0.079624 | 0.048599 |
| H | 0.446735 | -1.545488 | 1.23356700 | C | 2.619361 | -1.164951 | -0.393497 |
| C | 2.515415 | -1.233129 | -0.63590900 | H | 0.489355 | 0.270020 | 1.120824 |
| S | -1.623795 | 0.094537 | 1.75992600 | H | 0.626863 | 1.011187 | -0.475704 |
| C | -2.600757 | -1.492179 | -0.16079000 | C | 3.647292 | -0.233757 | 0.080153 |
| C | 3.327164 | -0.232372 | -1.20681400 | C | -0.903636 | -1.732628 | -0.891756 |
| C | 2.945912 | -1.820125 | 0.56933700 | C | 4.997998 | -0.597433 | -0.119518 |
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| C | -1.060355 | 1.467807 | 0.74830800 | C | 6.046603 | 0.222499 | 0.291711 |
| C | -2.392525 | -2.091172 | -1.34583400 | H | 5.219787 | -1.543282 | -0.609469 |
| C | 4.497867 | 0.194783 | -0.58000500 | C | 4.448999 | 1.818596 | 1.137278 |
| H | 3.025004 | 0.218887 | -2.14955500 | H | 2.383772 | 1.321443 | 0.916853 |
| C | 4.117927 | -1.393489 | 1.19885600 | C | 0.882851 | -3.406812 | -1.537327 |
| H | 2.381372 | -2.640690 | 1.00193400 | C | 5.777682 | 1.440310 | 0.923980 |
| C | 0.286123 | 1.837573 | 0.77294600 | H | 7.073944 | -0.089346 | 0.119915 |
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| C | -3.530843 | -2.404162 | -2.28014100 | H | 6.591402 | 2.083659 | 1.248456 |
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| H | 5.102928 | 0.972893 | -1.03915200 | H | -1.753256 | -2.304785 | -1.247039 |
| H | 4.428687 | -1.863950 | 2.12827200 | H | 1.553832 | -3.232509 | -2.388345 |
| C | 0.715646 | 2.892049 | -0.03510300 | H | 1.447635 | -3.981865 | -0.792146 |
| H | 0.982285 | 1.319923 | 1.42445300 | C | -1.078585 | -0.371581 | -0.251248 |
| C | -1.525559 | 3.187375 | -0.87257400 | C | -1.905627 | -0.512943 | 1.043138 |
| H | -3.021924 | 1.855847 | -0.06359000 | C | -1.788210 | 0.611801 | -1.194885 |
| H | -4.489035 | -2.052264 | -1.88281400 | O | -1.478947 | -0.393392 | 2.171258 |
| H | -3.377729 | -1.936767 | -3.26347300 | O | -2.060377 | 0.395580 | -2.355638 |
| H | -3.618723 | -3.486514 | -2.45596700 | O | -3.180436 | -0.838425 | 0.751911 |
| H | 5.809151 | -0.051772 | 1.12107200 | O | -2.039608 | 1.778952 | -0.565580 |
| C | -0.177355 | 3.582451 | -0.86753200 | C | -4.074287 | -1.042919 | 1.877485 |
| H | 1.763156 | 3.182934 | -0.01176800 | H | -3.663254 | -1.841469 | 2.503119 |
| H | -2.236410 | 3.713489 | -1.50618300 | H | -4.095075 | -0.123897 | 2.471669 |
| C | 0.286980 | 4.744360 | -1.71482500 | C | -5.439751 | -1.397078 | 1.319680 |
| H | 1.374740 | 4.739879 | -1.84020800 | H | -6.142493 | -1.558418 | 2.145495 |
| H | -0.170829 | 4.722595 | -2.71054600 | H | -5.829337 | -0.591005 | 0.688809 |
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| H | -3.354659 | 4.829246 | -1.013951 | H | 5.781567 | -2.743339 | 1.922236 |
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| | | | | H | 4.276770 | -1.413473 | 4.270894 |
| TS15 | | | | H | 5.630452 | -2.552552 | 4.431283 |
| C | 1.132906 | 0.471932 | -0.778240 | H | 5.897388 | -0.951689 | 3.707682 |
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| H | 2.421405 | 1.079045 | 0.889180 | Pd | -1.029503 | -0.101251 | -0.376583 |
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| C | 0.506489 | 2.827342 | 0.060672 | C | -4.150570 | -1.949434 | -0.636888 |
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| C | 0.404746 | 2.703397 | 1.455930 | C | -5.682878 | -2.000148 | -0.817108 |
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| C | 0.928538 | 5.210336 | 0.347571 | H | -2.376042 | -2.364744 | -1.837909 |
| H | 0.839074 | 4.214265 | -1.559243 | H | -3.834350 | -3.246170 | -2.336345 |
| C | 0.573377 | 3.813491 | 2.284873 | H | -4.280318 | -3.044162 | 1.285555 |
| H | 0.175857 | 1.733937 | 1.889960 | H | -4.023375 | -4.038965 | -0.143342 |
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| C | 0.837696 | 5.072247 | 1.734933 | H | -5.954596 | -3.023533 | -1.110762 |
| H | 1.131573 | 6.183097 | -0.093150 | H | -6.225780 | -1.775295 | 0.105779 |
| H | 0.491786 | 3.695744 | 3.362644 | H | -6.050930 | -1.337215 | -1.603845 |
| H | 0.966757 | 5.936272 | 2.381555 | H | -5.316778 | -1.601661 | 2.221718 |
| H | 0.147419 | 1.984373 | -1.897159 | C | -5.128235 | -0.540740 | 2.398077 |
| H | 3.400825 | -1.377145 | -2.463517 | C | -3.734518 | -0.093084 | 1.906205 |
| H | -0.098924 | -0.905664 | -3.115339 | H | -5.942058 | 0.030154 | 1.944193 |
| H | 0.583128 | 0.628895 | -3.667694 | H | -5.183744 | -0.380184 | 3.484024 |
| C | 3.364272 | -0.447095 | -0.382847 | C | -2.650878 | -0.933929 | 2.624396 |
| C | 4.481262 | 0.604683 | -0.573882 | C | -3.514731 | 1.368403 | 2.357157 |
| C | 3.951415 | -1.658029 | 0.350965 | H | -1.644643 | -0.609445 | 2.341388 |
| O | 4.359572 | 1.796968 | -0.389571 | H | -2.767911 | -0.796690 | 3.708612 |
| O | 4.091173 | -2.766793 | -0.116914 | H | -2.717707 | -1.999914 | 2.411024 |
| O | 5.608509 | 0.027349 | -1.033876 | H | -3.496290 | 1.390177 | 3.455230 |
| O | 4.303720 | -1.321468 | 1.610781 | H | -2.559581 | 1.770850 | 2.005383 |
| C | 6.722792 | 0.910103 | -1.322163 | H | -4.317685 | 2.037983 | 2.038612 |
| H | 6.400241 | 1.638260 | -2.073430 | H | -5.901344 | 1.777872 | 0.609677 |
| H | 6.976089 | 1.457084 | -0.408404 | C | -5.869229 | 1.377585 | -0.407335 |
| C | 7.872207 | 0.050173 | -1.814011 | C | -4.419675 | 1.184011 | -0.909331 |
| H | 8.734736 | 0.686681 | -2.044400 | H | -6.370247 | 2.110727 | -1.054708 |
| H | 8.174133 | -0.676883 | -1.052566 | H | -6.462731 | 0.462637 | -0.432237 |
| H | 7.594764 | -0.496549 | -2.721544 | C | -3.692700 | 2.543061 | -0.763400 |
| C | 4.881537 | -2.373496 | 2.424238 | C | -4.449101 | 0.903451 | -2.429848 |
| | | | | H | -3.506945 | 2.843073 | 0.267269 |

