

Supporting Information

Understanding the influence of metal centers on the mechanism and chemoselectivity of transition-metal-catalyzed cyclizations of dienyl aldehydes

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1. Detailed free energy profiles and additional results for Co(I) and (S,S)-BDPP ligand (L₁)

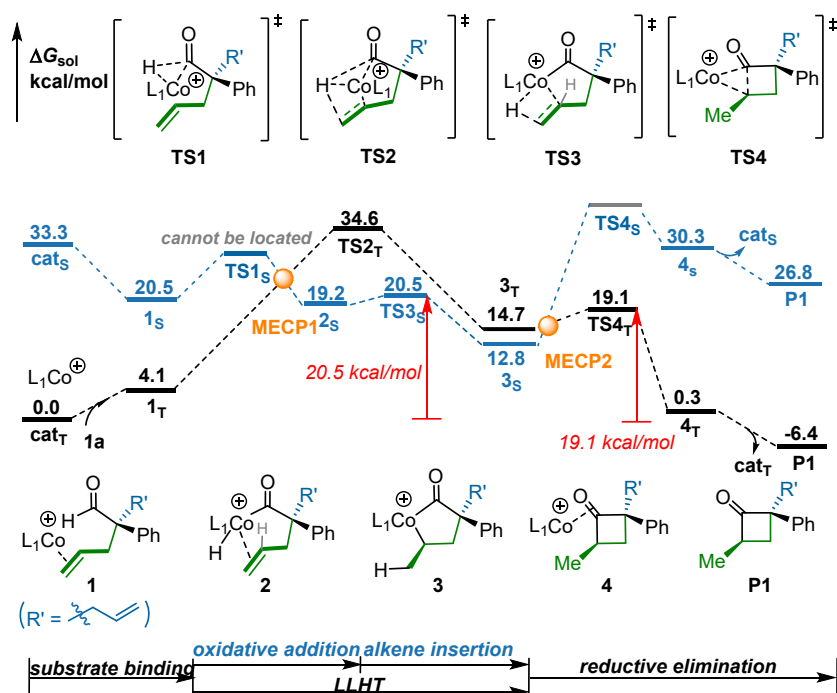


Fig. S1. Free energy profile for the formation of **P1** in the presence of Co(I) and (S,S)-BDPP ligand at the level of SMD(Acetonitrile)/B3LYP-D3(BJ)/def2-TZVPP//SMD(Acetonitrile)/B3LYP-D3(BJ)/def2-SVP. S and T refer to the singlet and triplet states, respectively.

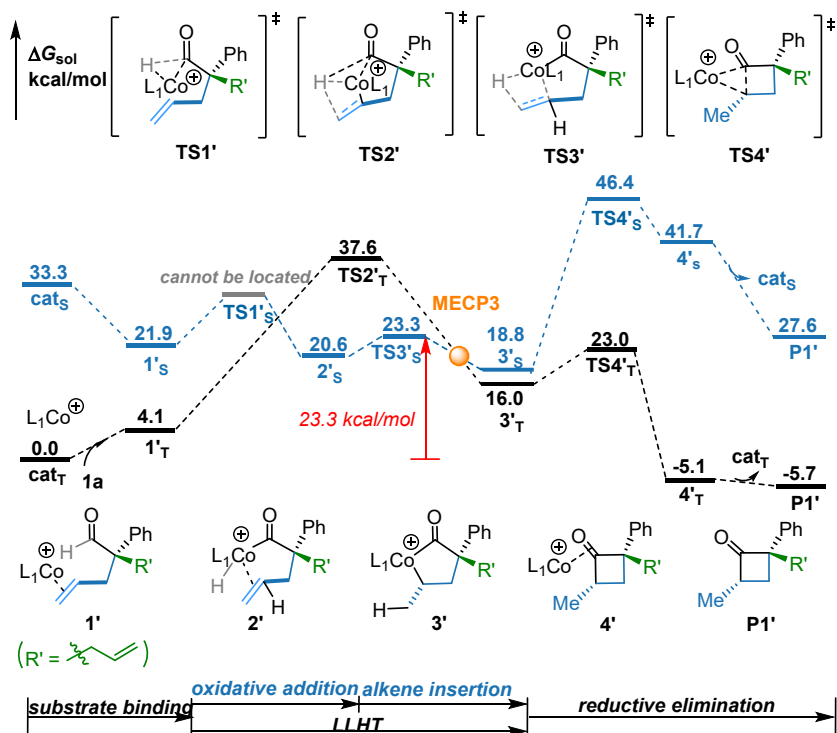


Fig. S2. Free energy profiles for the formation of **P1'** in the presence of Co(I) and (S,S)-BDPP ligand at the level of SMD(Acetonitrile)/B3LYP-D3(BJ)/def2-TZVPP//SMD(Acetonitrile)/B3LYP-D3(BJ)/def2-SVP. S and T refer to the singlet and triplet states, respectively.

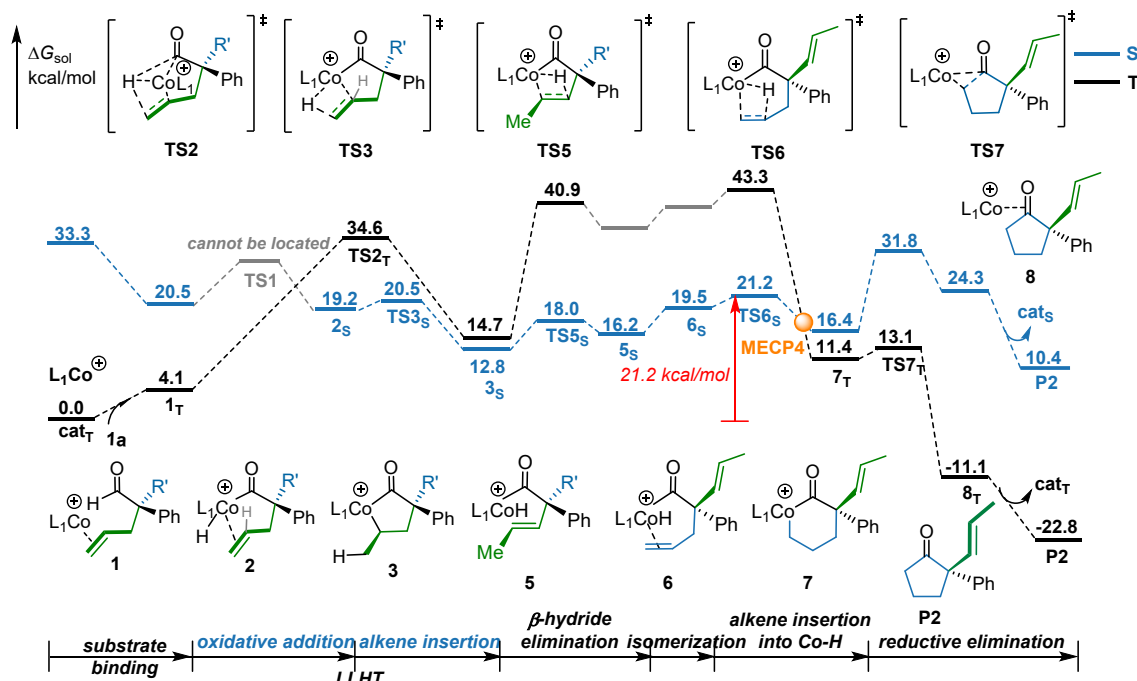


Fig. S3. Free energy profiles for the formation of **P2** in the presence of Co(I) and (*S,S*)-BDPP ligand at the level of SMD(Acetonitrile)/B3LYP-D3(BJ)/def2-TZVPP//SMD(Acetonitrile)/B3LYP-D3(BJ)/def2-SVP. S and T refer to the singlet and triplet states, respectively.

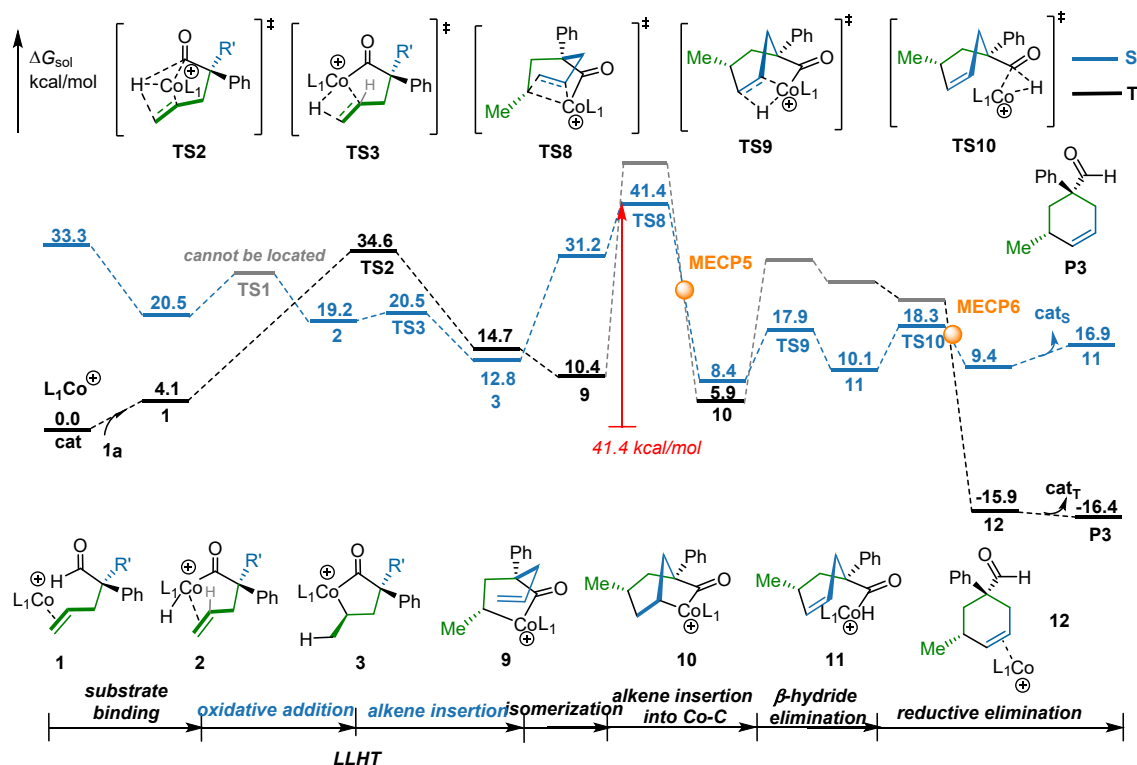


Fig. S4. Free energy profiles for the formation of **P3** in the presence of Co(I) and (*S,S*)-BDPP ligand at the level of SMD(Acetonitrile)/B3LYP-D3(BJ)/def2-TZVPP//SMD(Acetonitrile)/B3LYP-D3(BJ)/def2-SVP. S and T refer to the singlet and triplet states, respectively.

2. Comparison of three competitive pathways in the presence of (*S,S*)-BDPP ligand (L_1)

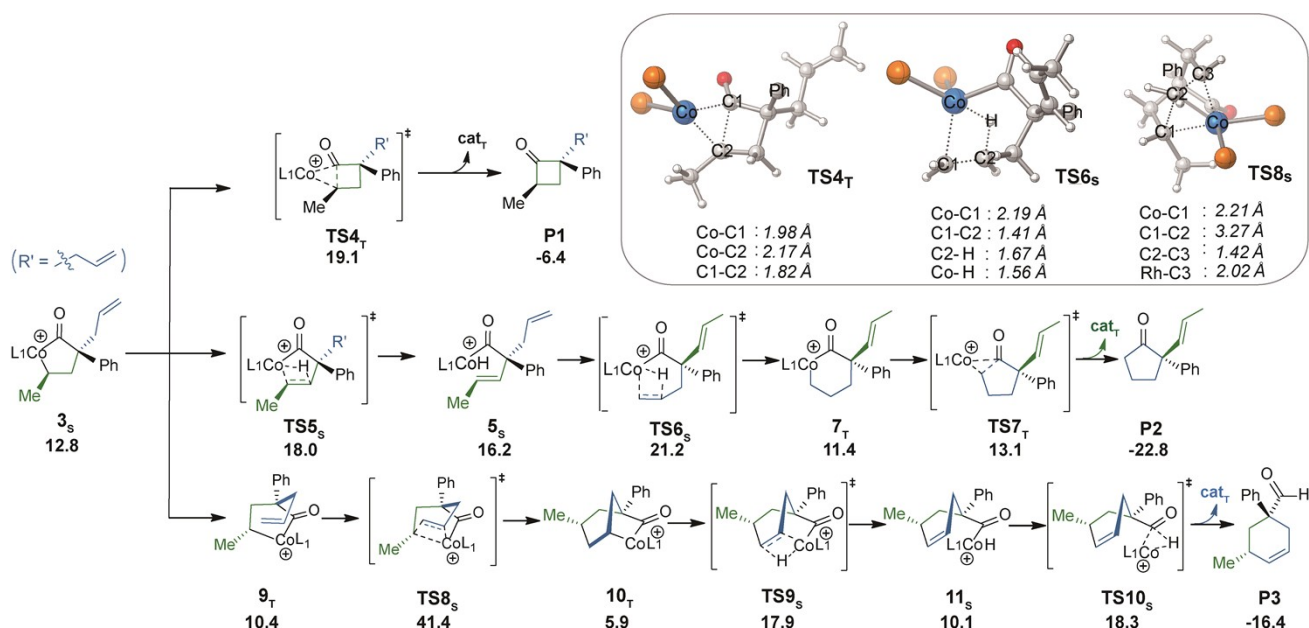


Fig. S5. Free energy profiles for three competitive pathways in the presence of Co(I) and (*S,S*)-BDPP ligand at the level of SMD(Acetonitrile)/B3LYP-D3(BJ)/def2-TZVPP//SMD(Acetonitrile)/B3LYP-D3(BJ)/def2-SVP. The subscripts S and T refer to the singlet and triplet states, respectively.

3. Detailed free energy profiles for Co(0) and (*S,S*)-BDPP ligand (L_1)

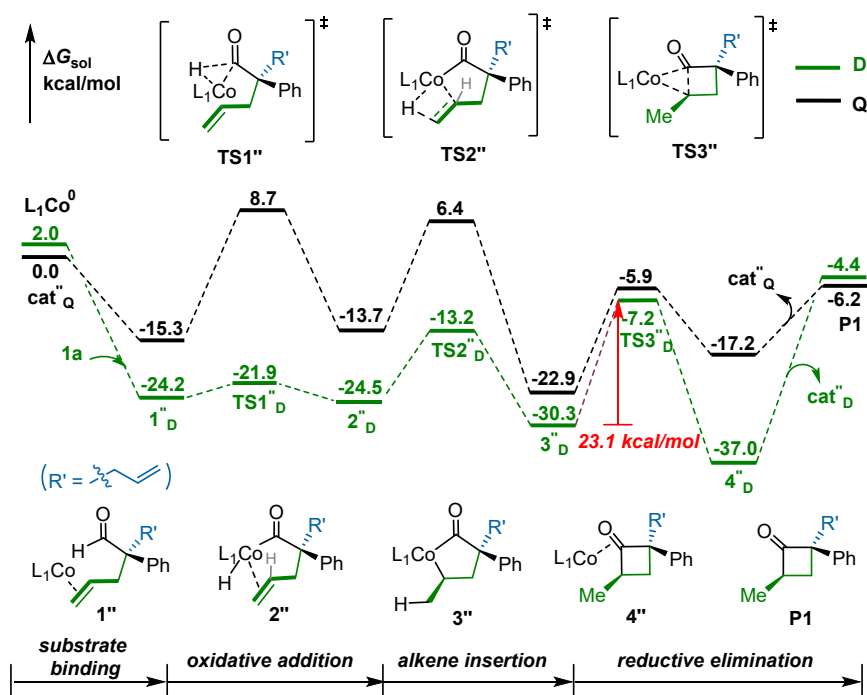


Fig. S6. Free energy profiles for the formation of **P1** in the presence of Co(0) and (*S,S*)-BDPP ligand at the level of SMD(Acetonitrile)/B3LYP-D3(BJ)/def2-TZVPP//SMD(Acetonitrile)/B3LYP-D3(BJ)/def2-SVP. D and Q refer to the doublet and quartet states, respectively.

4. The solvent effect on the chemoselectivity of the cyclization reactions of dienyl aldehydes.

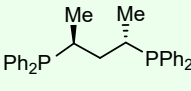
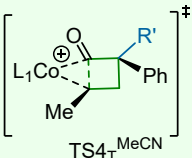
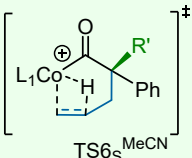
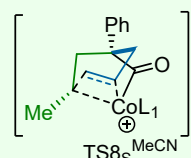
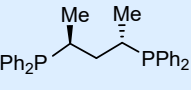
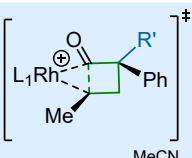
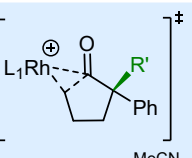

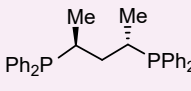
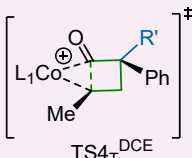
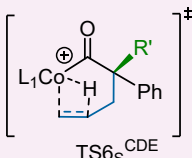
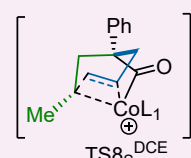
| Solvent | Metal | Ligand | Chemoselectivity-determining step for the formation of P1 | Chemoselectivity-determining step for the formation of P2 | Chemoselectivity-determining step for the formation of P3 |
|---------|-------|---|--|--|---|
| MeCN | Co |  $L_1=(S,S)\text{-BDPP}$ |  $TS4_{MeCN}$ 19.1 kcal/mol (<i>reductive elimination</i>) |  $TS6_{MeCN}$ 21.2 kcal/mol (<i>alkene insertion into Co-H</i>) |  $TS8_{MeCN}$ 41.1 kcal/mol (<i>alkene insertion into Co-C</i>) |
| MeCN | Rh |  $L_1=(S,S)\text{-BDPP}$ |  $TS4_{L_1Rh}^{MeCN}$ 31.3 kcal/mol (<i>reductive elimination</i>) |  $TS7_{L_1Rh}^{MeCN}$ 17.7 kcal/mol (<i>reductive elimination</i>) |  $TS8_{L_1Rh}^{MeCN}$ 34.0 kcal/mol (<i>alkene insertion into Co-C</i>) |
| DCE | Co |  $L_1=(S,S)\text{-BDPP}$ |  $TS4_{DCE}$ 15.8 kcal/mol (<i>reductive elimination</i>) |  $TS6_{DCE}$ 19.1 kcal/mol (<i>alkene insertion into Co-H</i>) |  $TS8_{DCE}$ 38.1 kcal/mol (<i>alkene insertion into Co-C</i>) |

Fig. S7. A comparison of the effects of ligands, transition metal centers, and solvents on the chemoselectivity of the cyclization reactions of dienyl aldehydes.

Since the Co- and Rh-catalyzed reactions differ in both ligand and solvent, we have also investigated the solvent effect on the chemoselectivity of the cyclization reactions of dienyl aldehydes. A comparison of the calculated results for $L_1Co(I)$ -catalyzed cyclization reactions in both MeCN and DCE indicates that the solvent is not a pivotal factor in regulating the reaction pathways.

5. Detailed free energy profiles and additional results for Rh(I) and (S,S)-BDPP ligand (L₁)

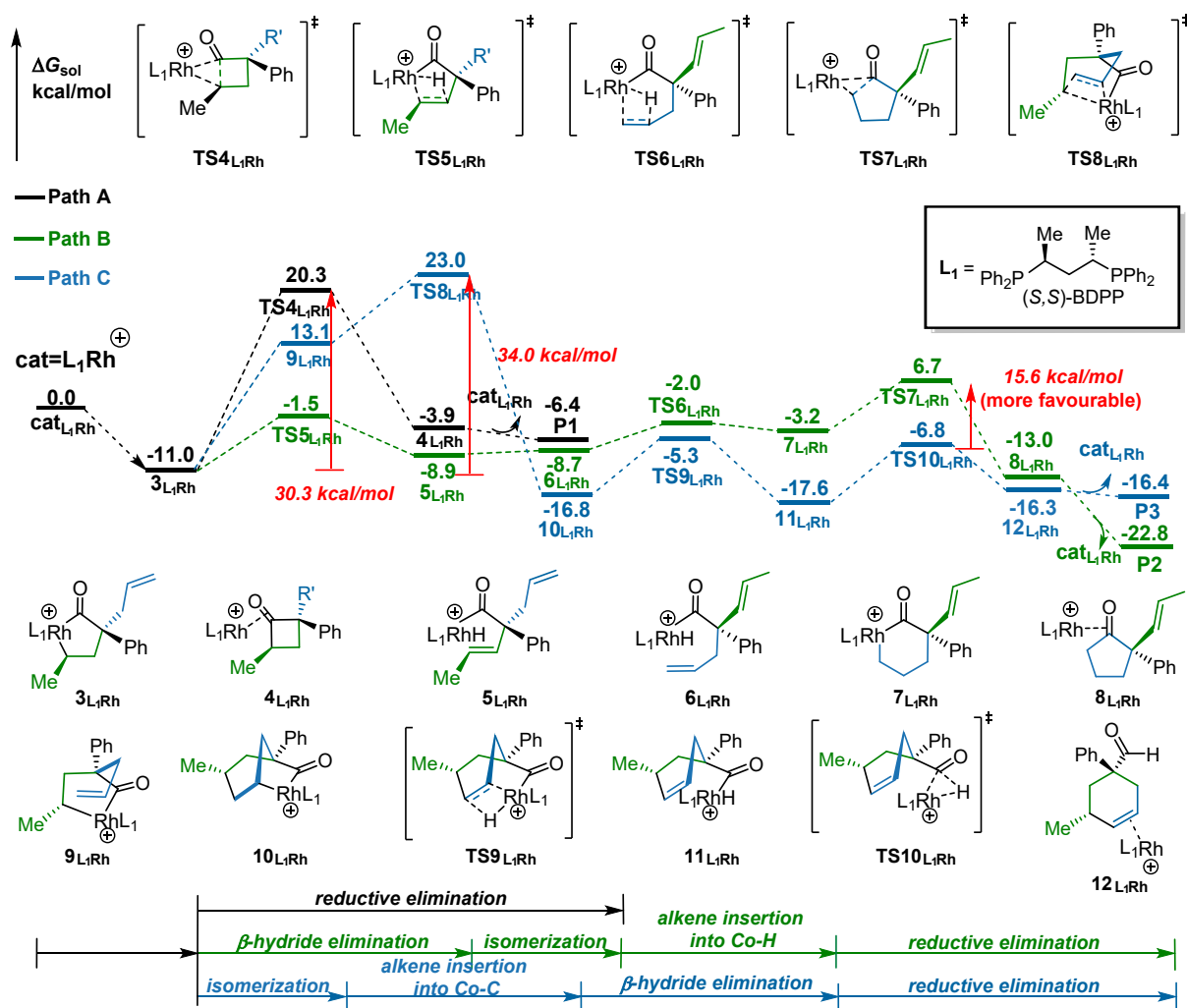


Fig. S8. Free energy profiles for the formation of **P1**, **P2** and **P3** in the presence of Rh(I) and (S,S)-BDPP ligand at the level of SMD(Acetonitrile)/B3LYP-D3(BJ)/def2-TZVPP//SMD(Acetonitrile)/B3LYP-D3(BJ)/def2-SVP/ECP28MDF_AVZDZ(Rh).

6. Detailed free energy profiles and additional results for Rh and (*R*)-MeO-BIPHEP ligand (L_2)

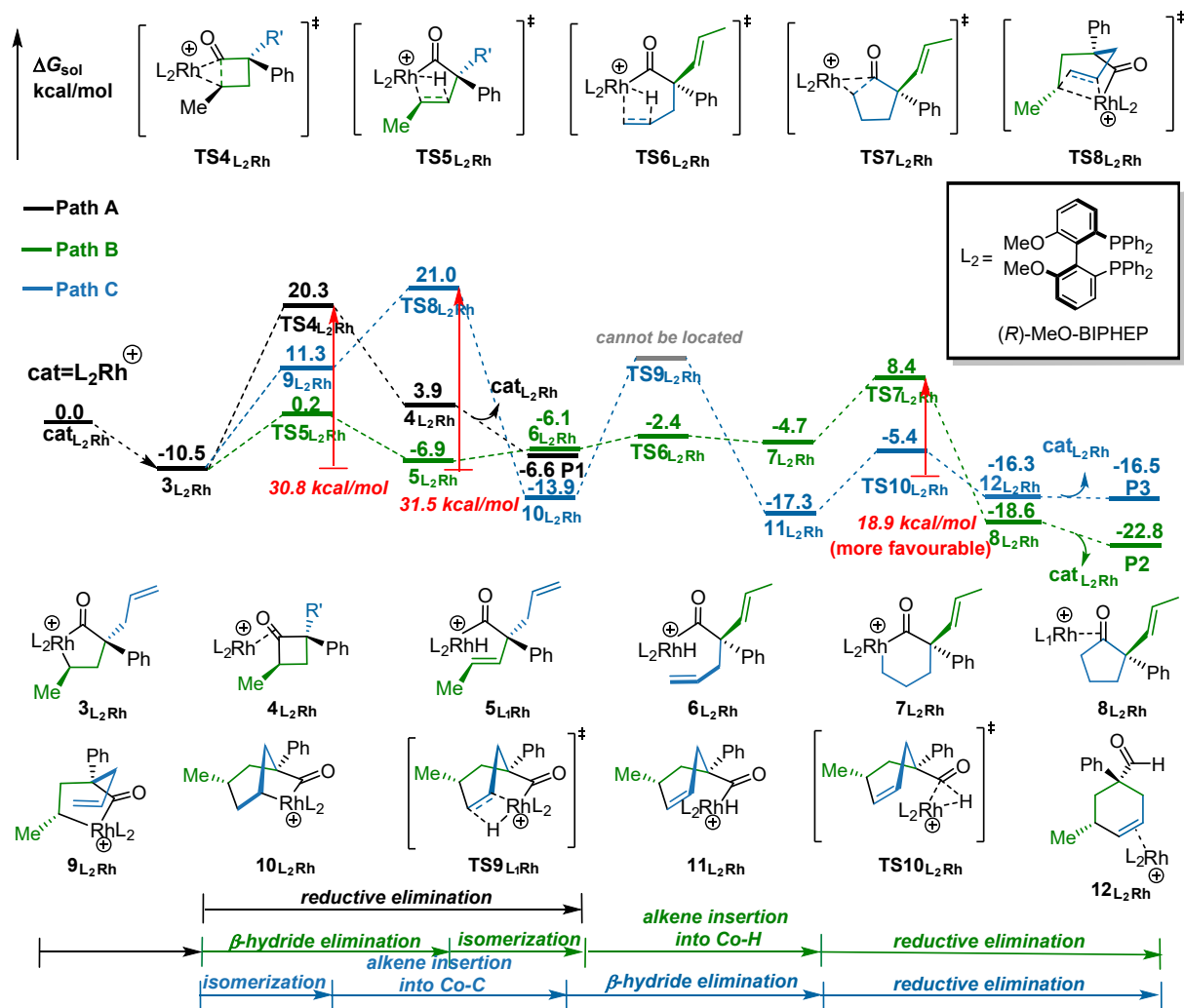


Fig. S9. Free energy profiles for the formation of **P1**, **P2** and **P3** in the presence of Rh(I) and (*R*)-MeO-BIPHEP ligand at the level of SMD(DiChloroEthane)/B3LYP-D3(BJ)/def2-TZVPP//SMD(DiChloroEthane)/B3LYP-D3(BJ)/def2-SVP/ECP28MDF_AVZDZ(Rh).

7. Electrostatic potential (ESP) surfaces and the surface areas for $3s$ and 3_{L1Rh}

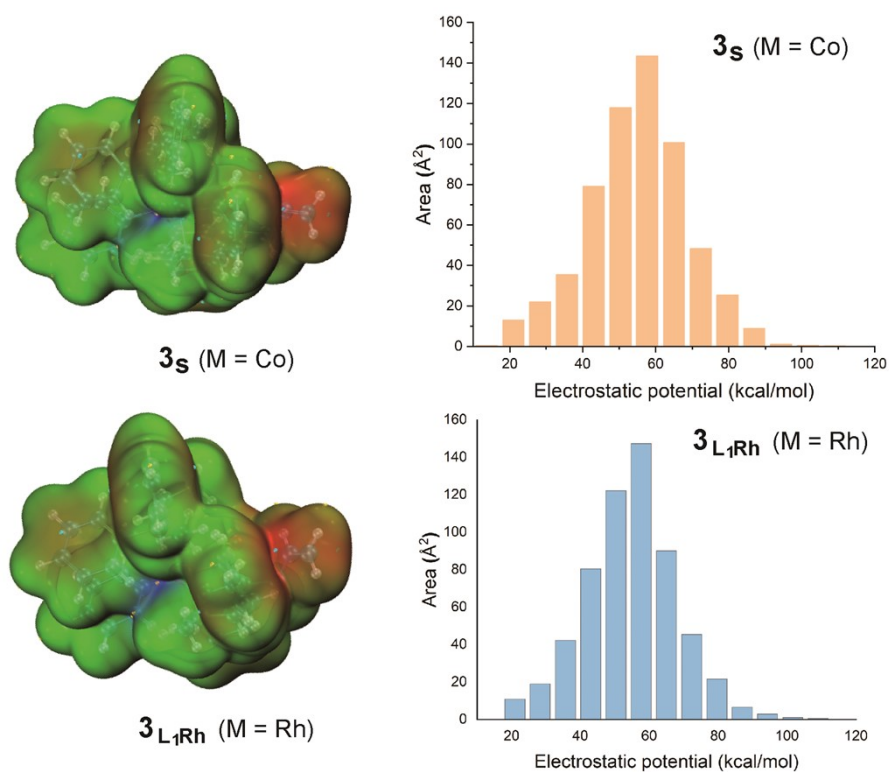


Fig. S10. Electrostatic potential (ESP) surfaces for $3s$ and 3_{L1Rh} .

8. ETS-NOCV analysis for the cobaltacycle intermediate $3s$ and rhodacycle intermediate 3_{L1Rh} .

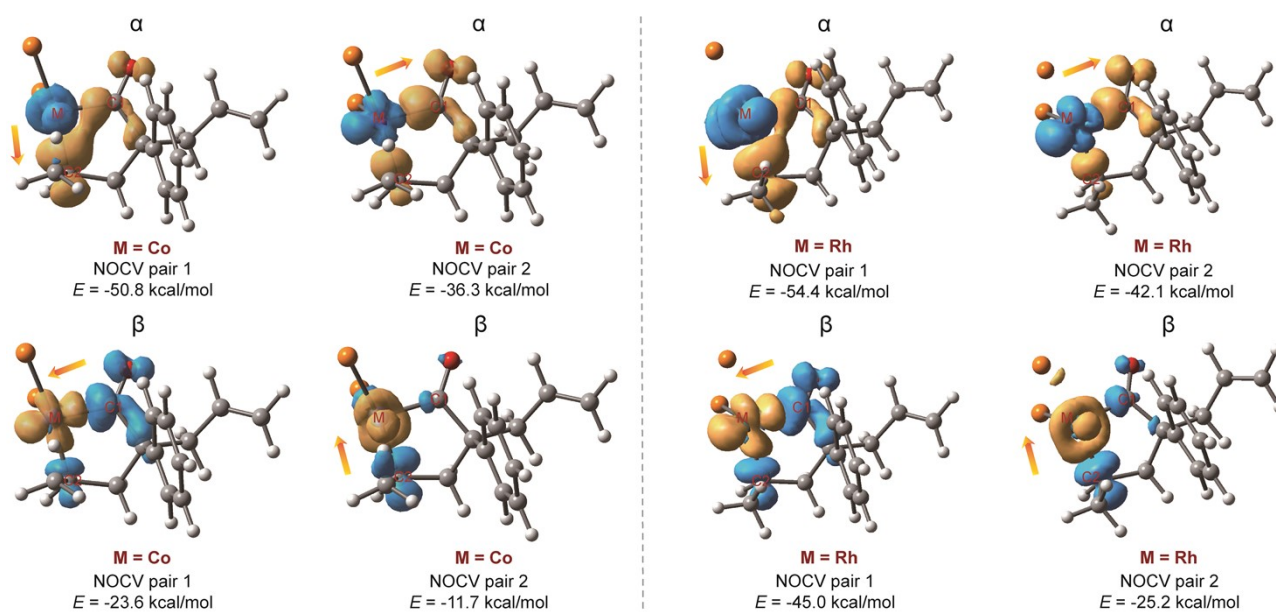


Fig. S11. The dominant orbital interactions revealed by the ETS-NOCV analysis for the cobaltacycle intermediate $3s$ and rhodacycle intermediate 3_{L1Rh} (isovalue = 0.003).

9. Results of the minimum energy crossing points

The minimum energy crossing points (MECPs) were searched at SMD(Acetonitrile)/B3LYP-D3(BJ)/def2-SVP level via sobMECP, which is a modified version of Harvey's MECP program by Tian Lu^[S1].

Table S1. Calculated energies of the MECPs

| Low-spin state (energies in a.u.) | High-spin state (energies in a.u.) | MECPs (energies in a.u.) |
|--|--|-----------------------------|
| 3_S-R (-3805.604041) | 3_T-R (-3805.593597) | MECP2 (-3805.586345) |
| 3_S-S (-3805.593866) | 3_T-S (-3805.590818) | MECP3 (-3805.586776) |
| 7_S-R (-3805.584757) | 7_T-R (-3805.584757) | MECP4 (-3805.584454) |
| 10_S-R (-3805.625725) | 10_T-R (-3805.624627) | MECP5 (-3805.622377) |
| 12_S-R (-3805.608419) | 12_T-R (-3805.644442) | MECP6 (-3805.607435) |

For the L₁Co(I)-catalyzed cyclization of **1a**, the reaction initiates on the triplet potential energy surface before reaching point B (see Fig. S12), which approximates the location of MECP1. Following this spin surface crossing, hydrogen transfer is completed via an alkene insertion step, as represented by transition state **TS3_S**. The changes of structures along the minimum energy path of triplet state and singlet states are shown in Fig. S12.

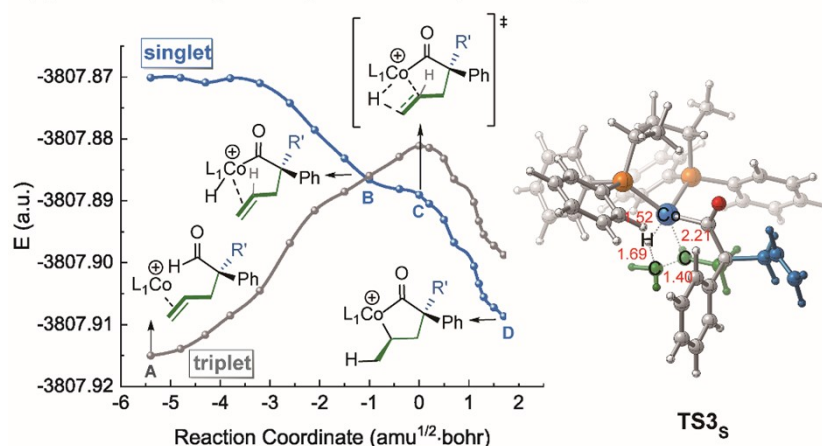


Fig. S12. Electronic energies along the minimum energy path of triplet state and singlet states.

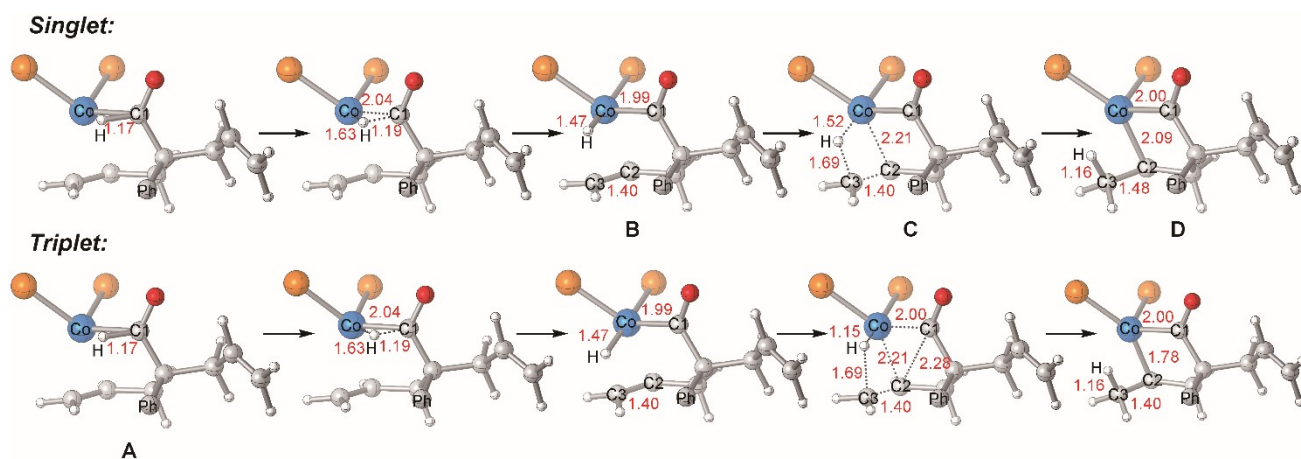


Fig. S13. The changes of structures along the minimum energy path of triplet state and singlet states.

References

[S1] (a) J. N. Harvey, M. Aschi, H. Schwarz and W. Koch, The singlet and triplet states of phenyl cation. A hybrid approach for locating minimum energy crossing points between non-interacting potential energy surfaces, *Theor. Chem. Acc.*, 1998, **99**, 95-99. (b) Tian Lu, sobMECP program, <http://sobereva.com/286>

10. Calculated energies and imaginary frequencies

Table S2. Calculated energies and imaginary frequencies for Co.

| Stationary point | Corrected thermal correction to Gibbs free energy at B3LYP-D3(BJ)/def2SVP (in a.u.) | Single-point energy including solvation energy at B3LYP-D3(BJ)/def2-TZVPP (in a.u.) | Imaginary frequencies (in cm^{-1}) |
|-------------------------|---|---|--|
| 1a | 0.211739 | -618.606239 | |
| P1 | 0.214437 | -618.619164 | |
| P1' | 0.214649 | -618.618217 | |
| P2 | 0.216625 | -618.647483 | |
| P3 | 0.218865 | -618.639413 | |
| cat_s | 0.441130 | -3189.252257 | |
| cat_T | 0.435279 | -3189.299400 | |
| 1_s | 0.683918 | -3807.906584 | |
| 1_T | 0.679416 | -3807.928093 | |
| TS2_T | 0.681060 | -3807.881149 | 742.04 <i>i</i> |
| 2_s | 0.688436 | -3807.913163 | |
| TS3_s | 0.686628 | -3807.909184 | 610.34 <i>i</i> |
| 3_s | 0.688832 | -3807.923681 | |
| 3_T | 0.683761 | -3807.915577 | |
| TS4_T | 0.683002 | -3807.907876 | 153.96 <i>i</i> |
| 4_s | 0.686350 | -3807.893306 | |
| 4_T | 0.682504 | -3807.937274 | |
| 1'_s | 0.684994 | -3807.905285 | |
| 1'_T | 0.679149 | -3807.926378 | |
| TS2'_T | 0.678528 | -3807.873952 | 896.66 <i>i</i> |
| 2'_s | 0.689422 | -3807.911881 | |
| TS3'_s | 0.689316 | -3807.907382 | 657.51 <i>i</i> |
| 3'_s | 0.688268 | -3807.913653 | |

| | | | |
|-------------------------|----------|--------------|-----------------|
| 3'_T | 0.682319 | -3807.912028 | |
| TS4'_s | 0.688916 | -3807.893306 | 306.57 <i>i</i> |
| TS4'_T | 0.679888 | -3807.898636 | 225.69 <i>i</i> |
| 4'_s | 0.684209 | -3807.873036 | |
| 4'_T | 0.680345 | -3807.943756 | |
| TS5_s | 0.682406 | -3807.908999 | 418.32 <i>i</i> |
| TS5_T | 0.677657 | -3807.867698 | 719.26 <i>i</i> |
| 5_s | 0.684979 | -3807.914486 | |
| 6_s | 0.686845 | -3807.911104 | |
| TS6_s | 0.684575 | -3807.906009 | 701.25 <i>i</i> |
| TS6_T | 0.680291 | -3807.866599 | 712.22 <i>i</i> |
| 7_s | 0.691820 | -3807.920454 | |
| 7_T | 0.682355 | -3807.919462 | |
| TS7_s | 0.687065 | -3807.891616 | 303.84 <i>i</i> |
| TS7_T | 0.681746 | -3807.916102 | 229.37 <i>i</i> |
| 8_s | 0.688368 | -3807.904834 | |
| 8_T | 0.681314 | -3807.954329 | |
| 9_s | 0.691049 | -3807.895750 | |
| 9_T | 0.681644 | -3807.920277 | |
| TS8_s | 0.694809 | -3807.884093 | 320.25 <i>i</i> |
| 10_s | 0.697501 | -3807.939380 | |
| 10_T | 0.693638 | -3807.939518 | |
| TS9_s | 0.686421 | -3807.913227 | 631.93 <i>i</i> |
| 11_s | 0.688597 | -3807.927702 | |
| TS10_s | 0.687948 | -3807.914000 | 836.47 <i>i</i> |
| 12_s | 0.688076 | -3807.928427 | |
| 12_T | 0.685401 | -3807.966006 | |
| cat"_D | 0.434605 | -3189.356467 | |
| cat"_Q | 0.434607 | -3189.359713 | |

| | | | |
|--------------------------------------|----------|--------------|-----------------|
| 1^{''}_D | 0.679211 | -3808.034033 | |
| 1^{''}_Q | 0.679093 | -3808.019666 | |
| TS1^{''}_D | 0.679953 | -3808.031154 | 742.97 <i>i</i> |
| TS1^{''}_Q | 0.671982 | -3807.974325 | 527.51 <i>i</i> |
| 2^{''}_D | 0.678977 | -3808.034341 | |
| 2^{''}_Q | 0.671583 | -3808.009681 | |
| TS2^{''}_D | 0.680978 | -3808.01819 | 709.81 <i>i</i> |
| TS2^{''}_Q | 0.670503 | -3807.97661 | 897.92 <i>i</i> |
| 3^{''}_D | 0.679301 | -3808.043858 | |
| 3^{''}_Q | 0.675640 | -3808.027731 | |
| TS3^{''}_D | 0.681045 | -3808.006838 | 115.37 <i>i</i> |
| TS3^{''}_Q | 0.678087 | -3807.996775 | 284.42 <i>i</i> |
| 4^{''}_D | 0.684589 | -3808.059836 | |
| 4^{''}_Q | 0.678150 | -3808.02182 | |
| cat_S^{DCE} | 0.443999 | -3189.244593 | |
| cat_T^{DCE} | 0.438384 | -3189.290882 | |
| TS4_T^{DCE} | 0.683427 | -3807.90169 | 160.97 <i>i</i> |
| TS6_S^{DCE} | 0.686214 | -3807.899194 | 689.87 <i>i</i> |
| TS8_S^{DCE} | 0.69735 | -3807.880183 | 318.98 <i>i</i> |

Table S3. Calculated energies and imaginary frequencies for Rh.

| Stationary point | Corrected thermal correction to Gibbs free energy at B3LYP-D3(BJ)/def2SVP ECP60MDF_AVDZ(Rh) (in a.u.) | Single-point energy including solvation energy at B3LYP-D3(BJ)/def2-TZVPP (in a.u.) | Imaginary frequencies (in cm ⁻¹) |
|-----------------------------|---|---|--|
| cat _{L1Rh} | 0.444477 | -1917.117249 | |
| 3 _{L1Rh} | 0.691140 | -2535.772158 | |
| TS4 _{L1Rh} | 0.688465 | -2535.720114 | 178.94 <i>i</i> |
| 4 _{L1Rh} | 0.684651 | -2535.754706 | |
| TS5 _{L1Rh} | 0.684051 | -2535.750430 | 758.81 <i>i</i> |
| 5 _{L1Rh} | 0.685126 | -2535.763304 | |
| 6 _{L1Rh} | 0.685655 | -2535.763438 | |
| TS6 _{L1Rh} | 0.685655 | -2535.752752 | 677.64 <i>i</i> |
| 7 _{L1Rh} | 0.692354 | -2535.761360 | |
| TS7 _{L1Rh} | 0.689055 | -2535.742223 | 386.57 <i>i</i> |
| 8 _{L1Rh} | 0.687098 | -2535.771788 | |
| 9 _{L1Rh} | 0.688226 | -2535.731297 | |
| TS8 _{L1Rh} | 0.695699 | -2535.722975 | 304.81 <i>i</i> |
| 10 _{L1Rh} | 0.701197 | -2535.791827 | |
| TS9 _{L1Rh} | 0.686184 | -2535.758611 | 483.42 <i>i</i> |
| 11 _{L1Rh} | 0.69001 | -2535.781975 | |
| TS10 _{L1Rh} | 0.68886 | -2535.763580 | 526.20 <i>i</i> |
| 12 _{L1Rh} | 0.692414 | -2535.782333 | |
| cat _{L2Rh} | 0.520221 | -2411.929072 | |
| 3 _{L2Rh} | 0.768403 | -3030.584948 | |
| TS4 _{L2Rh} | 0.763333 | -3030.530815 | 111.83 <i>i</i> |
| 4 _{L2Rh} | 0.769983 | -3030.563541 | |
| TS5 _{L2Rh} | 0.760154 | -3030.559563 | 722.56 <i>i</i> |
| 5 _{L2Rh} | 0.761618 | -3030.572440 | |
| 6 _{L2Rh} | 0.763136 | -3030.572616 | |
| TS6 _{L2Rh} | 0.76257 | -3030.566117 | 537.18 <i>i</i> |
| 7 _{L2Rh} | 0.766165 | -3030.573406 | |

| | | | |
|-----------------------------|----------|--------------|-----------------|
| TS7 _{L2Rh} | 0.764022 | -3030.550414 | 401.51 <i>i</i> |
| 8 _{L2Rh} | 0.767024 | -3030.596508 | |
| 9 _{L2Rh} | 0.764445 | -3030.546229 | |
| TS8 _{L2Rh} | 0.771202 | -3030.537586 | 299.01 <i>i</i> |
| 10 _{L2Rh} | 0.774128 | -3030.596028 | |
| 11 _{L2Rh} | 0.766123 | -3030.593483 | |
| TS10 _{L2Rh} | 0.766073 | -3030.574396 | 420.68 <i>i</i> |
| 12 _{L2Rh} | 0.766533 | -3030.592314 | |

11. Cartesian coordinates of all optimized structures

1a

| | | | |
|---|-------------|-------------|-------------|
| C | 0.77505500 | -0.45557000 | 0.06427100 |
| C | 1.39321400 | -1.19092100 | -0.95946800 |
| C | 2.74691700 | -1.53069600 | -0.88391000 |
| C | 3.51154300 | -1.14702300 | 0.22199600 |
| C | 2.91079200 | -0.41180400 | 1.24698800 |
| C | 1.55875800 | -0.06658600 | 1.16389800 |
| H | 0.82274400 | -1.49813000 | -1.83708100 |
| H | 3.20555600 | -2.10020900 | -1.69639200 |
| H | 4.56900000 | -1.41633900 | 0.28219400 |
| H | 3.49580000 | -0.09836500 | 2.11537100 |
| H | 1.11900700 | 0.52717300 | 1.96893200 |
| C | -0.68643200 | -0.01427900 | -0.04058300 |
| C | -1.25336600 | 0.16828800 | 1.36283400 |
| O | -1.79418200 | 1.16605100 | 1.77764300 |
| H | -1.16210600 | -0.74279000 | 2.00543400 |
| C | -1.56176500 | -1.14318900 | -0.67748500 |
| H | -1.38021200 | -2.07997100 | -0.12775300 |
| H | -1.20890800 | -1.29476700 | -1.70934800 |
| C | -0.80183300 | 1.29183700 | -0.87270400 |
| H | -1.85343800 | 1.62022800 | -0.83718200 |
| H | -0.56466600 | 1.04655800 | -1.91978100 |
| C | -3.03442800 | -0.84522000 | -0.70618200 |
| C | -3.95432700 | -1.49930700 | 0.01009800 |
| H | -3.35590200 | -0.03032700 | -1.36550200 |
| H | -5.01644100 | -1.24220300 | -0.05137100 |
| H | -3.67842400 | -2.31932300 | 0.68297700 |
| C | 0.07140400 | 2.41873900 | -0.40370700 |
| C | 1.07509600 | 2.94862500 | -1.10946600 |
| H | -0.15230600 | 2.81373600 | 0.59339800 |
| H | 1.67636000 | 3.77538900 | -0.71806800 |
| H | 1.33361200 | 2.57357200 | -2.10644700 |

P1

| | | | |
|---|------------|-------------|-------------|
| C | 0.73499800 | -0.39823600 | -0.14228200 |
| C | 1.44926000 | -1.04943800 | -1.16094200 |
| C | 2.73288000 | -1.54970500 | -0.92674000 |
| C | 3.32304500 | -1.40862300 | 0.33401700 |
| C | 2.61975200 | -0.76176200 | 1.35450500 |
| C | 1.33765500 | -0.25547400 | 1.11755500 |

| | | | |
|---|-------------|-------------|-------------|
| H | 0.99652800 | -1.16483200 | -2.14901400 |
| H | 3.27376600 | -2.05369500 | -1.73206400 |
| H | 4.32596400 | -1.80164600 | 0.51937400 |
| H | 3.07156000 | -0.64742100 | 2.34346000 |
| H | 0.79001300 | 0.24432900 | 1.91712400 |
| C | -0.63016600 | 0.18036000 | -0.43325700 |
| C | -1.68594000 | 0.10817900 | 0.68838600 |
| O | -1.65831800 | 0.32284100 | 1.87450400 |
| H | -2.88273000 | -2.46528800 | 0.60037600 |
| C | -1.61608600 | -0.68291200 | -1.29109800 |
| H | -1.30383500 | -1.73500000 | -1.34091800 |
| H | -1.81283900 | -0.30853200 | -2.30426500 |
| C | -0.51624100 | 1.63285400 | -0.98793700 |
| H | -1.53185800 | 1.97776600 | -1.24938700 |
| H | 0.06582900 | 1.58554200 | -1.92242500 |
| C | -2.74808100 | -0.46730000 | -0.24382400 |
| C | -3.54972800 | -1.65402500 | 0.26589400 |
| H | -3.42078700 | 0.35110000 | -0.55606600 |
| H | -4.18257700 | -1.36029200 | 1.11856900 |
| H | -4.20608600 | -2.05426100 | -0.52324100 |
| C | 0.10598200 | 2.60052100 | -0.02718100 |
| C | 1.27414100 | 3.22126200 | -0.21670300 |
| H | -0.45340000 | 2.78303300 | 0.89869300 |
| H | 1.67984800 | 3.91769500 | 0.52381300 |
| H | 1.86832300 | 3.05456900 | -1.12241600 |

P1'

| | | | |
|---|-------------|-------------|-------------|
| C | -1.18858000 | 0.53623600 | 0.79593700 |
| O | -1.16811700 | 0.47043800 | 1.99853400 |
| H | -2.67989100 | 3.03987500 | 1.02868000 |
| C | 1.14690500 | -0.09004500 | -0.14287800 |
| C | 1.99046800 | 0.18279300 | -1.23090700 |
| C | 3.38015200 | 0.17275600 | -1.07697000 |
| C | 3.94816100 | -0.10738000 | 0.16984700 |
| C | 3.11540100 | -0.38129300 | 1.25991400 |
| C | 1.72640800 | -0.37763300 | 1.10407200 |
| H | 1.55813300 | 0.40251900 | -2.20991500 |
| H | 4.02143600 | 0.38648000 | -1.93614800 |
| H | 5.03431000 | -0.11171200 | 0.29166500 |
| H | 3.54958200 | -0.59917400 | 2.23932100 |
| H | 1.07807700 | -0.58610500 | 1.95668200 |
| C | -0.35563800 | -0.13376500 | -0.32117400 |
| C | -0.80138400 | -1.60675200 | -0.55511200 |
| H | -0.41953900 | -2.20869500 | 0.28429600 |

| | | | | | | | |
|----|-------------|-------------|-------------|----------------|-------------|-------------|-------------|
| H | -0.28695700 | -1.94983700 | -1.46949500 | H | 2.50734200 | -2.76896800 | -1.23547200 |
| C | -0.99464800 | 0.90626300 | -1.30244300 | H | 2.43599700 | -2.07538600 | 1.46753800 |
| H | -1.45489400 | 0.48798600 | -2.20665000 | H | 3.51646100 | -1.20765400 | 0.35828400 |
| H | -0.28580200 | 1.69464200 | -1.58870900 | | | | |
| C | -2.28271700 | -1.81156700 | -0.69668800 | P3 | | | |
| C | -3.05098900 | -2.42080400 | 0.21216100 | C | 1.25700400 | 0.13096500 | -0.00482200 |
| H | -2.74675200 | -1.41727700 | -1.60874500 | C | 1.81388600 | -1.15864900 | -0.09014000 |
| H | -4.12891600 | -2.53989500 | 0.06432800 | C | 3.18770600 | -1.34218600 | -0.25260000 |
| H | -2.62699400 | -2.82546200 | 1.13832600 | C | 4.04080600 | -0.23599200 | -0.32534800 |
| C | -1.97609900 | 1.38868900 | -0.19391700 | C | 3.50376700 | 1.04918300 | -0.22703700 |
| C | -2.09155000 | 2.87443400 | 0.11205800 | C | 2.12596100 | 1.23141400 | -0.06380800 |
| H | -2.97667400 | 0.93938700 | -0.32090900 | H | 1.16327300 | -2.03237700 | -0.01827900 |
| H | -2.58937400 | 3.40779600 | -0.71345500 | H | 3.59381100 | -2.35475800 | -0.31851400 |
| H | -1.09615000 | 3.32436800 | 0.25905100 | H | 5.11714000 | -0.37638500 | -0.45216400 |
| | | | | H | 4.15922500 | 1.92255500 | -0.27575900 |
| P2 | | | | H | 1.73914400 | 2.24738100 | 0.01078400 |
| C | -0.62996000 | -0.21672800 | -0.18382700 | C | -0.26663900 | 0.27935400 | 0.15932600 |
| C | -1.62891900 | 0.15933200 | -1.09809600 | C | -0.56106600 | -0.41969900 | 1.48707700 |
| C | -2.96667500 | -0.17397700 | -0.88112200 | O | -0.93174000 | -1.56276500 | 1.61298400 |
| C | -3.33749300 | -0.89833400 | 0.25795200 | H | -3.04061600 | -1.75108800 | 0.52618700 |
| C | -2.35416600 | -1.28591000 | 1.16978300 | C | -1.00266400 | -0.38073700 | -1.02949300 |
| C | -1.01316900 | -0.94877800 | 0.94990200 | H | -0.72094100 | -1.44017800 | -1.10040500 |
| H | -1.35279400 | 0.72989800 | -1.98733600 | H | -0.61548500 | 0.10673800 | -1.93772300 |
| H | -3.72519900 | 0.13577200 | -1.60482400 | C | -0.71524200 | 1.74329100 | 0.29460200 |
| H | -4.38503800 | -1.15697800 | 0.43134100 | H | -0.30780800 | 2.33281400 | -0.54469500 |
| H | -2.62618900 | -1.85285100 | 2.06386200 | H | -0.28944600 | 2.18821500 | 1.20883600 |
| H | -0.27166300 | -1.25868100 | 1.68801500 | C | -2.54768200 | -0.26085600 | -1.00795900 |
| C | 0.83326100 | 0.13403100 | -0.49784900 | C | -3.27175500 | -1.52788500 | -0.52402600 |
| C | 1.72346200 | -0.15511100 | 0.75063800 | H | -2.86205300 | -0.11773200 | -2.05893300 |
| O | 1.81735800 | 0.56441100 | 1.71619500 | H | -4.36369000 | -1.40988800 | -0.62187900 |
| H | -0.47398900 | 1.88133200 | 1.34214300 | H | -2.97368400 | -2.39989400 | -1.12849900 |
| C | 1.01411200 | 1.56521000 | -0.96671600 | C | -2.21505500 | 1.85827100 | 0.31354500 |
| H | 1.65145100 | 1.67512100 | -1.85065300 | C | -3.02306600 | 0.95676000 | -0.25909100 |
| H | 0.94159900 | -2.70245200 | -0.39986400 | H | -0.34639600 | 0.21327500 | 2.38563200 |
| C | 1.39037700 | -0.89295500 | -1.52486600 | H | -4.10883800 | 1.09989700 | -0.21004300 |
| H | 2.27398100 | -0.45344900 | -2.01696300 | H | -2.64547400 | 2.73415100 | 0.81021800 |
| H | 0.65718800 | -1.13574000 | -2.30706300 | | | | |
| C | 0.51958700 | 2.68362200 | -0.41586000 | L ₁ | | | |
| C | -0.35831500 | 2.82033700 | 0.78979300 | P | 1.54980100 | -0.48813400 | -0.19841000 |
| H | 0.77417000 | 3.62744600 | -0.91541900 | C | 1.18373200 | -1.24413600 | 1.48891800 |
| H | 0.06026200 | 3.57213000 | 1.48106800 | C | -0.22172100 | -0.90134500 | 2.01935800 |
| H | -1.36042100 | 3.18764000 | 0.50150900 | C | -1.45391700 | -1.51039000 | 1.32184800 |
| C | 1.82125000 | -2.10567900 | -0.68940700 | P | -1.83685700 | -0.88224200 | -0.41520700 |
| C | 2.45964400 | -1.47047300 | 0.54871900 | C | -3.69655200 | -0.96376000 | -0.45277400 |

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|---|-------------|-------------|-------------|------------------|-------------|-------------|-------------|
| C | -4.31786400 | -0.38832000 | -1.57920800 | H | 3.46637600 | 3.76804800 | -1.79420200 |
| C | -5.70449000 | -0.41437600 | -1.73119400 | H | 2.80642400 | 5.10935900 | 0.21036000 |
| C | -6.50569800 | -1.03558000 | -0.76482500 | H | 1.63907700 | 3.98289600 | 2.11004100 |
| C | -5.90280700 | -1.62271500 | 0.34945300 | C | -1.40023000 | -3.04252500 | 1.27412300 |
| C | -4.51110300 | -1.58644300 | 0.50623700 | H | -2.33794700 | -3.47312300 | 0.89079400 |
| C | -1.67337800 | 0.95617100 | -0.25365800 | H | -0.58921700 | -3.39980400 | 0.62034600 |
| C | -1.02614800 | 1.66225100 | -1.27873600 | H | -1.22960900 | -3.45466200 | 2.28304400 |
| C | -2.19986800 | 1.67340800 | 0.83488200 | C | 2.25679800 | -1.03066700 | 2.55999700 |
| C | -2.06863400 | 3.06237400 | 0.89988900 | H | 2.30029200 | 0.01227600 | 2.90571100 |
| C | -1.42119800 | 3.75627700 | -0.13001200 | H | 2.03690700 | -1.65994600 | 3.43907800 |
| C | -0.90562400 | 3.05452000 | -1.22250000 | H | 3.25646100 | -1.30684100 | 2.19462500 |
| C | 3.16426600 | -1.31470400 | -0.55549700 | | | | |
| C | 4.42530900 | -0.78517000 | -0.23271400 | cat _s | | | |
| C | 5.59165100 | -1.49992000 | -0.52146100 | P | 1.46142100 | -0.35540400 | 0.21628700 |
| C | 5.51669700 | -2.75808400 | -1.12871200 | C | 1.24489200 | -0.58129900 | 2.05901800 |
| C | 4.26700400 | -3.29638500 | -1.45238200 | C | -0.12439300 | -0.11938100 | 2.59322700 |
| C | 3.10192000 | -2.57514700 | -1.17642400 | C | -1.37745700 | -0.77968800 | 1.99206700 |
| C | 2.03922200 | 1.26719900 | 0.06650900 | P | -1.56455700 | -0.39562900 | 0.17995000 |
| C | 1.66837200 | 2.03578600 | 1.18231700 | C | -3.19637400 | -1.09874400 | -0.26974300 |
| C | 2.68075800 | 1.92085000 | -1.00541800 | C | -3.18980600 | -2.22615500 | -1.10677600 |
| C | 2.96299400 | 3.28626100 | -0.95186500 | C | -4.39086300 | -2.82890700 | -1.49039900 |
| C | 2.59350800 | 4.03826800 | 0.16987800 | C | -5.60673700 | -2.30601200 | -1.03856500 |
| C | 1.94272400 | 3.40709700 | 1.23200500 | C | -5.61917700 | -1.18052400 | -0.20585600 |
| H | 1.19320900 | -2.31541000 | 1.22761500 | C | -4.41923300 | -0.57501200 | 0.17622600 |
| H | -0.34878000 | 0.18766100 | 2.09174300 | C | -1.77630600 | 1.42149000 | 0.05660600 |
| H | -0.25917800 | -1.26988700 | 3.05996400 | C | -1.34274100 | 2.01399400 | -1.14083400 |
| H | -2.30730400 | -1.21087900 | 1.94998300 | C | -2.31078800 | 2.23197100 | 1.07003100 |
| H | -3.70344900 | 0.09617000 | -2.34418800 | C | -2.41407800 | 3.61380700 | 0.88062100 |
| H | -6.16288100 | 0.04842400 | -2.60925700 | C | -1.99232400 | 4.19388600 | -0.32026300 |
| H | -7.59181700 | -1.06246000 | -0.88349700 | C | -1.45839500 | 3.39076200 | -1.33409700 |
| H | -6.51659700 | -2.11221100 | 1.11044000 | C | 3.01373800 | -1.26265100 | -0.13922700 |
| H | -4.07654300 | -2.04924600 | 1.39302900 | C | 4.29860200 | -0.70383000 | -0.05861600 |
| H | -0.60273900 | 1.11409600 | -2.12352800 | C | 5.42073900 | -1.48824400 | -0.33873400 |
| H | -2.72223100 | 1.14389800 | 1.63564100 | C | 5.26962000 | -2.83131600 | -0.70272800 |
| H | -2.47583600 | 3.60753700 | 1.75548000 | C | 3.99140200 | -3.39235500 | -0.79056800 |
| H | -1.31652500 | 4.84283900 | -0.07701500 | C | 2.86771600 | -2.60978300 | -0.51348500 |
| H | -0.39437800 | 3.58891900 | -2.02682000 | C | 1.84414100 | 1.40026100 | -0.15349600 |
| H | 4.49951200 | 0.19133800 | 0.24922900 | C | 1.52987100 | 2.47116300 | 0.69638700 |
| H | 6.56488400 | -1.07315000 | -0.26472900 | C | 2.33620500 | 1.68147800 | -1.44220100 |
| H | 6.42987800 | -3.31549800 | -1.35230800 | C | 2.52940200 | 2.99864200 | -1.85938700 |
| H | 4.19854900 | -4.27639000 | -1.93180000 | C | 2.22124700 | 4.05996900 | -0.99976400 |
| H | 2.12844100 | -2.99415900 | -1.44813500 | C | 1.72055900 | 3.79114100 | 0.27582000 |
| H | 1.14725300 | 1.57858800 | 2.02162000 | H | 1.27778800 | -1.68176600 | 2.12067100 |
| H | 2.95928500 | 1.35248900 | -1.89721400 | H | -0.21233500 | 0.97401000 | 2.51809500 |

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|------------------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | -0.13180400 | -0.34403800 | 3.67379600 | C | -1.84520000 | 1.36879200 | 0.02381400 |
| H | -2.25417900 | -0.35276800 | 2.50499800 | C | -1.42774400 | 2.03824400 | -1.13911600 |
| H | -2.23262500 | -2.63344200 | -1.44805900 | C | -2.27715700 | 2.12309100 | 1.12647400 |
| H | -4.37789400 | -3.70610700 | -2.14207700 | C | -2.29351100 | 3.51971800 | 1.06212000 |
| H | -6.54783700 | -2.77471100 | -1.33700900 | C | -1.88472600 | 4.17606800 | -0.10330900 |
| H | -6.56975500 | -0.77123700 | 0.14537600 | C | -1.45505500 | 3.43234400 | -1.20732300 |
| H | -4.43674000 | 0.30734800 | 0.82000300 | C | 3.26387000 | -1.21412500 | -0.13066500 |
| H | -0.88961400 | 1.37748800 | -1.90534300 | C | 4.46732200 | -0.54267300 | 0.13791700 |
| H | -2.64566800 | 1.79326900 | 2.01196800 | C | 5.69155400 | -1.18473100 | -0.06723800 |
| H | -2.82584500 | 4.23999900 | 1.67605500 | C | 5.72601000 | -2.50248600 | -0.53763700 |
| H | -2.07199700 | 5.27446900 | -0.46282500 | C | 4.53132300 | -3.17636300 | -0.81175800 |
| H | -1.11290100 | 3.84120600 | -2.26756500 | C | 3.30711400 | -2.53062600 | -0.61766500 |
| H | 4.42440900 | 0.34395800 | 0.22144700 | C | 1.88996100 | 1.32179300 | -0.13454400 |
| H | 6.41924300 | -1.04897300 | -0.27175300 | C | 1.61267100 | 2.32702000 | 0.80398500 |
| H | 6.15044100 | -3.43989200 | -0.92220900 | C | 2.31171000 | 1.70124700 | -1.42366600 |
| H | 3.86923800 | -4.43892000 | -1.08040500 | C | 2.47343500 | 3.04598000 | -1.75697500 |
| H | 1.86086000 | -3.03496800 | -0.58379600 | C | 2.20021300 | 4.04078900 | -0.81044400 |
| H | 1.11606800 | 2.29469200 | 1.68697000 | C | 1.76703100 | 3.67609300 | 0.46594100 |
| H | 2.56386700 | 0.86046700 | -2.12691900 | H | 1.22098300 | -1.92781400 | 1.89678300 |
| H | 2.91569000 | 3.19862300 | -2.86197600 | H | -0.20766800 | 0.76021700 | 2.29776000 |
| H | 2.36511200 | 5.09221000 | -1.32812700 | H | -0.19051300 | -0.54739700 | 3.46469300 |
| H | 1.46534800 | 4.61184400 | 0.95037400 | H | -2.26635300 | -0.59204900 | 2.36198700 |
| C | -1.39860400 | -2.30092700 | 2.16653500 | H | -2.78538800 | -2.53986400 | -1.65466300 |
| H | -2.38371300 | -2.71906300 | 1.91180800 | H | -5.07425200 | -3.44291500 | -2.07812700 |
| H | -0.65414300 | -2.78384500 | 1.51359300 | H | -7.04221400 | -2.42472100 | -0.93000100 |
| H | -1.17315200 | -2.56993000 | 3.21132200 | H | -6.71401500 | -0.51449500 | 0.63893200 |
| C | 2.40119300 | -0.03847200 | 2.90141300 | H | -4.43873200 | 0.37399600 | 1.06436300 |
| H | 2.43592300 | 1.06012300 | 2.90652100 | H | -1.06835800 | 1.45492200 | -1.99171500 |
| H | 2.28318300 | -0.37236500 | 3.94534500 | H | -2.59765800 | 1.62584900 | 2.04379100 |
| H | 3.37244500 | -0.40712600 | 2.54124800 | H | -2.62538300 | 4.09775400 | 1.92827700 |
| Co | -0.03276600 | -1.20728200 | -1.01275400 | H | -1.89360000 | 5.26792000 | -0.14829500 |
| | | | | H | -1.12395600 | 3.93972100 | -2.11645000 |
| cat _T | | | | H | 4.44889300 | 0.48552200 | 0.50544900 |
| P | 1.59837200 | -0.47528800 | 0.10663900 | H | 6.62398000 | -0.65428100 | 0.14252900 |
| C | 1.23884300 | -0.82499800 | 1.91070300 | H | 6.68521600 | -3.00156600 | -0.69680300 |
| C | -0.14620900 | -0.33328700 | 2.38293900 | H | 4.55310200 | -4.20228300 | -1.18792100 |
| C | -1.41247000 | -0.96663800 | 1.77355600 | H | 2.36892400 | -3.04234400 | -0.85325400 |
| P | -1.72879800 | -0.46267700 | 0.00037400 | H | 1.26230300 | 2.07688500 | 1.80350800 |
| C | -3.45910300 | -1.03102400 | -0.26639900 | H | 2.50895200 | 0.93113700 | -2.17502700 |
| C | -3.65290300 | -2.10213000 | -1.15220400 | H | 2.80563000 | 3.31996600 | -2.76154400 |
| C | -4.93546200 | -2.60682600 | -1.38798600 | H | 2.31727700 | 5.09532400 | -1.07173500 |
| C | -6.03767600 | -2.03611600 | -0.74446000 | H | 1.54012000 | 4.44448800 | 1.20886600 |
| C | -5.85338200 | -0.96361800 | 0.13660200 | C | -1.41169200 | -2.49577200 | 1.84372100 |
| C | -4.57108100 | -0.46339800 | 0.37599900 | H | -2.39315200 | -2.91117400 | 1.57043300 |

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|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | -0.66424400 | -2.92769800 | 1.15865700 | P | -0.65859000 | -1.72766900 | 0.50184700 |
| H | -1.17286000 | -2.83396100 | 2.86542900 | C | 0.67128200 | -2.98614200 | 0.38827500 |
| C | 2.34126800 | -0.39840100 | 2.88437500 | C | 1.85442200 | -2.68345800 | -0.29915900 |
| H | 2.44838400 | 0.69443100 | 2.94318900 | C | 2.89075200 | -3.61958600 | -0.37363300 |
| H | 2.09986600 | -0.76257600 | 3.89663100 | C | 2.74576100 | -4.86670500 | 0.23903700 |
| H | 3.31699500 | -0.81950200 | 2.60430300 | C | 1.56214600 | -5.17882800 | 0.92130200 |
| Co | -0.03480100 | -1.17562300 | -1.26502900 | C | 0.52678300 | -4.24555600 | 0.99445500 |
| | | | | C | -2.11901000 | -2.66162300 | -0.09428700 |
| 1s | | | | C | -2.09906700 | -3.06874300 | -1.44085400 |
| C | 4.22985500 | 0.18904900 | -0.54586400 | C | -3.24217500 | -2.95387000 | 0.69059700 |
| C | 4.79480600 | -0.30360300 | -1.73272400 | C | -4.33433900 | -3.62834900 | 0.13303900 |
| C | 5.83806800 | -1.23342200 | -1.69814600 | C | -4.31073500 | -4.02440200 | -1.20563800 |
| C | 6.33308700 | -1.69548100 | -0.47468700 | C | -3.18448800 | -3.74922600 | -1.99106400 |
| C | 5.78321900 | -1.20932100 | 0.71416800 | C | -1.51780300 | 3.12487200 | 0.08675400 |
| C | 4.74752400 | -0.27157200 | 0.67615400 | C | -2.37404700 | 3.80019400 | -0.79571900 |
| H | 4.42678100 | 0.04012900 | -2.70024100 | C | -2.20404900 | 5.16772200 | -1.03553000 |
| H | 6.26337500 | -1.60112300 | -2.63542900 | C | -1.17974900 | 5.87192600 | -0.39751600 |
| H | 7.14304800 | -2.42857400 | -0.44892800 | C | -0.31956800 | 5.20246200 | 0.48056300 |
| H | 6.16123300 | -1.55798500 | 1.67839300 | C | -0.48247500 | 3.83679500 | 0.71914600 |
| H | 4.34168500 | 0.10338400 | 1.61862800 | C | -3.34638500 | 0.88694000 | -0.19679900 |
| C | 3.09910400 | 1.22065900 | -0.56640200 | C | -4.50345700 | 1.38948600 | 0.42397900 |
| C | 2.22203000 | 0.97049400 | 0.65468600 | C | -3.47992800 | 0.01883800 | -1.29124700 |
| O | 1.95100900 | 1.77898700 | 1.51783000 | C | -4.74392500 | -0.36283900 | -1.74667500 |
| H | 1.83514300 | -0.07201900 | 0.72040300 | C | -5.88945900 | 0.12153800 | -1.10981400 |
| C | 2.18032100 | 1.00901100 | -1.80481700 | C | -5.76652700 | 1.00162700 | -0.02828700 |
| H | 2.06192500 | -0.07300700 | -1.99730700 | H | -0.46945900 | 1.26391600 | 2.38118200 |
| H | 2.69926100 | 1.40739000 | -2.69392400 | H | -2.89781000 | -0.59631300 | 2.20931800 |
| C | 3.66221300 | 2.66931400 | -0.58008800 | H | -2.03924000 | -0.32750200 | 3.71676400 |
| H | 2.80298300 | 3.36047100 | -0.54907900 | H | -1.31023900 | -2.40314800 | 2.71824800 |
| H | 4.16913300 | 2.81554700 | -1.54619000 | H | 1.97271300 | -1.70776800 | -0.76932200 |
| C | 0.81070000 | 1.62894300 | -1.67753000 | H | 3.80989100 | -3.36608700 | -0.90639400 |
| C | -0.27702300 | 1.19244900 | -2.44412400 | H | 3.55434700 | -5.59997000 | 0.18569500 |
| H | 0.76194900 | 2.61100100 | -1.19983600 | H | 1.44658800 | -6.15573700 | 1.39736200 |
| H | -1.15191700 | 1.83304900 | -2.58744400 | H | -0.39620200 | -4.49576500 | 1.52369100 |
| H | -0.13957000 | 0.41429700 | -3.20834200 | H | -1.22846500 | -2.84622400 | -2.06398000 |
| C | 4.60397000 | 3.00592800 | 0.53907600 | H | -3.28546900 | -2.66140600 | 1.73923800 |
| C | 5.90164000 | 3.28273900 | 0.37855200 | H | -5.20732400 | -3.84356300 | 0.75396500 |
| H | 4.17236000 | 3.01487500 | 1.54538700 | H | -5.16670900 | -4.54754500 | -1.63863400 |
| H | 6.54442200 | 3.52763500 | 1.23005900 | H | -3.15607800 | -4.05966200 | -3.03831600 |
| H | 6.37041300 | 3.27411500 | -0.61227600 | H | -3.17835500 | 3.26152800 | -1.29930300 |
| P | -1.64926400 | 1.31474100 | 0.34157000 | H | -2.87822100 | 5.68247500 | -1.72451800 |
| C | -1.54120600 | 1.08946500 | 2.19558800 | H | -1.04917000 | 6.94057100 | -0.58496700 |
| C | -1.90920800 | -0.34415200 | 2.62193100 | H | 0.48712100 | 5.74502200 | 0.97959600 |
| C | -0.89289100 | -1.46124400 | 2.32769900 | H | 0.21220400 | 3.32247700 | 1.38471100 |