| | | | | | | | |
|--------|-----------|-----------|-----------|----|-----------|-----------|-----------|
| H | -2.736581 | 2.545650 | -1.292425 | O | -4.352518 | 2.167263 | -0.675755 |
| H | -4.323060 | 3.316720 | -1.223072 | O | -1.602952 | 3.410693 | 0.140274 |
| H | -5.087430 | 0.061905 | -2.704029 | C | -5.688283 | 2.513537 | -0.225264 |
| H | -4.848398 | 1.791945 | -2.937748 | H | -6.204630 | 1.591242 | 0.058523 |
| H | -3.444435 | 0.722072 | -2.826402 | H | -5.599375 | 3.141668 | 0.666901 |
| O | -0.823243 | -2.171586 | -0.138366 | C | -6.384192 | 3.231157 | -1.366645 |
| C | 0.342285 | -2.785970 | 0.312515 | H | -7.400093 | 3.507306 | -1.060687 |
| H | 0.611032 | -2.464095 | 1.344576 | H | -5.848104 | 4.145163 | -1.644154 |
| H | 1.213076 | -2.551726 | -0.323851 | H | -6.453860 | 2.588954 | -2.251013 |
| C | 0.176880 | -4.312282 | 0.328831 | C | -1.101946 | 4.742089 | -0.147103 |
| H | -0.066212 | -4.677877 | -0.676491 | H | -1.663767 | 5.141968 | -0.997462 |
| H | 1.103977 | -4.800971 | 0.659637 | H | -0.051903 | 4.663956 | -0.442823 |
| H | -0.634184 | -4.612304 | 1.004292 | C | -1.283451 | 5.580275 | 1.104767 |
| | | | | H | -0.723349 | 5.159030 | 1.946489 |
| | | | | H | -0.916751 | 6.597149 | 0.921809 |
| | | | | H | -2.339267 | 5.641083 | 1.389462 |
| | | | | H | -2.363299 | -1.918168 | -3.239840 |
| | | | | H | -0.700417 | -3.053887 | 0.437738 |
| Int 17 | | | | Pd | 0.808507 | -0.681186 | -0.211218 |
| C | -1.255476 | -1.051648 | -0.021588 | P | 3.121550 | 0.206992 | 0.298887 |
| C | -1.324650 | 0.355195 | 0.541491 | C | 4.611246 | -0.915859 | -0.268183 |
| C | -1.350399 | -2.286777 | 0.876045 | C | 4.215204 | -2.391706 | -0.005534 |
| H | -1.664264 | 0.426186 | 1.577101 | C | 4.810503 | -0.770946 | -1.794421 |
| H | -0.277403 | 0.820636 | 0.569910 | C | 5.970306 | -0.634245 | 0.407839 |
| C | -2.737638 | -2.885416 | 1.095938 | H | 4.267288 | -2.655879 | 1.052132 |
| C | -2.406493 | 0.231600 | -1.602448 | H | 3.205753 | -2.624078 | -0.361256 |
| C | -2.976982 | -4.226850 | 0.760315 | H | 4.930353 | -3.040393 | -0.530702 |
| C | -3.785116 | -2.148122 | 1.670381 | H | 5.239454 | 0.192620 | -2.079317 |
| C | -1.943781 | -1.008815 | -1.333111 | H | 5.515423 | -1.545993 | -2.123198 |
| C | -4.223832 | -4.818346 | 0.986939 | H | 3.882705 | -0.920232 | -2.351604 |
| H | -2.175029 | -4.814558 | 0.318100 | H | 6.722316 | -1.301645 | -0.036518 |
| C | -5.033910 | -2.734525 | 1.895764 | H | 6.318515 | 0.391787 | 0.260943 |
| H | -3.635357 | -1.106637 | 1.939570 | H | 5.959179 | -0.842143 | 1.480462 |
| C | -2.122406 | -2.211760 | -2.212473 | H | 5.473404 | 1.955247 | -1.093814 |
| C | -5.259730 | -4.072144 | 1.555396 | C | 4.784537 | 2.545286 | -0.485488 |
| H | -4.383434 | -5.860359 | 0.719301 | C | 3.350175 | 1.975304 | -0.486868 |
| H | -5.830124 | -2.143213 | 2.342214 | H | 5.204835 | 2.628818 | 0.520402 |
| H | -6.230833 | -4.527686 | 1.733454 | H | 4.763919 | 3.556262 | -0.916859 |
| H | -0.916711 | -2.035730 | 1.853626 | C | 2.830644 | 1.904290 | -1.944731 |
| H | -2.892215 | 0.548036 | -2.518332 | C | 2.439820 | 2.992180 | 0.235863 |
| H | -1.222116 | -2.829742 | -2.214936 | H | 1.793150 | 1.556640 | -1.986197 |
| H | -2.944264 | -2.834411 | -1.836950 | H | 2.860787 | 2.912657 | -2.380154 |
| C | -2.204602 | 1.185160 | -0.444036 | H | 3.429743 | 1.255564 | -2.584315 |
| C | -3.569977 | 1.510403 | 0.199689 | H | 2.446553 | 3.928081 | -0.338851 |
| C | -1.555792 | 2.511711 | -0.867275 | | | | |
| O | -3.916319 | 1.209133 | 1.322934 | | | | |
| O | -1.056509 | 2.734330 | -1.948320 | | | | |

| | | | | | | | |
|------|-----------|-----------|-----------|----|-----------|-----------|-----------|
| H | 1.401787 | 2.649770 | 0.287066 | H | 6.394360 | -4.483205 | -1.811908 |
| H | 2.779971 | 3.231939 | 1.246023 | H | 1.043138 | -2.087842 | -1.740648 |
| H | 4.163094 | 2.354607 | 2.510438 | H | 2.795625 | 0.830989 | 2.566498 |
| C | 4.323877 | 1.307979 | 2.782003 | H | 1.675990 | -2.766119 | 2.308173 |
| C | 3.216688 | 0.377930 | 2.241739 | H | 3.364065 | -2.582445 | 1.838854 |
| H | 4.323308 | 1.258649 | 3.880215 | C | 2.048379 | 1.294429 | 0.458668 |
| H | 5.321799 | 1.019820 | 2.444032 | C | 3.374087 | 1.766416 | -0.180663 |
| C | 1.849135 | 0.882514 | 2.762913 | C | 1.214743 | 2.532080 | 0.815003 |
| C | 3.401449 | -1.021398 | 2.873637 | O | 3.816679 | 1.394349 | -1.247351 |
| H | 1.564985 | 1.863726 | 2.381063 | O | 0.702468 | 2.748444 | 1.890500 |
| H | 1.050795 | 0.173913 | 2.518590 | O | 3.998974 | 2.637707 | 0.631327 |
| H | 1.897268 | 0.959257 | 3.857948 | O | 1.135345 | 3.366795 | -0.243042 |
| H | 4.408913 | -1.419879 | 2.739881 | C | 5.283493 | 3.142771 | 0.180338 |
| H | 3.229996 | -0.937779 | 3.955522 | H | 5.953003 | 2.290520 | 0.027838 |
| H | 2.683342 | -1.747991 | 2.480241 | H | 5.139053 | 3.638625 | -0.784804 |
| O | 1.085269 | -2.579522 | -1.015523 | C | 5.799775 | 4.093405 | 1.244071 |
| C | 1.419034 | -2.680279 | -2.370043 | H | 6.772951 | 4.493484 | 0.936283 |
| H | 2.409621 | -2.239546 | -2.589679 | H | 5.112869 | 4.933998 | 1.389902 |
| H | 0.702233 | -2.145568 | -3.022327 | H | 5.926558 | 3.579909 | 2.203029 |
| C | 1.455957 | -4.158716 | -2.781719 | C | 0.449841 | 4.627226 | -0.029582 |
| H | 0.476120 | -4.628712 | -2.632748 | H | 0.924480 | 5.136538 | 0.815219 |
| H | 1.733636 | -4.261268 | -3.840224 | H | -0.588644 | 4.417795 | 0.243712 |
| H | 2.186468 | -4.706066 | -2.174102 | C | 0.552028 | 5.428911 | -1.313852 |
| | | | | H | 0.081549 | 4.898403 | -2.148369 |
| | | | | H | 0.043179 | 6.391667 | -1.186646 |
| TS16 | | | | H | 1.597793 | 5.624472 | -1.574123 |
| C | 1.518414 | -1.005468 | 0.035754 | H | 2.751052 | -1.721034 | 3.264556 |
| C | 1.364885 | 0.300168 | -0.500352 | H | 0.904491 | -3.024172 | -0.264822 |
| C | 1.533284 | -2.285835 | -0.777508 | Pd | -0.701072 | -0.546374 | 0.151626 |
| H | 1.427676 | 0.492859 | -1.565527 | P | -2.998581 | 0.049749 | -0.308124 |
| H | -0.239162 | 0.818233 | -0.518004 | C | -3.744755 | 1.065350 | 1.174477 |
| C | 2.915167 | -2.877089 | -1.039778 | C | -3.237325 | 0.420260 | 2.485434 |
| C | 2.395062 | 0.419382 | 1.648269 | C | -3.182852 | 2.504358 | 1.169096 |
| C | 3.135515 | -4.247699 | -0.838116 | C | -5.285792 | 1.147972 | 1.214996 |
| C | 3.974327 | -2.094118 | -1.524964 | H | -3.598655 | -0.596837 | 2.634086 |
| C | 2.148635 | -0.879656 | 1.379690 | H | -2.143488 | 0.398822 | 2.520255 |
| C | 4.378070 | -4.826371 | -1.115061 | H | -3.590649 | 1.025726 | 3.331544 |
| H | 2.324650 | -4.867382 | -0.460509 | H | -3.578832 | 3.115381 | 0.353988 |
| C | 5.218449 | -2.669237 | -1.800214 | H | -3.479600 | 2.990363 | 2.108137 |
| H | 3.833144 | -1.028288 | -1.684325 | H | -2.089354 | 2.515907 | 1.133882 |
| C | 2.498204 | -2.048553 | 2.250734 | H | -5.579783 | 1.763286 | 2.076854 |
| C | 5.426203 | -4.037369 | -1.597228 | H | -5.710034 | 1.615283 | 0.322859 |
| H | 4.525942 | -5.891280 | -0.951241 | H | -5.756769 | 0.171153 | 1.344516 |
| H | 6.025995 | -2.044915 | -2.175598 | H | -4.704690 | 2.600330 | -1.376818 |