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|----------------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | -4.42623900 | 2.09568500 | 1.25027600 | H | -4.24760100 | -1.47673200 | 1.47627800 |
| H | -2.58050300 | -0.36142400 | -1.77560400 | H | -6.38017300 | -2.61794000 | 1.16060200 |
| H | -4.83011900 | -1.04560800 | -2.59459500 | H | -6.19827400 | -2.48611500 | -0.69411300 |
| H | -6.88011000 | -0.18079700 | -1.45845400 | P | 0.84339500 | -1.70553900 | 0.54599000 |
| H | -6.66008800 | 1.39302900 | 0.46411300 | C | 1.63862200 | -1.64358400 | 2.24637600 |
| C | 0.44916900 | -1.21335900 | 3.02466800 | C | 2.61642500 | -0.47580500 | 2.49803500 |
| H | 1.14323400 | -2.05322600 | 2.88325300 | C | 2.14273200 | 0.98145300 | 2.32633900 |
| H | 0.94313900 | -0.29868900 | 2.66791600 | P | 1.85480700 | 1.46580200 | 0.54451800 |
| H | 0.27601300 | -1.09542200 | 4.10649400 | C | 1.53811500 | 3.26884400 | 0.62650200 |
| C | -2.34257000 | 2.09879900 | 3.02500800 | C | 0.21233900 | 3.69561200 | 0.45005400 |
| H | -3.41297000 | 1.84820200 | 3.03774600 | C | -0.10999300 | 5.05280700 | 0.53474100 |
| H | -1.98679700 | 2.06468200 | 4.06736100 | C | 0.89511200 | 5.99225600 | 0.78623800 |
| H | -2.23245400 | 3.13081700 | 2.66607900 | C | 2.22045700 | 5.57277300 | 0.95373600 |
| Co | -0.18912300 | 0.15124900 | -0.73744900 | C | 2.54351800 | 4.21574200 | 0.87453600 |
| | | | | C | 3.47871300 | 1.33596600 | -0.29448400 |
| I _T | | | | C | 3.49229400 | 1.33589800 | -1.69997800 |
| C | -4.77612400 | 1.12171000 | -0.73317200 | C | 4.69775700 | 1.24362700 | 0.39719600 |
| C | -5.38925800 | 1.47984000 | -1.94295000 | C | 5.90114200 | 1.13116600 | -0.30558100 |
| C | -6.62097100 | 2.14183900 | -1.95195300 | C | 5.90370400 | 1.12011600 | -1.70333400 |
| C | -7.26006800 | 2.46356400 | -0.75111600 | C | 4.69576800 | 1.23129500 | -2.39927400 |
| C | -6.65999200 | 2.11266600 | 0.46140700 | C | -0.16458700 | -3.24077600 | 0.66322000 |
| C | -5.43320100 | 1.44429400 | 0.46675600 | C | 0.25636300 | -4.47966100 | 0.15279300 |
| H | -4.91467300 | 1.23696500 | -2.89441900 | C | -0.55240700 | -5.61148100 | 0.28890400 |
| H | -7.08219700 | 2.40836100 | -2.90628300 | C | -1.78628300 | -5.52234500 | 0.94175800 |
| H | -8.22114200 | 2.98364800 | -0.76022000 | C | -2.20878400 | -4.29395800 | 1.45946600 |
| H | -7.14940000 | 2.35361900 | 1.40837600 | C | -1.40527500 | -3.15932200 | 1.31861300 |
| H | -4.99007200 | 1.16086000 | 1.42511500 | C | 2.10877600 | -2.11844300 | -0.71842200 |
| C | -3.46853000 | 0.33553300 | -0.68560800 | C | 3.49550500 | -2.07350400 | -0.50816400 |
| C | -2.65689000 | 0.77852800 | 0.51190600 | C | 1.63596200 | -2.39540500 | -2.01636500 |
| O | -2.00521000 | 0.01457200 | 1.21721800 | C | 2.52349500 | -2.62002900 | -3.06918200 |
| H | -2.61998300 | 1.87562400 | 0.69506800 | C | 3.90433600 | -2.56581800 | -2.84778100 |
| C | -2.52949400 | 0.68876800 | -1.88401600 | C | 4.38466600 | -2.29574400 | -1.56489900 |
| H | -2.39005400 | 1.78049000 | -1.91949300 | H | 0.74439200 | -1.47184300 | 2.87011400 |
| H | -3.05393200 | 0.40343900 | -2.81041500 | H | 3.53572100 | -0.63367800 | 1.92059500 |
| C | -3.73730400 | -1.19337700 | -0.65913600 | H | 2.91989600 | -0.56939600 | 3.55492300 |
| H | -2.76547100 | -1.70345200 | -0.57639300 | H | 2.95588100 | 1.62529300 | 2.69871600 |
| H | -4.17818000 | -1.47156700 | -1.62831700 | H | -0.56487200 | 2.95205900 | 0.24537800 |
| C | -1.18253500 | -0.00220200 | -1.88171500 | H | -1.14466700 | 5.37715000 | 0.39866800 |
| C | -0.00881000 | 0.66078500 | -2.15379300 | H | 0.64726100 | 7.05489300 | 0.84752500 |
| H | -1.19860100 | -1.09224400 | -1.97193400 | H | 3.00636400 | 6.30760800 | 1.14562200 |
| H | 0.88133800 | 0.11443500 | -2.46903200 | H | 3.57975500 | 3.89366500 | 1.00225800 |
| H | -0.00447900 | 1.74410700 | -2.31391700 | H | 2.55680300 | 1.41562700 | -2.25380700 |
| C | -4.61711000 | -1.66182200 | 0.46127700 | H | 4.72352200 | 1.26137000 | 1.48724300 |
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|------------------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | 6.84544100 | 1.02619000 | -2.24953300 | C | -0.96881800 | -0.81361600 | -2.05050900 |
| H | 4.68794500 | 1.22639000 | -3.49186600 | C | -0.76882400 | 0.53153500 | -2.36959200 |
| H | 1.22054000 | -4.56689200 | -0.35034600 | H | -0.21438500 | -1.53751200 | -2.37026900 |
| H | -0.21367400 | -6.56901500 | -0.11493100 | H | 0.15705200 | 0.82031800 | -2.87606300 |
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| H | -3.17441600 | -4.21284200 | 1.96406600 | C | -5.04415500 | -0.75114000 | 1.09966100 |
| H | -1.74974500 | -2.19903200 | 1.70272700 | C | -6.35434000 | -0.55632300 | 0.92021600 |
| H | 3.90348700 | -1.85859400 | 0.47640500 | H | -4.56749700 | -0.40428100 | 2.02206500 |
| H | 0.56123800 | -2.44186000 | -2.20650300 | H | -6.96965500 | -0.06436000 | 1.68020600 |
| H | 2.13435500 | -2.83390400 | -4.06773700 | H | -6.86079900 | -0.88133800 | 0.00400900 |
| H | 4.60080500 | -2.73312500 | -3.67296800 | P | 0.82184600 | -1.79839600 | 0.52473000 |
| H | 5.45999500 | -2.24936800 | -1.37863700 | C | 1.48582700 | -1.61762000 | 2.25763000 |
| C | 0.88031300 | 1.29129000 | 3.13671000 | C | 2.51761400 | -0.47716600 | 2.34711400 |
| H | 0.65907800 | 2.36854900 | 3.14275500 | C | 2.00060900 | 0.97403100 | 2.32287300 |
| H | -0.00472200 | 0.76992700 | 2.73875800 | P | 1.45622000 | 1.53130800 | 0.63550000 |
| H | 1.01898700 | 0.96850300 | 4.18126800 | C | 0.90033700 | 3.25446400 | 0.92042100 |
| C | 2.26819700 | -2.96910000 | 2.68449500 | C | -0.46243400 | 3.57409600 | 0.85275200 |
| H | 3.13655800 | -3.23771500 | 2.06465000 | C | -0.89597900 | 4.87483400 | 1.12508600 |
| H | 2.61565000 | -2.88963800 | 3.72769000 | C | 0.03093700 | 5.86400300 | 1.46539400 |
| H | 1.54790400 | -3.79735600 | 2.63315400 | C | 1.39389700 | 5.55020400 | 1.53287600 |
| Co | -0.11190700 | 0.33720800 | -0.00948400 | C | 1.82945700 | 4.25130900 | 1.26243300 |
| | | | | C | 2.95432900 | 1.73809700 | -0.39282600 |
| | | | | C | 2.75837300 | 2.12986000 | -1.72952100 |
| TS2 _T | | | | C | 4.25685700 | 1.50295000 | 0.06978500 |
| C | -3.66127400 | 0.75520700 | -1.06928900 | C | 5.34517200 | 1.64088700 | -0.79871700 |
| C | -4.25860600 | 0.78403500 | -2.33959700 | C | 5.14394300 | 2.02134900 | -2.12762800 |
| C | -4.88096300 | 1.94076100 | -2.81694600 | C | 3.84660500 | 2.27324400 | -2.59008000 |
| C | -4.91799700 | 3.09833100 | -2.03337100 | C | -0.29204300 | -3.24588200 | 0.58791600 |
| C | -4.34110600 | 3.07894300 | -0.76126500 | C | -0.30946700 | -4.18778600 | -0.45341000 |
| C | -3.72787000 | 1.91718000 | -0.28334500 | C | -1.24323800 | -5.22762200 | -0.44919900 |
| H | -4.24050300 | -0.10321700 | -2.97392300 | C | -2.16880300 | -5.33814100 | 0.59241900 |
| H | -5.33645100 | 1.93579900 | -3.81051000 | C | -2.15862600 | -4.40097700 | 1.63085200 |
| H | -5.39758000 | 4.00517700 | -2.40984600 | C | -1.23095400 | -3.35696500 | 1.62794000 |
| H | -4.37008300 | 3.97058000 | -0.12982600 | C | 2.22967200 | -2.30078900 | -0.53042800 |
| H | -3.30169900 | 1.92296500 | 0.71944800 | C | 2.94718300 | -3.49554300 | -0.34285800 |
| C | -3.03286100 | -0.53556400 | -0.52676600 | C | 2.61301500 | -1.42575800 | -1.55810400 |
| C | -1.94236800 | -0.14764500 | 0.51046700 | C | 3.71492100 | -1.71443100 | -2.36677200 |
| O | -2.15068200 | -0.04662400 | 1.69727100 | C | 4.43686400 | -2.89296600 | -2.16055000 |
| H | -0.60142500 | 1.37241300 | -0.91520600 | C | 4.04585200 | -3.78536700 | -1.15479600 |
| C | -2.29985500 | -1.37457400 | -1.60341200 | H | 0.59381700 | -1.34050500 | 2.84018800 |
| H | -2.95636900 | -1.52864600 | -2.47487000 | H | 3.29227700 | -0.62813000 | 1.57905100 |
| H | -2.12849000 | -2.37411500 | -1.18381600 | H | 3.03235200 | -0.59748600 | 3.31472100 |
| C | -4.14245200 | -1.42681600 | 0.11031500 | H | 2.84722100 | 1.62675200 | 2.58973100 |
| H | -3.63528900 | -2.27777500 | 0.59404700 | H | -1.18397800 | 2.80232000 | 0.58362100 |
| H | -4.74351400 | -1.83415800 | -0.71874500 | | | | |

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|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | -1.96082300 | 5.11331600 | 1.06783500 | H | -1.10161300 | -0.93217500 | 0.96458700 |
| H | -0.30627400 | 6.88200400 | 1.67578800 | C | -0.96612300 | 2.60556700 | 1.43568100 |
| H | 2.12124000 | 6.32246600 | 1.79505700 | H | -1.45195500 | 3.20362000 | 2.22221700 |
| H | 2.89522800 | 4.01572700 | 1.31343700 | H | -0.37923300 | 3.31467600 | 0.84032600 |
| H | 1.74746900 | 2.31946400 | -2.09815000 | C | -2.64044500 | 3.10839400 | -0.36925900 |
| H | 4.44025200 | 1.21189300 | 1.10421600 | H | -1.83166800 | 3.50198800 | -1.00557700 |
| H | 6.35579000 | 1.45080200 | -0.42937200 | H | -2.93432000 | 3.91502900 | 0.32111700 |
| H | 5.99616600 | 2.12459100 | -2.80359200 | C | -0.02857100 | 1.59696200 | 2.04612700 |
| H | 3.68224700 | 2.57811300 | -3.62638700 | C | -0.43745800 | 0.42711000 | 2.62985500 |
| H | 0.40264700 | -4.10981800 | -1.27612100 | H | 1.01898700 | 1.89197800 | 2.15347400 |
| H | -1.24629000 | -5.95307100 | -1.26640900 | H | 0.29496200 | -0.21308700 | 3.13115500 |
| H | -2.89822900 | -6.15167700 | 0.59483900 | H | -1.48802200 | 0.20588400 | 2.81342900 |
| H | -2.88249800 | -4.47658100 | 2.44573100 | C | -3.81578000 | 2.72608200 | -1.21862800 |
| H | -1.25379900 | -2.62072500 | 2.43262600 | C | -5.05648100 | 3.19243400 | -1.04572500 |
| H | 2.64181800 | -4.20797700 | 0.42368800 | H | -3.61361000 | 2.01355000 | -2.02446800 |
| H | 2.03774100 | -0.51407300 | -1.71752300 | H | -5.87964800 | 2.88581000 | -1.69894900 |
| H | 4.00589300 | -1.01643500 | -3.15493300 | H | -5.29597800 | 3.89822100 | -0.24205100 |
| H | 5.30072300 | -3.12353200 | -2.78895200 | P | 1.78783300 | 0.98435500 | -0.50039700 |
| H | 4.59969100 | -4.71495000 | -1.00263100 | C | 2.17685900 | 0.45233800 | -2.24689500 |
| C | 0.86998200 | 1.21636600 | 3.32991300 | C | 2.28776700 | -1.07884600 | -2.35606000 |
| H | 0.68756100 | 2.29026100 | 3.47494300 | C | 0.97001900 | -1.87220500 | -2.42007300 |
| H | -0.07636000 | 0.75458800 | 3.00850100 | P | 0.07712900 | -1.89378200 | -0.78843500 |
| H | 1.14698400 | 0.78512800 | 4.30534500 | C | -1.46094100 | -2.83787800 | -1.11595000 |
| C | 2.06804600 | -2.90563300 | 2.84409300 | C | -2.55707000 | -2.20607500 | -1.72925300 |
| H | 3.04190100 | -3.14490400 | 2.39246100 | C | -3.73556500 | -2.91514400 | -1.97053700 |
| H | 2.22840800 | -2.77093800 | 3.92592700 | C | -3.83415300 | -4.26232600 | -1.60689300 |
| H | 1.40062700 | -3.76803100 | 2.70595100 | C | -2.74385800 | -4.89914100 | -1.00812500 |
| Co | -0.09618800 | 0.11275600 | -0.23906500 | C | -1.56167000 | -4.19339900 | -0.76424300 |
| | | | | C | 1.06225800 | -2.98357600 | 0.31395900 |
| 2s | | | | C | 0.67481000 | -3.07844500 | 1.66492000 |
| C | -3.16386200 | 1.26951800 | 1.26219200 | C | 2.20576800 | -3.67652400 | -0.11346200 |
| C | -3.72775600 | 1.85367000 | 2.40664800 | C | 2.95623200 | -4.42938300 | 0.79438000 |
| C | -4.81634100 | 1.26190600 | 3.05404200 | C | 2.57194700 | -4.50737300 | 2.13553100 |
| C | -5.36525100 | 0.07045500 | 2.56996400 | C | 1.42257400 | -3.83685500 | 2.56644800 |
| C | -4.82148700 | -0.51361200 | 1.42298900 | C | 1.70411100 | 2.80828100 | -0.61758600 |
| C | -3.73943100 | 0.08654900 | 0.77475700 | C | 2.27763600 | 3.63689900 | 0.36026100 |
| H | -3.32076500 | 2.78416700 | 2.80595100 | C | 2.09509000 | 5.02150600 | 0.30935600 |
| H | -5.23554200 | 1.73675000 | 3.94483100 | C | 1.34013600 | 5.59559600 | -0.71739300 |
| H | -6.21198900 | -0.39513900 | 3.08032100 | C | 0.76871400 | 4.77687500 | -1.69660700 |
| H | -5.23951200 | -1.44078700 | 1.02239700 | C | 0.94524800 | 3.39255500 | -1.64720000 |
| H | -3.34474600 | -0.38511900 | -0.12239000 | C | 3.27158200 | 0.59793300 | 0.49869800 |
| C | -2.02846200 | 1.97141000 | 0.50810500 | C | 4.51443300 | 1.23070300 | 0.31788000 |
| C | -1.27477500 | 0.93411400 | -0.39462800 | C | 3.14854500 | -0.40234200 | 1.47742000 |
| O | -1.49645100 | 0.84528600 | -1.57931600 | C | 4.24977400 | -0.78032300 | 2.25004800 |

| | | | | | | | |
|------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | 5.48402900 | -0.15409400 | 2.05700900 | H | -5.56630500 | -0.34338000 | -3.76929500 |
| C | 5.61240100 | 0.85387600 | 1.09408100 | H | -6.48310700 | 1.52907400 | -2.39005800 |
| H | 1.29959200 | 0.79013500 | -2.81951900 | H | -5.50839800 | 1.97033700 | -0.12758200 |
| H | 2.93835100 | -1.45751600 | -1.55219600 | H | -3.66317300 | 0.58274900 | 0.71985200 |
| H | 2.82064200 | -1.29864300 | -3.29578500 | C | -2.41703100 | -1.56338500 | -0.46870400 |
| H | 1.22759200 | -2.92842100 | -2.59939500 | C | -1.46068000 | -0.67807200 | 0.41800700 |
| H | -2.48976800 | -1.15896000 | -2.02107000 | O | -1.67186000 | -0.52096800 | 1.59618000 |
| H | -4.58110600 | -2.40947800 | -2.44306400 | H | -0.84188700 | 1.05910100 | -1.30534600 |
| H | -4.75846800 | -4.81476900 | -1.79286000 | C | -1.53814200 | -2.26210600 | -1.53036200 |
| H | -2.81014300 | -5.95269000 | -0.72561900 | H | -2.16662000 | -2.72548800 | -2.30712800 |
| H | -0.72038900 | -4.70381400 | -0.29348800 | H | -1.02216600 | -3.09558300 | -1.03833700 |
| H | -0.21586700 | -2.55269300 | 2.01127000 | C | -3.08347500 | -2.68449200 | 0.39332100 |
| H | 2.52582000 | -3.64299800 | -1.15428100 | H | -2.26950800 | -3.22897900 | 0.89632200 |
| H | 3.84683600 | -4.95835600 | 0.44694400 | H | -3.54729800 | -3.38396000 | -0.32077400 |
| H | 3.16380700 | -5.09326600 | 2.84284600 | C | -0.49954000 | -1.35115900 | -2.13285300 |
| H | 1.10763600 | -3.89959700 | 3.61073800 | C | -0.80152500 | -0.07570300 | -2.61802300 |
| H | 2.86115500 | 3.20439000 | 1.17410600 | H | 0.46134100 | -1.79610900 | -2.40531800 |
| H | 2.54564300 | 5.65285000 | 1.07903400 | H | -0.04572400 | 0.45833700 | -3.20274100 |
| H | 1.19708300 | 6.67815800 | -0.75504100 | H | -1.83146400 | 0.24775600 | -2.77344800 |
| H | 0.17494500 | 5.21568600 | -2.50195300 | C | -4.10443200 | -2.26609900 | 1.40783100 |
| H | 0.47324600 | 2.77150000 | -2.40959900 | C | -5.39659600 | -2.60564400 | 1.36150100 |
| H | 4.62482700 | 2.02768400 | -0.41775200 | H | -3.73637700 | -1.65108200 | 2.23444900 |
| H | 2.18697800 | -0.89281700 | 1.63611800 | H | -6.09994800 | -2.28903900 | 2.13821900 |
| H | 4.13841000 | -1.56346300 | 3.00343100 | H | -5.80003600 | -3.21193300 | 0.54216800 |
| H | 6.34707000 | -0.44596000 | 2.66054900 | P | 1.45763100 | -1.33414500 | 0.50111700 |
| H | 6.57397600 | 1.35173700 | 0.94734000 | C | 1.80110500 | -0.93398400 | 2.29004400 |
| C | 0.07100000 | -1.41463400 | -3.57379000 | C | 2.28376100 | 0.51972400 | 2.45551600 |
| H | -0.72864500 | -2.14097400 | -3.77154700 | C | 1.23528800 | 1.64622900 | 2.40132300 |
| H | -0.39617000 | -0.44037000 | -3.37764000 | P | 0.50718300 | 1.86148400 | 0.70620300 |
| H | 0.67971500 | -1.32858000 | -4.48821400 | C | -0.71290800 | 3.21767300 | 0.89134400 |
| C | 3.42217900 | 1.12437900 | -2.82816700 | C | -1.98859600 | 3.10142300 | 0.32728500 |
| H | 4.34055600 | 0.71521700 | -2.38191000 | C | -2.91595500 | 4.14064500 | 0.45308100 |
| H | 3.46485500 | 0.93116400 | -3.91221400 | C | -2.57086800 | 5.30505900 | 1.14307200 |
| H | 3.41970500 | 2.21348900 | -2.67827100 | C | -1.29251000 | 5.43172400 | 1.70163900 |
| Co | 0.00030200 | -0.08490700 | 0.46964600 | C | -0.36566200 | 4.39589500 | 1.57603900 |
| | | | | C | 1.82125000 | 2.64614500 | -0.31871700 |
| | | | | C | 1.50666400 | 2.92797500 | -1.66127100 |
| TS3s | | | | C | 3.11054500 | 2.93658900 | 0.15189300 |
| C | -3.51944000 | -0.66230900 | -1.04437000 | C | 4.07116500 | 3.47735300 | -0.70872300 |
| C | -4.08905900 | -0.90934000 | -2.30358000 | C | 3.75496500 | 3.74163400 | -2.04353700 |
| C | -5.14634000 | -0.12973200 | -2.78306600 | C | 2.46518500 | 3.47352900 | -2.51559900 |
| C | -5.66090100 | 0.91627800 | -2.01249100 | C | 1.09013800 | -3.12483100 | 0.48013800 |
| C | -5.11426500 | 1.16372500 | -0.75060900 | C | 1.53300400 | -3.92904900 | -0.58260300 |
| C | -4.06268900 | 0.37798900 | -0.27216800 | C | 1.16454200 | -5.27508300 | -0.64976900 |
| H | -3.70967300 | -1.71471900 | -2.93285100 | | | | |

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|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | 0.35293100 | -5.83357000 | 0.34236100 | C | -3.59763300 | -0.28220700 | -0.91198900 |
| C | -0.08892500 | -5.03858100 | 1.40449000 | C | -4.41996000 | -0.51962600 | -2.02499200 |
| C | 0.27253400 | -3.69108100 | 1.47269700 | C | -5.34867800 | 0.43392200 | -2.44959400 |
| C | 3.02547500 | -1.16255400 | -0.43066100 | C | -5.47654800 | 1.64782300 | -1.76618600 |
| C | 4.18991600 | -1.87614500 | -0.09536100 | C | -4.67357900 | 1.88985000 | -0.64955000 |
| C | 3.05421300 | -0.28571300 | -1.52817900 | C | -3.74967700 | 0.93056500 | -0.22399600 |
| C | 4.23279600 | -0.09509500 | -2.25445900 | H | -4.33976200 | -1.46098400 | -2.57091900 |
| C | 5.39253200 | -0.78765000 | -1.89756400 | H | -5.97525800 | 0.22596400 | -3.32072200 |
| C | 5.36618200 | -1.68384100 | -0.82271300 | H | -6.19962400 | 2.39612200 | -2.09991100 |
| H | 0.81069400 | -1.04160400 | 2.75970400 | H | -4.76185600 | 2.83043700 | -0.10101600 |
| H | 3.09873700 | 0.71025900 | 1.74076800 | H | -3.14264800 | 1.14137300 | 0.65659600 |
| H | 2.74577700 | 0.58902400 | 3.45389800 | C | -2.65252300 | -1.37559900 | -0.40234800 |
| H | 1.77205700 | 2.58499100 | 2.61049900 | C | -1.52606700 | -0.72476700 | 0.45554000 |
| H | -2.25481900 | 2.19757600 | -0.21909500 | O | -1.60082900 | -0.66623200 | 1.65888100 |
| H | -3.90844200 | 4.03437400 | 0.00871300 | H | -0.94642100 | 0.88754100 | -1.76627300 |
| H | -3.29418000 | 6.11805600 | 1.24395400 | C | -1.87832800 | -2.12243800 | -1.50792200 |
| H | -1.01565500 | 6.34451600 | 2.23489000 | H | -2.54140800 | -2.39531500 | -2.34585100 |
| H | 0.63175100 | 4.51193700 | 2.00640800 | H | -1.51070900 | -3.06845300 | -1.08372700 |
| H | 0.50498400 | 2.71773000 | -2.04122800 | C | -3.48703800 | -2.39719900 | 0.42981600 |
| H | 3.38438600 | 2.74749600 | 1.18919500 | H | -2.77838100 | -3.09818000 | 0.89811600 |
| H | 5.07295200 | 3.69193400 | -0.32888400 | H | -4.08466000 | -2.97483900 | -0.29376700 |
| H | 4.50950900 | 4.15926600 | -2.71446200 | C | -0.69319700 | -1.30047800 | -1.96015500 |
| H | 2.20517600 | 3.68591700 | -3.55543800 | C | -0.96127500 | 0.04062800 | -2.56008500 |
| H | 2.16446200 | -3.50554000 | -1.36518600 | H | 0.06452600 | -1.89097200 | -2.48559400 |
| H | 1.51498400 | -5.88931300 | -1.48282100 | H | -0.20254100 | 0.35770700 | -3.28837000 |
| H | 0.06622800 | -6.88655100 | 0.28877600 | H | -1.97364500 | 0.19074800 | -2.96002600 |
| H | -0.72463700 | -5.46597400 | 2.18350700 | C | -4.39162800 | -1.81890000 | 1.47688700 |
| H | -0.09432200 | -3.08319000 | 2.30142600 | C | -5.72525900 | -1.90769100 | 1.45916000 |
| H | 4.17784300 | -2.59682000 | 0.72226100 | H | -3.89575600 | -1.29292000 | 2.29888800 |
| H | 2.15601400 | 0.25605600 | -1.82913200 | H | -6.33880100 | -1.47399900 | 2.25527900 |
| H | 4.23924500 | 0.59608900 | -3.10001700 | H | -6.25407500 | -2.41712800 | 0.64535100 |
| H | 6.31616400 | -0.63768500 | -2.46202000 | P | 1.31250200 | -1.43852100 | 0.48958400 |
| H | 6.26639300 | -2.24056100 | -0.55120600 | C | 1.56935300 | -1.06614100 | 2.29822700 |
| C | 0.14051200 | 1.48203700 | 3.46154100 | C | 2.08048200 | 0.36257800 | 2.58720200 |
| H | -0.46578700 | 2.39396000 | 3.55479700 | C | 1.09803400 | 1.53648500 | 2.42747200 |
| H | -0.53716500 | 0.65206000 | 3.22479200 | P | 0.60401400 | 1.75151900 | 0.64616900 |
| H | 0.60925800 | 1.28688900 | 4.43960400 | C | -0.40024000 | 3.29003700 | 0.61050800 |
| C | 2.77630900 | -1.88914600 | 2.98442000 | C | -1.42217400 | 3.41939500 | -0.34024000 |
| H | 3.81402400 | -1.68608300 | 2.68260600 | C | -2.16540800 | 4.60062000 | -0.42764100 |
| H | 2.71438500 | -1.73629400 | 4.07387600 | C | -1.89606000 | 5.66244100 | 0.43940300 |
| H | 2.55691300 | -2.94574700 | 2.77915500 | C | -0.87558500 | 5.54212300 | 1.39032700 |
| Co | -0.00639900 | 0.06089800 | -0.47554300 | C | -0.12870200 | 4.36565800 | 1.47452500 |
| | | | | C | 2.16599000 | 2.27996100 | -0.17533700 |
| | | | | C | 2.35643200 | 1.89241000 | -1.51082700 |

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| | | | | | | | |
|---|-------------|-------------|-------------|----------------|-------------|-------------|-------------|
| C | 3.15891200 | 3.04091200 | 0.46221700 | C | 2.40752400 | -2.12126300 | 3.03149500 |
| C | 4.32209900 | 3.39787500 | -0.22409400 | H | 3.46723200 | -2.09333300 | 2.74241100 |
| C | 4.50407500 | 3.00631700 | -1.55495600 | H | 2.35320600 | -1.92936900 | 4.11491300 |
| C | 3.51649600 | 2.25609800 | -2.19882500 | H | 2.03675600 | -3.13944300 | 2.85335100 |
| C | 0.85511700 | -3.21328500 | 0.44418500 | Co | -0.07453100 | -0.10709800 | -0.54049700 |
| C | 1.39778100 | -4.09601500 | -0.50145300 | | | | |
| C | 0.95053900 | -5.41908400 | -0.57049500 | 3 _T | | | |
| C | -0.03564400 | -5.87797800 | 0.30650400 | C | -3.44796800 | -1.39919100 | -1.11151600 |
| C | -0.57164700 | -5.00621900 | 1.25974600 | C | -3.99784700 | -1.88178200 | -2.30958500 |
| C | -0.13402100 | -3.68256600 | 1.32667300 | C | -4.85589500 | -1.08937200 | -3.07445300 |
| C | 2.89819500 | -1.28823800 | -0.42522800 | C | -5.18459600 | 0.20378000 | -2.65207600 |
| C | 4.12749300 | -1.01380100 | 0.19682100 | C | -4.65285000 | 0.69003000 | -1.45595000 |
| C | 2.86579700 | -1.39608300 | -1.82862700 | C | -3.79470100 | -0.10744500 | -0.69092600 |
| C | 4.02908300 | -1.25267600 | -2.58488600 | H | -3.75415400 | -2.88924700 | -2.65302400 |
| C | 5.24495000 | -0.97301200 | -1.95587600 | H | -5.27051800 | -1.48398300 | -4.00562800 |
| C | 5.28789700 | -0.85121300 | -0.56502600 | H | -5.85558400 | 0.82552300 | -3.24995700 |
| H | 0.53849700 | -1.13521900 | 2.67761600 | H | -4.90775000 | 1.69296000 | -1.10877000 |
| H | 2.98915300 | 0.57319700 | 2.00751300 | H | -3.40120200 | 0.28652300 | 0.24851800 |
| H | 2.39632400 | 0.36686700 | 3.64338600 | C | -2.57025600 | -2.30129100 | -0.25374800 |
| H | 1.66869100 | 2.44266200 | 2.68010200 | C | -1.68372500 | -1.47479300 | 0.68866800 |
| H | -1.64355400 | 2.59509800 | -1.01823800 | O | -1.67532400 | -1.57096000 | 1.89101300 |
| H | -2.96001400 | 4.68454100 | -1.17260600 | H | -1.43234500 | -0.52463700 | -2.63804700 |
| H | -2.47942600 | 6.58432400 | 0.37628200 | C | -1.43320400 | -2.97885700 | -1.05195200 |
| H | -0.65825700 | 6.37029400 | 2.06937000 | H | -1.82647800 | -3.46668800 | -1.95897400 |
| H | 0.67031300 | 4.29266000 | 2.21469800 | H | -1.01071200 | -3.77343400 | -0.41790900 |
| H | 1.59374200 | 1.29887800 | -2.01763800 | C | -3.44128900 | -3.33399200 | 0.50852500 |
| H | 3.03678100 | 3.36003000 | 1.49857300 | H | -2.76710700 | -3.90962200 | 1.16550300 |
| H | 5.09090000 | 3.98487600 | 0.28446200 | H | -3.86021800 | -4.03319500 | -0.23225600 |
| H | 5.41672200 | 3.28394600 | -2.08798800 | C | -0.34143000 | -1.96688000 | -1.37435800 |
| H | 3.65241500 | 1.94131600 | -3.23574000 | C | -0.52982000 | -1.15422400 | -2.65088300 |
| H | 2.17281500 | -3.76097600 | -1.19049500 | H | 0.63917900 | -2.45898500 | -1.38484800 |
| H | 1.38146400 | -6.09360400 | -1.31439100 | H | 0.33724800 | -0.50433300 | -2.84835300 |
| H | -0.38322000 | -6.91231300 | 0.25059100 | H | -0.62520800 | -1.83283000 | -3.52005200 |
| H | -1.34051900 | -5.35449100 | 1.95339800 | C | -4.54666400 | -2.73335300 | 1.32636300 |
| H | -0.57604000 | -3.01724900 | 2.06820500 | C | -5.85053700 | -2.89817400 | 1.08388100 |
| H | 4.20260000 | -0.92013900 | 1.27711800 | H | -4.23049000 | -2.10724300 | 2.16851700 |
| H | 1.92578400 | -1.58921400 | -2.34180100 | H | -6.61413300 | -2.43018300 | 1.71321300 |
| H | 3.97884500 | -1.34509200 | -3.67224200 | H | -6.20249900 | -3.50774600 | 0.24372300 |
| H | 6.15456700 | -0.84493500 | -2.54737100 | P | 2.06446400 | -0.80967400 | 0.48486600 |
| H | 6.23164800 | -0.63007800 | -0.06107900 | C | 2.53830700 | -0.20584000 | 2.19181200 |
| C | -0.09227900 | 1.47201000 | 3.38771900 | C | 2.23829400 | 1.27707300 | 2.48042100 |
| H | -0.71433100 | 2.37614600 | 3.31790600 | C | 0.76929900 | 1.73602700 | 2.54651400 |
| H | -0.73447900 | 0.60706700 | 3.19181700 | P | -0.06092700 | 1.77466200 | 0.88487900 |
| H | 0.28504100 | 1.40562700 | 4.42129200 | C | -1.51862600 | 2.87512900 | 1.06121800 |

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|---|-------------|-------------|-------------|------------------|-------------|-------------|-------------|
| C | -2.34467100 | 3.01428900 | -0.06777800 | H | 3.87584800 | -0.61782700 | -4.09566900 |
| C | -3.44113300 | 3.87737400 | -0.04043500 | H | 5.44949400 | 1.27068500 | -3.64800700 |
| C | -3.73691300 | 4.59943600 | 1.12114500 | H | 5.58523800 | 2.24315800 | -1.35227200 |
| C | -2.92348500 | 4.46105800 | 2.24876600 | C | -0.06456100 | 0.90705200 | 3.52922100 |
| C | -1.81507700 | 3.60820000 | 2.22050500 | H | -1.07170400 | 1.32560500 | 3.66732100 |
| C | 1.02045100 | 2.75632100 | -0.22065500 | H | -0.19169300 | -0.12783700 | 3.18423300 |
| C | 1.15812800 | 2.32642700 | -1.54848200 | H | 0.43212700 | 0.88980700 | 4.51282000 |
| C | 1.67536300 | 3.92392400 | 0.20157900 | C | 3.97032600 | -0.57081600 | 2.59675500 |
| C | 2.46631500 | 4.64259900 | -0.69767700 | H | 4.72046000 | 0.02085800 | 2.05297800 |
| C | 2.59417200 | 4.21214300 | -2.02400200 | H | 4.10525500 | -0.37066100 | 3.67195500 |
| C | 1.93497600 | 3.05637800 | -2.45089400 | H | 4.18487100 | -1.63480100 | 2.42391000 |
| C | 2.42976400 | -2.60194200 | 0.60816100 | Co | -0.24091700 | -0.38921600 | -0.07777600 |
| C | 3.59411300 | -3.18891800 | 0.09143300 | | | | |
| C | 3.81366300 | -4.56202800 | 0.23891800 | TS4 _T | | | |
| C | 2.87847900 | -5.35776500 | 0.90732100 | C | -3.39815900 | -1.47670800 | -0.65290500 |
| C | 1.71853800 | -4.77619700 | 1.43080100 | C | -4.41127100 | -1.16691900 | -1.57278800 |
| C | 1.49176300 | -3.40689100 | 1.27795900 | C | -5.54205200 | -0.44998300 | -1.17238000 |
| C | 3.22922000 | -0.16010300 | -0.76683200 | C | -5.67310700 | -0.02429300 | 0.15375700 |
| C | 4.11337800 | 0.90273200 | -0.52665900 | C | -4.66628900 | -0.32191900 | 1.07506500 |
| C | 3.15116700 | -0.69557200 | -2.06699300 | C | -3.54058100 | -1.04755500 | 0.67517400 |
| C | 3.94802900 | -0.18778000 | -3.09377200 | H | -4.32085300 | -1.49769800 | -2.61035000 |
| C | 4.82987800 | 0.86905200 | -2.84265200 | H | -6.32263200 | -0.21806600 | -1.90143600 |
| C | 4.90765900 | 1.41136700 | -1.55814000 | H | -6.55160300 | 0.54636600 | 0.46366500 |
| H | 1.85561100 | -0.81611700 | 2.80561600 | H | -4.75287700 | 0.01502200 | 2.11090600 |
| H | 2.79689900 | 1.92673100 | 1.79290200 | H | -2.76640400 | -1.28382700 | 1.40490600 |
| H | 2.65730600 | 1.47840100 | 3.48063400 | C | -2.22750400 | -2.34507100 | -1.06913600 |
| H | 0.79874300 | 2.78113600 | 2.89277100 | C | -0.92032000 | -2.02911000 | -0.32773900 |
| H | -2.12320500 | 2.45057000 | -0.97734900 | O | -0.52372200 | -2.49385900 | 0.72438700 |
| H | -4.06864300 | 3.98397100 | -0.92832700 | H | 0.55688900 | -1.06899000 | -3.82062700 |
| H | -4.59939000 | 5.26992900 | 1.14532200 | C | -1.58843300 | -2.03366500 | -2.44367800 |
| H | -3.14621400 | 5.02387700 | 3.15864000 | H | -1.93638900 | -1.07412100 | -2.85125900 |
| H | -1.18627900 | 3.53110600 | 3.10813700 | H | -1.74503000 | -2.81601200 | -3.19974800 |
| H | 0.66138300 | 1.40822400 | -1.86888700 | C | -2.59608100 | -3.85269400 | -0.93697700 |
| H | 1.56823600 | 4.27594200 | 1.23020300 | H | -1.71242500 | -4.43705400 | -1.24852000 |
| H | 2.98165400 | 5.54660800 | -0.36394300 | H | -3.39825900 | -4.05275600 | -1.66503900 |
| H | 3.21335000 | 4.77858500 | -2.72387900 | C | -0.13300200 | -1.91639000 | -1.96915800 |
| H | 2.03831200 | 2.71180300 | -3.48202000 | C | 0.74667300 | -0.93373700 | -2.74147100 |
| H | 4.33524000 | -2.57703900 | -0.42513400 | H | 0.37398000 | -2.88933500 | -1.90223400 |
| H | 4.72318600 | -5.00999900 | -0.16898900 | H | 0.49612300 | 0.13941400 | -2.56240300 |
| H | 3.05260200 | -6.43068800 | 1.01997100 | H | 1.81777800 | -1.07798100 | -2.55893800 |
| H | 0.98246800 | -5.39156400 | 1.95388700 | C | -3.02791200 | -4.28378900 | 0.43293700 |
| H | 0.57902400 | -2.96331600 | 1.68088100 | C | -4.26091000 | -4.69564900 | 0.74344600 |
| H | 4.18415400 | 1.35640500 | 0.45914600 | H | -2.26152800 | -4.23205300 | 1.21326800 |
| H | 2.46571700 | -1.51784000 | -2.28014700 | H | -4.52425100 | -4.99775400 | 1.76203100 |