| | | | |
|---|-----------|-----------|-----------|
| C | -4.535249 | 1.812944 | -2.116181 |
| C | -3.160327 | 1.129177 | -1.935336 |
| H | -5.374441 | 1.117494 | -2.070744 |
| H | -4.560888 | 2.292020 | -3.104872 |
| C | -2.081365 | 2.236774 | -1.973691 |
| C | -2.877177 | 0.245517 | -3.172293 |
| H | -1.075421 | 1.817666 | -2.043493 |
| H | -2.249892 | 2.844826 | -2.873327 |
| H | -2.108909 | 2.907103 | -1.115305 |
| H | -2.794102 | 0.898571 | -4.051709 |
| H | -1.930551 | -0.296346 | -3.075148 |
| H | -3.670276 | -0.474535 | -3.380865 |
| H | -5.322412 | -1.034204 | -2.316380 |
| C | -5.415082 | -1.368859 | -1.280421 |
| C | -4.053689 | -1.569764 | -0.581169 |
| H | -5.930317 | -2.338960 | -1.305718 |
| H | -6.068296 | -0.670440 | -0.749527 |
| C | -3.192860 | -2.566770 | -1.398084 |
| C | -4.310845 | -2.262505 | 0.775334 |
| H | -2.925752 | -2.204607 | -2.391862 |
| H | -2.284673 | -2.824800 | -0.846041 |
| H | -3.778705 | -3.486916 | -1.535507 |
| H | -4.998735 | -1.710735 | 1.420504 |
| H | -4.776672 | -3.236259 | 0.570388 |
| H | -3.371907 | -2.451284 | 1.295947 |
| O | -1.055019 | -2.446699 | 1.023019 |
| C | -1.069515 | -2.594016 | 2.410222 |
| H | -2.016031 | -2.231690 | 2.864462 |
| H | -0.273754 | -2.008088 | 2.911231 |
| C | -0.912090 | -4.072371 | 2.794697 |
| H | 0.040008 | -4.474342 | 2.425304 |
| H | -0.945685 | -4.203615 | 3.885927 |
| H | -1.717863 | -4.667622 | 2.347633 |

Int 18

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|---|-----------|-----------|-----------|
| C | 1.153086 | -1.380699 | -0.462446 |
| C | 0.477016 | -0.287382 | -0.058509 |
| C | 2.642074 | -1.628850 | -0.412843 |
| H | 0.880352 | 0.609736 | 0.391651 |
| C | 3.467825 | -0.472360 | 0.113100 |
| C | -1.061381 | -1.883605 | -0.889548 |
| C | 4.054420 | 0.448463 | -0.766132 |
| C | 3.654042 | -0.293004 | 1.491539 |

| | | | |
|---|-----------|-----------|-----------|
| C | 0.184523 | -2.388803 | -0.981279 |
| C | 4.807378 | 1.522690 | -0.283336 |
| H | 3.920653 | 0.323078 | -1.838946 |
| C | 4.405113 | 0.779333 | 1.979473 |
| H | 3.202668 | -0.996540 | 2.188133 |
| C | 0.578344 | -3.729326 | -1.526955 |
| C | 4.985124 | 1.691328 | 1.092552 |
| H | 5.257242 | 2.224035 | -0.981961 |
| H | 4.538470 | 0.900695 | 3.051675 |
| H | 5.572865 | 2.524070 | 1.470620 |
| H | 2.989114 | -1.896578 | -1.421317 |
| H | -1.985648 | -2.348244 | -1.210471 |
| H | 1.246937 | -3.627839 | -2.392382 |
| H | 1.115088 | -4.327363 | -0.778286 |
| C | -1.008360 | -0.492561 | -0.288488 |
| C | -1.814173 | -0.470460 | 1.023315 |
| C | -1.532944 | 0.587884 | -1.251520 |
| O | -1.347149 | -0.432360 | 2.139642 |
| O | -1.849121 | 0.411126 | -2.406931 |
| O | -3.136700 | -0.533990 | 0.759129 |
| O | -1.564813 | 1.786963 | -0.633312 |
| C | -4.025793 | -0.545004 | 1.905370 |
| H | -3.773867 | -1.407970 | 2.530000 |
| H | -3.844033 | 0.361309 | 2.491768 |
| C | -5.447935 | -0.613738 | 1.381432 |
| H | -6.149349 | -0.624138 | 2.223981 |
| H | -5.678659 | 0.252487 | 0.752147 |
| H | -5.606627 | -1.522035 | 0.790361 |
| C | -2.012913 | 2.914588 | -1.428395 |
| H | -3.023778 | 2.701617 | -1.790619 |
| H | -1.354464 | 3.007424 | -2.297914 |
| C | -1.967730 | 4.145623 | -0.542834 |
| H | -0.950634 | 4.334840 | -0.183511 |
| H | -2.300215 | 5.020665 | -1.113594 |
| H | -2.625213 | 4.030980 | 0.325615 |
| H | -0.300754 | -4.297764 | -1.846473 |
| H | 2.825820 | -2.521089 | 0.204312 |

TS17

| | | | |
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| S | 4.374119 | 1.348657 | -0.410840 |
| O | 5.363085 | 2.141261 | 0.327683 |
| O | 3.819666 | 1.795243 | -1.691890 |
| N | 3.043003 | 1.170727 | 0.630241 |

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|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 5.064337 | -0.292599 | -0.660871 | C | 0.521892 | -2.668576 | -0.014912 |
| C | 4.620738 | -1.071682 | -1.731776 | H | 1.229460 | -2.378845 | 0.790352 |
| C | 1.840869 | 0.496203 | 0.070992 | H | 0.996115 | -2.345631 | -0.966942 |
| C | 0.699592 | 0.679043 | 1.054503 | C | 0.445754 | -4.202447 | -0.023155 |
| C | 3.305439 | 0.972990 | 2.005762 | H | -0.190337 | -4.554686 | -0.844253 |
| C | 6.021229 | -0.783991 | 0.234248 | H | 1.445269 | -4.643911 | -0.145353 |
| C | 2.408501 | 0.469101 | 2.871082 | H | 0.017790 | -4.568086 | 0.918617 |
| C | -0.008565 | 2.940892 | -0.001201 | P | -3.592577 | -0.558784 | -0.146436 |
| C | -0.129858 | 1.832512 | 0.996128 | C | -4.463587 | -0.905533 | 1.559809 |
| C | -0.137231 | 2.761989 | -1.386940 | C | -3.513065 | -1.787212 | 2.406257 |
| C | 1.011775 | 0.079370 | 2.420337 | C | -4.633619 | 0.415104 | 2.344108 |
| C | 6.526237 | -2.070015 | 0.050936 | C | -5.844100 | -1.591668 | 1.472320 |
| C | 6.091908 | -2.879386 | -1.012694 | H | -3.326113 | -2.767694 | 1.970423 |
| C | 5.138292 | -2.358231 | -1.898624 | H | -2.540983 | -1.304030 | 2.546200 |
| C | 0.265330 | 4.229374 | 0.486334 | H | -3.969068 | -1.937724 | 3.394878 |
| C | 0.033524 | 3.835052 | -2.263144 | H | -5.398716 | 1.070017 | 1.920074 |
| C | 2.734531 | 0.298351 | 4.331519 | H | -4.951577 | 0.168798 | 3.366110 |
| C | 0.324127 | 5.109749 | -1.768202 | H | -3.693794 | 0.971671 | 2.418777 |
| C | 0.436546 | 5.304037 | -0.388988 | H | -6.244347 | -1.703205 | 2.489803 |
| C | 6.642086 | -4.275588 | -1.188890 | H | -6.571395 | -1.011192 | 0.899407 |
| H | 3.898720 | -0.668483 | -2.434349 | H | -5.789237 | -2.592558 | 1.039233 |
| H | 2.049618 | -0.570158 | -0.065070 | H | -6.421121 | 1.024249 | 0.050781 |
| H | 1.635048 | 0.945139 | -0.897395 | C | -6.032592 | 0.888038 | -0.962030 |
| H | 4.281727 | 1.319803 | 2.325763 | C | -4.488676 | 0.951556 | -1.008015 |
| H | 6.380332 | -0.157436 | 1.044076 | H | -6.439498 | -0.042462 | -1.361196 |
| H | -0.503111 | 2.173676 | 1.961492 | H | -6.435200 | 1.709222 | -1.571030 |
| H | -0.389243 | 1.777865 | -1.774433 | C | -4.052585 | 2.292080 | -0.368452 |
| H | 0.916462 | -1.015443 | 2.397445 | C | -4.040098 | 1.042445 | -2.485259 |
| H | 0.279052 | 0.428647 | 3.161044 | H | -2.995811 | 2.501414 | -0.550220 |
| H | 7.277380 | -2.448892 | 0.740787 | H | -4.629996 | 3.097892 | -0.842088 |
| H | 4.797465 | -2.962297 | -2.736164 | H | -4.233516 | 2.350791 | 0.704826 |
| H | 0.361546 | 4.388125 | 1.558334 | H | -4.408022 | 1.990952 | -2.898990 |
| H | -0.062600 | 3.674335 | -3.333845 | H | -2.949464 | 1.047184 | -2.579530 |
| H | 2.068119 | 0.900664 | 4.966453 | H | -4.440797 | 0.241798 | -3.109377 |
| H | 3.766742 | 0.590916 | 4.554136 | H | -5.429664 | -1.484613 | -2.666152 |
| H | 2.606104 | -0.748031 | 4.644937 | C | -5.190301 | -2.278474 | -1.954504 |
| H | 0.458678 | 5.944231 | -2.451278 | C | -3.801612 | -2.115772 | -1.300374 |
| H | 0.659434 | 6.291058 | 0.007987 | H | -5.190229 | -3.221617 | -2.518312 |
| H | 7.738515 | -4.278109 | -1.165074 | H | -6.000431 | -2.340916 | -1.222300 |
| H | 6.323483 | -4.714854 | -2.139592 | C | -2.718144 | -2.027470 | -2.403895 |
| H | 6.298981 | -4.938619 | -0.383910 | C | -3.494549 | -3.404852 | -0.502339 |
| H | -1.763862 | 1.369490 | 0.645045 | H | -2.838966 | -1.168573 | -3.066248 |
| Pd | -1.246634 | -0.097789 | 0.376848 | H | -1.723776 | -2.000467 | -1.949920 |
| O | -0.742076 | -2.118285 | 0.155618 | H | -2.788946 | -2.930453 | -3.026673 |