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|---|-------------|-------------|-------------|----|-------------|-------------|-------------|
| H | -5.05437300 | -4.74424400 | -0.01118800 | H | 3.64917700 | -2.14408800 | -1.55393800 |
| P | 2.09764300 | -0.69474400 | 0.45304100 | H | 4.25637900 | -4.52313900 | -1.83597100 |
| C | 2.01265200 | -0.27082400 | 2.27192300 | H | 3.64417500 | -6.19354000 | -0.08166200 |
| C | 1.52289300 | 1.17524000 | 2.50326800 | H | 2.40552700 | -5.44633000 | 1.95317600 |
| C | 0.02688000 | 1.51814200 | 2.29576900 | H | 1.76884800 | -3.08007800 | 2.22679000 |
| P | -0.43596500 | 1.73643300 | 0.50941100 | H | 5.09023100 | -0.84650900 | 0.78718400 |
| C | -2.14339700 | 2.40730000 | 0.47336900 | H | 2.20272000 | 1.50831400 | -1.37876900 |
| C | -2.87377500 | 2.25037500 | -0.71571700 | H | 4.02586700 | 2.93231900 | -2.28296600 |
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| C | -4.70194100 | 3.53127500 | 0.21981600 | H | 6.91634300 | 0.56190600 | -0.11754600 |
| C | -3.98397400 | 3.68149300 | 1.41056200 | C | -0.90622200 | 0.49072100 | 2.94604400 |
| C | -2.70526500 | 3.13090300 | 1.53626800 | H | -1.95165300 | 0.82835600 | 2.93921800 |
| C | 0.50588300 | 3.18554400 | -0.11564800 | H | -0.86184300 | -0.47959400 | 2.43124700 |
| C | 0.52690000 | 3.39056700 | -1.50606700 | H | -0.60931100 | 0.33212700 | 3.99537700 |
| C | 1.17732500 | 4.09028200 | 0.71905300 | C | 3.32167600 | -0.50058300 | 3.03085300 |
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| C | 1.89850800 | 5.36385300 | -1.21546500 | H | 3.13818400 | -0.42254000 | 4.11488500 |
| C | 1.21398300 | 4.47542800 | -2.05266200 | H | 3.75042200 | -1.49305800 | 2.83266800 |
| C | 2.67456700 | -2.43183500 | 0.36356400 | Co | -0.01792800 | -0.27932700 | -0.54952600 |
| C | 3.36994800 | -2.86268100 | -0.78070000 | | | | |
| C | 3.71499100 | -4.20719400 | -0.94065000 | 4s | | | |
| C | 3.37226100 | -5.14220800 | 0.04102400 | C | -1.97032600 | 2.25036300 | 0.77625800 |
| C | 2.67888900 | -4.72294100 | 1.18084200 | C | -3.35422200 | 2.00493500 | 0.85724500 |
| C | 2.32603400 | -3.38033600 | 1.33957200 | C | -4.15552300 | 2.06951500 | -0.27701800 |
| C | 3.51249900 | 0.26223600 | -0.20887400 | C | -3.59058500 | 2.34446700 | -1.53211900 |
| C | 4.85036400 | -0.00956300 | 0.13007000 | C | -2.22595500 | 2.59021500 | -1.63344900 |
| C | 3.23405000 | 1.31585600 | -1.09124700 | C | -1.41416500 | 2.56269400 | -0.48455200 |
| C | 4.26349500 | 2.11091200 | -1.60298300 | H | -3.80226400 | 1.77526900 | 1.82514300 |
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| H | 1.25602400 | -0.97001900 | 2.65784300 | H | -1.77863700 | 2.83330000 | -2.59907300 |
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| H | -0.13435800 | 2.49184400 | 2.78425000 | C | 0.19138900 | 1.44280500 | 1.87920200 |
| H | -2.44891200 | 1.67723100 | -1.54331900 | O | 1.19866300 | 1.72137100 | 1.15564700 |
| H | -4.70237300 | 2.68838400 | -1.77354100 | H | 0.14298100 | -0.74454600 | 4.72438800 |
| H | -5.70018600 | 3.96529700 | 0.12409000 | C | -1.45592300 | 1.36130800 | 3.21621700 |
| H | -4.41757500 | 4.23707500 | 2.24579600 | H | -2.14042800 | 0.55035200 | 2.93324800 |
| H | -2.14919200 | 3.27461300 | 2.46461600 | H | -1.84028100 | 1.87497200 | 4.10733800 |
| H | 0.00964200 | 2.68986300 | -2.16644500 | C | -0.81484100 | 3.73442600 | 2.47857300 |
| H | 1.16419600 | 3.96624100 | 1.80244300 | H | -0.23048600 | 3.67130100 | 3.41276500 |
| H | 2.40383300 | 5.86270000 | 0.82785900 | H | -1.78660200 | 4.19167400 | 2.72880400 |
| H | 2.44769000 | 6.20662800 | -1.64216200 | C | 0.01199200 | 0.85008300 | 3.27712800 |
| H | 1.22422300 | 4.62199300 | -3.13537500 | C | 0.27256700 | -0.59808900 | 3.63988900 |

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|---|-------------|-------------|-------------|----------------|-------------|-------------|-------------|
| H | 0.60833300 | 1.50558100 | 3.93927400 | H | -5.95836000 | -1.08806800 | -2.42652700 |
| H | -0.43275100 | -1.26507800 | 3.12795000 | H | -3.51996400 | -0.98972000 | -2.77210900 |
| H | 1.29619200 | -0.90539000 | 3.37952900 | H | 0.52999100 | -1.93147900 | 1.40965600 |
| C | -0.07367400 | 4.59454300 | 1.50016700 | H | -2.26123000 | -3.76930800 | -1.30531800 |
| C | -0.56246900 | 5.70329600 | 0.93546200 | H | -1.83782400 | -5.97187100 | -0.25130000 |
| H | 0.93861300 | 4.26232400 | 1.24374200 | H | -0.25282500 | -6.16209500 | 1.66715300 |
| H | 0.03060900 | 6.29561800 | 0.23149800 | H | 0.93203400 | -4.12650400 | 2.50284900 |
| H | -1.57517300 | 6.05955100 | 1.15653800 | H | 4.84549900 | 0.36478500 | -0.40501600 |
| P | 1.90110300 | -0.24053700 | -0.73303400 | H | 6.18711700 | 2.35109900 | -1.01833400 |
| C | 1.80040000 | -0.99035000 | -2.44709900 | H | 5.09468000 | 4.33201400 | -2.07047300 |
| C | 0.63828500 | -1.96418300 | -2.68780100 | H | 2.63674700 | 4.29820100 | -2.51875700 |
| C | -0.78383700 | -1.37817400 | -2.56917100 | H | 1.29029000 | 2.31231500 | -1.90162400 |
| P | -1.20872000 | -1.06277000 | -0.78302000 | H | 2.62112500 | -3.15790400 | -0.71301900 |
| C | -3.03971000 | -1.05794700 | -0.65619800 | H | 3.21096800 | 0.33526300 | 1.76119800 |
| C | -3.57844300 | -1.13969500 | 0.63965000 | H | 4.45151100 | -1.04861100 | 3.40716900 |
| C | -4.95749500 | -1.20668900 | 0.83196400 | H | 4.79230400 | -3.48657800 | 2.98708600 |
| C | -5.82018300 | -1.18476300 | -0.27004700 | H | 3.86564800 | -4.52590700 | 0.91591100 |
| C | -5.29223700 | -1.10215200 | -1.56039800 | C | -0.97080800 | -0.12431300 | -3.42757900 |
| C | -3.90757300 | -1.04178200 | -1.75518400 | H | -2.01024000 | 0.22715800 | -3.43101000 |
| C | -0.88186200 | -2.70012800 | -0.01087200 | H | -0.34900200 | 0.70771700 | -3.06884500 |
| C | 0.01037100 | -2.81627200 | 1.05622600 | H | -0.68152500 | -0.33997000 | -4.46921900 |
| C | -1.55079600 | -3.84636800 | -0.47893000 | C | 3.13154500 | -1.54184300 | -2.96715200 |
| C | -1.31758600 | -5.08469100 | 0.11828600 | H | 3.37038600 | -2.52708900 | -2.54521800 |
| C | -0.42653500 | -5.19133900 | 1.19607900 | H | 3.06598900 | -1.65791500 | -4.06096400 |
| C | 0.23435800 | -4.05583200 | 1.66558600 | H | 3.97052400 | -0.86405900 | -2.75313300 |
| C | 2.97234100 | 1.20556200 | -1.10092600 | Co | -0.03386000 | 0.63293600 | 0.02378200 |
| C | 4.35288200 | 1.22372700 | -0.86217300 | | | | |
| C | 5.11136100 | 2.34700600 | -1.21055100 | 4 _T | | | |
| C | 4.49994200 | 3.45534800 | -1.80221300 | C | -2.35306600 | 2.37362500 | 0.60582000 |
| C | 3.12303100 | 3.43741300 | -2.05334700 | C | -3.74366300 | 2.20348000 | 0.63752100 |
| C | 2.36456600 | 2.31955400 | -1.70439200 | C | -4.47735700 | 2.10656800 | -0.54784800 |
| C | 2.87292500 | -1.30273400 | 0.38588400 | C | -3.83077500 | 2.17521900 | -1.78618300 |
| C | 3.04696500 | -2.67759500 | 0.16636900 | C | -2.44619900 | 2.35872500 | -1.83047800 |
| C | 3.37460600 | -0.72570300 | 1.56756900 | C | -1.71411700 | 2.46394600 | -0.64381000 |
| C | 4.06458700 | -1.50813500 | 2.49449400 | H | -4.25803300 | 2.13360100 | 1.59839100 |
| C | 4.25270500 | -2.87486700 | 2.25996800 | H | -5.55917500 | 1.96089100 | -0.50361800 |
| C | 3.73926900 | -3.45609700 | 1.09765100 | H | -4.40413300 | 2.08695300 | -2.71201200 |
| H | 1.58920800 | -0.07713800 | -3.02376800 | H | -1.93112800 | 2.42349700 | -2.79082500 |
| H | 0.74123800 | -2.85160100 | -2.04616700 | H | -0.63571300 | 2.63519400 | -0.68934400 |
| H | 0.74484100 | -2.32500900 | -3.72473100 | C | -1.54202900 | 2.48687300 | 1.87453700 |
| H | -1.48177600 | -2.15932000 | -2.90956500 | C | -0.21647700 | 1.70170200 | 1.91754300 |
| H | -2.91332300 | -1.15902700 | 1.50616500 | O | 0.87036100 | 1.88632100 | 1.30548100 |
| H | -5.36082200 | -1.27233900 | 1.84538500 | H | -0.70532700 | -0.76180000 | 4.42490000 |
| H | -6.90164500 | -1.23441000 | -0.12139800 | C | -1.97979300 | 1.62468300 | 3.10184800 |

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|---|-------------|-------------|-------------|-----|-------------|-------------|-------------|
| H | -2.69032100 | 0.83462000 | 2.82580000 | H | 1.67301900 | -0.00479500 | -3.03216300 |
| H | -2.37818600 | 2.19253100 | 3.95268600 | H | 1.26171400 | -2.80309000 | -1.83801400 |
| C | -1.31144300 | 3.97792200 | 2.26449500 | H | 1.17279600 | -2.43238000 | -3.55267800 |
| H | -0.78332300 | 3.99027900 | 3.23388200 | H | -1.02448400 | -2.52622800 | -2.83548200 |
| H | -2.30118900 | 4.43739800 | 2.42039700 | H | -2.93921800 | -0.90561100 | 1.36443400 |
| C | -0.53602000 | 1.06809100 | 3.26634900 | H | -5.40990700 | -0.98970900 | 1.52855600 |
| C | -0.33701700 | -0.42723200 | 3.44176800 | H | -6.77694600 | -1.58016900 | -0.47684900 |
| H | 0.02294800 | 1.62148200 | 4.04233600 | H | -5.64248600 | -2.11094000 | -2.63414000 |
| H | -0.88293500 | -0.98374800 | 2.66503900 | H | -3.18256900 | -2.07191600 | -2.79375600 |
| H | 0.72895700 | -0.69462800 | 3.37075900 | H | 0.79867200 | -2.15765300 | 1.43449800 |
| C | -0.51993400 | 4.76358100 | 1.26194200 | H | -2.01436100 | -4.21516900 | -1.11118300 |
| C | -0.98948400 | 5.79725100 | 0.55658300 | H | -1.42334400 | -6.36469000 | -0.02277300 |
| H | 0.51371500 | 4.43390200 | 1.10612500 | H | 0.26851100 | -6.41899500 | 1.80950700 |
| H | -0.36058500 | 6.33122600 | -0.16285900 | H | 1.38233000 | -4.30507700 | 2.53566600 |
| H | -2.02156700 | 6.14731200 | 0.67251000 | H | 4.98928600 | 0.68357700 | -0.41617700 |
| P | 2.07754900 | -0.03270700 | -0.74451400 | H | 6.23575500 | 2.76256600 | -0.93510600 |
| C | 2.03852000 | -0.84763600 | -2.42430800 | H | 5.04475500 | 4.73467900 | -1.89215200 |
| C | 1.02175900 | -1.99854400 | -2.54994100 | H | 2.58852700 | 4.61060200 | -2.32445100 |
| C | -0.47988900 | -1.64537300 | -2.45874000 | H | 1.33538800 | 2.53888100 | -1.78951100 |
| P | -1.04932900 | -1.43620000 | -0.69628600 | H | 3.21544000 | -2.86257400 | -0.70514900 |
| C | -2.88256700 | -1.47592800 | -0.72422100 | H | 3.01346200 | 0.60668300 | 1.86608700 |
| C | -3.53035700 | -1.17847600 | 0.48719600 | H | 4.17862300 | -0.65875000 | 3.65272200 |
| C | -4.92160500 | -1.22573300 | 0.58002800 | H | 4.86029400 | -3.03149400 | 3.26663300 |
| C | -5.68653300 | -1.55454100 | -0.54366200 | H | 4.36420200 | -4.11650600 | 1.07484000 |
| C | -5.05090400 | -1.84911500 | -1.75339900 | C | -0.85533300 | -0.42356000 | -3.29903000 |
| C | -3.65551400 | -1.81821500 | -1.84455300 | H | -1.94220100 | -0.27848500 | -3.35187000 |
| C | -0.63989800 | -3.04109900 | 0.09046100 | H | -0.42283100 | 0.49749900 | -2.88440400 |
| C | 0.31206800 | -3.07837300 | 1.11802000 | H | -0.47872000 | -0.54482100 | -4.32782600 |
| C | -1.26356800 | -4.23267600 | -0.31771900 | C | 3.41118300 | -1.23329900 | -2.98343300 |
| C | -0.93380000 | -5.44152800 | 0.29732100 | H | 3.83070900 | -2.12251400 | -2.49363500 |
| C | 0.01690000 | -5.47165800 | 1.32613100 | H | 3.31598800 | -1.46218600 | -4.05740600 |
| C | 0.63899900 | -4.28985600 | 1.73546400 | H | 4.13714800 | -0.41371700 | -2.87963100 |
| C | 3.07804000 | 1.46605600 | -1.07283500 | Co | -0.01350200 | 0.38965800 | 0.26301900 |
| C | 4.45823800 | 1.54125700 | -0.83313500 | | | | |
| C | 5.16074200 | 2.71435100 | -1.12622000 | l's | | | |
| C | 4.49344700 | 3.81900600 | -1.66427500 | C | -4.22586600 | 0.96760400 | -0.22907400 |
| C | 3.11704500 | 3.74971900 | -1.90758800 | C | -4.75064300 | 0.20201100 | -1.28273800 |
| C | 2.41214800 | 2.58211600 | -1.60750600 | C | -5.93963200 | -0.51904400 | -1.13355800 |
| C | 3.07219700 | -1.01945700 | 0.43360000 | C | -6.63688500 | -0.48859500 | 0.07547500 |
| C | 3.44277600 | -2.35761100 | 0.23198500 | C | -6.13545600 | 0.27982700 | 1.13078000 |
| C | 3.33415700 | -0.42117100 | 1.68277900 | C | -4.94903900 | 1.00102900 | 0.97760100 |
| C | 3.97938900 | -1.13803200 | 2.69097800 | H | -4.23727000 | 0.15438800 | -2.24222300 |
| C | 4.35967100 | -2.46830600 | 2.47525400 | H | -6.31714500 | -1.11036500 | -1.97164300 |
| C | 4.08586700 | -3.07399700 | 1.24690400 | H | -7.56336800 | -1.05577800 | 0.19482500 |

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|---|-------------|-------------|-------------|----------------|-------------|-------------|-------------|
| H | -6.67243400 | 0.32201200 | 2.08193000 | C | -2.58012100 | -2.20753000 | 0.90516100 |
| H | -4.58258200 | 1.59786900 | 1.81207400 | C | 1.41495500 | -2.80369100 | -0.24503400 |
| C | -2.95802200 | 1.80887900 | -0.38800100 | C | 1.58783400 | -4.10056700 | 0.27075200 |
| C | -1.98040400 | 1.62660300 | 0.77676800 | C | 2.25731200 | -2.35769400 | -1.27384800 |
| O | -2.18219400 | 1.03977600 | 1.81855000 | C | 3.27922500 | -3.17672800 | -1.76048700 |
| H | -0.99577300 | 2.13524100 | 0.61310900 | C | 3.46371200 | -4.45373400 | -1.22447600 |
| C | -2.15486700 | 1.48043200 | -1.66871000 | C | 2.61161100 | -4.91655800 | -0.21443500 |
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| H | -2.80731300 | 1.63095600 | -2.54675000 | H | 2.50222200 | -1.58778600 | 2.12639800 |
| C | -3.39348100 | 3.32023500 | -0.41875200 | H | 1.85185200 | -1.10338000 | 3.68418100 |
| H | -3.95184600 | 3.52352800 | 0.50973000 | H | 3.03297800 | 0.74779500 | 2.71603300 |
| H | -4.10289800 | 3.42542300 | -1.25425300 | H | 0.65066100 | 2.86955600 | -1.08735300 |
| C | -1.56025400 | 0.09213900 | -1.65270800 | H | 0.89505500 | 5.32590800 | -1.37697900 |
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| H | -2.22487700 | -0.69432200 | -1.29294700 | H | 4.11805600 | 5.34046600 | 1.49844200 |
| H | -0.25947300 | -1.33983400 | -2.64179200 | H | 3.89214300 | 2.88227900 | 1.77025400 |
| H | 0.06646100 | 0.43211600 | -3.06049600 | H | 3.23542100 | 1.13268600 | -2.07410300 |
| C | -2.29078300 | 4.32944200 | -0.56051800 | H | 4.39447100 | -0.63092300 | 1.70392800 |
| C | -2.14331200 | 5.13707000 | -1.61570900 | H | 6.49379600 | -1.42068900 | 0.68786700 |
| H | -1.58104400 | 4.40943500 | 0.27141200 | H | 6.99541100 | -0.94565800 | -1.70897000 |
| H | -1.34058600 | 5.87892600 | -1.66280400 | H | 5.36034900 | 0.35114400 | -3.08225700 |
| H | -2.83008600 | 5.09029800 | -2.46863200 | H | -0.71151800 | -3.84201900 | -1.44353500 |
| P | 0.12431100 | -1.66579100 | 0.37531500 | H | -2.90218800 | -4.91632600 | -1.86617800 |
| C | 0.34245600 | -1.50175800 | 2.22649500 | H | -4.89876500 | -4.27057300 | -0.51458800 |
| C | 1.73431700 | -0.95534800 | 2.59791500 | H | -4.68169900 | -2.52483200 | 1.25613500 |
| C | 2.02130400 | 0.53579300 | 2.33597200 | H | -2.51533300 | -1.42158000 | 1.65897500 |
| P | 2.04540300 | 0.90301900 | 0.51721500 | H | 0.91562500 | -4.48269300 | 1.03881300 |
| C | 2.24622100 | 2.71762200 | 0.36686400 | H | 2.10798300 | -1.36182500 | -1.68687300 |
| C | 1.40976400 | 3.41264400 | -0.51846800 | H | 3.93252300 | -2.81082700 | -2.55545100 |
| C | 1.54845100 | 4.79492300 | -0.68189100 | H | 4.26588800 | -5.09476400 | -1.59858500 |
| C | 2.51830400 | 5.48858400 | 0.04628900 | H | 2.74229900 | -5.92112000 | 0.19524800 |
| C | 3.35712500 | 4.79865400 | 0.93127300 | C | 1.03120000 | 1.45357800 | 3.06022800 |
| C | 3.22777100 | 3.41766500 | 1.08736600 | H | 1.33519800 | 2.50756500 | 2.99547000 |
| C | 3.65962300 | 0.30438000 | -0.11557700 | H | 0.00946100 | 1.36769200 | 2.66270500 |
| C | 3.95200400 | 0.57587500 | -1.46436700 | H | 0.99612800 | 1.17866400 | 4.12708100 |
| C | 4.58671200 | -0.41132000 | 0.65384400 | C | 0.06310200 | -2.78095800 | 3.02264300 |
| C | 5.78116800 | -0.85951200 | 0.07849800 | H | 0.89964000 | -3.49058500 | 2.94657200 |
| C | 6.06289900 | -0.59187600 | -1.26272500 | H | -0.04998600 | -2.52049400 | 4.08733200 |
| C | 5.14588000 | 0.13388900 | -2.03308000 | H | -0.85481500 | -3.29125900 | 2.70198200 |
| C | -1.44861900 | -2.57623400 | 0.15485400 | Co | 0.14485800 | 0.26874200 | -0.57824300 |
| C | -1.57687000 | -3.55239000 | -0.84494600 | | | | |
| C | -2.81444200 | -4.15844300 | -1.08374300 | I _T | | | |
| C | -3.93183300 | -3.79773200 | -0.32619300 | C | 2.23868800 | -1.65783200 | 0.69201000 |
| C | -3.81027600 | -2.82224500 | 0.66954700 | O | 2.25482200 | -2.22881000 | 1.75526700 |

| | | | | | | | |
|---|-------------|-------------|-------------|----|-------------|-------------|-------------|
| H | 1.92960200 | -0.57283500 | 0.65851600 | H | 2.15041900 | 3.21222500 | -0.60440300 |
| P | 0.01221300 | 1.83902200 | 0.87214000 | H | 4.55942100 | 3.53393200 | -0.14486700 |
| C | -1.00498100 | 1.95611500 | 2.43110500 | H | 5.53305300 | 2.80299800 | 2.03464800 |
| C | -2.44763300 | 1.46246300 | 2.18660300 | H | 4.06248500 | 1.74083500 | 3.74987200 |
| C | -2.69652200 | -0.05669500 | 2.03561500 | H | 1.65804900 | 1.40338100 | 3.29551800 |
| P | -2.25955500 | -0.71945000 | 0.34349100 | H | 0.36529300 | 4.82944000 | 0.81575900 |
| C | -2.70339500 | -2.49437200 | 0.44312800 | H | -1.70263700 | 1.77715100 | -1.42640700 |
| C | -1.66651700 | -3.41900000 | 0.64967300 | H | -2.70962900 | 3.51730800 | -2.88239700 |
| C | -1.94776500 | -4.78250000 | 0.76713400 | H | -2.16518600 | 5.92731600 | -2.49733200 |
| C | -3.26871200 | -5.23224200 | 0.67198200 | H | -0.62027500 | 6.56814800 | -0.64829600 |
| C | -4.30605000 | -4.31588200 | 0.46256500 | C | -1.96449800 | -0.88254500 | 3.09826800 |
| C | -4.02688700 | -2.95127400 | 0.34843000 | H | -2.33545500 | -1.91647800 | 3.13166300 |
| C | -3.48663500 | -0.02420700 | -0.82238200 | H | -0.87904200 | -0.92241800 | 2.91023700 |
| C | -3.24054500 | -0.21028000 | -2.19439900 | H | -2.11670400 | -0.43552800 | 4.09386800 |
| C | -4.62225700 | 0.69698200 | -0.42427700 | C | -1.00731700 | 3.34972600 | 3.06097100 |
| C | -5.48844400 | 1.23233200 | -1.38351600 | H | -1.57720500 | 4.06496900 | 2.44847400 |
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| C | -4.11122300 | 0.31620100 | -3.14927200 | H | 0.01144800 | 3.74462200 | 3.18983200 |
| C | 1.72366400 | 2.30481100 | 1.31957100 | Co | -0.02410700 | -0.30267300 | 0.02534100 |
| C | 2.56092300 | 2.89617500 | 0.35641300 | C | 3.77104200 | -1.32790600 | -1.21191800 |
| C | 3.92153900 | 3.07597200 | 0.61493600 | C | 3.98557600 | -1.20359600 | -2.59359100 |
| C | 4.46773100 | 2.66463800 | 1.83519000 | C | 5.01900700 | -0.40561700 | -3.08794700 |
| C | 3.64386300 | 2.06865500 | 2.79511200 | C | 5.85843400 | 0.28912000 | -2.20984900 |
| C | 2.28185100 | 1.88532400 | 2.53969100 | C | 5.65955700 | 0.16889900 | -0.83299000 |
| C | -0.61511500 | 3.18069300 | -0.20068600 | C | 4.62800300 | -0.63712000 | -0.34057300 |
| C | -0.31000000 | 4.53657500 | 0.01012000 | H | 3.33755900 | -1.72773500 | -3.29747600 |
| C | -1.47574700 | 2.82758700 | -1.25186100 | H | 5.16625000 | -0.32203100 | -4.16772700 |
| C | -2.03786900 | 3.80971300 | -2.07177600 | H | 6.66249700 | 0.91889200 | -2.59840600 |
| C | -1.73236700 | 5.15630100 | -1.85496700 | H | 6.30609100 | 0.70398700 | -0.13368900 |
| C | -0.86472700 | 5.51639500 | -0.81678900 | H | 4.49842400 | -0.71883700 | 0.74136800 |
| H | -0.50450600 | 1.26148900 | 3.12226300 | C | 2.66557000 | -2.23402300 | -0.65367900 |
| H | -2.88005900 | 2.01063900 | 1.33412000 | C | 3.25366100 | -3.66576000 | -0.45697300 |
| H | -3.03290600 | 1.77704500 | 3.06697100 | H | 3.98500400 | -3.61625300 | 0.36313700 |
| H | -3.77848500 | -0.22058000 | 2.16192200 | H | 3.81133100 | -3.90623900 | -1.37598900 |
| H | -0.63489800 | -3.06681900 | 0.72504500 | C | 1.41320000 | -2.30148200 | -1.57158500 |
| H | -1.13177900 | -5.49101300 | 0.92758300 | H | 0.71633500 | -3.02840100 | -1.12983200 |
| H | -3.49113400 | -6.29873200 | 0.75830100 | H | 1.71930700 | -2.76282800 | -2.52695600 |
| H | -5.33845200 | -4.66646200 | 0.38700600 | C | 2.25750600 | -4.76703500 | -0.20391200 |
| H | -4.84022900 | -2.24069600 | 0.18337100 | C | 2.02358300 | -5.34539600 | 0.97827400 |
| H | -2.35550700 | -0.76467300 | -2.51383300 | H | 1.70656800 | -5.12732400 | -1.08055400 |
| H | -4.84425200 | 0.84907700 | 0.63242400 | H | 1.30674600 | -6.16671400 | 1.07744300 |
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| H | -3.90790300 | 0.16381800 | -4.21200900 | C | 1.03843300 | 0.26480400 | -1.78409000 |

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|-------------------|-------------|-------------|-------------|----|-------------|-------------|-------------|
| H | -0.26887100 | -1.25143300 | -2.48421300 | H | -5.60662400 | -4.08118600 | -0.23429500 |
| H | 0.47351300 | 1.05622400 | -2.28158200 | H | -4.76573500 | -1.75163500 | -0.24629000 |
| H | 2.03418700 | 0.53753000 | -1.42886700 | H | -2.41055000 | -0.31216800 | -2.48850900 |
| TS2' _T | | | | H | -4.44226400 | 1.18350800 | 1.02476000 |
| C | 1.37374300 | -1.51959500 | 0.47687800 | H | -5.98295600 | 2.45390400 | -0.41315500 |
| O | 1.68877700 | -1.54690100 | 1.64599000 | H | -5.76985400 | 2.34991000 | -2.89712200 |
| H | 1.35451500 | 0.26883600 | -0.88968900 | H | -3.98383000 | 0.93691600 | -3.92575000 |
| P | 0.33967900 | 1.81209900 | 0.72250700 | H | 2.37179100 | 3.16719500 | -0.89918200 |
| C | -0.44033000 | 1.81000400 | 2.41603300 | H | 4.80681300 | 3.50328600 | -0.61285100 |
| C | -1.93475100 | 1.44898100 | 2.35176900 | H | 5.95594300 | 2.67755600 | 1.44371600 |
| C | -2.31884400 | -0.02965000 | 2.13252300 | H | 4.64181300 | 1.49015500 | 3.20198000 |
| P | -2.08094400 | -0.59321900 | 0.37167300 | H | 2.21245700 | 1.14658200 | 2.92245000 |
| C | -2.75103700 | -2.29836700 | 0.34495300 | H | 0.76285100 | 4.76574000 | 0.98691000 |
| C | -1.89819600 | -3.36183800 | 0.67965800 | H | -1.47479400 | 2.04006200 | -1.50396800 |
| C | -2.37664900 | -4.67391200 | 0.69261900 | H | -2.48528000 | 3.95913500 | -2.70741100 |
| C | -3.70993300 | -4.93694300 | 0.36167800 | H | -1.87907100 | 6.29499600 | -2.05481300 |
| C | -4.56392200 | -3.88172900 | 0.02513400 | H | -0.24740400 | 6.68305400 | -0.20995700 |
| C | -4.08986400 | -2.56684600 | 0.01743600 | C | -1.59616300 | -0.97389200 | 3.09942700 |
| C | -3.29992800 | 0.34942600 | -0.62595700 | H | -2.03784500 | -1.97982600 | 3.08298000 |
| C | -3.19556500 | 0.28709300 | -2.02653500 | H | -0.52566600 | -1.07142900 | 2.86504100 |
| C | -4.31934600 | 1.12750300 | -0.05649900 | H | -1.68692000 | -0.58474900 | 4.12650700 |
| C | -5.19974100 | 1.84573900 | -0.87206600 | C | -0.24020400 | 3.12242500 | 3.17722900 |
| C | -5.08247700 | 1.78505500 | -2.26281100 | H | -0.84604600 | 3.93067900 | 2.74079000 |
| C | -4.08155700 | 0.99534400 | -2.83916700 | H | -0.56374100 | 2.98840000 | 4.22201700 |
| C | 2.11347600 | 2.15983200 | 1.00522700 | H | 0.81022000 | 3.44603400 | 3.18855200 |
| C | 2.86218800 | 2.80780700 | 0.00799800 | Co | 0.06433500 | -0.21848900 | -0.26935800 |
| C | 4.23606100 | 2.99536300 | 0.16821400 | C | 3.26528800 | -1.85308100 | -1.14585000 |
| C | 4.88044100 | 2.53031200 | 1.31963000 | C | 3.76241400 | -2.26370400 | -2.39485900 |
| C | 4.14440700 | 1.86692700 | 2.30504400 | C | 4.95053200 | -1.73809600 | -2.90735200 |
| C | 2.76767100 | 1.67945200 | 2.15015200 | C | 5.67319800 | -0.78799400 | -2.17872000 |
| C | -0.31121100 | 3.26848200 | -0.16378100 | C | 5.19691900 | -0.37967800 | -0.93121700 |
| C | 0.04070500 | 4.58337900 | 0.19019200 | C | 4.00746400 | -0.90810300 | -0.41867100 |
| C | -1.21292800 | 3.05661100 | -1.21679800 | H | 3.21808300 | -3.00378100 | -2.98361000 |
| C | -1.77995700 | 4.14020600 | -1.89311900 | H | 5.31193000 | -2.07402100 | -3.88273800 |
| C | -1.43895300 | 5.44503300 | -1.52746800 | H | 6.60097800 | -0.37248500 | -2.57975800 |
| C | -0.52408000 | 5.66373200 | -0.49011700 | H | 5.74842800 | 0.35846500 | -0.34582100 |
| H | 0.09804000 | 1.00715100 | 2.94111900 | H | 3.66309100 | -0.56953800 | 0.55816200 |
| H | -2.43350900 | 2.09945700 | 1.61687200 | C | 1.98693500 | -2.49322500 | -0.57644400 |
| H | -2.36348600 | 1.72657700 | 3.32901400 | C | 2.42889900 | -3.82626100 | 0.09764600 |
| H | -3.40108300 | -0.11514400 | 2.31990900 | H | 3.15726400 | -3.56802000 | 0.88015100 |
| H | -0.85764900 | -3.16657800 | 0.93744200 | H | 2.96644500 | -4.40638300 | -0.67138000 |
| H | -1.70244800 | -5.49165200 | 0.95710900 | C | 0.88367000 | -2.70800900 | -1.64168900 |
| H | -4.08298900 | -5.96406200 | 0.36416300 | H | 0.10697600 | -3.35275600 | -1.21165400 |
| | | | | H | 1.28130200 | -3.26171300 | -2.50870000 |

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|-----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| C | 1.34127400 | -4.68235900 | 0.67730600 | H | 0.38577300 | 0.85011500 | 2.99395200 |
| C | 1.15673300 | -4.89626600 | 1.98382800 | H | -1.85231500 | 2.47147800 | 1.67725700 |
| H | 0.66959000 | -5.17223500 | -0.03691700 | H | -1.85289900 | 2.07966200 | 3.38761800 |
| H | 0.35611200 | -5.54632100 | 2.34992400 | H | -3.27244900 | 0.51774800 | 2.34622500 |
| H | 1.79734400 | -4.42244100 | 2.73514400 | H | -1.48514700 | -2.90950100 | 1.26657400 |
| C | 0.21231200 | -1.43348600 | -2.10996500 | H | -2.77046900 | -5.01436600 | 1.29701500 |
| C | 0.91028100 | -0.25703700 | -2.39290000 | H | -5.10405200 | -5.07231700 | 0.40024600 |
| H | -0.81507500 | -1.53261700 | -2.46699600 | H | -6.12704100 | -2.98730500 | -0.51262500 |
| H | 0.37643200 | 0.57570000 | -2.86250100 | H | -4.84641100 | -0.87201400 | -0.52928600 |
| H | 1.99427800 | -0.25316000 | -2.52114600 | H | -2.46622600 | 0.17566100 | -2.44871700 |
| | | | | H | -4.02450300 | 2.01700300 | 1.14467600 |
| 2's | | | | H | -5.31961500 | 3.58683300 | -0.23234000 |
| C | 0.91841700 | -1.40424300 | 0.32675600 | H | -5.21183100 | 3.47383400 | -2.72306700 |
| O | 1.24249400 | -1.31133300 | 1.48549000 | H | -3.78674200 | 1.73659000 | -3.81833200 |
| H | 1.30973800 | 0.33498900 | -1.12441800 | H | 3.01990800 | 2.30877300 | -0.93206000 |
| P | 0.77430700 | 1.54361200 | 0.75635100 | H | 5.47444800 | 2.20504400 | -0.64904200 |
| C | 0.03350000 | 1.73916700 | 2.45114000 | H | 6.45743500 | 1.30976100 | 1.46516400 |
| C | -1.50308000 | 1.72237400 | 2.40488700 | H | 4.95013900 | 0.52364800 | 3.29222200 |
| C | -2.19547800 | 0.36593800 | 2.17337900 | H | 2.50096600 | 0.64002000 | 3.02336100 |
| P | -2.07743600 | -0.19519000 | 0.40038200 | H | 1.91615500 | 4.31636900 | 0.99147400 |
| C | -3.07150000 | -1.73868100 | 0.36909300 | H | -0.98964600 | 2.22816200 | -1.43376400 |
| C | -2.50189200 | -2.91679800 | 0.87822300 | H | -1.48803600 | 4.31954100 | -2.64824700 |
| C | -3.22966600 | -4.10789700 | 0.89493200 | H | -0.29333500 | 6.43139900 | -2.04410400 |
| C | -4.53495300 | -4.13946700 | 0.39306800 | H | 1.41043800 | 6.41191100 | -0.22297400 |
| C | -5.10766800 | -2.97149000 | -0.11904000 | C | -1.71751700 | -0.70981800 | 3.15586400 |
| C | -4.38344000 | -1.77521400 | -0.12991800 | H | -2.40410300 | -1.56626200 | 3.17786800 |
| C | -3.12584000 | 0.98542500 | -0.54566700 | H | -0.71290600 | -1.08383900 | 2.91501100 |
| C | -3.08378700 | 0.92123300 | -1.95038400 | H | -1.68804200 | -0.28150700 | 4.17091700 |
| C | -3.94755300 | 1.94843200 | 0.06004200 | C | 0.52364500 | 2.99324700 | 3.18089700 |
| C | -4.69035900 | 2.83924600 | -0.72121900 | H | 0.08886200 | 3.90340700 | 2.74175400 |
| C | -4.63277500 | 2.77420200 | -2.11554600 | H | 0.20329600 | 2.94426900 | 4.23404300 |
| C | -3.83341500 | 1.80422000 | -2.72888200 | H | 1.61771300 | 3.09375200 | 3.16561400 |
| C | 2.58412100 | 1.50098200 | 1.03265500 | Co | 0.00395100 | -0.06087600 | -0.56775700 |
| C | 3.43766000 | 1.92833000 | 0.00228300 | C | 2.58810400 | -2.34281200 | -1.30025200 |
| C | 4.82267200 | 1.86704200 | 0.15994800 | C | 2.83193800 | -2.89274800 | -2.56827900 |
| C | 5.37288100 | 1.36312300 | 1.34326400 | C | 4.04726000 | -2.67750700 | -3.22474000 |
| C | 4.52897100 | 0.92336200 | 2.36662700 | C | 5.04807600 | -1.90988100 | -2.62310500 |
| C | 3.14071500 | 0.99332000 | 2.21535600 | C | 4.82076500 | -1.36387500 | -1.35703900 |
| C | 0.47857200 | 3.12676900 | -0.11821000 | C | 3.60495600 | -1.57939600 | -0.70295100 |
| C | 1.15726900 | 4.31360700 | 0.20831800 | H | 2.07087200 | -3.49722000 | -3.06264100 |
| C | -0.46570600 | 3.14271800 | -1.15689400 | H | 4.20938400 | -3.11508800 | -4.21313900 |
| C | -0.74748200 | 4.32567200 | -1.84501800 | H | 5.99810500 | -1.74021000 | -3.13586900 |
| C | -0.07804900 | 5.50462100 | -1.50645600 | H | 5.59100700 | -0.76305200 | -0.86970100 |
| C | 0.87697300 | 5.49434100 | -0.48292400 | H | 3.45458200 | -1.14497100 | 0.28570500 |

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|-------|-------------|-------------|-------------|----|-------------|-------------|-------------|
| C | 1.29953800 | -2.66264400 | -0.52279300 | C | 3.16517100 | 1.07089300 | 2.07999500 |
| C | 1.66749200 | -3.85302700 | 0.41902400 | C | 0.34471200 | 3.17232100 | -0.08446900 |
| H | 2.48821600 | -3.51802100 | 1.06840400 | C | 0.89878500 | 4.39515600 | 0.33327300 |
| H | 2.07157400 | -4.64293300 | -0.23619100 | C | -0.53273800 | 3.15682400 | -1.17841500 |
| C | 0.08244500 | -2.98391500 | -1.41079900 | C | -0.88154400 | 4.34296200 | -1.82969200 |
| H | -0.68880800 | -3.44484000 | -0.78534600 | C | -0.34344800 | 5.55752100 | -1.39629400 |
| H | 0.33693400 | -3.73894900 | -2.17144700 | C | 0.55225400 | 5.57959400 | -0.32020000 |
| C | 0.56672400 | -4.43878300 | 1.25435600 | H | 0.39971500 | 0.75608200 | 2.92608300 |
| C | 0.46999400 | -4.31457500 | 2.58191700 | H | -1.88689700 | 2.39737500 | 1.72647700 |
| H | -0.19292700 | -5.02338400 | 0.72304800 | H | -1.85480400 | 1.96056100 | 3.42528000 |
| H | -0.34675500 | -4.78138800 | 3.14127700 | H | -3.28606100 | 0.43176000 | 2.33337600 |
| H | 1.20125700 | -3.73550600 | 3.15520000 | H | -1.50319400 | -2.99407800 | 1.22319700 |
| C | -0.52122400 | -1.76052700 | -2.05213800 | H | -2.79462200 | -5.09903300 | 1.17961700 |
| C | 0.19479600 | -0.77651200 | -2.68280800 | H | -5.10903500 | -5.12776900 | 0.23316700 |
| H | -1.61208100 | -1.74438700 | -2.11972700 | H | -6.10613700 | -3.01940400 | -0.65351200 |
| H | -0.33223200 | 0.03545600 | -3.19501700 | H | -4.81816700 | -0.90876300 | -0.59779700 |
| H | 1.25546300 | -0.87573000 | -2.90386800 | H | -2.37179800 | 0.14213100 | -2.45560100 |
| | | | | H | -4.01678900 | 1.93933300 | 1.12012300 |
| | | | | H | -5.27515000 | 3.53033400 | -0.26703400 |
| | | | | H | -5.10625900 | 3.45014800 | -2.75553800 |
| | | | | H | -3.65788100 | 1.72538100 | -3.83905300 |
| TS3's | | | | H | 2.87020400 | 2.55213600 | -0.98146700 |
| C | 0.91673800 | -1.40912300 | 0.37047100 | H | 5.33659200 | 2.56198500 | -0.78075800 |
| O | 1.22518300 | -1.31905500 | 1.53395200 | H | 6.43400800 | 1.61267600 | 1.25164300 |
| H | 1.16242800 | 0.28524900 | -1.45503100 | H | 5.03174300 | 0.64359100 | 3.07427300 |
| P | 0.72626700 | 1.57518700 | 0.72631600 | H | 2.57065700 | 0.63395300 | 2.88179500 |
| C | 0.02165900 | 1.67082700 | 2.44774200 | H | 1.61444300 | 4.42356000 | 1.15548100 |
| C | -1.51729600 | 1.63335900 | 2.42791200 | H | -0.94495200 | 2.20989700 | -1.52431200 |
| C | -2.20681100 | 0.27882600 | 2.17416900 | H | -1.57090500 | 4.31234900 | -2.67660700 |
| P | -2.06442900 | -0.26838200 | 0.39970900 | H | -0.61144200 | 6.48801500 | -1.90300200 |
| C | -3.06566500 | -1.80266000 | 0.31863400 | H | 0.98723200 | 6.52611300 | 0.00998400 |
| C | -2.51121900 | -2.99307700 | 0.81379600 | C | -1.74478900 | -0.80750500 | 3.15266700 |
| C | -3.24221300 | -4.18202900 | 0.78847600 | H | -2.42616600 | -1.66860700 | 3.14660100 |
| C | -4.53672600 | -4.19720000 | 0.25873000 | H | -0.73249400 | -1.17167700 | 2.93052800 |
| C | -5.09499300 | -3.01588100 | -0.23894900 | H | -1.74178400 | -0.39295600 | 4.17380400 |
| C | -4.36699500 | -1.82235800 | -0.20874300 | C | 0.50160400 | 2.88471800 | 3.24832700 |
| C | -3.07827500 | 0.92984400 | -0.56149600 | H | 0.03195100 | 3.81108400 | 2.88553300 |
| C | -3.00249000 | 0.88293900 | -1.96585300 | H | 0.21287600 | 2.75622500 | 4.30396400 |
| C | -3.91262200 | 1.88633600 | 0.03693300 | H | 1.59195400 | 3.01461200 | 3.21067500 |
| C | -4.63503700 | 2.78832700 | -0.75026200 | Co | -0.03070600 | -0.09184100 | -0.55254100 |
| C | -4.54342900 | 2.74124400 | -2.14357000 | C | 2.67745200 | -2.34303200 | -1.18788100 |
| C | -3.73120600 | 1.77788100 | -2.75027600 | C | 3.03140100 | -3.00729000 | -2.37428700 |
| C | 2.54360700 | 1.61465900 | 0.94606400 | C | 4.27424600 | -2.79514700 | -2.97591700 |
| C | 3.33922800 | 2.14229400 | -0.08452600 | C | 5.19606800 | -1.91590400 | -2.39976600 |
| C | 4.73005600 | 2.14623900 | 0.02735300 | | | | |
| C | 5.34480000 | 1.61222300 | 1.16508200 | | | | |
| C | 4.55952200 | 1.07038900 | 2.18615500 | | | | |

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|-----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | 4.86210400 | -1.26106600 | -1.21228200 | C | 4.81175100 | -2.20950000 | -1.91308900 |
| C | 3.61771300 | -1.47563100 | -0.61155600 | C | 3.97882500 | -1.27828000 | -2.54208600 |
| H | 2.33324500 | -3.69997300 | -2.84600200 | C | -2.19481300 | -2.10541100 | 0.62868200 |
| H | 4.52108800 | -3.32222500 | -3.90113400 | C | -2.58786900 | -3.25319700 | -0.07547800 |
| H | 6.16755500 | -1.74653200 | -2.87072700 | C | -3.92852600 | -3.64834800 | -0.08577200 |
| H | 5.57011300 | -0.57580200 | -0.74272500 | C | -4.88750300 | -2.90378200 | 0.60634200 |
| H | 3.38705600 | -0.95755700 | 0.31806600 | C | -4.49907600 | -1.76380300 | 1.31805400 |
| C | 1.34556200 | -2.65806900 | -0.48200000 | C | -3.16176700 | -1.36522400 | 1.33013500 |
| C | 1.66324600 | -3.86523600 | 0.45507900 | C | 0.47874400 | -2.89841200 | -0.15828300 |
| H | 2.45624300 | -3.54449700 | 1.14517100 | C | 0.79419700 | -4.08019300 | 0.53355800 |
| H | 2.09409600 | -4.64482100 | -0.19556300 | C | 0.86548700 | -2.76842800 | -1.50138700 |
| C | 0.18000700 | -2.94233200 | -1.44968500 | C | 1.56019500 | -3.79681800 | -2.14132700 |
| H | -0.64768000 | -3.37736300 | -0.87771300 | C | 1.88190100 | -4.96378900 | -1.44392100 |
| H | 0.46084000 | -3.70493300 | -2.19418300 | C | 1.49716700 | -5.10288000 | -0.10628200 |
| C | 0.52749600 | -4.46502700 | 1.22859800 | H | -0.50518100 | -0.41010900 | 2.65914500 |
| C | 0.39549200 | -4.40102400 | 2.55743500 | H | 2.06185700 | -1.96925900 | 2.08359000 |
| H | -0.22589300 | -5.00937100 | 0.64797600 | H | 1.71051100 | -1.35855300 | 3.68922500 |
| H | -0.44504700 | -4.87692100 | 3.07205200 | H | 3.21328200 | 0.12703500 | 2.56740200 |
| H | 1.12130300 | -3.86430000 | 3.17725600 | H | 2.08098100 | 2.57671400 | -1.62562500 |
| C | -0.32625300 | -1.68336700 | -2.11046400 | H | 3.43961200 | 4.59351700 | -2.08746900 |
| C | 0.52125800 | -0.71320400 | -2.66116900 | H | 5.13774000 | 5.36645800 | -0.42669800 |
| H | -1.38683100 | -1.65839100 | -2.37079100 | H | 5.48938200 | 4.06976500 | 1.67636200 |
| H | 0.07520900 | 0.07823200 | -3.27338700 | H | 4.16777600 | 2.03444600 | 2.12200100 |
| H | 1.57087300 | -0.92305000 | -2.86842000 | H | 2.48757200 | 0.25304000 | -2.28103500 |
| | | | | H | 4.04401000 | -1.54066100 | 1.33641100 |
| 3's | | | | H | 5.46840400 | -3.02424100 | -0.02003300 |
| C | -1.22333100 | 1.33015700 | 0.43976800 | H | 5.45206100 | -2.86429700 | -2.50901500 |
| O | -1.43777600 | 1.41741200 | 1.62445100 | H | 3.96423300 | -1.20141300 | -3.63194200 |
| H | -2.35523600 | -1.64131800 | -2.25719800 | H | -1.85155500 | -3.83827600 | -0.62749500 |
| P | -0.45911200 | -1.52611700 | 0.60239800 | H | -4.22287200 | -4.54175600 | -0.64186600 |
| C | 0.00561500 | -1.35044700 | 2.40513400 | H | -5.93582800 | -3.21171200 | 0.59356300 |
| C | 1.52195200 | -1.17521000 | 2.61892200 | H | -5.24147400 | -1.17645500 | 1.86298100 |
| C | 2.14330100 | 0.20274800 | 2.31689400 | H | -2.87456300 | -0.47392500 | 1.88587500 |
| P | 2.04279800 | 0.62766300 | 0.51761400 | H | 0.48629000 | -4.21411900 | 1.56879700 |
| C | 3.01209100 | 2.17251000 | 0.28670800 | H | 0.62517000 | -1.85767900 | -2.05015400 |
| C | 2.83187300 | 2.89700700 | -0.90127100 | H | 1.85841500 | -3.67908800 | -3.18512300 |
| C | 3.59547100 | 4.03649600 | -1.16047700 | H | 2.43204200 | -5.76591200 | -1.94181300 |
| C | 4.54638100 | 4.46880000 | -0.23025300 | H | 1.74129700 | -6.01513200 | 0.44330700 |
| C | 4.74103300 | 3.74424000 | 0.94960700 | C | 1.51883000 | 1.31633700 | 3.16879200 |
| C | 3.98532600 | 2.59592500 | 1.20461100 | H | 2.05906700 | 2.26676700 | 3.06333400 |
| C | 3.15358100 | -0.54046500 | -0.37559200 | H | 0.46988400 | 1.49742200 | 2.90186200 |
| C | 3.14841100 | -0.45775200 | -1.77895800 | H | 1.55877000 | 1.02436100 | 4.23072900 |
| C | 4.00208000 | -1.46418200 | 0.24967800 | C | -0.54177600 | -2.44256700 | 3.33306200 |
| C | 4.81857100 | -2.30106600 | -0.51891900 | H | 0.05185200 | -3.36609300 | 3.28011100 |

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|-----------------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | -0.48445800 | -2.07952100 | 4.37167300 | C | 4.10436800 | 4.86094000 | 0.45325500 |
| H | -1.58972400 | -2.69397500 | 3.12349200 | C | 4.88863500 | 3.76320600 | 0.82972000 |
| Co | -0.01573600 | 0.30363300 | -0.49891700 | C | 4.33970600 | 2.48004300 | 0.83356200 |
| C | -3.42923400 | 2.07585300 | -0.65617000 | C | 3.49736600 | -0.37035500 | -0.42203400 |
| C | -4.13853200 | 2.22993600 | -1.85836300 | C | 3.60403300 | -0.14925800 | -1.80702500 |
| C | -5.53374800 | 2.16668800 | -1.88490700 | C | 4.33664400 | -1.31353200 | 0.18660900 |
| C | -6.25336700 | 1.95312100 | -0.70550500 | C | 5.25450700 | -2.03762200 | -0.58230300 |
| C | -5.56023100 | 1.82318000 | 0.50067200 | C | 5.35231400 | -1.81636500 | -1.95787200 |
| C | -4.16427500 | 1.89247000 | 0.52541600 | C | 4.52914000 | -0.86268200 | -2.56849200 |
| H | -3.60344600 | 2.39341900 | -2.79403900 | C | -2.04225300 | -2.25507500 | 0.75953200 |
| H | -6.05972800 | 2.28246400 | -2.83608100 | C | -2.49621400 | -3.37435900 | 0.04513300 |
| H | -7.34451100 | 1.89599100 | -0.72618100 | C | -3.84037000 | -3.75304200 | 0.10868500 |
| H | -6.10678400 | 1.66737700 | 1.43433800 | C | -4.74232700 | -3.02361300 | 0.88887500 |
| H | -3.63960400 | 1.80046300 | 1.47505500 | C | -4.29582000 | -1.90547500 | 1.60107400 |
| C | -1.90266900 | 2.22065600 | -0.64477000 | C | -2.95772500 | -1.51490900 | 1.52866600 |
| C | -1.60780800 | 3.71803000 | -0.31797800 | C | 0.62903100 | -2.93198400 | -0.22580000 |
| H | -2.16456500 | 3.96678400 | 0.59738100 | C | 0.79285100 | -4.25081500 | 0.23349700 |
| H | -2.04823900 | 4.30732300 | -1.14002500 | C | 1.24528800 | -2.54451400 | -1.42731100 |
| C | -1.22154900 | 1.70264900 | -1.93094100 | C | 2.02632400 | -3.44891000 | -2.15077300 |
| H | -0.15556800 | 2.03573600 | -1.89755500 | C | 2.20149500 | -4.75134800 | -1.67584300 |
| H | -1.57730000 | 2.18058500 | -2.85930000 | C | 1.58024100 | -5.15166300 | -0.48698800 |
| C | -0.16313400 | 4.07519400 | -0.14485800 | H | -0.28900200 | -0.72420300 | 2.82944500 |
| C | 0.40745400 | 4.35548600 | 1.03099500 | H | 2.31813400 | -2.05095000 | 1.92073200 |
| H | 0.45244300 | 4.08709200 | -1.04911700 | H | 2.06086900 | -1.53592600 | 3.57717800 |
| H | 1.47094700 | 4.59701000 | 1.10653100 | H | 3.36464700 | 0.11846800 | 2.53983200 |
| H | -0.17233700 | 4.35217300 | 1.96022800 | H | 1.16977100 | 3.23988400 | -0.18614900 |
| C | -1.24967100 | 0.17819300 | -1.98035700 | H | 2.15782200 | 5.52759400 | -0.21262900 |
| C | -2.54964500 | -0.56375000 | -2.16113900 | H | 4.53762600 | 5.86420100 | 0.44502500 |
| H | -0.51326900 | -0.18104600 | -2.72691500 | H | 5.93307100 | 3.90881400 | 1.11657300 |
| H | -3.06207300 | -0.23887000 | -3.08543900 | H | 4.95687800 | 1.62381100 | 1.11641500 |
| H | -3.25375900 | -0.42609200 | -1.33200800 | H | 2.95630600 | 0.58694200 | -2.29101100 |
| | | | | H | 4.28920300 | -1.49435700 | 1.26040100 |
| 3' _T | | | | H | 5.89807200 | -2.77594500 | -0.09783000 |
| C | -1.44170000 | 1.69782500 | 0.11417100 | H | 6.06937300 | -2.38470000 | -2.55512100 |
| O | -1.44113300 | 1.97320800 | 1.28532100 | H | 4.60266900 | -0.68131600 | -3.64350300 |
| H | -1.33188700 | -1.65563100 | -2.26526100 | H | -1.80330900 | -3.95165300 | -0.56848400 |
| P | -0.32348200 | -1.64475400 | 0.65207200 | H | -4.18218400 | -4.62480600 | -0.45493100 |
| C | 0.26359500 | -1.59053800 | 2.43179600 | H | -5.79221400 | -3.32223200 | 0.93937500 |
| C | 1.77701100 | -1.31507000 | 2.53448800 | H | -4.99511900 | -1.32635700 | 2.20667800 |
| C | 2.29810500 | 0.11070000 | 2.26233500 | H | -2.62566000 | -0.62569200 | 2.06946000 |
| P | 2.24384500 | 0.61941500 | 0.47214800 | H | 0.29769500 | -4.58142100 | 1.14633200 |
| C | 2.99697600 | 2.28849400 | 0.46760600 | H | 1.11133000 | -1.52261900 | -1.78898800 |
| C | 2.21442300 | 3.38928000 | 0.09425900 | H | 2.50514900 | -3.13088700 | -3.07887700 |
| C | 2.76949800 | 4.67322800 | 0.08490500 | H | 2.81928700 | -5.45909800 | -2.23416200 |

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|-------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | 1.70751800 | -6.17292300 | -0.11963200 | C | -0.48380800 | 1.52525500 | 2.33768800 |
| C | 1.57438400 | 1.16918200 | 3.10261100 | C | -1.65441600 | 0.61408200 | 2.74470800 |
| H | 2.09317400 | 2.13753200 | 3.06020800 | C | -1.61188500 | -0.86779200 | 2.33269100 |
| H | 0.54017700 | 1.32865500 | 2.76234300 | P | -1.73801700 | -1.05644700 | 0.49770100 |
| H | 1.54243600 | 0.84706000 | 4.15593300 | C | -2.14115400 | -2.81083700 | 0.14880100 |
| C | -0.10527800 | -2.81651600 | 3.27201000 | C | -1.93754400 | -3.27782900 | -1.15869600 |
| H | 0.53424100 | -3.67771500 | 3.02970600 | C | -2.31267100 | -4.57612100 | -1.50989200 |
| H | 0.04803900 | -2.58491000 | 4.33865800 | C | -2.89901700 | -5.41653400 | -0.55748000 |
| H | -1.15452900 | -3.11500200 | 3.13941900 | C | -3.11629600 | -4.94999800 | 0.74304700 |
| Co | 0.00521900 | 0.47224800 | -0.39494900 | C | -2.74271500 | -3.65040400 | 1.09699000 |
| C | -3.79910500 | 1.63551500 | -0.74299000 | C | -3.35385200 | -0.32766200 | 0.00214900 |
| C | -4.56949900 | 1.15985700 | -1.81523100 | C | -3.53787200 | -0.02082100 | -1.35442500 |
| C | -5.86191300 | 0.66689300 | -1.60989100 | C | -4.43167300 | -0.19091200 | 0.88960800 |
| C | -6.41719600 | 0.64880200 | -0.32828200 | C | -5.66848200 | 0.26720500 | 0.42631200 |
| C | -5.66602800 | 1.13302600 | 0.74626400 | C | -5.84461600 | 0.57458400 | -0.92586300 |
| C | -4.37344300 | 1.61809100 | 0.53993300 | C | -4.77687600 | 0.42449800 | -1.81661900 |
| H | -4.17078900 | 1.16983200 | -2.82875600 | C | 1.12395600 | 2.98239800 | 0.42789900 |
| H | -6.43673600 | 0.29818300 | -2.46327200 | C | 0.97185500 | 4.11940500 | -0.38300000 |
| H | -7.42693300 | 0.26281300 | -0.16856700 | C | 1.96972100 | 5.09742600 | -0.43266700 |
| H | -6.08502400 | 1.12947600 | 1.75542500 | C | 3.12896200 | 4.96167100 | 0.33396900 |
| H | -3.80058900 | 1.98775600 | 1.39124100 | C | 3.27755000 | 3.84483300 | 1.16261600 |
| C | -2.41224900 | 2.26888600 | -0.95200400 | C | 2.28675600 | 2.86369500 | 1.21180900 |
| C | -2.58880200 | 3.80789200 | -0.78210700 | C | -1.58252800 | 2.46531900 | -0.37583300 |
| H | -3.15435500 | 3.99523100 | 0.14158600 | C | -2.70769900 | 3.02965700 | 0.24163100 |
| H | -3.22997900 | 4.13150500 | -1.62069400 | C | -1.49118800 | 2.49014800 | -1.78076900 |
| C | -1.69976800 | 1.86576700 | -2.25157000 | C | -2.48662600 | 3.09615300 | -2.54697600 |
| H | -0.89880500 | 2.59536900 | -2.43584600 | C | -3.60344400 | 3.65969600 | -1.92243400 |
| H | -2.36962000 | 1.91920700 | -3.12433300 | C | -3.71443200 | 3.61665200 | -0.53046400 |
| C | -1.33028700 | 4.62570400 | -0.76639500 | H | 0.45515800 | 1.03747800 | 2.64390800 |
| C | -0.92476400 | 5.34561400 | 0.28457700 | H | -2.60204400 | 1.06791700 | 2.42306000 |
| H | -0.73010100 | 4.63917500 | -1.68363000 | H | -1.67870300 | 0.62623300 | 3.84714600 |
| H | -0.01456400 | 5.95040200 | 0.25075700 | H | -2.50521300 | -1.33782900 | 2.77017600 |
| H | -1.49553800 | 5.35868700 | 1.21980600 | H | -1.48410800 | -2.62065600 | -1.90489400 |
| C | -1.06755000 | 0.48969200 | -2.09438900 | H | -2.14368600 | -4.93339000 | -2.52857500 |
| C | -1.92613300 | -0.73324000 | -2.32913500 | H | -3.18902700 | -6.43422700 | -0.82987800 |
| H | -0.12421200 | 0.41276100 | -2.67371700 | H | -3.57864000 | -5.60116400 | 1.48888600 |
| H | -2.36762500 | -0.70011700 | -3.34437800 | H | -2.92423400 | -3.30061100 | 2.11454700 |
| H | -2.75708500 | -0.81767800 | -1.61774900 | H | -2.70470700 | -0.12814100 | -2.05149600 |
| | | | | H | -4.32386300 | -0.44562900 | 1.94470200 |
| | | | | H | -6.49947300 | 0.37788600 | 1.12734000 |
| TS4's | | | | H | -6.81244200 | 0.93236800 | -1.28548100 |
| C | 2.01353700 | -0.56564400 | -0.07035700 | H | -4.90521800 | 0.66673600 | -2.87392800 |
| O | 2.21807500 | -0.03886900 | 1.02301600 | H | 0.07585200 | 4.25519200 | -0.98670300 |
| H | 2.38743500 | 2.18049600 | -1.55669900 | H | 1.83283800 | 5.97113700 | -1.07453000 |
| P | -0.18002700 | 1.67791800 | 0.49986500 | | | | |

| | | | | | | | |
|----|-------------|-------------|-------------|------------------|-------------|-------------|-------------|
| H | 3.90946800 | 5.72548400 | 0.29324300 | H | 3.77832800 | 1.10129300 | -1.32550600 |
| H | 4.17506200 | 3.73194800 | 1.77583300 | | | | |
| H | 2.42838400 | 1.99302700 | 1.84635900 | TS4 _T | | | |
| H | -2.81673100 | 3.01410800 | 1.32466600 | C | 2.01305100 | -0.80620100 | 0.00389500 |
| H | -0.62960900 | 2.03948900 | -2.27919200 | O | 2.13367000 | -0.27991400 | 1.09035300 |
| H | -2.39644200 | 3.11538900 | -3.63561800 | H | 2.00553000 | 1.83281700 | -1.92476200 |
| H | -4.39184800 | 4.12222000 | -2.52098500 | P | -0.11556400 | 1.85093100 | 0.50328200 |
| H | -4.59087800 | 4.04237100 | -0.03646400 | C | -0.68690100 | 1.71216700 | 2.28734400 |
| C | -0.37250700 | -1.60165000 | 2.85392100 | C | -2.04411000 | 0.99068100 | 2.40989200 |
| H | -0.43317900 | -2.68164500 | 2.66000700 | C | -2.11233800 | -0.54012000 | 2.21075500 |
| H | 0.54900800 | -1.22840400 | 2.38617500 | P | -2.01762700 | -1.05390600 | 0.43005700 |
| H | -0.29141000 | -1.45534400 | 3.94326300 | C | -2.41204100 | -2.84835700 | 0.38326900 |
| C | -0.58370700 | 2.86619800 | 3.07505600 | C | -1.98866900 | -3.57321000 | -0.74206500 |
| H | -1.52995000 | 3.38460700 | 2.86578500 | C | -2.28898400 | -4.93146300 | -0.86532300 |
| H | -0.54433600 | 2.67804600 | 4.15997900 | C | -3.00977900 | -5.58185100 | 0.14136700 |
| H | 0.24038600 | 3.54589400 | 2.82393100 | C | -3.44128500 | -4.86398700 | 1.26164200 |
| Co | 0.08177000 | -0.26087400 | -0.55962300 | C | -3.15206500 | -3.50145700 | 1.38029700 |
| C | 4.35767500 | -1.42365200 | -0.46796100 | C | -3.50555600 | -0.38585300 | -0.41620200 |
| C | 5.28348800 | -1.39420700 | -1.52136500 | C | -3.55255800 | -0.50837200 | -1.81562400 |
| C | 6.64391300 | -1.16818300 | -1.28202000 | C | -4.59243100 | 0.19123200 | 0.25551100 |
| C | 7.10793200 | -0.96813300 | 0.01980800 | C | -5.69638200 | 0.65966800 | -0.46541400 |
| C | 6.19783700 | -1.00894700 | 1.08173600 | C | -5.73382400 | 0.53926900 | -1.85680800 |
| C | 4.84233000 | -1.24086400 | 0.84028300 | C | -4.66124500 | -0.05562400 | -2.53085100 |
| H | 4.95411400 | -1.54767400 | -2.54916800 | C | 1.37430600 | 2.92170700 | 0.59291000 |
| H | 7.34169500 | -1.14824800 | -2.12332400 | C | 1.60052800 | 3.92051900 | -0.36944600 |
| H | 8.16927100 | -0.78643100 | 0.20733900 | C | 2.78588900 | 4.66108800 | -0.36327800 |
| H | 6.54562600 | -0.86053900 | 2.10758600 | C | 3.76366800 | 4.41705500 | 0.60532800 |
| H | 4.14168100 | -1.26352200 | 1.67415400 | C | 3.54624200 | 3.42726700 | 1.56954800 |
| C | 2.86910000 | -1.72869400 | -0.69092800 | C | 2.36408300 | 2.68317300 | 1.56314600 |
| C | 2.64933200 | -3.17892100 | -0.22036600 | C | -1.34854200 | 2.89608000 | -0.35902400 |
| H | 3.08777900 | -3.30094300 | 0.78172300 | C | -1.70348700 | 4.19242500 | 0.05768800 |
| H | 3.25582900 | -3.80876100 | -0.89867300 | C | -1.95621500 | 2.36142800 | -1.50387700 |
| C | 2.35170100 | -1.32959300 | -2.09240500 | C | -2.92300100 | 3.08671200 | -2.20641600 |
| H | 1.49707500 | -1.95467100 | -2.38860300 | C | -3.28866500 | 4.36194200 | -1.76945200 |
| H | 3.07350900 | -1.32848900 | -2.91693700 | C | -2.67191600 | 4.91569600 | -0.64057100 |
| C | 1.24580000 | -3.69377500 | -0.21134300 | H | 0.09573000 | 1.08196000 | 2.73629700 |
| C | 0.72858100 | -4.42588400 | 0.78000900 | H | -2.77902400 | 1.50059100 | 1.76861100 |
| H | 0.63529400 | -3.49365400 | -1.09726100 | H | -2.38740400 | 1.16366300 | 3.44335800 |
| H | -0.28540800 | -4.82551900 | 0.72986700 | H | -3.09725700 | -0.85559700 | 2.58901800 |
| H | 1.31182900 | -4.65616700 | 1.67889200 | H | -1.41206400 | -3.07148700 | -1.52297600 |
| C | 1.87999900 | 0.06963000 | -1.64755100 | H | -1.95023200 | -5.48486100 | -1.74455300 |
| C | 2.83459400 | 1.23222800 | -1.87294900 | H | -3.23677500 | -6.64706900 | 0.05235400 |
| H | 0.90236500 | 0.35494100 | -2.11595400 | H | -4.00986200 | -5.36606900 | 2.04834900 |
| H | 3.07375100 | 1.30781400 | -2.94672800 | H | -3.50696300 | -2.95631500 | 2.25669300 |

| | | | | | | | |
|----|-------------|-------------|-------------|-----|-------------|-------------|-------------|
| H | -2.70976000 | -0.95520800 | -2.34916100 | H | 0.69468300 | -3.87006200 | -0.67984800 |
| H | -4.59556300 | 0.27955600 | 1.34235900 | H | -0.30581800 | -4.32694200 | 1.49420500 |
| H | -6.53304800 | 1.11714800 | 0.06834900 | H | 1.29022600 | -3.86651700 | 2.34752100 |
| H | -6.59734500 | 0.90728000 | -2.41615800 | C | 1.65288100 | -0.30317100 | -1.78286500 |
| H | -4.68335100 | -0.15554100 | -3.61872900 | C | 2.53551400 | 0.88958800 | -2.10484800 |
| H | 0.85089900 | 4.12072000 | -1.13677500 | H | 0.67328300 | -0.16683300 | -2.29357300 |
| H | 2.94337700 | 5.43307700 | -1.12076900 | H | 2.82196800 | 0.85560500 | -3.17043800 |
| H | 4.69037300 | 4.99619000 | 0.61049600 | H | 3.46293800 | 0.90437800 | -1.51339200 |
| H | 4.30293900 | 3.22952500 | 2.33303700 | | | | |
| H | 2.21915700 | 1.90910700 | 2.31561400 | 4's | | | |
| H | -1.21073200 | 4.64777300 | 0.91634800 | C | -2.45893200 | 0.21770800 | 0.18799000 |
| H | -1.66737000 | 1.36612800 | -1.84054700 | O | -2.29731000 | -0.19414600 | 1.31645900 |
| H | -3.39133900 | 2.65051200 | -3.09110100 | H | -2.59001800 | -2.33011200 | -1.25796200 |
| H | -4.04771700 | 4.93108200 | -2.31200700 | P | 0.52493200 | -1.66369500 | 0.49578700 |
| H | -2.94381800 | 5.91977500 | -0.30543600 | C | 0.81183500 | -1.47638100 | 2.33371000 |
| C | -1.02436200 | -1.27785600 | 3.00074400 | C | 2.02798400 | -0.57840200 | 2.62275900 |
| H | -1.19856600 | -2.36203300 | 3.01931200 | C | 1.93984500 | 0.91477700 | 2.25381900 |
| H | -0.02517000 | -1.10941500 | 2.57168000 | P | 1.82757300 | 1.17951700 | 0.42109700 |
| H | -1.01224400 | -0.91883500 | 4.04253300 | C | 1.77053800 | 2.99060900 | 0.14523500 |
| C | -0.73931700 | 3.03178800 | 3.06305500 | C | 1.07237700 | 3.45669600 | -0.97850400 |
| H | -1.62292900 | 3.62525400 | 2.78608800 | C | 1.04781900 | 4.82165800 | -1.27828700 |
| H | -0.81402900 | 2.81724400 | 4.14182700 | C | 1.71441000 | 5.72955100 | -0.45058300 |
| H | 0.15539000 | 3.64944400 | 2.90405100 | C | 2.41757000 | 5.26866200 | 0.66904400 |
| Co | 0.08682900 | -0.37316000 | -0.35889900 | C | 2.45370600 | 3.90400800 | 0.96311900 |
| C | 4.38170400 | -1.55824400 | -0.59450900 | C | 3.49239400 | 0.82020600 | -0.28216700 |
| C | 5.22284700 | -2.06464000 | -1.59970800 | C | 3.67043000 | 1.08604200 | -1.65145400 |
| C | 6.59865400 | -1.82184200 | -1.57724400 | C | 4.57042600 | 0.31335400 | 0.45587800 |
| C | 7.16381600 | -1.06593000 | -0.54579500 | C | 5.79556200 | 0.05576400 | -0.17043800 |
| C | 6.33910400 | -0.56908400 | 0.46684500 | C | 5.96242400 | 0.31856500 | -1.53159500 |
| C | 4.96332000 | -0.81974000 | 0.44775600 | C | 4.89587600 | 0.84461200 | -2.26998500 |
| H | 4.80247400 | -2.65981100 | -2.41273400 | C | -0.68248900 | -3.03937300 | 0.32718500 |
| H | 7.23024300 | -2.22478300 | -2.37321800 | C | -0.55630800 | -3.94694100 | -0.73764400 |
| H | 8.23863100 | -0.86876900 | -0.53051500 | C | -1.50432600 | -4.95644700 | -0.92514000 |
| H | 6.76613200 | 0.01978200 | 1.28278400 | C | -2.58760900 | -5.07446600 | -0.04964800 |
| H | 4.33588900 | -0.42907200 | 1.24797000 | C | -2.71669200 | -4.17759800 | 1.01602700 |
| C | 2.88691400 | -1.90038700 | -0.63317200 | C | -1.77360800 | -3.16486300 | 1.20354500 |
| C | 2.70858500 | -3.28495800 | 0.04147700 | C | 2.03132700 | -2.38300400 | -0.26345600 |
| H | 3.22152400 | -3.25626500 | 1.01508200 | C | 2.76829500 | -3.42862700 | 0.31715500 |
| H | 3.25119400 | -4.01133900 | -0.58865100 | C | 2.42021100 | -1.88757500 | -1.51676800 |
| C | 2.25378400 | -1.69180500 | -2.03025500 | C | 3.53132800 | -2.41665400 | -2.17744900 |
| H | 1.46009900 | -2.42579400 | -2.22321500 | C | 4.27454300 | -3.43921900 | -1.58258700 |
| H | 2.96065600 | -1.71847100 | -2.86874600 | C | 3.88988300 | -3.94464200 | -0.33537200 |
| C | 1.29113700 | -3.73365300 | 0.22784000 | H | -0.10728000 | -0.95685700 | 2.64597300 |
| C | 0.72917700 | -3.98705400 | 1.41422900 | H | 2.91711200 | -1.04251000 | 2.17207300 |

| | | | | | | | |
|----|-------------|-------------|-------------|----------------|-------------|-------------|-------------|
| H | 2.19363500 | -0.61282300 | 3.71252500 | H | -3.70484700 | 2.59335900 | 1.35081700 |
| H | 2.87486200 | 1.38703800 | 2.59484200 | H | -3.96817800 | 3.39628700 | -0.20258400 |
| H | 0.53968000 | 2.74711300 | -1.61885700 | C | -2.52759000 | 1.17434100 | -1.72124200 |
| H | 0.49849800 | 5.17620900 | -2.15368500 | H | -1.70326200 | 1.89206200 | -1.82869800 |
| H | 1.68923300 | 6.79801500 | -0.67829500 | H | -3.11915900 | 1.16331800 | -2.64406200 |
| H | 2.94402400 | 5.97630500 | 1.31425100 | C | -1.94424200 | 3.41288600 | 0.44016100 |
| H | 3.01775600 | 3.55450800 | 1.83056500 | C | -1.39273800 | 3.87306500 | 1.56647000 |
| H | 2.83966800 | 1.47954400 | -2.24201000 | H | -1.41881800 | 3.57830900 | -0.50397800 |
| H | 4.47582500 | 0.11196100 | 1.52242000 | H | -0.43496500 | 4.39918500 | 1.55325900 |
| H | 6.62358900 | -0.34939000 | 0.41640000 | H | -1.87827900 | 3.74023600 | 2.53960200 |
| H | 6.92015500 | 0.11600300 | -2.01711200 | C | -2.03126400 | -0.21657600 | -1.23196800 |
| H | 5.01682700 | 1.05673000 | -3.33510700 | C | -2.82378700 | -1.40480300 | -1.79366800 |
| H | 0.28139500 | -3.86371300 | -1.43162100 | H | -0.95817100 | -0.50699000 | -1.54157100 |
| H | -1.39432400 | -5.65233400 | -1.76046400 | H | -2.57559300 | -1.54316900 | -2.85726600 |
| H | -3.32902000 | -5.86381300 | -0.19602100 | H | -3.90333600 | -1.21953700 | -1.71336500 |
| H | -3.56006400 | -4.26276500 | 1.70572900 | | | | |
| H | -1.90054900 | -2.46155400 | 2.02415500 | 4 ^T | | | |
| H | 2.46466000 | -3.85487500 | 1.27195300 | C | 2.35787400 | -1.04718600 | -1.05606900 |
| H | 1.84534100 | -1.07210900 | -1.96128100 | O | 1.37939800 | -0.98984500 | -0.33090000 |
| H | 3.82430100 | -2.01846500 | -3.15115400 | H | 0.84904600 | 0.51057300 | -3.03038600 |
| H | 5.15219900 | -3.84609300 | -2.09098100 | P | -0.38997200 | 1.78451500 | 0.15079700 |
| H | 4.46231200 | -4.75111700 | 0.12950500 | C | -0.47338100 | 1.52901100 | 2.00673300 |
| C | 0.75743200 | 1.59934800 | 2.94725400 | C | -1.72850800 | 0.72739100 | 2.40652400 |
| H | 0.81665700 | 2.69200300 | 2.86618100 | C | -1.74794100 | -0.79297900 | 2.14269800 |
| H | -0.20491500 | 1.28504400 | 2.51731400 | P | -2.02912700 | -1.22061500 | 0.34640300 |
| H | 0.75610900 | 1.33690500 | 4.01753700 | C | -2.10020500 | -3.05982800 | 0.37217800 |
| C | 0.93232000 | -2.77029700 | 3.14820500 | C | -1.05286800 | -3.77030600 | -0.23383100 |
| H | 1.94591600 | -3.19178000 | 3.08716300 | C | -1.05025800 | -5.16883900 | -0.22807900 |
| H | 0.74076900 | -2.54255600 | 4.20919800 | C | -2.09696300 | -5.86678400 | 0.38187900 |
| H | 0.21912800 | -3.54466200 | 2.83809600 | C | -3.14615000 | -5.16403600 | 0.98676200 |
| Co | 0.04262800 | 0.23983300 | -0.45187300 | C | -3.14954600 | -3.76714300 | 0.98088300 |
| C | -4.77486000 | 0.93673400 | -0.46058100 | C | -3.77913700 | -0.77318600 | 0.00006700 |
| C | -5.57472900 | 1.33177600 | -1.54372600 | C | -4.17311900 | -0.78326100 | -1.35042500 |
| C | -6.92843100 | 0.98865200 | -1.59370300 | C | -4.71322200 | -0.38997800 | 0.97396000 |
| C | -7.50565200 | 0.24456500 | -0.55932000 | C | -6.00930700 | -0.01456800 | 0.60268700 |
| C | -6.71917500 | -0.14401200 | 0.52885000 | C | -6.39087700 | -0.02843100 | -0.74140300 |
| C | -5.36562000 | 0.20331300 | 0.57939200 | C | -5.46954100 | -0.42165200 | -1.71955000 |
| H | -5.13936700 | 1.91415900 | -2.35841100 | C | 1.16460200 | 2.72312100 | -0.10781700 |
| H | -7.53451300 | 1.30367800 | -2.44709200 | C | 1.26454800 | 3.71077200 | -1.10304900 |
| H | -8.56293800 | -0.02872700 | -0.60135400 | C | 2.49802900 | 4.29536200 | -1.40299000 |
| H | -7.15901500 | -0.72302900 | 1.34494300 | C | 3.65196500 | 3.90030700 | -0.71795500 |
| H | -4.76033900 | -0.10335700 | 1.43421000 | C | 3.56361500 | 2.91405900 | 0.27001600 |
| C | -3.30819600 | 1.37303800 | -0.37859300 | C | 2.33152000 | 2.32734900 | 0.56892300 |
| C | -3.27441300 | 2.73406800 | 0.34638800 | C | -1.73017200 | 2.98037400 | -0.22406100 |