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| H | -4.273705 | -3.651803 | 0.223384 | H | 3.657277 | 0.724092 | 4.532667 |
| H | -3.454172 | -4.237272 | -1.219050 | H | 2.570086 | -0.671411 | 4.669980 |
| H | -2.521588 | -3.335523 | -0.010040 | H | 1.271710 | 5.796721 | -2.409663 |
| | | | | H | 0.018843 | 3.816294 | -3.253223 |
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| Int 19 | | | | H | 5.990243 | -5.108895 | -0.860478 |
| S | 4.320738 | 1.244687 | -0.456251 | H | 7.537030 | -4.514544 | -0.235050 |
| O | 5.277159 | 2.096720 | 0.259586 | H | -1.252499 | 1.612660 | 0.798151 |
| O | 3.774621 | 1.618798 | -1.763593 | Pd | -1.218222 | -0.185891 | 0.331937 |
| N | 2.983219 | 1.067362 | 0.572655 | O | -0.924972 | -2.177510 | -0.003776 |
| C | 5.063302 | -0.384494 | -0.627143 | C | 0.331073 | -2.775546 | -0.122764 |
| C | 4.652204 | -1.224445 | -1.667893 | H | 0.984536 | -2.559982 | 0.744788 |
| C | 1.794652 | 0.355328 | 0.026346 | H | 0.873895 | -2.422440 | -1.021735 |
| C | 0.628460 | 0.504008 | 0.987217 | C | 0.168292 | -4.297710 | -0.223397 |
| C | 3.229950 | 0.949236 | 1.958491 | H | -0.433746 | -4.565749 | -1.099656 |
| C | 6.023973 | -0.806744 | 0.294787 | H | 1.148420 | -4.786526 | -0.313814 |
| C | 2.342964 | 0.442878 | 2.833011 | H | -0.334144 | -4.689540 | 0.669194 |
| C | 0.260426 | 2.928816 | 0.034261 | P | -3.702408 | -0.442583 | -0.140466 |
| C | -0.113512 | 1.826080 | 1.002541 | C | -4.543293 | -0.924652 | 1.549430 |
| C | 0.959711 | 4.050888 | 0.500061 | C | -3.631400 | -1.960468 | 2.252752 |
| C | 0.983673 | -0.048908 | 2.367301 | C | -4.580411 | 0.305931 | 2.484011 |
| C | 6.569479 | -2.086447 | 0.172106 | C | -5.973143 | -1.497992 | 1.452510 |
| C | 6.170749 | -2.952350 | -0.856642 | H | -3.552766 | -2.905072 | 1.716250 |
| C | 5.207793 | -2.498782 | -1.773594 | H | -2.614831 | -1.576297 | 2.382715 |
| C | -0.078809 | 2.863480 | -1.323892 | H | -4.050062 | -2.172779 | 3.246647 |
| C | 1.322539 | 5.078064 | -0.374068 | H | -5.302301 | 1.063622 | 2.169948 |
| C | 2.647463 | 0.363701 | 4.305966 | H | -4.882065 | -0.029702 | 3.485349 |
| C | 0.985403 | 5.000005 | -1.728202 | H | -3.595798 | 0.776080 | 2.582248 |
| C | 0.282861 | 3.888666 | -2.201199 | H | -6.343401 | -1.696430 | 2.468425 |
| C | 6.760742 | -4.337491 | -0.986319 | H | -6.676431 | -0.808232 | 0.979250 |
| H | 3.925130 | -0.872835 | -2.392701 | H | -6.008337 | -2.445159 | 0.909593 |
| H | 2.030700 | -0.709136 | -0.090993 | H | -6.401270 | 1.295850 | 0.374473 |
| H | 1.582645 | 0.780732 | -0.952877 | C | -6.067243 | 1.265406 | -0.666010 |
| H | 4.182854 | 1.358533 | 2.275796 | C | -4.528573 | 1.205247 | -0.786734 |
| H | 6.356584 | -0.135844 | 1.080075 | H | -6.567119 | 0.429432 | -1.159652 |
| H | -0.180489 | 2.218393 | 2.023823 | H | -6.423811 | 2.189149 | -1.143213 |
| H | 1.234693 | 4.114328 | 1.550604 | C | -3.936362 | 2.415308 | -0.023098 |
| H | 0.971766 | -1.148942 | 2.350068 | C | -4.143976 | 1.433669 | -2.267232 |
| H | 0.218957 | 0.243376 | 3.100724 | H | -2.870126 | 2.537845 | -0.230837 |
| H | 7.323994 | -2.412159 | 0.884399 | H | -4.437177 | 3.327275 | -0.375969 |
| H | 4.893020 | -3.149273 | -2.586887 | H | -4.073202 | 2.368190 | 1.057396 |
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| H | 1.874458 | 5.935327 | 0.002664 | H | -3.062271 | 1.369030 | -2.423294 |
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| C | -3.011707 | -1.701018 | -2.574312 | H | 7.574921 | -1.493028 | 1.233370 |
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| H | -4.579836 | -3.511910 | -0.083833 | H | 3.958899 | 3.206945 | 2.732295 |
| H | -3.842931 | -3.979731 | -1.611668 | H | 2.870391 | 2.253730 | 3.760246 |
| H | -2.822780 | -3.277865 | -0.342782 | H | -0.851749 | 7.015124 | 0.879720 |
| | | | | H | 1.090612 | 6.409838 | -0.558600 |
| | | | | H | 7.356831 | -4.858882 | 0.187780 |
| Int 20 | | | | H | 6.285288 | -4.709471 | 1.583040 |
| S | 4.198801 | 0.635785 | -1.636068 | H | 7.832374 | -3.847379 | 1.562678 |
| O | 5.146638 | 1.754879 | -1.677532 | H | 0.415056 | 1.856816 | -1.634785 |
| O | 3.508266 | 0.161612 | -2.840587 | Pd | -1.116999 | -0.090971 | 0.215328 |
| N | 2.971739 | 1.097391 | -0.560138 | O | -0.812039 | -1.625812 | 1.533230 |
| C | 5.041301 | -0.772594 | -0.903584 | C | 0.439322 | -2.198926 | 1.769990 |
| C | 4.598069 | -2.068590 | -1.189662 | H | 1.193283 | -1.453685 | 2.087013 |
| C | 1.820616 | 0.171808 | -0.394684 | H | 0.848880 | -2.691539 | 0.864625 |
| C | 0.688938 | 0.925020 | 0.290805 | C | 0.322112 | -3.246242 | 2.885212 |
| C | 3.333855 | 1.842572 | 0.590271 | H | -0.369790 | -4.047006 | 2.598974 |
| C | 6.111817 | -0.559034 | -0.032030 | H | 1.302149 | -3.696130 | 3.097447 |
| C | 2.516114 | 2.011330 | 1.643548 | H | -0.055078 | -2.782651 | 3.804541 |
| C | -0.290132 | 3.308625 | -0.205058 | P | -3.466851 | -0.910616 | -0.278894 |
| C | -0.038043 | 1.879277 | -0.637397 | C | -4.642308 | -0.605450 | 1.243016 |
| C | -1.380775 | 3.659823 | 0.601448 | C | -3.849358 | -0.933028 | 2.531920 |
| C | 1.117922 | 1.415838 | 1.667468 | C | -4.996617 | 0.895970 | 1.332970 |
| C | 6.736083 | -1.658326 | 0.561338 | C | -5.960907 | -1.408001 | 1.244443 |
| C | 6.308427 | -2.967953 | 0.298802 | H | -3.604278 | -1.989414 | 2.631220 |
| C | 5.233682 | -3.153112 | -0.587074 | H | -2.906537 | -0.381362 | 2.582636 |
| C | 0.594470 | 4.315664 | -0.619220 | H | -4.466513 | -0.650063 | 3.396372 |
| C | -1.583130 | 4.986159 | 0.993671 | H | -5.685003 | 1.222761 | 0.549865 |
| C | 2.931353 | 2.839083 | 2.831189 | H | -5.495325 | 1.075703 | 2.294692 |
| C | -0.694662 | 5.982405 | 0.579154 | H | -4.104645 | 1.530978 | 1.306674 |
| C | 0.394889 | 5.642348 | -0.228882 | H | -6.543286 | -1.125794 | 2.133088 |
| C | 6.984281 | -4.155923 | 0.943163 | H | -6.583727 | -1.204809 | 0.369593 |
| H | 3.782734 | -2.220607 | -1.889478 | H | -5.795270 | -2.486065 | 1.301441 |
| H | 2.125942 | -0.687376 | 0.215376 | H | -6.344822 | 0.262062 | -1.254261 |
| H | 1.532057 | -0.177806 | -1.386889 | C | -5.758658 | -0.228387 | -2.036129 |
| H | 4.303046 | 2.324686 | 0.526671 | C | -4.239853 | -0.026933 | -1.841407 |