| | | | | | | | |
|----|-------------|-------------|-------------|------------------|-------------|-------------|-------------|
| C | -1.72935900 | 4.32310700 | 0.19397000 | H | 6.25362400 | -0.12359100 | -0.60532100 |
| C | -2.82912400 | 2.49557600 | -0.95041600 | H | 7.29242400 | 0.89796500 | 1.40008900 |
| C | -3.92173600 | 3.32089400 | -1.23151200 | H | 6.07711600 | 0.89714900 | 3.58152800 |
| C | -3.91834000 | 4.65001400 | -0.79958000 | H | 3.82065600 | -0.16333800 | 3.73571500 |
| C | -2.81750200 | 5.15051600 | -0.09336800 | H | 2.79338800 | -1.20159200 | 1.73188800 |
| H | 0.41919400 | 0.92037500 | 2.21739600 | C | 3.82683900 | -1.38247000 | -0.79381300 |
| H | -2.61992500 | 1.20366600 | 1.96685700 | C | 4.05999500 | -2.92266300 | -0.72670600 |
| H | -1.83959600 | 0.84611500 | 3.49788000 | H | 3.70975200 | -3.27004200 | 0.25738000 |
| H | -2.60806100 | -1.20371100 | 2.69558900 | H | 5.15292000 | -3.06844300 | -0.76378400 |
| H | -0.23514200 | -3.22102000 | -0.70712300 | C | 4.11714200 | -0.74369400 | -2.19810800 |
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| H | -2.09814900 | -6.95975100 | 0.38375600 | H | 4.54443900 | 0.26339500 | -2.10938800 |
| H | -3.96659900 | -5.70780600 | 1.46208800 | C | 3.39428400 | -3.71999100 | -1.81108500 |
| H | -3.97486300 | -3.22506600 | 1.44895400 | C | 2.37003900 | -4.55396900 | -1.60337600 |
| H | -3.44954000 | -1.06753100 | -2.12026000 | H | 3.78074600 | -3.58665400 | -2.82862400 |
| H | -4.44248600 | -0.37804400 | 2.03045000 | H | 1.90784800 | -5.11176800 | -2.42346500 |
| H | -6.72378700 | 0.28924900 | 1.37189000 | H | 1.96249800 | -4.71304000 | -0.59973900 |
| H | -7.40303900 | 0.26758800 | -1.02793100 | C | 2.58878700 | -0.68897400 | -2.50462700 |
| H | -5.75936100 | -0.43570900 | -2.77318500 | C | 1.95154900 | 0.58601000 | -3.03641800 |
| H | 0.37572100 | 4.02256100 | -1.65522100 | H | 2.28074600 | -1.55649100 | -3.11511500 |
| H | 2.55688700 | 5.06321600 | -2.17874500 | H | 2.26361800 | 0.76549300 | -4.07677500 |
| H | 4.61587800 | 4.35787700 | -0.95383400 | H | 2.24049500 | 1.45619000 | -2.43072400 |
| H | 4.45609400 | 2.59132100 | 0.80993300 | | | | |
| H | 2.29088900 | 1.54748800 | 1.32969200 | TS5 _s | | | |
| H | -0.87376300 | 4.72886400 | 0.73519900 | C | 3.67652100 | 0.64943200 | -0.77578700 |
| H | -2.82648100 | 1.45924700 | -1.28901400 | C | 4.32766700 | 0.18146400 | -1.92802400 |
| H | -4.77236000 | 2.92251900 | -1.78991700 | C | 5.64003900 | -0.29309100 | -1.86465800 |
| H | -4.76917200 | 5.30033600 | -1.01805000 | C | 6.32393700 | -0.31090300 | -0.64469300 |
| H | -2.80716900 | 6.19245900 | 0.23640300 | C | 5.68609800 | 0.15961400 | 0.50641900 |
| C | -0.48462900 | -1.50038700 | 2.64481400 | C | 4.37501100 | 0.64162300 | 0.44054400 |
| H | -0.61732200 | -2.59178700 | 2.65838500 | H | 3.80412800 | 0.18140900 | -2.88630400 |
| H | 0.38811900 | -1.27836700 | 2.01284400 | H | 6.12836800 | -0.65494600 | -2.77307300 |
| H | -0.25460300 | -1.17621500 | 3.67305400 | H | 7.34793300 | -0.68899500 | -0.59259500 |
| C | -0.38082100 | 2.81789500 | 2.82462000 | H | 6.21006900 | 0.15350600 | 1.46556400 |
| H | -1.30342200 | 3.41150300 | 2.74007600 | H | 3.88701300 | 1.00424300 | 1.34450600 |
| H | -0.24175500 | 2.57144600 | 3.89028000 | C | 2.26264600 | 1.20646700 | -0.88271000 |
| H | 0.46429500 | 3.44889200 | 2.51239000 | C | 1.37237600 | 0.89615900 | 0.33601700 |
| Co | -0.48295300 | -0.20043900 | -0.91733900 | O | 1.57234000 | 1.16193900 | 1.49417000 |
| C | 4.44827600 | -0.72778100 | 0.42228300 | H | -0.16644700 | -1.17336100 | -3.45346600 |
| C | 5.71710500 | -0.13651100 | 0.34587200 | C | 1.40302100 | 0.51155400 | -1.95296900 |
| C | 6.30308300 | 0.43992700 | 1.47720600 | H | 1.20882300 | 1.02429900 | -2.89974400 |
| C | 5.62366700 | 0.43856500 | 2.69928200 | H | -0.01512400 | 1.29364800 | -1.41533500 |
| C | 4.36035800 | -0.15655500 | 2.78530300 | C | 2.28308800 | 2.74417100 | -1.13037300 |
| C | 3.78044100 | -0.74283600 | 1.65753100 | H | 1.23365000 | 3.07825300 | -1.20708400 |

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|---|-------------|-------------|-------------|------------------|-------------|-------------|-------------|
| H | 2.75472300 | 2.90393300 | -2.11280800 | H | 2.45728100 | -1.35670800 | 1.53944400 |
| C | 1.25332400 | -0.87846500 | -1.83716300 | H | 4.46661200 | -2.77764800 | 1.48269500 |
| C | 0.63610300 | -1.71109100 | -2.92557000 | H | 4.32029500 | -5.13190800 | 0.65366700 |
| H | 1.95945500 | -1.40042700 | -1.18894200 | H | 2.12465100 | -6.03431700 | -0.11575300 |
| H | 1.40640200 | -1.98097900 | -3.67092100 | H | 0.10100900 | -4.61752100 | -0.05190100 |
| H | 0.22477000 | -2.65138100 | -2.53153400 | H | -1.83345500 | -1.41798400 | -1.70182200 |
| C | 2.98728700 | 3.54747100 | -0.08052700 | H | -1.87473200 | -4.15000600 | 1.64786300 |
| C | 4.06244700 | 4.30863200 | -0.30501400 | H | -3.82117200 | -5.31484900 | 0.66520500 |
| H | 2.57011000 | 3.49358400 | 0.93012600 | H | -4.78508300 | -4.54542400 | -1.50293300 |
| H | 4.53029800 | 4.88738800 | 0.49741500 | H | -3.77617800 | -2.58932400 | -2.68479000 |
| H | 4.51282500 | 4.38304100 | -1.30131800 | H | -3.09585800 | 3.43582500 | -0.92649500 |
| P | -1.62725900 | 1.25844200 | 0.50495800 | H | -2.74979100 | 5.87950000 | -1.02914100 |
| C | -1.86345300 | 0.88694200 | 2.31048900 | H | -0.92015700 | 6.94965700 | 0.28963700 |
| C | -2.07851800 | -0.61314100 | 2.60133500 | H | 0.55366300 | 5.53642300 | 1.72853900 |
| C | -0.84338600 | -1.53029300 | 2.51957100 | H | 0.22009700 | 3.09278100 | 1.82883400 |
| P | -0.31271000 | -1.75091300 | 0.74067800 | H | -4.48200000 | 0.36411800 | 1.14533100 |
| C | 1.12164000 | -2.89338900 | 0.77846600 | H | -2.04739200 | 1.28367600 | -2.31193800 |
| C | 2.36690300 | -2.38790700 | 1.19837200 | H | -3.94845300 | 0.71289000 | -3.79231700 |
| C | 3.50793700 | -3.18966200 | 1.15900900 | H | -6.10829100 | -0.06999600 | -2.81033700 |
| C | 3.42556600 | -4.50569400 | 0.69064200 | H | -6.34914800 | -0.23907100 | -0.33324000 |
| C | 2.19625300 | -5.01078100 | 0.26032000 | C | 0.27944800 | -1.11616400 | 3.47249500 |
| C | 1.04909300 | -4.21046800 | 0.30073900 | H | 1.04060300 | -1.90402500 | 3.55792600 |
| C | -1.71184300 | -2.70035500 | 0.03644000 | H | 0.78028800 | -0.19137600 | 3.15956400 |
| C | -2.25818000 | -2.27717800 | -1.18457900 | H | -0.14613200 | -0.95590600 | 4.47671300 |
| C | -2.28488800 | -3.80056400 | 0.69826900 | C | -2.90807500 | 1.76707300 | 3.00503400 |
| C | -3.38327000 | -4.46039300 | 0.14355300 | H | -3.93605000 | 1.49903500 | 2.72333100 |
| C | -3.92254000 | -4.02933700 | -1.07415100 | H | -2.81882300 | 1.63753900 | 4.09552800 |
| C | -3.35795000 | -2.93728700 | -1.73810600 | H | -2.76086900 | 2.83283000 | 2.77987900 |
| C | -1.45681400 | 3.08561600 | 0.45076200 | Co | -0.04378300 | 0.10482500 | -0.52211800 |
| C | -2.28992600 | 3.88555600 | -0.34584700 | | | | |
| C | -2.09435400 | 5.26918900 | -0.40287500 | TS5 _T | | | |
| C | -1.07208600 | 5.86862100 | 0.33734500 | C | 3.87201800 | 0.68545800 | -0.78318500 |
| C | -0.24687800 | 5.07743900 | 1.14363400 | C | 4.38299500 | 0.26516500 | -2.02203000 |
| C | -0.43604000 | 3.69570300 | 1.20160400 | C | 5.61896300 | -0.38123300 | -2.10574100 |
| C | -3.12564100 | 0.87867700 | -0.47391200 | C | 6.36875700 | -0.61938400 | -0.94940300 |
| C | -4.34469900 | 0.44589700 | 0.06905300 | C | 5.87586100 | -0.19335500 | 0.28712200 |
| C | -2.99613200 | 0.96471900 | -1.87450900 | C | 4.64145300 | 0.45843500 | 0.36867900 |
| C | -4.06496300 | 0.63764500 | -2.70863900 | H | 3.80921900 | 0.44288400 | -2.93402200 |
| C | -5.27419800 | 0.19984000 | -2.15819000 | H | 5.99585200 | -0.70260600 | -3.08009800 |
| C | -5.40899100 | 0.10434300 | -0.77108900 | H | 7.33236200 | -1.13090300 | -1.01300800 |
| H | -0.87552600 | 1.17002900 | 2.70845400 | H | 6.45352800 | -0.36862000 | 1.19826800 |
| H | -2.88348300 | -1.01781800 | 1.96993900 | H | 4.26888700 | 0.78832000 | 1.33821200 |
| H | -2.44835800 | -0.68391300 | 3.63740800 | C | 2.54467200 | 1.42329900 | -0.71088700 |
| H | -1.17907900 | -2.53452300 | 2.82114300 | C | 1.74462000 | 1.15687600 | 0.60817100 |

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|---|-------------|-------------|-------------|----------------|-------------|-------------|-------------|
| O | 2.06220800 | 1.55631100 | 1.70443600 | C | -4.08465600 | 0.52082900 | -2.88126300 |
| H | -0.27916100 | -0.31570200 | -3.45585400 | C | -5.22500400 | -0.14584100 | -2.41769100 |
| C | 1.50082000 | 0.94989400 | -1.74585900 | C | -5.36864900 | -0.40595000 | -1.05320000 |
| H | 1.21732400 | 1.64251900 | -2.54630600 | H | -1.22619000 | 1.25436400 | 2.69510900 |
| H | 0.34063500 | 1.57659000 | -0.85392200 | H | -2.92917200 | -1.21553000 | 2.04087700 |
| C | 2.74458600 | 2.95989100 | -0.88121000 | H | -2.45784300 | -0.75388400 | 3.66648500 |
| H | 1.74753100 | 3.42999700 | -0.79811500 | H | -1.04060500 | -2.49949600 | 2.91092400 |
| H | 3.09962800 | 3.12739500 | -1.91084100 | H | 2.53316700 | -1.32975200 | 1.12385300 |
| C | 1.26237300 | -0.41906800 | -1.92846400 | H | 4.50785100 | -2.81377100 | 1.15834300 |
| C | 0.55744500 | -0.95747900 | -3.14053100 | H | 4.22779400 | -5.27825200 | 0.83374600 |
| H | 1.92806800 | -1.11580200 | -1.41042900 | H | 1.94832800 | -6.22580700 | 0.47461700 |
| H | 1.27155400 | -1.01214600 | -3.98279800 | H | -0.02958200 | -4.74393100 | 0.44119900 |
| H | 0.18001500 | -1.97491400 | -2.97391200 | H | -1.57998900 | -1.53500400 | -1.82797400 |
| C | 3.68304300 | 3.59637700 | 0.09764400 | H | -2.10455500 | -3.94927900 | 1.71219400 |
| C | 4.84772100 | 4.16345800 | -0.23134300 | H | -3.98892400 | -5.12392200 | 0.62709600 |
| H | 3.37063900 | 3.57299800 | 1.14655900 | H | -4.66425200 | -4.53821200 | -1.70123200 |
| H | 5.49431300 | 4.62053500 | 0.52428000 | H | -3.44533800 | -2.73804300 | -2.93060400 |
| H | 5.19813600 | 4.19098500 | -1.26945300 | H | -3.79318400 | 3.24381500 | -0.54272800 |
| P | -1.84227300 | 1.18833200 | 0.44645700 | H | -3.73177000 | 5.71959200 | -0.51643900 |
| C | -2.13031200 | 0.80337800 | 2.25319400 | H | -1.77976900 | 6.91819400 | 0.47171300 |
| C | -2.14427100 | -0.69735700 | 2.61068500 | H | 0.11672300 | 5.61162500 | 1.43938500 |
| C | -0.82537300 | -1.49139000 | 2.52253000 | H | 0.06910300 | 3.13791300 | 1.40113100 |
| P | -0.29913400 | -1.76176400 | 0.75294900 | H | -4.51896600 | -0.22117900 | 0.90974400 |
| C | 1.10967100 | -2.93183600 | 0.80243700 | H | -2.20125000 | 1.42678900 | -2.35321500 |
| C | 2.39857700 | -2.40377700 | 0.99585200 | H | -3.96046400 | 0.72195700 | -3.94800400 |
| C | 3.51367100 | -3.24278400 | 1.01346000 | H | -5.99503600 | -0.46927400 | -3.12207400 |
| C | 3.35528700 | -4.62033500 | 0.82847200 | H | -6.25063800 | -0.93520800 | -0.68513700 |
| C | 2.07787300 | -5.15146500 | 0.62694300 | C | 0.30358300 | -0.89106900 | 3.36188300 |
| C | 0.95812600 | -4.31396700 | 0.61122700 | H | 1.16619400 | -1.57126500 | 3.41320200 |
| C | -1.69523200 | -2.67012600 | 0.00215000 | H | 0.66165200 | 0.07064200 | 2.96823600 |
| C | -2.09139600 | -2.33629100 | -1.30068700 | H | -0.05597900 | -0.73005100 | 4.39129400 |
| C | -2.38974000 | -3.67747500 | 0.69445200 | C | -3.34414200 | 1.53142400 | 2.84107600 |
| C | -3.45368800 | -4.34305100 | 0.08149700 | H | -4.29462400 | 1.10750400 | 2.48766900 |
| C | -3.83146300 | -4.01466800 | -1.22534900 | H | -3.32549700 | 1.43738500 | 3.93865200 |
| C | -3.14807200 | -3.01074500 | -1.91609800 | H | -3.33670200 | 2.60249700 | 2.59444300 |
| C | -1.86165300 | 3.01984300 | 0.41658600 | Co | 0.15622900 | 0.23513200 | -0.18615200 |
| C | -2.93040200 | 3.75627200 | -0.11453000 | | | | |
| C | -2.89624600 | 5.15438500 | -0.09614900 | 5 _s | | | |
| C | -1.80339800 | 5.82575200 | 0.45921900 | C | 3.62977500 | 0.96362700 | -0.67638200 |
| C | -0.74014300 | 5.09440400 | 1.00081000 | C | 4.43228200 | 0.40657000 | -1.68504900 |
| C | -0.76550400 | 3.69871700 | 0.97751600 | C | 5.75812200 | 0.04673400 | -1.43113100 |
| C | -3.24198900 | 0.67403000 | -0.60367900 | C | 6.30915000 | 0.23773500 | -0.16034400 |
| C | -4.38503500 | 0.00231500 | -0.14698400 | C | 5.52405200 | 0.80534400 | 0.84679000 |
| C | -3.09637300 | 0.92019700 | -1.98257700 | C | 4.19968300 | 1.17173300 | 0.58909400 |

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|---|-------------|-------------|-------------|----|-------------|-------------|-------------|
| H | 4.01864400 | 0.24506700 | -2.68205400 | C | -3.17201100 | 4.89792600 | -0.35978200 |
| H | 6.36134100 | -0.38930600 | -2.23153800 | C | -2.21337200 | 5.70393900 | 0.25908200 |
| H | 7.34321500 | -0.05209400 | 0.04198900 | C | -1.15196700 | 5.10934000 | 0.94990100 |
| H | 5.94172000 | 0.96516500 | 1.84405600 | C | -1.04500700 | 3.71898200 | 1.01457800 |
| H | 3.59858400 | 1.61101300 | 1.38364500 | C | -3.24352500 | 0.39617400 | -0.44348400 |
| C | 2.19842200 | 1.39362400 | -0.99325900 | C | -4.30391100 | -0.30118300 | 0.15436100 |
| C | 1.22201400 | 1.21468700 | 0.19083400 | C | -3.21602900 | 0.52662500 | -1.84609700 |
| O | 1.33121200 | 1.67919900 | 1.29910700 | C | -4.23675200 | -0.01454200 | -2.62754000 |
| H | 0.22522800 | -1.20277400 | -3.71146600 | C | -5.28934100 | -0.70994400 | -2.02320300 |
| C | 1.51997900 | 0.53947300 | -2.07440500 | C | -5.31825300 | -0.85205700 | -0.63393500 |
| H | 1.14537200 | 1.04679100 | -2.96669200 | H | -1.04383700 | 1.23430000 | 2.66731700 |
| H | -0.41467400 | 1.43149300 | -1.35274300 | H | -2.64079700 | -1.32865600 | 2.12694400 |
| C | 2.15725200 | 2.89139100 | -1.43836100 | H | -2.16271700 | -0.82383300 | 3.73726600 |
| H | 1.10463300 | 3.12721600 | -1.67239400 | H | -0.64697500 | -2.47588300 | 2.91515100 |
| H | 2.73051800 | 2.95676300 | -2.37641800 | H | 2.70929500 | -0.97573000 | 1.46175600 |
| C | 1.50340800 | -0.82467900 | -2.00378300 | H | 4.84547600 | -2.19164000 | 1.36337900 |
| C | 0.95937800 | -1.71775900 | -3.07406400 | H | 4.90804100 | -4.56467100 | 0.57424200 |
| H | 2.10830600 | -1.30751300 | -1.23439000 | H | 2.78808500 | -5.69450100 | -0.10261800 |
| H | 1.79188200 | -2.05945900 | -3.71540300 | H | 0.63809600 | -4.48301700 | 0.00690300 |
| H | 0.49690000 | -2.62051000 | -2.65031400 | H | -1.50475100 | -1.68491200 | -1.73481100 |
| C | 2.68212200 | 3.87682400 | -0.44015700 | H | -1.40619300 | -4.11057300 | 1.83997700 |
| C | 3.78263100 | 4.61489800 | -0.61426900 | H | -3.18526800 | -5.55044700 | 0.90479500 |
| H | 2.10748300 | 3.98153900 | 0.48595100 | H | -4.12219400 | -5.08301200 | -1.35905000 |
| H | 4.11783900 | 5.32958200 | 0.14382300 | H | -3.26476100 | -3.14503600 | -2.68047000 |
| H | 4.38909500 | 4.53095000 | -1.52311300 | H | -3.83259900 | 2.89225000 | -0.78047600 |
| P | -1.81915400 | 1.07834300 | 0.47718800 | H | -4.01029400 | 5.35244600 | -0.89350400 |
| C | -1.95855100 | 0.74020400 | 2.30059900 | H | -2.29488200 | 6.79244000 | 0.20831600 |
| C | -1.88071500 | -0.75291000 | 2.67371000 | H | -0.39972200 | 5.73020800 | 1.44268900 |
| C | -0.51274300 | -1.44736200 | 2.54557500 | H | -0.21372900 | 3.26902700 | 1.55612800 |
| P | -0.03798300 | -1.66056600 | 0.75242200 | H | -4.35324500 | -0.42873300 | 1.23347300 |
| C | 1.50898400 | -2.64935500 | 0.77212200 | H | -2.39208400 | 1.05728900 | -2.32693300 |
| C | 2.71033200 | -2.01735500 | 1.14334600 | H | -4.20476800 | 0.10008900 | -3.71354800 |
| C | 3.92341500 | -2.70361500 | 1.07915300 | H | -6.08339800 | -1.14368900 | -2.63564800 |
| C | 3.95723500 | -4.02943400 | 0.63331900 | H | -6.13448200 | -1.39685500 | -0.15399300 |
| C | 2.77041800 | -4.66171400 | 0.25409700 | C | 0.57488700 | -0.78608500 | 3.39494400 |
| C | 1.55207800 | -3.97703100 | 0.31946500 | H | 1.46186600 | -1.42852600 | 3.48018200 |
| C | -1.32686100 | -2.79447200 | 0.11297100 | H | 0.89203100 | 0.18312700 | 2.98886800 |
| C | -1.86059300 | -2.53876700 | -1.15893100 | H | 0.18464900 | -0.62305400 | 4.41283600 |
| C | -1.81184800 | -3.88723100 | 0.85146800 | C | -3.15251300 | 1.43504600 | 2.96598800 |
| C | -2.81324200 | -4.70414800 | 0.32225600 | H | -4.11210300 | 0.97328600 | 2.69432400 |
| C | -3.33734100 | -4.44269300 | -0.94897100 | H | -3.04518500 | 1.35993200 | 4.05987100 |
| C | -2.85734200 | -3.36033400 | -1.69071800 | H | -3.20229700 | 2.50135300 | 2.70557300 |
| C | -2.00052100 | 2.90344300 | 0.38233700 | Co | -0.09805000 | 0.21618700 | -0.57130000 |
| C | -3.07028600 | 3.50431800 | -0.29775900 | | | | |

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|----------------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 6 _s | | | | C | 3.33850500 | -0.95925200 | -1.36121400 |
| C | -3.51783200 | 1.36255400 | -0.93483500 | C | 4.43168000 | -0.59577700 | 0.76164600 |
| C | -4.45715100 | 1.51741900 | 0.09882600 | C | 5.47397700 | -1.43707400 | 0.36465000 |
| C | -5.67210400 | 0.83107300 | 0.07517700 | C | 5.45421100 | -2.03817500 | -0.89747500 |
| C | -5.96707000 | -0.04248400 | -0.97647100 | C | 4.38341400 | -1.79465100 | -1.76102400 |
| C | -5.03551600 | -0.21712500 | -2.00203000 | C | -2.00069300 | -2.30292100 | 0.72808200 |
| C | -3.82240900 | 0.47964700 | -1.98216200 | C | -2.26932400 | -3.56310400 | 0.17172200 |
| H | -4.23093600 | 2.18621900 | 0.93008600 | C | -3.55957700 | -4.09910800 | 0.22990500 |
| H | -6.38951300 | 0.97444100 | 0.88712600 | C | -4.59016500 | -3.38997700 | 0.85133000 |
| H | -6.91449600 | -0.58660100 | -0.99298900 | C | -4.32467300 | -2.13825300 | 1.41595200 |
| H | -5.24983800 | -0.89896500 | -2.82877300 | C | -3.04131000 | -1.59360700 | 1.35389500 |
| H | -3.12205700 | 0.32561500 | -2.80159700 | C | 0.72571000 | -2.82824300 | -0.15853000 |
| C | -2.17952400 | 2.11452400 | -0.85405400 | C | 1.69416800 | -3.60670700 | 0.49340500 |
| C | -1.30123200 | 1.20370000 | 0.07776000 | C | 0.56709700 | -2.96056200 | -1.55241000 |
| O | -1.56088900 | 1.14910000 | 1.25752800 | C | 1.34577500 | -3.86723500 | -2.27193700 |
| H | -2.74762100 | 6.02595800 | 0.51891900 | C | 2.30678900 | -4.64025200 | -1.61346300 |
| C | -2.39917500 | 3.50568900 | -0.28207200 | C | 2.48066100 | -4.50423100 | -0.23352400 |
| H | -3.03592500 | 4.12163300 | -0.93084200 | H | -0.57065000 | -0.54329200 | 2.73041000 |
| H | -1.26504700 | -0.45326300 | -1.24560800 | H | 2.29400200 | -1.53653500 | 2.27095300 |
| C | -1.49215300 | 2.30756300 | -2.23003500 | H | 1.72251500 | -0.84829200 | 3.78009800 |
| H | -0.84912700 | 3.19493200 | -2.14998200 | H | 2.95687800 | 0.77538700 | 2.51130900 |
| H | -2.25655800 | 2.52785200 | -2.98976300 | H | 0.54223200 | 3.27096400 | 0.02825700 |
| C | -1.88408400 | 4.06123000 | 0.81988100 | H | 1.28533000 | 5.60337200 | -0.28287100 |
| C | -2.10633200 | 5.48456700 | 1.23191800 | H | 3.72477700 | 6.13417700 | -0.42361600 |
| H | -1.25611000 | 3.46214500 | 1.48394900 | H | 5.40129500 | 4.29516300 | -0.24156100 |
| H | -2.57296600 | 5.54069400 | 2.23125500 | H | 4.66081800 | 1.95855400 | 0.08253200 |
| H | -1.14506900 | 6.02283800 | 1.31052400 | H | 2.49881900 | -0.79924800 | -2.03373100 |
| C | -0.62604000 | 1.16148500 | -2.67743400 | H | 4.47776500 | -0.13797400 | 1.75010000 |
| C | 0.73427500 | 1.22347200 | -2.55349500 | H | 6.30587300 | -1.62250500 | 1.04841100 |
| H | -1.07136900 | 0.36128400 | -3.27239900 | H | 6.26886100 | -2.69891000 | -1.20376600 |
| H | 1.36117200 | 0.46013100 | -3.02178600 | H | 4.35010100 | -2.26682700 | -2.74509200 |
| H | 1.23104800 | 2.13285900 | -2.21319100 | H | -1.47492200 | -4.13634800 | -0.30649500 |
| P | -0.31894500 | -1.57033000 | 0.66048400 | H | -3.75438000 | -5.08044800 | -0.20974800 |
| C | 0.13301100 | -1.34252900 | 2.45070100 | H | -5.59761100 | -3.81064000 | 0.89728400 |
| C | 1.56487900 | -0.82813800 | 2.68867700 | H | -5.12303200 | -1.57537300 | 1.90356600 |
| C | 1.90891600 | 0.59840200 | 2.22690000 | H | -2.85313200 | -0.61300300 | 1.78950400 |
| P | 1.93346200 | 0.73740100 | 0.36286200 | H | 1.84796000 | -3.52350400 | 1.56743000 |
| C | 2.54729700 | 2.44836200 | 0.09150800 | H | -0.17529500 | -2.35035400 | -2.07244000 |
| C | 1.60890300 | 3.48772800 | -0.02069100 | H | 1.20708600 | -3.96271300 | -3.35136700 |
| C | 2.02897400 | 4.80717100 | -0.19843700 | H | 2.92439600 | -5.34404800 | -2.17645700 |
| C | 3.39407900 | 5.10294200 | -0.27762900 | H | 3.23476900 | -5.09996300 | 0.28588100 |
| C | 4.33338600 | 4.07265100 | -0.17553200 | C | 1.07826200 | 1.68227700 | 2.91635300 |
| C | 3.91476900 | 2.75087300 | 0.00836200 | H | 1.43266400 | 2.68887600 | 2.65204400 |
| C | 3.34817000 | -0.34629100 | -0.09936800 | H | 0.01410500 | 1.61662100 | 2.66603900 |

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|------------------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | 1.18446300 | 1.56929000 | 4.00764500 | C | 2.75952400 | 2.36079500 | 0.35043900 |
| C | -0.17396200 | -2.56678200 | 3.32062900 | C | 1.91408400 | 3.47004100 | 0.52456500 |
| H | 0.50715600 | -3.40573900 | 3.11916500 | C | 2.41183000 | 4.76771700 | 0.39896200 |
| H | -0.05581100 | -2.29000300 | 4.38049700 | C | 3.75981300 | 4.97342900 | 0.08457900 |
| H | -1.20383100 | -2.92223300 | 3.17999700 | C | 4.60340300 | 3.87496200 | -0.10151200 |
| Co | -0.01885000 | 0.12273300 | -0.72259500 | C | 4.10866100 | 2.57291600 | 0.03005600 |
| | | | | C | 3.31729900 | -0.47456700 | -0.09698800 |
| TS6 _s | | | | C | 3.13027600 | -1.09887800 | -1.34273800 |
| C | -3.51617900 | 1.41663400 | -0.88587100 | C | 4.46476800 | -0.78423300 | 0.65290900 |
| C | -4.42096000 | 2.03738800 | -0.01316800 | C | 5.40260100 | -1.69755000 | 0.16570200 |
| C | -5.69077700 | 1.49515700 | 0.20989700 | C | 5.20876200 | -2.31076600 | -1.07632300 |
| C | -6.07624600 | 0.31497800 | -0.43022200 | C | 4.07161400 | -2.00815000 | -1.82998900 |
| C | -5.16980500 | -0.33218200 | -1.27438400 | C | -2.13388600 | -2.07698500 | 0.69651200 |
| C | -3.90081500 | 0.20721700 | -1.49017000 | C | -2.60993600 | -3.24554900 | 0.08451900 |
| H | -4.13607700 | 2.96377000 | 0.48620200 | C | -3.94030400 | -3.64153600 | 0.25895300 |
| H | -6.38360700 | 2.00531900 | 0.88416500 | C | -4.80220800 | -2.88488600 | 1.05541400 |
| H | -7.06962600 | -0.10730900 | -0.26010900 | C | -4.33423000 | -1.71540900 | 1.66279800 |
| H | -5.44447500 | -1.27190800 | -1.75871700 | C | -3.01421300 | -1.30579400 | 1.47845900 |
| H | -3.20521000 | -0.32986700 | -2.13577100 | C | 0.50607000 | -2.93194800 | -0.25080800 |
| C | -2.11681100 | 2.01685100 | -1.13747700 | C | 1.43686100 | -3.77263800 | 0.37862500 |
| C | -1.18603800 | 1.29198900 | -0.06893400 | C | 0.28858000 | -3.07541700 | -1.63515200 |
| O | -1.43012800 | 1.45047700 | 1.10373500 | C | 0.97146100 | -4.04880200 | -2.36515300 |
| H | -2.16515200 | 6.17728500 | -0.67429600 | C | 1.89955100 | -4.87940600 | -1.72902300 |
| C | -2.11804000 | 3.52218100 | -0.89956400 | C | 2.13075500 | -4.73602100 | -0.35882400 |
| H | -2.58838000 | 4.06896800 | -1.72659900 | H | -0.53706800 | -0.62794300 | 2.72043500 |
| H | -0.87373600 | -0.24705300 | -1.76293600 | H | 2.24571700 | -1.77675400 | 2.15245700 |
| C | -1.67066200 | 1.76672600 | -2.61335100 | H | 1.73005700 | -1.22710100 | 3.73630400 |
| H | -1.53371600 | 2.73685200 | -3.11322700 | H | 3.03884100 | 0.46569500 | 2.68486300 |
| H | -2.45898000 | 1.24928500 | -3.16846600 | H | 0.85904800 | 3.31954700 | 0.74919700 |
| C | -1.64739400 | 4.23333900 | 0.13074400 | H | 1.74081700 | 5.61865900 | 0.53872000 |
| C | -1.69420700 | 5.72832100 | 0.21408200 | H | 4.14966900 | 5.98881800 | -0.02071100 |
| H | -1.20629200 | 3.71768700 | 0.98689000 | H | 5.65561400 | 4.02791300 | -0.35395300 |
| H | -2.25386400 | 6.05632200 | 1.10776100 | H | 4.77967900 | 1.72705300 | -0.12428100 |
| H | -0.67748700 | 6.14748000 | 0.31648300 | H | 2.23898200 | -0.88930500 | -1.93730100 |
| C | -0.37473100 | 1.00488600 | -2.75233000 | H | 4.63591700 | -0.31316500 | 1.62213700 |
| C | 0.81225300 | 1.56643900 | -2.24810000 | H | 6.28947300 | -1.93002200 | 0.76017200 |
| H | -0.30584900 | 0.27474200 | -3.56550400 | H | 5.94230500 | -3.02727800 | -1.45388800 |
| H | 1.78181300 | 1.21351200 | -2.60859900 | H | 3.90739600 | -2.48891300 | -2.79646100 |
| H | 0.79302800 | 2.56940800 | -1.81549600 | H | -1.94550700 | -3.86464400 | -0.51911200 |
| P | -0.37586800 | -1.56065500 | 0.58363800 | H | -4.29657200 | -4.55527500 | -0.22314500 |
| C | 0.09777400 | -1.46458200 | 2.38803300 | H | -5.83892800 | -3.19976500 | 1.19663400 |
| C | 1.56458700 | -1.07699700 | 2.65654300 | H | -5.00495000 | -1.10847900 | 2.27440200 |
| C | 1.99250900 | 0.37005100 | 2.35569200 | H | -2.67257100 | -0.38110800 | 1.94337500 |
| P | 2.03438900 | 0.68640800 | 0.52084700 | H | 1.64025000 | -3.68422900 | 1.44343100 |

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|------------------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | -0.41920700 | -2.41742900 | -2.14366100 | H | 0.84766300 | -0.40140300 | -2.99483200 |
| H | 0.78623800 | -4.15015800 | -3.43713700 | H | 0.68310400 | 1.43951400 | -2.73709900 |
| H | 2.44563400 | -5.63262400 | -2.30197100 | P | 0.16112600 | -1.76670900 | 0.60828700 |
| H | 2.85889700 | -5.37557300 | 0.14543900 | C | 0.64677800 | -1.54162000 | 2.40135300 |
| C | 1.16780100 | 1.41538600 | 3.11049500 | C | 1.92534600 | -0.70933000 | 2.63526000 |
| H | 1.62984400 | 2.41063200 | 3.04777200 | C | 1.92060000 | 0.79220500 | 2.28487100 |
| H | 0.14380900 | 1.48974500 | 2.72296400 | P | 1.89822000 | 1.09224000 | 0.44716600 |
| H | 1.11934800 | 1.13687600 | 4.17591500 | C | 2.09407800 | 2.89904900 | 0.24328400 |
| C | -0.30812500 | -2.70134800 | 3.19969700 | C | 1.00041100 | 3.62440200 | -0.25400400 |
| H | 0.32829000 | -3.57074700 | 2.98351000 | C | 1.07947500 | 5.01238800 | -0.39551100 |
| H | -0.20459000 | -2.47416400 | 4.27286300 | C | 2.25521900 | 5.68220300 | -0.04470100 |
| H | -1.35164800 | -2.99132600 | 3.01743200 | C | 3.35104400 | 4.96221600 | 0.44675900 |
| Co | 0.17127400 | 0.18236600 | -0.68114400 | C | 3.27462200 | 3.57497800 | 0.59125900 |
| | | | | C | 3.45373100 | 0.33113900 | -0.15897100 |
| | | | | C | 3.49184800 | -0.21846700 | -1.44914300 |
| TS6 _T | | | | C | 4.61232200 | 0.28109900 | 0.63653900 |
| C | -3.98704900 | 0.82495900 | -0.78229900 | C | 5.78047000 | -0.30619700 | 0.14462500 |
| C | -4.84246000 | 1.06681500 | 0.30865600 | C | 5.80911400 | -0.84764300 | -1.14437600 |
| C | -5.96630300 | 0.27150200 | 0.53207800 | C | 4.66212100 | -0.79984700 | -1.94109900 |
| C | -6.26169000 | -0.79090500 | -0.33078400 | C | -1.36433900 | -2.77340500 | 0.71161200 |
| C | -5.42067100 | -1.04335800 | -1.41538000 | C | -1.42066400 | -4.11858900 | 0.31815000 |
| C | -4.29321100 | -0.24398700 | -1.63827200 | C | -2.62109800 | -4.82919300 | 0.41829500 |
| H | -4.61608900 | 1.88755600 | 0.98954100 | C | -3.76851500 | -4.20800400 | 0.91991800 |
| H | -6.61668500 | 0.48199200 | 1.38502700 | C | -3.71467200 | -2.86869800 | 1.32176700 |
| H | -7.13972800 | -1.41716400 | -0.15490000 | C | -2.52227400 | -2.15112100 | 1.21284200 |
| H | -5.63552600 | -1.87030600 | -2.09676300 | C | 1.37291100 | -2.78410100 | -0.30276300 |
| H | -3.66217000 | -0.47095700 | -2.49614400 | C | 2.57542700 | -3.27228200 | 0.23005900 |
| C | -2.73456200 | 1.69759700 | -0.94720100 | C | 1.09886000 | -2.98908600 | -1.66905100 |
| C | -1.75617200 | 1.20458400 | 0.18064700 | C | 2.00340400 | -3.67553100 | -2.47890700 |
| O | -2.05200700 | 1.28961200 | 1.35019800 | C | 3.20431500 | -4.15236200 | -1.94069500 |
| H | -3.67667900 | 5.76688700 | -0.68697400 | C | 3.48569100 | -3.94876100 | -0.58797900 |
| C | -3.09021400 | 3.16551200 | -0.80541300 | H | -0.21473200 | -0.95818100 | 2.76705300 |
| H | -3.77108600 | 3.52293200 | -1.58916600 | H | 2.78518500 | -1.19530900 | 2.15333900 |
| H | -1.34332800 | -0.27516400 | -1.04582900 | H | 2.12482700 | -0.76373800 | 3.71864700 |
| C | -2.01537500 | 1.50472700 | -2.30692200 | H | 2.88597200 | 1.19595000 | 2.62800900 |
| H | -1.38049800 | 2.38656000 | -2.47077600 | H | 0.08419400 | 3.09653300 | -0.52500900 |
| H | -2.75067400 | 1.48291900 | -3.12453400 | H | 0.22089600 | 5.56700900 | -0.78139200 |
| C | -2.64339200 | 4.03655700 | 0.10690900 | H | 2.32104700 | 6.76728000 | -0.15646800 |
| C | -3.00778200 | 5.48908000 | 0.14258300 | H | 4.27135500 | 5.48498500 | 0.71860000 |
| H | -1.97159200 | 3.69106500 | 0.89794500 | H | 4.13581400 | 3.02250700 | 0.97244400 |
| H | -3.50760700 | 5.74814400 | 1.09279200 | H | 2.59691700 | -0.20494400 | -2.06527800 |
| H | -2.10468600 | 6.12215000 | 0.08792300 | H | 4.61520800 | 0.69571900 | 1.64531300 |
| C | -1.11854200 | 0.26997600 | -2.38898200 | H | 6.67236600 | -0.34077900 | 0.77487800 |
| C | 0.26211600 | 0.43812700 | -2.61617500 | H | 6.72309800 | -1.31053700 | -1.52431600 |
| H | -1.56286700 | -0.66286600 | -2.75856100 | | | | |

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|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | 4.67046400 | -1.22792800 | -2.94580500 | C | -2.35229000 | 5.16819500 | 0.41788100 |
| H | -0.52926800 | -4.61700100 | -0.06626200 | H | -2.66055600 | 3.11514400 | 1.17604500 |
| H | -2.65579700 | -5.87584700 | 0.10577300 | H | -3.31998500 | 5.58851100 | 0.74577800 |
| H | -4.70485700 | -4.76603900 | 0.99712000 | H | -1.62230700 | 5.43650700 | 1.20017400 |
| H | -4.60685200 | -2.37474700 | 1.71191300 | C | -0.72892500 | 0.62979000 | -2.69969300 |
| H | -2.49389100 | -1.10452300 | 1.52076500 | C | 0.31057100 | 1.51685300 | -2.11832300 |
| H | 2.82186800 | -3.12703300 | 1.27998000 | H | -0.50148900 | 0.24976500 | -3.70837900 |
| H | 0.16953400 | -2.60751900 | -2.09921600 | H | 1.30114500 | 1.46781300 | -2.58947300 |
| H | 1.77495900 | -3.82960700 | -3.53624000 | H | 0.02115400 | 2.54687200 | -1.89126000 |
| H | 3.92018500 | -4.67773500 | -2.57736500 | P | 0.04483600 | -1.72588700 | 0.53792500 |
| H | 4.42239100 | -4.31410000 | -0.16063100 | C | 0.38725900 | -1.49716700 | 2.36066300 |
| C | 0.80829300 | 1.58141200 | 2.97615800 | C | 1.67595800 | -0.71572200 | 2.67959900 |
| H | 0.93752300 | 2.66369700 | 2.82580900 | C | 1.71621800 | 0.78789600 | 2.35354300 |
| H | -0.18903800 | 1.30980800 | 2.60544400 | P | 1.72530900 | 1.08554500 | 0.51721700 |
| H | 0.84154000 | 1.38668400 | 4.06047000 | C | 2.10550000 | 2.86627100 | 0.31793300 |
| C | 0.68593700 | -2.85334200 | 3.19234700 | C | 1.07334300 | 3.80401700 | 0.48675500 |
| H | 1.55157600 | -3.47584600 | 2.92383500 | C | 1.32886500 | 5.16832600 | 0.33473000 |
| H | 0.76012000 | -2.62832800 | 4.26855900 | C | 2.61403400 | 5.61083100 | 0.00321700 |
| H | -0.22401600 | -3.44959700 | 3.03476000 | C | 3.64222700 | 4.68202200 | -0.17578100 |
| Co | -0.06611700 | 0.31552900 | -0.42036300 | C | 3.39188100 | 3.31522800 | -0.01988500 |
| | | | | C | 3.25249000 | 0.22627400 | -0.04999000 |
| 7s | | | | C | 3.28702700 | -0.34402200 | -1.33353100 |
| C | -3.90218700 | 1.01254000 | -0.73419900 | C | 4.39019300 | 0.11864800 | 0.76884700 |
| C | -4.97121500 | 1.86277900 | -0.42402600 | C | 5.53011700 | -0.54739600 | 0.31377400 |
| C | -6.25152800 | 1.34899600 | -0.18223600 | C | 5.55333100 | -1.11083800 | -0.96591600 |
| C | -6.48542400 | -0.02563300 | -0.24494700 | C | 4.42996000 | -1.00448700 | -1.78919200 |
| C | -5.42491100 | -0.88531500 | -0.55317400 | C | -1.49225900 | -2.73636200 | 0.56685900 |
| C | -4.15231600 | -0.36943800 | -0.79619000 | C | -1.62370500 | -3.92314500 | -0.17091500 |
| H | -4.81373700 | 2.93949300 | -0.37804800 | C | -2.80606600 | -4.66740600 | -0.10960700 |
| H | -7.06968900 | 2.03518500 | 0.05198800 | C | -3.86444100 | -4.24572600 | 0.69954000 |
| H | -7.48458800 | -0.42661600 | -0.05707400 | C | -3.73922900 | -3.06499500 | 1.43784800 |
| H | -5.58681000 | -1.96399100 | -0.60139200 | C | -2.56897500 | -2.30860500 | 1.36493300 |
| H | -3.33677400 | -1.05415200 | -1.03676500 | C | 1.29921800 | -2.79376700 | -0.26360200 |
| C | -2.48996600 | 1.51545900 | -1.07902800 | C | 2.35953500 | -3.43530900 | 0.39370500 |
| C | -1.46499200 | 0.86754200 | -0.03297200 | C | 1.19877700 | -2.90817400 | -1.66418200 |
| O | -1.77210200 | 0.82784000 | 1.13254000 | C | 2.11351100 | -3.67668700 | -2.38385900 |
| H | -2.06145900 | 5.66348600 | -0.52109400 | C | 3.16513500 | -4.31566900 | -1.71926400 |
| C | -2.32412600 | 3.02178500 | -0.89286300 | C | 3.28938400 | -4.18482200 | -0.33385000 |
| H | -2.10724900 | 3.58882700 | -1.80419200 | H | -0.46868200 | -0.86638500 | 2.64737700 |
| H | -0.73826200 | -0.41299300 | -2.14346800 | H | 2.54184000 | -1.21909000 | 2.22710600 |
| C | -2.16262000 | 1.10812800 | -2.54112900 | H | 1.82278200 | -0.79356400 | 3.76974700 |
| H | -2.34691300 | 1.96495300 | -3.20661800 | H | 2.69884400 | 1.15673500 | 2.68653200 |
| H | -2.83687300 | 0.30648500 | -2.86610300 | H | 0.06417600 | 3.46522300 | 0.72028500 |
| C | -2.45197400 | 3.68421200 | 0.26340800 | H | 0.51869100 | 5.88767300 | 0.46752200 |

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|----------------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | 2.81095300 | 6.67856200 | -0.12070200 | C | -2.54689500 | 3.37666400 | -1.41185200 |
| H | 4.64755000 | 5.01835200 | -0.44119400 | H | -3.21017400 | 3.59938600 | -2.25764300 |
| H | 4.20358800 | 2.60268700 | -0.16812200 | H | 0.03795600 | 1.23060900 | -3.62676900 |
| H | 2.41659800 | -0.28196300 | -1.98616900 | C | -1.78707800 | 1.25866900 | -2.49133700 |
| H | 4.40124300 | 0.55746100 | 1.76715600 | H | -2.50259000 | 1.37353300 | -3.31903200 |
| H | 6.40481200 | -0.62426300 | 0.96403400 | H | -1.65649100 | 0.17501000 | -2.32184000 |
| H | 6.44497300 | -1.63475900 | -1.31860700 | C | -2.01229100 | 4.39040300 | -0.72284800 |
| H | 4.43456200 | -1.44645300 | -2.78741000 | C | -2.24864700 | 5.83899800 | -1.02232900 |
| H | -0.80177700 | -4.28226000 | -0.79068100 | H | -1.35769500 | 4.17778000 | 0.12827600 |
| H | -2.89174100 | -5.58881700 | -0.69094000 | H | -2.69011300 | 6.35527600 | -0.15155500 |
| H | -4.78439700 | -4.83291000 | 0.75313300 | H | -1.29659700 | 6.35603500 | -1.23686500 |
| H | -4.56405200 | -2.71900100 | 2.06477800 | C | -0.42176500 | 1.86399900 | -2.85117500 |
| H | -2.50181400 | -1.37694600 | 1.92672700 | C | 0.51283200 | 1.97936800 | -1.64655700 |
| H | 2.48047100 | -3.35501400 | 1.47238900 | H | -0.57579400 | 2.85788600 | -3.30710200 |
| H | 0.39603300 | -2.38893200 | -2.19394600 | H | 1.56216100 | 1.78120300 | -1.91254000 |
| H | 2.01415100 | -3.76302900 | -3.46849800 | H | 0.47504300 | 2.96914300 | -1.17407800 |
| H | 3.89242600 | -4.90567100 | -2.28209500 | P | -0.28430800 | -1.61618400 | 0.68994800 |
| H | 4.11543300 | -4.67028700 | 0.19115300 | C | 0.43593400 | -1.87806900 | 2.39133600 |
| C | 0.65225900 | 1.60444500 | 3.09096100 | C | 1.92950800 | -1.52454500 | 2.52759600 |
| H | 0.83387400 | 2.68344300 | 2.98540100 | C | 2.33796500 | -0.04298600 | 2.40568500 |
| H | -0.36086400 | 1.39009200 | 2.73063500 | P | 2.29138400 | 0.56279900 | 0.64383300 |
| H | 0.69944100 | 1.36439700 | 4.16561500 | C | 3.09415600 | 2.20586800 | 0.69040700 |
| C | 0.31628500 | -2.79005500 | 3.18165200 | C | 2.28917600 | 3.31554100 | 1.00516100 |
| H | 1.19321600 | -3.43181300 | 3.01816100 | C | 2.84495800 | 4.59502900 | 1.06434600 |
| H | 0.28891500 | -2.53458400 | 4.25320000 | C | 4.20549400 | 4.78158700 | 0.79561000 |
| H | -0.58259100 | -3.37893900 | 2.95492700 | C | 5.00747600 | 3.68374200 | 0.46983400 |
| Co | 0.12832700 | 0.18556200 | -0.71555700 | C | 4.45656900 | 2.39959200 | 0.41757200 |
| | | | | C | 3.39839200 | -0.54425800 | -0.29569300 |
| 7 _T | | | | C | 2.98306400 | -0.91592700 | -1.58524600 |
| C | -3.69613000 | 1.25765400 | -0.77658500 | C | 4.60168000 | -1.05914900 | 0.21482000 |
| C | -4.44080800 | 1.87183700 | 0.24457200 | C | 5.37642000 | -1.92567700 | -0.56068000 |
| C | -5.68110900 | 1.36338000 | 0.63292800 | C | 4.96101600 | -2.28142500 | -1.84880300 |
| C | -6.20075900 | 0.22481300 | 0.00866400 | C | 3.76332300 | -1.77466400 | -2.36169900 |
| C | -5.45974900 | -0.40633300 | -0.99200000 | C | -2.04252000 | -2.04741000 | 0.95450400 |
| C | -4.21570600 | 0.10233000 | -1.37948500 | C | -2.62500000 | -3.22461800 | 0.46421300 |
| H | -4.04463700 | 2.76339600 | 0.73218300 | C | -3.95413600 | -3.52963100 | 0.77522300 |
| H | -6.24538600 | 1.86050700 | 1.42611600 | C | -4.70209100 | -2.67187700 | 1.58567300 |
| H | -7.17233200 | -0.17440900 | 0.30980400 | C | -4.12537400 | -1.49385600 | 2.07233600 |
| H | -5.84656700 | -1.30605400 | -1.47646900 | C | -2.80695600 | -1.17425400 | 1.74893900 |
| H | -3.65970500 | -0.41242900 | -2.16211000 | C | 0.36034900 | -2.83910600 | -0.50717400 |
| C | -2.35740900 | 1.87939300 | -1.20488600 | C | 1.36624200 | -3.77681600 | -0.23238900 |
| C | -1.32938100 | 1.58721200 | -0.09306200 | C | -0.13637400 | -2.73668100 | -1.82141700 |
| O | -1.39283200 | 1.96201800 | 1.05274700 | C | 0.35026600 | -3.56683700 | -2.83117100 |
| H | -2.91963100 | 5.97809200 | -1.88421500 | C | 1.35328200 | -4.50080100 | -2.54756400 |

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|------------------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | 1.85909600 | -4.60032900 | -1.24958400 | H | -8.09209500 | -0.96544900 | -0.36591900 |
| H | -0.14298100 | -1.13655500 | 2.96598100 | H | -6.24439900 | -2.57292200 | 0.12879300 |
| H | 2.53336100 | -2.13745500 | 1.84285900 | H | -3.90154300 | -1.82534800 | 0.12143700 |
| H | 2.22316200 | -1.83807000 | 3.54348800 | C | -2.90820100 | 0.78278800 | -0.50288200 |
| H | 3.39409400 | 0.02132800 | 2.71248400 | C | -1.87023700 | -0.32138500 | -0.09026900 |
| H | 1.22361600 | 3.17661700 | 1.19931700 | O | -2.01868500 | -0.92626500 | 0.97504800 |
| H | 2.21146000 | 5.44995500 | 1.31310400 | H | -2.72313500 | 3.76717500 | 2.41121700 |
| H | 4.63881600 | 5.78401200 | 0.83505000 | C | -2.80501300 | 1.88848800 | 0.52571600 |
| H | 6.06936600 | 3.82488600 | 0.25354100 | H | -2.86305500 | 1.51551300 | 1.55311200 |
| H | 5.09195000 | 1.55106600 | 0.15938200 | H | -0.50517100 | 0.72498700 | -2.36448900 |
| H | 2.03185000 | -0.54163800 | -1.97037700 | C | -2.60625800 | 1.17672200 | -1.97656600 |
| H | 4.93711400 | -0.79016200 | 1.21837100 | H | -2.28717500 | 2.22145600 | -2.06735900 |
| H | 6.30954600 | -2.32566900 | -0.15659100 | H | -3.50885000 | 1.06367800 | -2.59002300 |
| H | 5.56956600 | -2.96100200 | -2.45044500 | C | -2.70821800 | 3.20572100 | 0.32155500 |
| H | 3.42750200 | -2.05932800 | -3.36096300 | C | -2.64826600 | 4.22868200 | 1.41443100 |
| H | -2.04164000 | -3.91161900 | -0.15089700 | H | -2.65994900 | 3.59538900 | -0.70005900 |
| H | -4.40201000 | -4.44806600 | 0.38769900 | H | -1.70661000 | 4.80040300 | 1.36709300 |
| H | -5.73936900 | -2.91373300 | 1.82918000 | H | -3.46491600 | 4.96546600 | 1.31362700 |
| H | -4.71053000 | -0.81181600 | 2.69194900 | C | -1.51508700 | 0.23565700 | -2.49780100 |
| H | -2.36913900 | -0.24398700 | 2.11702800 | C | -1.55486900 | -1.03717000 | -1.68042800 |
| H | 1.78437900 | -3.87078300 | 0.76792300 | H | -1.54901900 | 0.07432000 | -3.58482400 |
| H | -0.90988600 | -2.00019600 | -2.05617800 | H | -0.77640000 | -1.77553400 | -1.92835000 |
| H | -0.04833100 | -3.47779000 | -3.84460000 | H | -2.50807800 | -1.57725900 | -1.70592500 |
| H | 1.74320000 | -5.14417000 | -3.33992700 | P | 0.80094300 | -1.77484100 | 0.54316900 |
| H | 2.64847900 | -5.32034200 | -1.02178400 | C | 0.99088200 | -1.49617400 | 2.36533300 |
| C | 1.51589900 | 0.88418000 | 3.30582600 | C | 1.78850700 | -0.22320200 | 2.69830900 |
| H | 1.97891200 | 1.87761600 | 3.38790300 | C | 1.19225900 | 1.13022100 | 2.27107900 |
| H | 0.49087000 | 1.02327800 | 2.92905600 | P | 1.20118200 | 1.35418900 | 0.42738000 |
| H | 1.45391900 | 0.45857100 | 4.32049600 | C | 0.81612300 | 3.12612100 | 0.12855300 |
| C | 0.12222000 | -3.25680100 | 2.98167400 | C | 0.26705500 | 3.49016000 | -1.10837200 |
| H | 0.70065800 | -4.05922300 | 2.50261000 | C | 0.06685300 | 4.83549600 | -1.42643700 |
| H | 0.37748600 | -3.25808200 | 4.05359800 | C | 0.41177400 | 5.83051400 | -0.50715700 |
| H | -0.94458700 | -3.50519000 | 2.88970200 | C | 0.96015900 | 5.47395200 | 0.72949200 |
| Co | 0.17027400 | 0.42881300 | -0.35941200 | C | 1.16500900 | 4.12908300 | 1.04732600 |
| | | | | C | 2.97795800 | 1.34296300 | -0.05199500 |
| TS7 _s | | | | C | 3.28011300 | 1.08443100 | -1.39765900 |
| C | -4.35332500 | 0.22539500 | -0.41129800 | C | 4.01897700 | 1.65001300 | 0.83823300 |
| C | -5.40574300 | 1.11881100 | -0.68196100 | C | 5.34147000 | 1.68331300 | 0.38753000 |
| C | -6.73673700 | 0.70009300 | -0.66953000 | C | 5.63551700 | 1.42308700 | -0.95456800 |
| C | -7.05127000 | -0.63237300 | -0.37864500 | C | 4.60093000 | 1.12835200 | -1.84773600 |
| C | -6.01768100 | -1.52875300 | -0.10270600 | C | -0.09525300 | -3.37260800 | 0.38153100 |
| C | -4.68229900 | -1.10521400 | -0.11601900 | C | 0.23163900 | -4.28307800 | -0.63713400 |
| H | -5.17518000 | 2.16294900 | -0.90519200 | C | -0.49735700 | -5.46513100 | -0.79560600 |
| H | -7.53206800 | 1.41836400 | -0.88568900 | C | -1.55864300 | -5.75836700 | 0.06408900 |

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|------------------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | -1.88285200 | -4.86331600 | 1.08862700 | O | -1.80669500 | 0.16007600 | 0.99067200 |
| C | -1.16171600 | -3.67805300 | 1.24703200 | H | -4.08023300 | 4.47922700 | 2.29056900 |
| C | 2.41273600 | -2.05369100 | -0.28115700 | P | 0.57239800 | -1.86575000 | 0.63806600 |
| C | 3.63735200 | -2.23919700 | 0.37682300 | C | 1.20848100 | -1.54878400 | 2.36548900 |
| C | 2.39563500 | -2.02271500 | -1.68901500 | C | 2.42195400 | -0.59697400 | 2.35379800 |
| C | 3.56691800 | -2.21623400 | -2.42073100 | C | 2.17640300 | 0.90982900 | 2.12908200 |
| C | 4.78171900 | -2.40645300 | -1.75607700 | P | 1.83124500 | 1.35989300 | 0.35771800 |
| C | 4.81428000 | -2.40608700 | -0.35918300 | C | 1.71626800 | 3.18715600 | 0.39501000 |
| H | -0.05835900 | -1.33002900 | 2.65285000 | C | 0.47368600 | 3.78621000 | 0.15058400 |
| H | 2.81618600 | -0.32031300 | 2.31978100 | C | 0.33788600 | 5.17665100 | 0.20395600 |
| H | 1.87565100 | -0.19088600 | 3.79712300 | C | 1.44758400 | 5.97447700 | 0.49707000 |
| H | 1.86887800 | 1.90075200 | 2.66951800 | C | 2.69325700 | 5.38030600 | 0.73664000 |
| H | -0.01007900 | 2.71518800 | -1.82348300 | C | 2.83025300 | 3.99152300 | 0.68562200 |
| H | -0.36554400 | 5.10506600 | -2.39297500 | C | 3.36660700 | 1.06152700 | -0.59515000 |
| H | 0.25260500 | 6.88338000 | -0.75236100 | C | 3.24606300 | 1.09098100 | -1.99634000 |
| H | 1.23096000 | 6.24681100 | 1.45290600 | C | 4.61562100 | 0.78777000 | -0.02035000 |
| H | 1.60505100 | 3.87217900 | 2.01238300 | C | 5.72428300 | 0.53778600 | -0.83652600 |
| H | 2.47475300 | 0.84261500 | -2.09452800 | C | 5.59780500 | 0.56860700 | -2.22789200 |
| H | 3.81243400 | 1.86910800 | 1.88683300 | C | 4.35573600 | 0.85262300 | -2.80803600 |
| H | 6.14549200 | 1.91576200 | 1.09022000 | C | -0.88263000 | -2.95688200 | 0.83478400 |
| H | 6.67069800 | 1.44793100 | -1.30356300 | C | -1.20959900 | -3.87518800 | -0.17902300 |
| H | 4.82338200 | 0.91832900 | -2.89634000 | C | -2.40642900 | -4.59386500 | -0.12763100 |
| H | 1.05966700 | -4.08145300 | -1.31582400 | C | -3.29592800 | -4.40534100 | 0.93508400 |
| H | -0.22772900 | -6.15929900 | -1.59525400 | C | -2.97839500 | -3.49442200 | 1.94763400 |
| H | -2.12841700 | -6.68255600 | -0.05995400 | C | -1.78351200 | -2.77186700 | 1.89756200 |
| H | -2.70656500 | -5.08574900 | 1.77142200 | C | 1.84131100 | -2.90556100 | -0.17323600 |
| H | -1.44074500 | -2.98866500 | 2.04018400 | C | 2.08856000 | -4.24644400 | 0.17150500 |
| H | 3.69099400 | -2.24796100 | 1.46381200 | C | 2.60871700 | -2.30816100 | -1.18504500 |
| H | 1.45793500 | -1.83729700 | -2.21728100 | C | 3.62408500 | -3.02288000 | -1.82709400 |
| H | 3.53323300 | -2.19586700 | -3.51247800 | C | 3.87178100 | -4.35092300 | -1.47004700 |
| H | 5.70424300 | -2.54121600 | -2.32571300 | C | 3.09858600 | -4.96210400 | -0.47505900 |
| H | 5.76212700 | -2.53933600 | 0.16753000 | H | 0.36653700 | -1.04289200 | 2.86131700 |
| C | -0.20283600 | 1.37501200 | 2.85082400 | H | 3.17854500 | -0.97220400 | 1.64627700 |
| H | -0.56268600 | 2.38800700 | 2.62422800 | H | 2.88705100 | -0.67745500 | 3.35047900 |
| H | -0.93861000 | 0.66025900 | 2.46086000 | H | 3.11416400 | 1.42764600 | 2.38776400 |
| H | -0.16411300 | 1.26718800 | 3.94704000 | H | -0.38981100 | 3.15930400 | -0.07360700 |
| C | 1.51612000 | -2.70164100 | 3.15318200 | H | -0.63606800 | 5.63441000 | 0.01536800 |
| H | 2.59626200 | -2.84875100 | 3.01534600 | H | 1.34504600 | 7.06179800 | 0.53662900 |
| H | 1.34102300 | -2.52988200 | 4.22721600 | H | 3.56220800 | 6.00345300 | 0.96250000 |
| H | 1.00878900 | -3.63528700 | 2.87542200 | H | 3.80553000 | 3.53375100 | 0.86794700 |
| Co | -0.04300000 | -0.12654500 | -0.65308900 | H | 2.27100300 | 1.28988900 | -2.45168000 |
| | | | | H | 4.73694900 | 0.76335300 | 1.06333800 |
| TS7 _T | | | | H | 6.69186000 | 0.31768100 | -0.37890600 |
| C | -1.79305900 | 0.48483500 | -0.17897800 | H | 6.46543600 | 0.36902600 | -2.86141600 |

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|----|-------------|-------------|-------------|----------------|-------------|-------------|-------------|
| H | 4.24971600 | 0.87745800 | -3.89526000 | C | -3.12133300 | 4.28543500 | 1.77873200 |
| H | -0.53055800 | -4.02575000 | -1.02032700 | H | -3.35481500 | 2.08277300 | 1.74251700 |
| H | -2.64523100 | -5.30262700 | -0.92447100 | H | -2.93580300 | 5.10168300 | 1.06368300 |
| H | -4.23312300 | -4.96587600 | 0.97399900 | H | -2.33957200 | 4.32662100 | 2.55847100 |
| H | -3.66781800 | -3.33854900 | 2.78105300 | | | | |
| H | -1.56438400 | -2.05221400 | 2.68630500 | 8 _s | | | |
| H | 1.48489500 | -4.73657400 | 0.93662300 | C | -1.81719700 | -0.70978700 | -0.51969900 |
| H | 2.40981600 | -1.27454100 | -1.46670200 | O | -1.27320700 | -0.89620300 | 0.64137700 |
| H | 4.21570800 | -2.53962900 | -2.60820600 | H | -5.05637200 | 2.59196800 | 2.43875600 |
| H | 4.66225600 | -4.91537500 | -1.97102500 | P | 1.90515900 | -1.22784900 | 0.39605100 |
| H | 3.28365100 | -6.00388400 | -0.20156000 | C | 1.93969900 | -0.84739700 | 2.22292900 |
| C | 1.06012700 | 1.47585000 | 3.01475300 | C | 2.11693400 | 0.66008400 | 2.48279900 |
| H | 1.06276000 | 2.57509200 | 3.00705900 | C | 0.90294500 | 1.57585200 | 2.22696400 |
| H | 0.06364300 | 1.14104800 | 2.68850500 | P | 0.48023300 | 1.72816000 | 0.43319300 |
| H | 1.20630400 | 1.14464700 | 4.05553200 | C | -0.62147400 | 3.18205400 | 0.24229500 |
| C | 1.53848300 | -2.82276300 | 3.14605900 | C | -1.10580200 | 3.44170900 | -1.05174700 |
| H | 2.44058200 | -3.31156800 | 2.74838500 | C | -1.86019100 | 4.58546800 | -1.30791000 |
| H | 1.73519100 | -2.56832000 | 4.20042900 | C | -2.14110400 | 5.48491900 | -0.27181500 |
| H | 0.71438900 | -3.55072300 | 3.12325600 | C | -1.65637700 | 5.23541000 | 1.01389400 |
| Co | 0.06056600 | 0.15261800 | -0.54118200 | C | -0.89519700 | 4.09017100 | 1.27329800 |
| C | -4.21546200 | 0.72027300 | -0.84051200 | C | 1.94354900 | 2.36505300 | -0.46623100 |
| C | -5.27914100 | 1.39810800 | -1.46179200 | C | 2.09529300 | 1.98129800 | -1.80915600 |
| C | -6.56178500 | 0.84990300 | -1.49252200 | C | 2.86778300 | 3.24698900 | 0.11159000 |
| C | -6.81041700 | -0.39443100 | -0.90060800 | C | 3.94529000 | 3.71986100 | -0.64310800 |
| C | -5.76296600 | -1.07493800 | -0.27850700 | C | 4.09447400 | 3.33282000 | -1.97935400 |
| C | -4.47613400 | -0.52324300 | -0.24726600 | C | 3.16372700 | 2.46795600 | -2.56440400 |
| H | -5.10115800 | 2.37260800 | -1.92213900 | C | 1.27222100 | -2.94332800 | 0.24779500 |
| H | -7.37233300 | 1.39759100 | -1.98023900 | C | 1.39787700 | -3.59087600 | -0.99543300 |
| H | -7.81413900 | -0.82600900 | -0.92386700 | C | 0.81494700 | -4.84007600 | -1.20891700 |
| H | -5.93792300 | -2.04680300 | 0.19023200 | C | 0.08236400 | -5.45719600 | -0.18751000 |
| H | -3.68559400 | -1.07983700 | 0.25379300 | C | -0.06070300 | -4.81453100 | 1.04433100 |
| C | -2.82336800 | 1.38314700 | -0.87325500 | C | 0.52829700 | -3.56413600 | 1.26232500 |
| C | -2.31495000 | 1.50982200 | -2.31782700 | C | 3.68070900 | -1.35476100 | -0.05974300 |
| H | -1.37193400 | 2.08368100 | -2.29224900 | C | 4.36765900 | -2.58145100 | -0.07498200 |
| H | -3.02338100 | 2.07104700 | -2.94295600 | C | 4.39109800 | -0.17699000 | -0.34685100 |
| C | -2.85255100 | 2.74364300 | -0.18381200 | C | 5.75502300 | -0.22338000 | -0.64768000 |
| H | -1.43575600 | 0.16269800 | -3.76906200 | C | 6.42718000 | -1.44852500 | -0.67274400 |
| H | -2.61982800 | 3.59861000 | -0.82791900 | C | 5.72929400 | -2.62608900 | -0.38423100 |
| C | -2.05276600 | 0.10122200 | -2.85988100 | H | 0.93753600 | -1.14032900 | 2.56767600 |
| C | -1.36693500 | -0.75433100 | -1.79785900 | H | 2.99902800 | 1.03713300 | 1.94214200 |
| H | -3.01073100 | -0.36016000 | -3.14796700 | H | 2.35481000 | 0.77305100 | 3.55373500 |
| H | -0.42367800 | -1.20454600 | -2.16037900 | H | 1.20525100 | 2.58527800 | 2.54791700 |
| H | -1.98391700 | -1.57251200 | -1.41085200 | H | -0.89354900 | 2.73956900 | -1.86157800 |
| C | -3.12814700 | 2.94800300 | 1.10897400 | H | -2.23431700 | 4.77408900 | -2.31695600 |