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|------|-----------|-----------|-----------|----|-----------|-----------|-----------|
| H | -6.049725 | -1.279962 | -2.070327 | C | -0.538758 | 4.399150 | -0.935667 |
| H | -6.056825 | 0.226386 | -2.991399 | C | -2.268295 | 4.585203 | 1.243470 |
| C | -3.967809 | 1.495320 | -1.768692 | C | 2.933817 | 2.895239 | 2.952784 |
| C | -3.509572 | -0.511878 | -3.115579 | C | -1.970183 | 5.728810 | 0.495280 |
| H | -2.897604 | 1.716864 | -1.771206 | C | -1.104203 | 5.631057 | -0.597295 |
| H | -4.396595 | 1.967455 | -2.663164 | C | 6.821167 | -4.051250 | 0.854944 |
| H | -4.410937 | 1.983504 | -0.901260 | H | 3.790445 | -1.904753 | -2.018967 |
| H | -3.819958 | 0.122029 | -3.957182 | H | 2.115260 | -0.442830 | 0.097272 |
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| H | -3.750338 | -1.542116 | -3.384439 | H | 4.343377 | 2.491801 | 0.651791 |
| H | -4.744750 | -3.032993 | -2.394624 | H | 6.455488 | 0.591857 | 0.257886 |
| C | -4.622479 | -3.416393 | -1.378523 | H | 0.118577 | 1.951292 | -1.635283 |
| C | -3.399448 | -2.823879 | -0.647653 | H | -1.953027 | 2.463040 | 1.473527 |
| H | -4.482005 | -4.503235 | -1.462444 | H | 0.995344 | 0.771282 | 2.357998 |
| H | -5.557568 | -3.252368 | -0.835338 | H | 0.422276 | 2.391959 | 2.038988 |
| C | -2.123639 | -3.089866 | -1.485238 | H | 7.480275 | -1.426641 | 1.270378 |
| C | -3.204470 | -3.602861 | 0.673660 | H | 4.816747 | -3.923369 | -1.004149 |
| H | -2.134673 | -2.610117 | -2.465262 | H | 0.137072 | 4.331811 | -1.785377 |
| H | -1.230689 | -2.759003 | -0.946637 | H | -2.950079 | 4.648382 | 2.087942 |
| H | -2.036884 | -4.172520 | -1.653154 | H | 2.293888 | 3.772098 | 3.127672 |
| H | -4.106556 | -3.624120 | 1.290353 | H | 3.972397 | 3.240057 | 2.898006 |
| H | -2.969467 | -4.645929 | 0.418664 | H | 2.837792 | 2.252211 | 3.839619 |
| H | -2.371581 | -3.194028 | 1.251392 | H | -2.415351 | 6.685193 | 0.757074 |
| | | | | H | -0.869192 | 6.511556 | -1.189736 |
| | | | | H | 6.270629 | -4.338030 | 1.761258 |
| | | | | H | 7.862647 | -3.877515 | 1.146135 |
| | | | | H | 6.795978 | -4.908258 | 0.173162 |
| | | | | H | -1.473438 | 1.029063 | -0.999890 |
| TS18 | | | | Pd | -1.106100 | 0.006433 | 0.158091 |
| S | 4.259291 | 0.924864 | -1.602504 | O | -0.632054 | -1.274651 | 1.752590 |
| O | 5.236598 | 2.017579 | -1.561177 | C | 0.579331 | -1.943416 | 1.896304 |
| O | 3.591485 | 0.527317 | -2.846885 | H | 1.453626 | -1.260687 | 1.893924 |
| N | 3.012097 | 1.369080 | -0.541034 | H | 0.763389 | -2.665352 | 1.069888 |
| C | 5.041061 | -0.539502 | -0.913821 | C | 0.609398 | -2.715321 | 3.223531 |
| C | 4.580382 | -1.807249 | -1.281333 | H | -0.197413 | -3.457401 | 3.261638 |
| C | 1.840179 | 0.462083 | -0.458101 | H | 1.567811 | -3.238418 | 3.353175 |
| C | 0.721219 | 1.203643 | 0.256587 | H | 0.471134 | -2.025680 | 4.065296 |
| C | 3.360902 | 2.033443 | 0.661635 | P | -3.225392 | -1.120740 | -0.295009 |
| C | 6.084715 | -0.396128 | 0.005419 | C | -4.451182 | -0.996901 | 1.213670 |
| C | 2.522844 | 2.158126 | 1.704947 | C | -3.649227 | -1.173167 | 2.525202 |
| C | -0.819283 | 3.247398 | -0.181703 | C | -5.058523 | 0.423193 | 1.267708 |
| C | -0.141917 | 1.975130 | -0.576911 | C | -5.611260 | -2.015743 | 1.198725 |
| C | -1.700813 | 3.355021 | 0.905665 | H | -3.252861 | -2.178851 | 2.655053 |
| C | 1.102928 | 1.618403 | 1.666925 | H | -2.797376 | -0.491984 | 2.587362 |
| C | 6.660922 | -1.537442 | 0.563709 | | | | |
| C | 6.210929 | -2.822584 | 0.222021 | | | | |
| C | 5.168941 | -2.936772 | -0.711497 | | | | |

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| H | -4.327384 | -0.969256 | 3.365903 | C | -0.226311 | 3.841504 | -0.636739 |
| H | -5.794178 | 0.603611 | 0.480331 | S | 3.545370 | -0.066337 | 1.509080 |
| H | -5.581724 | 0.535550 | 2.226437 | C | 1.991365 | -0.557414 | -0.649532 |
| H | -4.292203 | 1.203762 | 1.219732 | C | -0.149446 | 4.105842 | 0.743843 |
| H | -6.253067 | -1.823932 | 2.070146 | C | -0.484539 | 4.918766 | -1.509017 |
| H | -6.240089 | -1.937677 | 0.308564 | O | 2.903785 | -1.227473 | 2.152192 |
| H | -5.262494 | -3.047499 | 1.281667 | O | 3.850964 | 1.135044 | 2.297635 |
| H | -6.250790 | -0.510109 | -1.322511 | C | 5.044971 | -0.651661 | 0.714454 |
| C | -5.569015 | -0.892835 | -2.086647 | C | 1.127584 | 0.267541 | -1.632116 |
| C | -4.120377 | -0.396316 | -1.876932 | C | -0.292649 | 5.408184 | 1.225407 |
| H | -5.654838 | -1.980705 | -2.106890 | H | -0.037915 | 3.288513 | 1.446262 |
| H | -5.931607 | -0.517664 | -3.053689 | C | -0.622737 | 6.219432 | -1.027028 |
| C | -4.161371 | 1.150537 | -1.828081 | H | -0.566274 | 4.728986 | -2.577458 |
| C | -3.289294 | -0.751179 | -3.131464 | C | 5.311696 | -2.019073 | 0.665296 |
| H | -3.160823 | 1.586100 | -1.775537 | C | 5.947234 | 0.278218 | 0.185974 |
| H | -4.627809 | 1.508030 | -2.756134 | C | -0.193885 | -0.428587 | -1.977124 |
| H | -4.743710 | 1.550109 | -0.998654 | C | 1.958364 | 0.651064 | -2.876041 |
| H | -3.701522 | -0.201570 | -3.988156 | C | -0.520770 | 6.470359 | 0.345646 |
| H | -2.241353 | -0.452104 | -3.023709 | H | -0.238715 | 5.590006 | 2.295752 |
| H | -3.325539 | -1.812584 | -3.384726 | H | -0.813103 | 7.035291 | -1.719853 |
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| C | -3.897670 | -3.807347 | -1.369892 | H | 4.607795 | -2.721594 | 1.099732 |
| C | -2.811488 | -2.994049 | -0.635432 | C | 7.120980 | -0.178720 | -0.407167 |
| H | -3.564116 | -4.852905 | -1.426369 | H | 5.732330 | 1.340440 | 0.247575 |
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| C | -2.500038 | -3.697130 | 0.705454 | H | 2.190407 | -0.246752 | -3.463765 |
| H | -1.585006 | -2.586521 | -2.445778 | H | 1.401095 | 1.339508 | -3.520640 |
| H | -0.682924 | -2.550565 | -0.921844 | H | 2.901399 | 1.134896 | -2.592275 |
| H | -1.221713 | -4.095301 | -1.605446 | H | -0.631149 | 7.482386 | 0.726648 |
| H | -3.398604 | -3.891973 | 1.296733 | C | 7.415157 | -1.552879 | -0.477705 |
| H | -2.048738 | -4.673458 | 0.480422 | H | 6.707610 | -3.525727 | 0.028929 |
| H | -1.793095 | -3.112766 | 1.301124 | H | 7.825576 | 0.541638 | -0.817279 |
| | | | | C | 8.699654 | -2.027896 | -1.116126 |
| | | | | H | 9.574377 | -1.657201 | -0.566685 |
| Int 21 | | | | H | 8.756694 | -3.120852 | -1.137535 |
| Pd | -1.423092 | 0.261092 | -0.457785 | H | 8.788824 | -1.664901 | -2.147601 |
| P | -2.650521 | -1.747189 | -0.002199 | H | -0.419747 | 2.398972 | -2.236394 |
| C | 0.781701 | 1.507238 | -0.776969 | C | -1.642870 | -3.429141 | 0.187485 |
| C | 1.617519 | 1.508749 | 0.487104 | C | -0.544831 | -3.588859 | -0.887871 |
| C | -0.014172 | 2.513057 | -1.230761 | C | -0.886534 | -3.431805 | 1.536591 |
| N | 2.641181 | 0.475593 | 0.182898 | C | -2.529196 | -4.695034 | 0.103706 |
| H | 2.099990 | 2.470369 | 0.679954 | H | -0.908158 | -3.506964 | -1.912137 |
| H | 1.015557 | 1.245489 | 1.368548 | H | 0.262080 | -2.871437 | -0.743851 |

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|---|-----------|-----------|-----------|------|-----------|-----------|-----------|
| H | -0.110892 | -4.591689 | -0.774288 | | | | |
| H | -1.541868 | -3.544145 | 2.400874 | TS19 | | | |
| H | -0.199545 | -4.288576 | 1.540350 | Pd | 1.339757 | 0.597073 | 0.592912 |
| H | -0.279947 | -2.531029 | 1.672937 | P | 3.188696 | -0.943114 | -0.308219 |
| H | -1.909993 | -5.561741 | 0.373230 | C | -0.978242 | 0.404973 | 1.064801 |
| H | -3.382984 | -4.685524 | 0.779697 | C | -1.803793 | -0.132793 | -0.097831 |
| H | -2.896343 | -4.871869 | -0.910969 | C | -0.377478 | 1.721534 | 1.091516 |
| H | -3.555354 | -3.556694 | 2.573906 | N | -2.307908 | -1.420011 | 0.410505 |
| C | -4.289642 | -2.823463 | 2.234378 | H | -2.612953 | 0.592129 | -0.288298 |
| C | -3.654177 | -1.532695 | 1.670212 | H | -1.257639 | -0.291048 | -1.026183 |
| H | -4.971722 | -3.311458 | 1.532764 | C | -0.755418 | 2.786624 | 0.121801 |
| H | -4.882008 | -2.540252 | 3.114898 | S | -3.410941 | -2.295696 | -0.500717 |
| C | -2.706677 | -0.925883 | 2.735830 | C | -2.444339 | -1.349052 | 1.872765 |
| C | -4.792437 | -0.509067 | 1.470860 | C | -0.708157 | 2.626649 | -1.276054 |
| H | -2.360106 | 0.060839 | 2.418684 | C | -1.184606 | 4.029853 | 0.623420 |
| H | -3.284670 | -0.800751 | 3.662734 | O | -3.616698 | -3.553465 | 0.225128 |
| H | -1.852247 | -1.559519 | 2.974794 | O | -2.904569 | -2.260481 | -1.876849 |
| H | -5.227004 | -0.298023 | 2.457288 | C | -4.961371 | -1.385656 | -0.467082 |
| H | -4.407130 | 0.429177 | 1.078151 | C | -1.283879 | -0.434123 | 2.270698 |
| H | -5.602966 | -0.882370 | 0.839799 | C | -1.104266 | 3.654366 | -2.131904 |
| H | -5.773509 | -2.452376 | -0.406778 | H | -0.316476 | 1.706278 | -1.697447 |
| C | -5.130156 | -2.852738 | -1.192667 | C | -1.574551 | 5.063950 | -0.231343 |
| C | -3.907291 | -1.954062 | -1.479299 | H | -1.215098 | 4.185318 | 1.699911 |
| H | -5.737734 | -2.910583 | -2.106522 | C | -5.902116 | -1.660262 | 0.528935 |
| H | -4.854574 | -3.874204 | -0.922452 | C | -5.202955 | -0.394706 | -1.426154 |
| C | -4.409730 | -0.545595 | -1.874671 | C | 0.070783 | -0.924727 | 1.818598 |
| C | -3.176759 | -2.519803 | -2.717831 | C | -1.394882 | 0.179051 | 3.655268 |
| H | -4.972390 | -0.050690 | -1.083017 | C | -1.543419 | 4.878508 | -1.615622 |
| H | -3.577852 | 0.109999 | -2.153263 | H | -1.049033 | 3.505371 | -3.207610 |
| H | -5.073382 | -0.642802 | -2.745096 | H | -1.900036 | 6.013687 | 0.186429 |
| H | -2.906581 | -3.572820 | -2.607793 | C | -7.089379 | -0.925044 | 0.566223 |
| H | -3.856389 | -2.451758 | -3.577954 | H | -5.717428 | -2.454740 | 1.244991 |
| H | -2.278370 | -1.947289 | -2.963797 | C | -6.392844 | 0.329509 | -1.371146 |
| O | -2.403476 | 1.517049 | 0.908833 | H | -4.479594 | -0.214212 | -2.214848 |
| C | -3.253474 | 2.491126 | 0.376795 | H | 0.860881 | -0.733113 | 2.543789 |
| H | -4.122059 | 2.044785 | -0.154564 | H | 0.089837 | -1.886416 | 1.325664 |
| H | -2.750400 | 3.128339 | -0.375076 | H | -1.451129 | -0.611023 | 4.414595 |
| C | -3.798429 | 3.398147 | 1.488511 | H | -0.525487 | 0.800322 | 3.892327 |
| H | -2.974256 | 3.897450 | 2.009997 | H | -2.292738 | 0.803256 | 3.742952 |
| H | -4.466108 | 4.167868 | 1.075472 | H | -1.843134 | 5.680869 | -2.284985 |
| H | -4.358537 | 2.810035 | 2.226016 | C | -7.353239 | 0.079569 | -0.376172 |
| H | 2.748007 | -1.162961 | -1.157984 | H | -7.825741 | -1.144737 | 1.335742 |
| H | 1.362916 | -1.211127 | -0.032414 | H | -6.582540 | 1.096136 | -2.119240 |
| | | | | C | -8.642355 | 0.866888 | -0.340666 |

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|---|-----------|-----------|-----------|--------|-----------|-----------|-----------|
| H | -9.240690 | 0.685480 | -1.242598 | C | 2.583372 | 3.271536 | 1.041056 |
| H | -9.253854 | 0.596614 | 0.526041 | H | 3.191960 | 2.918907 | 1.901362 |
| H | -8.447627 | 1.945398 | -0.293790 | H | 1.615985 | 3.601721 | 1.466072 |
| H | -0.243094 | 2.117476 | 2.099590 | C | 3.269567 | 4.499645 | 0.427991 |
| C | 2.551304 | -2.478618 | -1.345556 | H | 2.664972 | 4.897661 | -0.395421 |
| C | 1.293557 | -3.074430 | -0.673931 | H | 3.399702 | 5.290013 | 1.181255 |
| C | 2.073984 | -2.005975 | -2.738583 | H | 4.256796 | 4.237565 | 0.028605 |
| C | 3.575389 | -3.618757 | -1.541164 | H | -3.399664 | -0.892074 | 2.180901 |
| H | 1.461944 | -3.418380 | 0.347642 | H | -2.373262 | -2.351092 | 2.303971 |
| H | 0.467988 | -2.359294 | -0.672336 | | | | |
| H | 0.963736 | -3.943805 | -1.258270 | | | | |
| H | 2.893265 | -1.730371 | -3.404677 | Int 22 | | | |
| H | 1.531029 | -2.832800 | -3.215598 | Pd | -1.463545 | 0.100891 | 0.564241 |
| H | 1.381690 | -1.160577 | -2.668674 | P | -3.645516 | -0.327345 | -0.622955 |
| H | 3.136887 | -4.370758 | -2.212366 | C | 1.357173 | 1.120243 | 0.302462 |
| H | 4.510848 | -3.284811 | -1.993222 | C | 2.296332 | 0.327536 | -0.608345 |
| H | 3.813235 | -4.130702 | -0.604970 | C | 0.490462 | 0.415858 | 1.306360 |
| H | 4.889392 | -1.428709 | -3.045894 | N | 3.291249 | 1.331182 | -1.031284 |
| C | 5.395228 | -0.820137 | -2.292485 | H | 2.757155 | -0.498313 | -0.043961 |
| C | 4.421183 | 0.043242 | -1.461350 | H | 1.820547 | -0.081429 | -1.503430 |
| H | 6.018748 | -1.478228 | -1.681568 | C | 0.385627 | -1.023549 | 1.452420 |
| H | 6.070962 | -0.142927 | -2.833513 | S | 4.576696 | 0.870102 | -1.993451 |
| C | 3.586867 | 0.924601 | -2.425650 | C | 3.475718 | 2.348576 | 0.016794 |
| C | 5.258776 | 1.021361 | -0.605847 | C | 0.215676 | -1.863150 | 0.310790 |
| H | 2.948553 | 1.612954 | -1.866669 | C | 0.239896 | -1.626826 | 2.741364 |
| H | 4.287365 | 1.524697 | -3.024381 | O | 5.277572 | 2.105858 | -2.359567 |
| H | 2.983605 | 0.346802 | -3.127101 | O | 4.022908 | -0.041107 | -3.002246 |
| H | 5.811951 | 1.679284 | -1.290453 | C | 5.692551 | -0.091889 | -0.957477 |
| H | 4.609073 | 1.650031 | 0.005899 | C | 2.106550 | 2.418613 | 0.680223 |
| H | 6.001243 | 0.517157 | 0.017960 | C | -0.024574 | -3.245267 | 0.470589 |
| H | 6.287922 | -1.423156 | 0.529190 | H | 0.418781 | -1.478595 | -0.682778 |
| C | 5.605487 | -2.182434 | 0.916206 | C | 0.005888 | -2.981037 | 2.874892 |
| C | 4.199363 | -1.621727 | 1.218413 | H | 0.339378 | -0.997499 | 3.622223 |
| H | 6.042418 | -2.560041 | 1.851878 | C | 6.712220 | 0.553830 | -0.253743 |
| H | 5.584282 | -3.014968 | 0.208595 | C | 5.516440 | -1.476213 | -0.847864 |
| C | 4.333204 | -0.461138 | 2.235346 | C | 0.932100 | 2.478849 | -0.252707 |
| C | 3.399253 | -2.732978 | 1.936313 | C | 2.058790 | 3.063741 | 2.047213 |
| H | 4.935092 | 0.368478 | 1.864376 | C | -0.124415 | -3.805249 | 1.733802 |
| H | 3.354376 | -0.055621 | 2.513207 | H | -0.113580 | -3.872506 | -0.412486 |
| H | 4.816189 | -0.842594 | 3.146081 | H | -0.074361 | -3.418249 | 3.867210 |
| H | 3.347549 | -3.661233 | 1.362808 | C | 7.551601 | -0.195901 | 0.574220 |
| H | 3.906392 | -2.967835 | 2.882179 | H | 6.860948 | 1.622132 | -0.374602 |
| H | 2.380826 | -2.422091 | 2.184107 | C | 6.363281 | -2.207873 | -0.016299 |
| O | 2.428952 | 2.277759 | 0.069773 | H | 4.743240 | -1.970661 | -1.427129 |

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|---|-----------|-----------|-----------|------|-----------|-----------|-----------|
| H | -0.003723 | 2.860881 | 0.147896 | H | -5.821904 | 0.227863 | -2.879411 |
| H | 1.105383 | 2.667847 | -1.310535 | C | -3.462418 | 2.390468 | -1.478705 |
| H | 2.406718 | 4.103536 | 1.987372 | C | -3.065324 | 0.702994 | -3.232543 |
| H | 1.040930 | 3.088925 | 2.447698 | H | -4.048691 | 2.768904 | -0.643333 |
| H | 2.700404 | 2.537630 | 2.767133 | H | -2.422513 | 2.358449 | -1.146292 |
| H | -0.296313 | -4.871947 | 1.850197 | H | -3.543839 | 3.115453 | -2.300895 |
| C | 7.391308 | -1.582403 | 0.709282 | H | -3.423873 | -0.152712 | -3.809392 |
| H | 8.350412 | 0.306391 | 1.115009 | H | -3.088174 | 1.572057 | -3.903150 |
| H | 6.230054 | -3.284839 | 0.062705 | H | -2.018724 | 0.532883 | -2.958129 |
| C | 8.306536 | -2.393631 | 1.597054 | O | -2.011641 | 2.002723 | 1.260621 |
| H | 8.876596 | -3.127188 | 1.012803 | C | -2.044252 | 2.223727 | 2.639019 |
| H | 9.023705 | -1.755546 | 2.123231 | H | -1.078638 | 1.996546 | 3.136177 |
| H | 7.737067 | -2.952666 | 2.349997 | H | -2.795861 | 1.586628 | 3.148604 |
| H | 0.423982 | 0.948189 | 2.252762 | C | -2.384790 | 3.694482 | 2.918934 |
| C | -3.768604 | -2.085362 | -1.465940 | H | -3.362353 | 3.952803 | 2.494934 |
| C | -2.464771 | -2.362693 | -2.252540 | H | -2.413177 | 3.888479 | 4.000483 |
| C | -3.834737 | -3.162007 | -0.358097 | H | -1.636780 | 4.355531 | 2.464735 |
| C | -4.957307 | -2.298408 | -2.427659 | H | 4.232970 | 2.047237 | 0.760813 |
| H | -2.357820 | -1.747486 | -3.145433 | H | 3.789307 | 3.291590 | -0.441054 |
| H | -1.582303 | -2.214136 | -1.628438 | | | | |
| H | -2.471196 | -3.411352 | -2.581004 | | | | |
| H | -4.790484 | -3.169397 | 0.170051 | TS20 | | | |
| H | -3.719146 | -4.149926 | -0.824686 | Pd | 1.243682 | 0.416938 | 0.285481 |
| H | -3.029329 | -3.048323 | 0.374213 | P | 3.160906 | -1.267750 | -0.104016 |
| H | -4.952563 | -3.344515 | -2.766009 | C | -1.199952 | 0.899193 | -0.452769 |
| H | -5.926500 | -2.111724 | -1.960387 | C | -2.653507 | 1.024835 | -0.919350 |
| H | -4.884249 | -1.675471 | -3.322923 | C | -0.345754 | 1.906484 | 0.310505 |
| H | -6.410005 | -1.865827 | 0.175384 | N | -2.940842 | -0.393680 | -1.233495 |
| C | -6.433456 | -0.780837 | 0.306627 | H | -3.289011 | 1.415455 | -0.108724 |
| C | -5.063813 | -0.193565 | 0.705356 | H | -2.797160 | 1.633230 | -1.813745 |
| H | -6.834962 | -0.333703 | -0.606822 | C | -0.001115 | 3.203135 | -0.319807 |
| H | -7.149879 | -0.571650 | 1.113640 | S | -4.451799 | -0.871724 | -1.754001 |
| C | -4.569018 | -0.901834 | 1.991123 | C | -2.105129 | -1.337711 | -0.442896 |
| C | -5.262779 | 1.292213 | 1.083110 | C | -0.276301 | 3.506706 | -1.670825 |
| H | -3.623719 | -0.474859 | 2.340050 | C | 0.626859 | 4.205901 | 0.451495 |
| H | -5.318361 | -0.754943 | 2.781362 | O | -4.310961 | -2.277244 | -2.154483 |
| H | -4.429681 | -1.977152 | 1.870418 | O | -4.913964 | 0.164730 | -2.682805 |
| H | -5.880471 | 1.336355 | 1.990734 | C | -5.537038 | -0.829817 | -0.318518 |
| H | -4.308970 | 1.785234 | 1.287215 | C | -1.073430 | -0.432174 | 0.237641 |
| H | -5.793623 | 1.853419 | 0.309883 | C | 0.065775 | 4.743548 | -2.222556 |
| H | -6.074122 | 1.518427 | -1.694592 | H | -0.771741 | 2.776033 | -2.302674 |
| C | -5.408428 | 1.158255 | -2.482457 | C | 0.968543 | 5.439671 | -0.097935 |
| C | -3.947513 | 1.017863 | -2.002812 | H | 0.857372 | 4.001975 | 1.492184 |
| H | -5.440142 | 1.901417 | -3.291791 | C | -5.710401 | -1.981243 | 0.453786 |

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|---|-----------|-----------|-----------|------|-----------|-----------|-------------|
| C | -6.182708 | 0.364063 | 0.025357 | H | 3.499749 | 1.621194 | -0.880331 |
| C | -0.198388 | 0.258109 | -1.389797 | H | 5.073376 | 1.635241 | -1.689327 |
| C | -0.953377 | -0.699404 | 1.731000 | H | 3.750291 | 0.690475 | -2.372175 |
| C | 0.692724 | 5.718079 | -1.441774 | H | 6.063910 | 1.204589 | 0.385128 |
| H | -0.166536 | 4.946004 | -3.265542 | H | 4.544232 | 0.995708 | 1.278906 |
| H | 1.453589 | 6.187806 | 0.524638 | H | 5.829980 | -0.248274 | 1.349449 |
| C | -6.525891 | -1.926975 | 1.587357 | H | 5.809970 | -2.256071 | 1.462093 |
| H | -5.237411 | -2.910780 | 0.153274 | C | 5.011367 | -2.999862 | 1.426328 |
| C | -6.991747 | 0.398978 | 1.160120 | C | 3.605436 | -2.361493 | 1.444291 |
| H | -6.071123 | 1.241338 | -0.603900 | H | 5.121053 | -3.632048 | 2.319074 |
| H | 0.575620 | 0.893299 | -1.833622 | H | 5.178320 | -3.636710 | 0.554336 |
| H | -0.515361 | -0.540280 | -2.051071 | C | 3.467379 | -1.481930 | 2.708062 |
| H | -0.540386 | -1.695547 | 1.923781 | C | 2.569265 | -3.496275 | 1.608805 |
| H | -0.347361 | 0.026558 | 2.273227 | H | 4.133261 | -0.620882 | 2.715414 |
| H | -1.970101 | -0.686982 | 2.160511 | H | 2.447703 | -1.104113 | 2.816110 |
| H | 0.957097 | 6.681242 | -1.870664 | H | 3.698479 | -2.100137 | 3.587101 |
| C | -7.175230 | -0.741576 | 1.960699 | H | 2.685321 | -4.293015 | 0.870597 |
| H | -6.667608 | -2.825973 | 2.182815 | H | 2.711745 | -3.951921 | 2.597968 |
| H | -7.498843 | 1.325103 | 1.422471 | H | 1.539990 | -3.124594 | 1.566111 |
| C | -8.068784 | -0.688151 | 3.178137 | O | 2.451191 | 1.446821 | 1.615869 |
| H | -7.766139 | 0.116931 | 3.858945 | C | 1.963333 | 1.773764 | 2.880755 |
| H | -9.111500 | -0.496260 | 2.894340 | H | 1.737200 | 0.872029 | 3.488336 |
| H | -8.042821 | -1.629401 | 3.736390 | H | 1.016843 | 2.348340 | 2.839227 |
| H | -0.632598 | 2.027253 | 1.357206 | C | 2.997120 | 2.615689 | 3.640432 |
| C | 2.803851 | -2.474740 | -1.599560 | H | 3.221868 | 3.534985 | 3.086517 |
| C | 1.392075 | -3.085207 | -1.421324 | H | 2.622026 | 2.888398 | 4.636935 |
| C | 2.751763 | -1.655392 | -2.910388 | H | 3.933976 | 2.059748 | 3.765307 |
| C | 3.802747 | -3.635957 | -1.794830 | H | -2.690498 | -1.841275 | 0.338763 |
| H | 1.338323 | -3.814395 | -0.612693 | H | -1.706530 | -2.115812 | -1.099324 |
| H | 0.643857 | -2.313202 | -1.234671 | | | | |
| H | 1.116118 | -3.609211 | -2.346654 | Sub2 | | | |
| H | 3.729319 | -1.281133 | -3.220061 | C | 1.885715 | 0.672078 | 0.12456000 |
| H | 2.387060 | -2.308167 | -3.714840 | C | 0.717882 | 1.443679 | 0.70813300 |
| H | 2.063783 | -0.807922 | -2.840372 | C | 2.930264 | 0.356453 | 0.93053000 |
| H | 3.517798 | -4.195175 | -2.697499 | N | -0.542186 | 0.977962 | 0.09243700 |
| H | 4.832037 | -3.298544 | -1.932264 | H | 0.649239 | 1.301713 | 1.78685500 |
| H | 3.784195 | -4.345835 | -0.963888 | H | 0.860337 | 2.521644 | 0.51459300 |
| H | 5.557770 | -1.259363 | -2.304094 | C | 4.225022 | -0.255715 | 0.57757300 |
| C | 5.849006 | -0.913040 | -1.309212 | S | -1.962052 | 1.450362 | 0.90472800 |
| C | 4.714686 | -0.178118 | -0.564069 | C | -0.576190 | 1.185845 | -1.36315400 |
| H | 6.237963 | -1.767702 | -0.748616 | C | 4.792350 | -1.203330 | 1.45301800 |
| H | 6.681847 | -0.209554 | -1.448101 | C | 4.959716 | 0.103283 | -0.56935900 |
| C | 4.212389 | 1.002068 | -1.433641 | O | -2.510134 | 2.696681 | 0.34139300 |
| C | 5.312986 | 0.469397 | 0.707093 | O | -1.651993 | 1.366378 | 2.33865100 |

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| C | 1.380723 | -1.085553 | -0.08477400 | C | -5.125588 | 0.428352 | -0.76717100 |
| C | -0.106964 | -1.361057 | -0.00171900 | H | -3.967624 | 1.244807 | 0.86608700 |
| C | 2.252043 | -2.122098 | -0.17306500 | H | 7.625628 | -2.164510 | -0.51822700 |
| N | -0.699212 | -0.414596 | 0.95832100 | C | -5.399741 | -0.691085 | -1.56740100 |
| H | -0.571669 | -1.239097 | -0.99698400 | H | -4.871772 | -2.750405 | -1.94084800 |
| H | -0.296674 | -2.374219 | 0.35327100 | H | -5.685563 | 1.347967 | -0.92167000 |
| C | 3.720960 | -2.091029 | -0.25266000 | C | -6.479282 | -0.644262 | -2.62319500 |
| S | -2.152245 | -0.859798 | 1.69731500 | H | -6.237962 | -1.292376 | -3.47268200 |
| C | -0.567888 | 0.996721 | 0.57821800 | H | -7.440260 | -0.985104 | -2.21478100 |
| C | 4.513615 | -1.163244 | 0.45230500 | H | -6.626896 | 0.372889 | -3.00128800 |
| C | 4.380645 | -3.067163 | -1.02732800 | H | 1.820245 | -3.122619 | -0.21733200 |
| O | -2.444524 | 0.198380 | 2.67046700 | C | 1.726537 | 0.324759 | -0.14784200 |
| O | -1.993323 | -2.262262 | 2.09446200 | H | 2.740058 | 0.588035 | -0.43410900 |
| C | -3.437711 | -0.800264 | 0.43732900 | H | -1.281138 | 1.268912 | -0.22275800 |
| C | 0.834501 | 1.314879 | 0.10231700 | H | -0.825749 | 1.593492 | 1.45515500 |
| C | 5.905977 | -1.189245 | 0.35295100 | C | 1.170959 | 2.744118 | -0.10147500 |
| H | 4.038734 | -0.445553 | 1.11392300 | C | 2.014577 | 3.135099 | -1.16116300 |
| C | 5.770830 | -3.089618 | -1.13088600 | C | 0.668797 | 3.753161 | 0.74365100 |
| H | 3.788590 | -3.807587 | -1.56123100 | C | 2.358688 | 4.472575 | -1.35420500 |
| C | -3.694107 | -1.932078 | -0.34279900 | H | 2.383218 | 2.382627 | -1.85264600 |
| C | -4.153939 | 0.382750 | 0.23367100 | C | 1.012366 | 5.092374 | 0.54941100 |
| C | 6.541369 | -2.145144 | -0.44461600 | H | 0.027407 | 3.495091 | 1.58111700 |
| H | 6.496240 | -0.468258 | 0.91322700 | C | 1.859585 | 5.459762 | -0.49884900 |
| H | 6.253965 | -3.847175 | -1.74306200 | H | 3.007629 | 4.745584 | -2.18267500 |
| C | -4.669131 | -1.867687 | -1.33830500 | H | 0.620024 | 5.848727 | 1.22456700 |
| H | -3.153763 | -2.854367 | -0.15483400 | H | 2.123598 | 6.503000 | -0.65134900 |