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|----|-------------|-------------|-------------|----------------|-------------|-------------|-------------|
| H | -2.73507800 | 6.38042900 | -0.46975300 | H | -3.17475300 | 2.14732500 | -0.53084100 |
| H | -1.86938500 | 5.93434300 | 1.82623000 | C | -2.37283000 | -1.12259900 | -2.83924500 |
| H | -0.51857700 | 3.92323100 | 2.28243800 | C | -1.45505500 | -1.60134100 | -1.69935300 |
| H | 1.38165700 | 1.28842600 | -2.26550500 | H | -3.13266600 | -1.89407900 | -3.03345200 |
| H | 2.75523700 | 3.56682900 | 1.14946300 | H | -0.35974300 | -1.51668100 | -1.97002200 |
| H | 4.66996700 | 4.39757200 | -0.18551300 | H | -1.55021700 | -2.66991300 | -1.44702800 |
| H | 4.93771000 | 3.70608800 | -2.56541900 | C | -3.81560700 | 1.27613600 | 1.26851600 |
| H | 3.27607900 | 2.16243500 | -3.60723000 | C | -4.02463600 | 2.53679800 | 2.04805200 |
| H | 1.95036900 | -3.10976800 | -1.80663100 | H | -4.03704100 | 0.34038000 | 1.79601400 |
| H | 0.92643600 | -5.33118500 | -2.17874500 | H | -3.83352200 | 3.43275000 | 1.44001700 |
| H | -0.37927400 | -6.43331500 | -0.35542700 | H | -3.35980500 | 2.57436100 | 2.92924400 |
| H | -0.63538600 | -5.28537600 | 1.84573900 | | | | |
| H | 0.39552200 | -3.07950800 | 2.22963300 | 8 _T | | | |
| H | 3.84297500 | -3.50865700 | 0.15845600 | C | -2.01374700 | -0.64101600 | -0.43049900 |
| H | 3.87815000 | 0.78131200 | -0.33056000 | O | -1.57309600 | -0.80946200 | 0.71858100 |
| H | 6.28924800 | 0.70397200 | -0.86818900 | H | -4.13336700 | 4.15808600 | 1.59454300 |
| H | 7.49208300 | -1.48699900 | -0.91524900 | P | 1.26922700 | -1.74847700 | 0.40940100 |
| H | 6.24840700 | -3.58779900 | -0.39470800 | C | 1.42913900 | -1.30502400 | 2.21706700 |
| C | -0.33935100 | 1.15440900 | 3.02467500 | C | 2.10283100 | 0.06906300 | 2.40730700 |
| H | -1.13041500 | 1.91473600 | 2.97522500 | C | 1.28353500 | 1.35255200 | 2.14080800 |
| H | -0.76768900 | 0.21659400 | 2.64830500 | P | 1.06796000 | 1.72770600 | 0.33221100 |
| H | -0.06375700 | 1.02208800 | 4.08311300 | C | 0.37823100 | 3.43493000 | 0.25969900 |
| C | 2.98768400 | -1.66250900 | 2.98083800 | C | -0.23367100 | 3.83732800 | -0.93886000 |
| H | 4.00669100 | -1.33493000 | 2.72376200 | C | -0.73320900 | 5.13351900 | -1.08315300 |
| H | 2.85219400 | -1.52568900 | 4.06608900 | C | -0.63091800 | 6.04329100 | -0.02604100 |
| H | 2.91304900 | -2.73801700 | 2.76252000 | C | -0.01388300 | 5.65390500 | 1.16691800 |
| Co | 0.05524900 | -0.18834600 | -0.53586000 | C | 0.49442800 | 4.35933800 | 1.30859900 |
| C | -4.27999400 | -1.08095700 | -0.46946300 | C | 2.75154500 | 2.06803600 | -0.33037800 |
| C | -4.05639200 | -2.22671700 | 0.30728400 | C | 2.90249400 | 2.06094100 | -1.72771000 |
| C | -5.10125300 | -3.11343200 | 0.59713600 | C | 3.86260400 | 2.35841600 | 0.47424600 |
| C | -6.38832000 | -2.86948900 | 0.11558600 | C | 5.10700100 | 2.61602100 | -0.11006100 |
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| C | -5.58179400 | -0.84450300 | -0.94436300 | C | 4.14166200 | 2.33323000 | -2.31031500 |
| H | -3.06185700 | -2.43548300 | 0.70297500 | C | 0.40482800 | -3.36317400 | 0.37318000 |
| H | -4.90114500 | -3.99914200 | 1.20586000 | C | 0.60280800 | -4.21653700 | -0.72651000 |
| H | -7.20369500 | -3.56127200 | 0.34151800 | C | -0.15727000 | -5.37935700 | -0.87131400 |
| H | -7.62880600 | -1.51918100 | -1.03731000 | C | -1.13180700 | -5.70483000 | 0.07828600 |
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| C | -3.17148200 | -0.05459000 | -0.78435200 | C | -0.57872600 | -3.69507700 | 1.31974400 |
| C | -3.04546000 | 0.16087700 | -2.31260600 | C | 2.96579100 | -2.14082100 | -0.16088000 |
| H | -2.38979300 | 1.03062200 | -2.47821400 | C | 3.68416000 | -3.27427500 | 0.26142000 |
| H | -4.00625600 | 0.36876600 | -2.80231900 | C | 3.56786500 | -1.25127000 | -1.06267400 |
| C | -3.39895000 | 1.21866900 | -0.00203100 | C | 4.87467800 | -1.46256400 | -1.51198400 |
| H | -1.83135500 | -0.94991000 | -3.78002300 | C | 5.58820400 | -2.58064500 | -1.07268500 |

| | | | | | | | |
|----|-------------|-------------|-------------|----------------|-------------|-------------|-------------|
| C | 4.98725100 | -3.48920600 | -0.19230000 | H | -5.50987700 | 1.21591200 | -1.75536600 |
| H | 0.38348700 | -1.24011600 | 2.55148100 | C | -3.09874000 | 0.38361100 | -0.81143300 |
| H | 3.04848800 | 0.09212700 | 1.84258100 | C | -2.84553700 | 0.48073800 | -2.33900800 |
| H | 2.39500200 | 0.12396700 | 3.46925700 | H | -1.94892100 | 1.10409300 | -2.50069600 |
| H | 1.87815700 | 2.17887300 | 2.56042700 | H | -3.67574400 | 0.94244800 | -2.88828300 |
| H | -0.32014800 | 3.12864200 | -1.76632700 | C | -2.87806200 | 1.68247900 | -0.08068800 |
| H | -1.21029700 | 5.43024000 | -2.02038100 | H | -2.05445500 | -1.02451700 | -3.74379800 |
| H | -1.02968100 | 7.05511500 | -0.13224100 | H | -1.99246100 | 2.23086500 | -0.40549400 |
| H | 0.07470700 | 6.36199900 | 1.99459000 | C | -2.55680500 | -0.96503500 | -2.76828100 |
| H | 0.98280100 | 4.08058200 | 2.24358600 | C | -1.70135000 | -1.52751800 | -1.62749800 |
| H | 2.04404500 | 1.82706500 | -2.36343200 | H | -3.49744400 | -1.53184600 | -2.83856600 |
| H | 3.77089900 | 2.38631900 | 1.56100900 | H | -0.60747300 | -1.50002400 | -1.89052600 |
| H | 5.96827200 | 2.83052000 | 0.52751700 | H | -1.86049900 | -2.58632300 | -1.37443300 |
| H | 6.22425800 | 2.80440900 | -1.95339900 | C | -3.60089800 | 2.17485800 | 0.93212400 |
| H | 4.24524700 | 2.32243700 | -3.39804500 | C | -3.28703700 | 3.45063800 | 1.65184400 |
| H | 1.35180600 | -3.96776600 | -1.48189900 | H | -4.48390200 | 1.62526000 | 1.27802500 |
| H | 0.01126700 | -6.03225400 | -1.73144300 | H | -2.39400200 | 3.94452800 | 1.24358900 |
| H | -1.72831100 | -6.61338900 | -0.03502300 | H | -3.11655100 | 3.26256600 | 2.72675900 |
| H | -2.09770500 | -5.10473400 | 1.91935900 | | | | |
| H | -0.76747200 | -3.04337100 | 2.17255800 | 9 _s | | | |
| H | 3.22273300 | -3.99851400 | 0.93418600 | C | 3.95178900 | -2.07118100 | 0.96432600 |
| H | 3.00711500 | -0.38537200 | -1.41137900 | C | 4.27299500 | -1.72130800 | 2.28912200 |
| H | 5.32917600 | -0.75325100 | -2.20781700 | C | 5.57792200 | -1.83075800 | 2.77019100 |
| H | 6.60959800 | -2.75216800 | -1.42171100 | C | 6.59969600 | -2.29788200 | 1.93513200 |
| H | 5.53777200 | -4.37224500 | 0.14182700 | C | 6.29684200 | -2.65098900 | 0.61905200 |
| C | -0.08402400 | 1.34112000 | 2.83643900 | C | 4.98672700 | -2.53672000 | 0.13848200 |
| H | -0.55664700 | 2.33287100 | 2.81555800 | H | 3.48999500 | -1.35283000 | 2.95420500 |
| H | -0.77818100 | 0.63384800 | 2.36301400 | H | 5.79926900 | -1.54911100 | 3.80297900 |
| H | 0.04110200 | 1.05201900 | 3.89283900 | H | 7.62253100 | -2.38604500 | 2.31000100 |
| C | 2.14733000 | -2.36367000 | 3.05616100 | H | 7.08249100 | -3.02104000 | -0.04488300 |
| H | 3.22503800 | -2.38454500 | 2.83482100 | H | 4.78599600 | -2.82248100 | -0.89407200 |
| H | 2.03210900 | -2.12633700 | 4.12646200 | C | 2.52104100 | -1.91945300 | 0.48185700 |
| H | 1.74359100 | -3.37257000 | 2.88969000 | C | 1.99641800 | -0.45339900 | 0.61500900 |
| Co | 0.06255300 | -0.08559700 | -0.70456900 | O | 2.63148600 | 0.44904900 | 1.09418100 |
| C | -4.47694300 | -0.22861300 | -0.51663300 | H | -0.19699600 | 0.07843200 | 1.61839100 |
| C | -4.65223700 | -1.32402000 | 0.34106900 | C | 1.49855600 | -2.72999700 | 1.33155000 |
| C | -5.92951700 | -1.83657900 | 0.59852600 | H | 1.83783600 | -2.77230600 | 2.37779100 |
| C | -7.05407200 | -1.25715200 | 0.00856600 | H | 1.46841900 | -3.76293400 | 0.95532100 |
| C | -6.89218600 | -0.15630600 | -0.84064900 | C | 2.32392700 | -2.28699100 | -1.00090800 |
| C | -5.61751100 | 0.34965300 | -1.09962900 | H | 2.54965200 | -3.35208700 | -1.15464500 |
| H | -3.79229200 | -1.78837800 | 0.82472700 | H | 3.03401000 | -1.70486300 | -1.61049400 |
| H | -6.03979500 | -2.69418200 | 1.26710700 | C | 0.12042300 | -2.09118200 | 1.26120300 |
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|---|-------------|-------------|-------------|----------------|-------------|-------------|-------------|
| H | -1.23637000 | -0.98889500 | 2.56358400 | H | 1.81958500 | 4.20304100 | -0.61365100 |
| H | 0.52587000 | -0.77965500 | 2.96119600 | H | 1.13053400 | 2.03898500 | 1.93164200 |
| C | 0.93645900 | -1.99467900 | -1.48856500 | H | -1.39933300 | 4.16819500 | -0.85316000 |
| C | 0.16864800 | -2.81191200 | -2.21530400 | H | -1.92584400 | 5.82430800 | 0.88952000 |
| H | 0.61689600 | -0.90289700 | -1.50922400 | H | -0.94018400 | 5.61439200 | 3.17178500 |
| H | -0.79931200 | -2.49278000 | -2.59783100 | H | 0.60694200 | 3.72031900 | 3.68122700 |
| H | 0.50160800 | -3.82506400 | -2.46288000 | H | -2.90964600 | -2.53350200 | 1.66442500 |
| P | -2.22709800 | -0.57294500 | -0.38224900 | H | -3.66027100 | -4.88490700 | 1.59276100 |
| C | -2.77235500 | 0.25845600 | -1.96220200 | H | -4.09930600 | -5.99936000 | -0.60001700 |
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| P | 0.29472300 | 1.64771300 | -0.78795600 | H | -5.04657800 | -1.06368100 | 0.49054300 |
| C | 1.95220200 | 2.18413400 | -1.39388800 | H | -1.82975500 | 1.62866700 | 1.51272900 |
| C | 2.75483700 | 1.28733800 | -2.11753600 | H | -3.29561500 | 2.77701100 | 3.12848300 |
| C | 4.00289000 | 1.68018700 | -2.60343900 | H | -5.65558500 | 2.01003200 | 3.44462600 |
| C | 4.46984500 | 2.97813500 | -2.37073500 | H | -6.51312700 | 0.08172700 | 2.11121300 |
| C | 3.67578500 | 3.87932000 | -1.65672400 | C | -0.28030000 | 1.22273700 | -3.51173200 |
| C | 2.42398900 | 3.48680400 | -1.17173000 | H | 0.69667300 | 1.59967800 | -3.84180500 |
| C | -0.11683000 | 2.96473500 | 0.42544500 | H | -0.18492800 | 0.13993500 | -3.34178800 |
| C | 0.45081800 | 2.86306300 | 1.70863100 | H | -0.99245900 | 1.36828000 | -4.33999300 |
| C | -0.96143800 | 4.04667700 | 0.13728500 | C | -4.28665300 | 0.22349500 | -2.18801900 |
| C | -1.25771000 | 4.99227700 | 1.12456800 | H | -4.80428500 | 0.89960200 | -1.49137800 |
| C | -0.70370200 | 4.87610000 | 2.40173800 | H | -4.50789300 | 0.56518100 | -3.21204100 |
| C | 0.16012300 | 3.81279800 | 2.68834400 | H | -4.71547400 | -0.78026300 | -2.06748400 |
| C | -2.89305600 | -2.28088000 | -0.49106300 | Co | 0.12784600 | -0.47252600 | 0.10801000 |
| C | -3.08419400 | -3.00960700 | 0.69754600 | | | | |
| C | -3.51484000 | -4.33715900 | 0.65848300 | 9 _T | | | |
| C | -3.76142800 | -4.96071700 | -0.56901200 | C | -3.63400500 | -1.53174600 | 1.01434200 |
| C | -3.57849800 | -4.24480800 | -1.75503600 | C | -4.66948400 | -1.99386600 | 0.18708700 |
| C | -3.14777200 | -2.91534700 | -1.71734700 | C | -5.97779700 | -1.52899000 | 0.34772400 |
| C | -3.32408600 | 0.19934500 | 0.88181500 | C | -6.27641800 | -0.58884500 | 1.33703000 |
| C | -4.65325900 | -0.22424300 | 1.06422700 | C | -5.25299500 | -0.12115000 | 2.16660000 |
| C | -2.85259800 | 1.28282400 | 1.63819800 | C | -3.94705100 | -0.59252600 | 2.01096000 |
| C | -3.68545000 | 1.93471900 | 2.55236100 | H | -4.46090500 | -2.72913800 | -0.59087700 |
| C | -5.00316600 | 1.50584600 | 2.72737100 | H | -6.76633600 | -1.90310800 | -0.31016500 |
| C | -5.48335900 | 0.42370700 | 1.98119200 | H | -7.29830200 | -0.22138400 | 1.45922500 |
| H | -2.27606300 | -0.31913400 | -2.75697400 | H | -5.46983000 | 0.61689800 | 2.94314200 |
| H | -2.61834200 | 2.24100900 | -1.10750900 | H | -3.16104200 | -0.22331700 | 2.67004500 |
| H | -2.82145300 | 2.19690200 | -2.84866700 | C | -2.23010800 | -2.12256600 | 0.88364400 |
| H | -0.67349400 | 3.04925800 | -2.47117100 | C | -1.11541700 | -1.08950400 | 1.13674100 |
| H | 2.40795500 | 0.27367900 | -2.31108200 | O | -0.92359600 | -0.49213400 | 2.16669900 |
| H | 4.61384300 | 0.96659200 | -3.16168000 | H | 1.13648200 | -2.51605600 | -2.31051900 |
| H | 5.44998100 | 3.28486900 | -2.74413300 | C | -1.88522900 | -2.64397000 | -0.51555100 |
| H | 4.03067200 | 4.89612000 | -1.47075400 | H | -2.40375800 | -2.03056600 | -1.26687200 |

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|---|-------------|-------------|-------------|------------------|-------------|-------------|-------------|
| H | -2.22861600 | -3.68386900 | -0.65316000 | H | 1.91147000 | 2.76632100 | -1.16325300 |
| C | -2.10167000 | -3.22009600 | 2.00037300 | H | 2.23391600 | 2.78372600 | -2.88681100 |
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| H | -2.30127400 | -2.71781500 | 2.96136300 | H | 2.41478500 | -2.93609300 | -0.20508200 |
| C | -0.38678900 | -2.52492400 | -0.74242500 | H | 4.09803100 | -4.77008100 | -0.30715800 |
| C | 0.04221800 | -2.50187100 | -2.19827700 | H | 6.50366400 | -4.23061300 | -0.68572600 |
| H | 0.17791300 | -3.27813700 | -0.17310000 | H | 7.22111500 | -1.85733200 | -0.95158100 |
| H | -0.35088700 | -3.39334800 | -2.72527000 | H | 5.54290900 | -0.02743500 | -0.84071100 |
| H | -0.35123200 | -1.62162800 | -2.73363900 | H | 2.49042200 | -0.49966300 | 2.37836300 |
| C | -0.79026200 | -3.94243800 | 2.08661000 | H | 4.00691300 | 2.64227400 | -0.18320500 |
| C | -0.63404100 | -5.25384400 | 1.87943400 | H | 4.67067800 | 3.93860000 | 1.80624400 |
| H | 0.08601900 | -3.33901100 | 2.35416600 | H | 4.26156500 | 3.03659800 | 4.09550900 |
| H | 0.34405100 | -5.73565900 | 1.97435300 | H | 3.18566000 | 0.80000500 | 4.37237600 |
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| P | -0.57236700 | 1.24481300 | -0.89960800 | H | -5.52615300 | 1.70492500 | -0.55003700 |
| C | 0.37590400 | 1.85265400 | -2.40068800 | H | -5.96597700 | 0.57495600 | -2.73006600 |
| C | 1.85475000 | 2.14562100 | -2.07149200 | H | -4.04811300 | -0.25584500 | -4.09915300 |
| C | 2.83964200 | 0.96077000 | -1.98039900 | H | -1.72833300 | 0.06741900 | -3.31250200 |
| P | 2.60264600 | -0.04819900 | -0.44129700 | H | -1.83201800 | 3.98321700 | -0.87629700 |
| C | 3.86707000 | -1.36903700 | -0.53088500 | H | 0.67189900 | 1.55958900 | 1.67188700 |
| C | 3.46778100 | -2.70386700 | -0.37576500 | H | 0.85596700 | 3.43446400 | 3.28265700 |
| C | 4.41530300 | -3.73174300 | -0.43048600 | H | -0.30935100 | 5.59607700 | 2.81631900 |
| C | 5.76281600 | -3.42839500 | -0.64153800 | H | -1.65492100 | 5.85309800 | 0.73187700 |
| C | 6.16645900 | -2.09515100 | -0.79211700 | C | 2.79337100 | 0.05686300 | -3.21604400 |
| C | 5.22409500 | -1.06736800 | -0.73328900 | H | 3.62468000 | -0.66216600 | -3.21989800 |
| C | 3.19624900 | 0.97871100 | 0.95676800 | H | 1.85642200 | -0.51521300 | -3.27474900 |
| C | 2.97659900 | 0.47136500 | 2.25009300 | H | 2.87227500 | 0.67183300 | -4.12699900 |
| C | 3.81652300 | 2.22696500 | 0.80689200 | C | -0.25779400 | 3.06930200 | -3.08089800 |
| C | 4.19570500 | 2.96293200 | 1.93479300 | H | -0.11090200 | 3.98188700 | -2.48436200 |
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| C | 3.36403200 | 1.20348300 | 3.37271700 | H | -1.33525700 | 2.93962700 | -3.25555500 |
| C | -2.30013000 | 1.08845200 | -1.48494900 | Co | 0.36748700 | -0.79127500 | -0.08164200 |
| C | -3.38448800 | 1.52826800 | -0.70922600 | | | | |
| C | -4.69414600 | 1.35310600 | -1.16283000 | TS8 _s | | | |
| C | -4.94002200 | 0.71669000 | -2.38205300 | C | -3.99563400 | -2.03485100 | -0.90851900 |
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| C | -2.55557900 | 0.43524700 | -2.70345300 | C | -5.57842100 | -1.82465800 | -2.75506200 |
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| C | -1.23023900 | 3.86035500 | 0.02441600 | C | -6.35903800 | -2.54906900 | -0.59004700 |
| C | 0.17449300 | 2.50350300 | 1.45945100 | C | -5.05663700 | -2.44593700 | -0.08707200 |
| C | 0.27123100 | 3.56075700 | 2.36870100 | H | -3.47431400 | -1.40430000 | -2.91262500 |
| C | -0.38138600 | 4.76797100 | 2.10674000 | H | -5.77338600 | -1.57573600 | -3.80153700 |
| C | -1.13571200 | 4.91341100 | 0.93603200 | H | -7.64399000 | -2.31547800 | -2.31685800 |
| H | 0.32413200 | 1.00219700 | -3.09669200 | H | -7.16677900 | -2.87668200 | 0.06970900 |

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|---|-------------|-------------|-------------|-----------------|-------------|-------------|-------------|
| H | -4.87747800 | -2.69690600 | 0.95878800 | C | 3.31945900 | 0.29912000 | -0.94802600 |
| C | -2.57516800 | -1.90988600 | -0.39587700 | C | 4.68617700 | 0.00445600 | -1.11057100 |
| C | -1.94871500 | -0.51066800 | -0.60923700 | C | 2.72250100 | 1.22483400 | -1.81490900 |
| O | -2.51037200 | 0.41109700 | -1.14375700 | C | 3.46861400 | 1.85535300 | -2.81496200 |
| H | 0.30561200 | -0.22299000 | -1.65252100 | C | 4.82545700 | 1.56069500 | -2.96546300 |
| C | -1.60106000 | -2.86679900 | -1.14946000 | C | 5.43062500 | 0.63114400 | -2.11161700 |
| H | -1.88203100 | -2.90467900 | -2.21192500 | H | 2.47543100 | -0.13466200 | 2.76091500 |
| H | -1.71314100 | -3.88574600 | -0.75072200 | H | 2.48857800 | 2.39805700 | 1.04033400 |
| C | -2.43483800 | -2.01674400 | 1.14184100 | H | 2.75468400 | 2.42209400 | 2.77473500 |
| H | -2.66079300 | -3.04176600 | 1.48131900 | H | 0.50901700 | 3.01785100 | 2.45108200 |
| H | -3.16389800 | -1.34293600 | 1.60952700 | H | -2.25316100 | 0.33008800 | 2.75539300 |
| C | -0.14671700 | -2.39182400 | -1.03428200 | H | -4.49072400 | 0.98011500 | 3.54814200 |
| C | 0.27562400 | -1.30742600 | -2.01905900 | H | -5.58626400 | 3.04679000 | 2.66574100 |
| H | 0.57906100 | -3.20672800 | -1.07818300 | H | -4.38768600 | 4.45074500 | 0.98388400 |
| H | 1.28928100 | -1.47240500 | -2.40218700 | H | -2.14805700 | 3.80191800 | 0.18723600 |
| H | -0.43655800 | -1.22810500 | -2.85324800 | H | -0.97903800 | 1.73427000 | -2.00349600 |
| C | -1.01365200 | -1.63711400 | 1.51870700 | H | 1.05300500 | 4.18099400 | 0.91931100 |
| C | -0.03821800 | -2.53317300 | 0.99798900 | H | 1.55926700 | 5.83835300 | -0.81633200 |
| H | -0.83536800 | -1.17882400 | 2.49242600 | H | 0.81151500 | 5.47620600 | -3.17086500 |
| H | 0.96597700 | -2.51620900 | 1.41076000 | H | -0.47847800 | 3.41525200 | -3.74925900 |
| H | -0.35680400 | -3.55550600 | 0.78824300 | H | 3.11730600 | -2.46038600 | -1.56891300 |
| P | 2.32778000 | -0.45864700 | 0.40607500 | H | 3.97909500 | -4.76989100 | -1.40062200 |
| C | 2.87703600 | 0.46535600 | 1.93071800 | H | 4.47577200 | -5.76724700 | 0.83501500 |
| C | 2.24412500 | 1.86463100 | 1.97168000 | H | 4.09119100 | -4.41812500 | 2.90011400 |
| C | 0.73913600 | 1.95482400 | 2.28177400 | H | 3.21326000 | -2.12166100 | 2.74312600 |
| P | -0.35222900 | 1.50092000 | 0.82902800 | H | 5.17318000 | -0.72040500 | -0.45825900 |
| C | -2.02625600 | 2.01654800 | 1.41440200 | H | 1.66784700 | 1.46327500 | -1.71279300 |
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| C | -4.59035600 | 2.76031900 | 2.31892400 | H | 6.49094000 | 0.39186500 | -2.22463800 |
| C | -3.91931800 | 3.54533600 | 1.37791900 | C | 0.37884800 | 1.20797100 | 3.56777000 |
| C | -2.64740000 | 3.17786200 | 0.92821400 | H | -0.62767200 | 1.46354300 | 3.92202900 |
| C | 0.02830500 | 2.80718100 | -0.42099500 | H | 0.43431300 | 0.11721800 | 3.45068300 |
| C | -0.40747300 | 2.62382200 | -1.74502900 | H | 1.09122600 | 1.49470700 | 4.35828100 |
| C | 0.72374200 | 3.98373100 | -0.09981700 | C | 4.39455100 | 0.57191400 | 2.09161500 |
| C | 1.00685400 | 4.93463900 | -1.08501400 | H | 4.82548400 | 1.25910900 | 1.34841700 |
| C | 0.58599700 | 4.73351900 | -2.40173000 | H | 4.62427000 | 0.97405600 | 3.09168200 |
| C | -0.13263600 | 3.57855200 | -2.72565900 | H | 4.90106700 | -0.39813700 | 1.99424500 |
| C | 3.11082600 | -2.11346400 | 0.57189300 | Co | -0.12495000 | -0.58592300 | 0.03368100 |
| C | 3.32488600 | -2.88400100 | -0.58498000 | | | | |
| C | 3.81429400 | -4.18806200 | -0.49044800 | 10 _s | | | |
| C | 4.09278100 | -4.74655100 | 0.76150400 | C | -3.71673500 | -1.84989200 | -0.69578400 |
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| C | 3.38685100 | -2.68520400 | 1.82541400 | C | -5.67772500 | -1.52659200 | -2.11283900 |

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|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | -6.51585900 | -1.56013000 | -0.99322600 | C | -0.36413400 | 3.81042100 | -2.28988100 |
| C | -5.95480900 | -1.74757700 | 0.27216800 | C | 3.43741300 | -1.68781600 | 0.53730000 |
| C | -4.57139400 | -1.88825700 | 0.41789300 | C | 3.95294300 | -2.21587800 | -0.65990900 |
| H | -3.65756100 | -1.64075000 | -2.84759200 | C | 4.58103300 | -3.46256000 | -0.67225200 |
| H | -6.10200100 | -1.38316000 | -3.11027000 | C | 4.70085600 | -4.20196700 | 0.50935000 |
| H | -7.59644100 | -1.44243700 | -1.10781600 | C | 4.19219500 | -3.68345400 | 1.70337700 |
| H | -6.59479700 | -1.77508900 | 1.15792200 | C | 3.56241600 | -2.43550700 | 1.71937000 |
| H | -4.16242200 | -2.01554800 | 1.41999600 | C | 3.37471600 | 0.91021100 | -0.71223300 |
| C | -2.21151900 | -1.98059600 | -0.54247500 | C | 4.77601400 | 1.01363500 | -0.75732400 |
| C | -1.42483700 | -0.80778700 | -1.18187200 | C | 2.60343500 | 1.63716000 | -1.62899700 |
| O | -1.72237000 | -0.29510400 | -2.24123700 | C | 3.21003700 | 2.48073900 | -2.56315000 |
| H | 0.71193800 | -1.51321100 | -1.94381900 | C | 4.60281700 | 2.58979200 | -2.59446300 |
| C | -1.68445000 | -3.25038200 | -1.28624400 | C | 5.38295100 | 1.85103000 | -1.69520100 |
| H | -2.01841100 | -3.22991200 | -2.33450200 | H | 2.40634800 | -0.17017000 | 2.84646100 |
| H | -2.17308200 | -4.11308800 | -0.80578800 | H | 1.85534500 | 2.55374600 | 1.56894200 |
| C | -1.70739100 | -2.03443700 | 0.90508600 | H | 1.97998300 | 2.29549500 | 3.30080500 |
| H | -2.03011900 | -2.97303700 | 1.38959600 | H | -0.30365900 | 2.36242300 | 2.87455400 |
| H | -2.13009700 | -1.21031500 | 1.49387400 | H | -2.39320900 | 1.45736700 | 3.33466500 |
| C | -0.15551700 | -3.44502000 | -1.22538500 | H | -4.80427300 | 1.76486100 | 3.60615000 |
| C | 0.63817100 | -2.59295000 | -2.21569600 | H | -6.30529100 | 1.86811400 | 1.61217000 |
| H | 0.03693400 | -4.49340200 | -1.50720000 | H | -5.32177700 | 1.66076800 | -0.67716800 |
| H | 1.67826900 | -2.94150600 | -2.28196500 | H | -2.91166600 | 1.33469700 | -0.96521100 |
| H | 0.19335700 | -2.59059600 | -3.22230100 | H | -0.74461700 | 1.70815900 | -2.01229400 |
| C | -0.19434200 | -1.94925200 | 0.83879300 | H | -0.00321900 | 4.02127100 | 1.57422100 |
| C | 0.37152700 | -3.22047500 | 0.19778800 | H | 0.28703700 | 6.04405000 | 0.20355800 |
| H | 0.26606900 | -1.78608700 | 1.82059200 | H | 0.05934800 | 5.93284900 | -2.27896600 |
| H | 1.46820400 | -3.22371300 | 0.19145400 | H | -0.47545500 | 3.75278100 | -3.37521600 |
| H | 0.06374100 | -4.06478600 | 0.84407000 | H | 3.85804800 | -1.65466100 | -1.59121900 |
| P | 2.46173600 | -0.14038700 | 0.47324400 | H | 4.97537700 | -3.85929200 | -1.61098100 |
| C | 2.67474600 | 0.63771400 | 2.15255000 | H | 5.18977500 | -5.17907700 | 0.49873500 |
| C | 1.69509400 | 1.80259300 | 2.35644400 | H | 4.28183100 | -4.25333400 | 2.63140800 |
| C | 0.19559600 | 1.45695400 | 2.49551900 | H | 3.15874400 | -2.05985700 | 2.66052800 |
| P | -0.63889500 | 1.17107600 | 0.85740400 | H | 5.39325500 | 0.43204800 | -0.07136700 |
| C | -2.45654400 | 1.33567500 | 1.16042000 | H | 1.51865700 | 1.54406000 | -1.59485800 |
| C | -3.01405000 | 1.47560200 | 2.44180900 | H | 2.59284000 | 3.04722600 | -3.26455400 |
| C | -4.39126600 | 1.66176400 | 2.59981000 | H | 5.08526000 | 3.24481300 | -3.32422300 |
| C | -5.22958000 | 1.72534400 | 1.48510100 | H | 6.47261100 | 1.92805600 | -1.72644300 |
| C | -4.68031000 | 1.61048400 | 0.20518700 | C | -0.03293800 | 0.33312600 | 3.51394500 |
| C | -3.30913900 | 1.41657700 | 0.04384000 | H | -1.08682400 | 0.05096800 | 3.61903500 |
| C | -0.37077100 | 2.70927600 | -0.12203000 | H | 0.51784900 | -0.57719700 | 3.25387400 |
| C | -0.51361100 | 2.65459300 | -1.51995300 | H | 0.32756200 | 0.66960500 | 4.49894600 |
| C | -0.09386500 | 3.94142200 | 0.49067200 | C | 4.10893000 | 1.06857700 | 2.45774200 |
| C | 0.06406600 | 5.09263800 | -0.28536500 | H | 4.41014600 | 1.93084400 | 1.84435300 |
| C | -0.06630900 | 5.03029100 | -1.67608100 | H | 4.18221200 | 1.36771500 | 3.51602000 |

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|-----------------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | 4.82844000 | 0.25458000 | 2.28688000 | C | -4.69261500 | 1.59392200 | 0.25582800 |
| Co | 0.24095600 | -0.45699000 | -0.33588900 | C | -3.32153500 | 1.40370500 | 0.07264700 |
| | | | | C | -0.25969100 | 3.00970800 | -0.29902800 |
| 10 _T | | | | C | -0.47094300 | 2.88191400 | -1.68269100 |
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| C | -4.36418900 | -1.85965900 | -1.79323700 | C | 0.38344300 | 5.32521600 | -0.63082800 |
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| C | -4.50475700 | -2.04483500 | 0.60556200 | C | 3.93749500 | -2.29319700 | -0.45503300 |
| H | -3.77590400 | -1.84894600 | -2.71061500 | C | 4.52577800 | -3.55855600 | -0.40253300 |
| H | -6.22284300 | -1.51255200 | -2.83241100 | C | 4.54999800 | -4.27441600 | 0.79911200 |
| H | -7.59788400 | -1.51051200 | -0.74524000 | C | 3.98402400 | -3.71593100 | 1.94898800 |
| H | -6.47706400 | -1.85820100 | 1.46079100 | C | 3.39510800 | -2.44917500 | 1.90136100 |
| H | -4.04109600 | -2.18520700 | 1.58203300 | C | 3.32598900 | 0.81198200 | -0.70489200 |
| C | -2.21114300 | -2.23330500 | -0.49714300 | C | 4.72105600 | 0.98979100 | -0.71374800 |
| C | -1.43976200 | -1.06153400 | -1.14909700 | C | 2.55396900 | 1.39979700 | -1.71858300 |
| O | -1.73669100 | -0.52379100 | -2.18959600 | C | 3.15301200 | 2.18488800 | -2.70727700 |
| H | 0.74891300 | -2.04616300 | -2.22660900 | C | 4.53720500 | 2.37488200 | -2.69715800 |
| C | -1.77652000 | -3.51199600 | -1.28344100 | C | 5.31941400 | 1.76966900 | -1.70520900 |
| H | -2.17381100 | -3.46505900 | -2.30844800 | H | 2.28089900 | -0.02773500 | 2.91932700 |
| H | -2.28633600 | -4.35067000 | -0.78224900 | H | 2.02158300 | 2.64690900 | 1.44549200 |
| C | -1.61031000 | -2.29558800 | 0.90997900 | H | 2.07020100 | 2.49427400 | 3.19280500 |
| H | -1.95046900 | -3.20426700 | 1.43958200 | H | -0.15765700 | 2.73304200 | 2.77956800 |
| H | -1.93928800 | -1.42891300 | 1.50412000 | H | -2.21517400 | 2.65356400 | 3.05436500 |
| C | -0.25958800 | -3.80491500 | -1.32519400 | H | -4.63273500 | 2.95499100 | 3.38063000 |
| C | 0.51139500 | -3.09868900 | -2.44990700 | H | -6.24562600 | 2.28030900 | 1.59846700 |
| H | -0.17854500 | -4.88340900 | -1.54062400 | H | -5.38561400 | 1.29787200 | -0.53452200 |
| H | 1.47660000 | -3.60380600 | -2.61540900 | H | -2.96769300 | 0.97768400 | -0.86400600 |
| H | -0.04735900 | -3.11519300 | -3.39920900 | H | -0.79731300 | 1.92429500 | -2.09658700 |
| C | -0.09779800 | -2.29910000 | 0.74695400 | H | 0.30828400 | 4.37088600 | 1.29784300 |
| C | 0.39264100 | -3.55789700 | 0.04767400 | H | 0.71707800 | 6.27965700 | -0.21626700 |
| H | 0.43376200 | -2.14762500 | 1.69915400 | H | 0.35717800 | 6.04033400 | -2.67223000 |
| H | 1.48736500 | -3.55310500 | -0.05406000 | H | -0.42251200 | 3.85954900 | -3.60585600 |
| H | 0.15297900 | -4.40920700 | 0.71531000 | H | 3.91238300 | -1.75082900 | -1.40222500 |
| P | 2.43428400 | -0.16192800 | 0.55906400 | H | 4.96396200 | -3.98836800 | -1.30664500 |
| C | 2.64547000 | 0.70904900 | 2.18869000 | H | 5.00833100 | -5.26550000 | 0.83861100 |
| C | 1.76539800 | 1.96782700 | 2.27332000 | H | 3.99788200 | -4.26894300 | 2.89133900 |
| C | 0.23396400 | 1.78576300 | 2.37931600 | H | 2.94885300 | -2.03474200 | 2.80686800 |
| P | -0.60628700 | 1.54023400 | 0.74041600 | H | 5.34142000 | 0.50875900 | 0.04337500 |
| C | -2.40687600 | 1.76379100 | 1.07690900 | H | 1.47573600 | 1.23759500 | -1.73056500 |
| C | -2.89491700 | 2.33557100 | 2.26377500 | H | 2.53593400 | 2.64469300 | -3.48264600 |
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| C | -5.17205500 | 2.14192200 | 1.44882600 | H | 6.40359300 | 1.90637200 | -1.70525300 |

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|------------------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | -0.16122600 | 0.65059200 | 3.33258400 | C | -2.10817500 | 1.74036200 | -2.32564200 |
| H | -1.24018200 | 0.64071700 | 3.53652800 | C | -0.58122900 | 1.89024500 | -2.45905400 |
| H | 0.10759100 | -0.33497800 | 2.92591200 | P | 0.35100200 | 1.57071100 | -0.87747900 |
| H | 0.36115800 | 0.77507000 | 4.29456600 | C | 2.08200900 | 1.91036600 | -1.38937400 |
| C | 4.09789500 | 1.04472300 | 2.53079400 | C | 2.88439300 | 0.84479700 | -1.82748400 |
| H | 4.48174300 | 1.85574600 | 1.89451600 | C | 4.19578100 | 1.07147800 | -2.24545400 |
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| H | 4.76138700 | 0.17464700 | 2.42110900 | C | 3.92303700 | 3.43600100 | -1.80275300 |
| Co | 0.20347800 | -0.54164200 | -0.22014900 | C | 2.60768400 | 3.20918900 | -1.38340100 |
| | | | | C | -0.07521200 | 2.95179900 | 0.25298400 |
| TS9 _s | | | | C | 0.37923300 | 2.87533400 | 1.58185900 |
| C | 3.80600100 | -2.03351800 | 0.80332600 | C | -0.85390700 | 4.05110200 | -0.13970000 |
| C | 4.73772100 | -1.27480700 | 1.53792300 | C | -1.19368000 | 5.04142700 | 0.78836500 |
| C | 6.10118300 | -1.32242300 | 1.24111800 | C | -0.75321100 | 4.95049300 | 2.11083000 |
| C | 6.57263200 | -2.13374200 | 0.20352900 | C | 0.04328100 | 3.86833900 | 2.50241500 |
| C | 5.66196400 | -2.89737900 | -0.53023300 | C | -2.93131200 | -2.22136400 | -0.89367000 |
| C | 4.29564500 | -2.84678400 | -0.23321100 | C | -3.54655100 | -2.90536900 | 0.16802600 |
| H | 4.39090100 | -0.62155100 | 2.33725000 | C | -3.94699000 | -4.23591300 | 0.01676200 |
| H | 6.80094800 | -0.71882800 | 1.82523600 | C | -3.73647600 | -4.90232400 | -1.19363900 |
| H | 7.64002000 | -2.17121000 | -0.02837500 | C | -3.11555900 | -4.23194500 | -2.25284500 |
| H | 6.01248900 | -3.54053200 | -1.34177100 | C | -2.71050500 | -2.90388300 | -2.10365600 |
| H | 3.61251900 | -3.45340800 | -0.82765400 | C | -3.33249200 | 0.26686500 | 0.56676600 |
| C | 2.32208300 | -1.91989900 | 1.09567800 | C | -4.72665400 | 0.07563400 | 0.58891700 |
| C | 1.80429400 | -0.47330000 | 0.79638300 | C | -2.75288600 | 1.12785500 | 1.51211500 |
| O | 2.41886100 | 0.48890300 | 1.19712100 | C | -3.54328900 | 1.79567600 | 2.45150400 |
| H | 0.70305500 | 0.30206700 | 3.33017200 | C | -4.92667800 | 1.60174400 | 2.46370400 |
| C | 1.98426200 | -2.13078000 | 2.59681400 | C | -5.51479200 | 0.73808200 | 1.53228200 |
| H | 2.62993800 | -1.49587200 | 3.21696200 | H | -2.13694500 | -0.29378800 | -3.04082300 |
| H | 2.22839100 | -3.17617700 | 2.84000500 | H | -2.48735100 | 2.30089100 | -1.45696400 |
| C | 1.43269000 | -2.86368100 | 0.28354200 | H | -2.54467000 | 2.23205700 | -3.21116300 |
| H | 1.62894100 | -3.92113400 | 0.53905600 | H | -0.37301400 | 2.94462500 | -2.69938800 |
| H | 1.63312600 | -2.76768700 | -0.79815700 | H | 2.48728300 | -0.17322400 | -1.82449000 |
| C | 0.49642700 | -1.83636800 | 2.93787200 | H | 4.81427000 | 0.23087200 | -2.56939400 |
| C | 0.30575000 | -0.60060800 | 3.81795700 | H | 5.74961600 | 2.54822800 | -2.54805500 |
| H | 0.10780300 | -2.70215300 | 3.50009600 | H | 4.32763500 | 4.45112000 | -1.78774600 |
| H | -0.76171900 | -0.42810700 | 4.03043800 | H | 1.99635400 | 4.04734300 | -1.04234700 |
| H | 0.82917200 | -0.72282500 | 4.77876800 | H | 1.00833000 | 2.03744800 | 1.88113000 |
| C | -0.00038200 | -2.49408200 | 0.52279700 | H | -1.20528900 | 4.15357600 | -1.16599000 |
| C | -0.39307100 | -1.81287200 | 1.69833000 | H | -1.80726000 | 5.88794300 | 0.47074000 |
| H | -0.75365000 | -3.00326300 | -0.07887300 | H | -1.02533000 | 5.72297900 | 2.83420300 |
| H | -0.40290600 | -0.34953000 | 1.41010700 | H | 0.40228800 | 3.79396700 | 3.53187200 |
| H | -1.46366400 | -1.82067700 | 1.93422200 | H | -3.71391600 | -2.40151700 | 1.12098500 |
| P | -2.24786000 | -0.53391400 | -0.67992500 | H | -4.42692500 | -4.75238700 | 0.85164300 |
| C | -2.66678600 | 0.31086600 | -2.29052900 | H | -4.05245600 | -5.94165300 | -1.31149800 |

| | | | | | | | |
|-----------------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | -2.94294600 | -4.74542900 | -3.20192400 | C | -0.08001500 | -2.69335800 | -0.26006000 |
| H | -2.21336800 | -2.40357000 | -2.93705000 | C | 0.37875500 | -2.37652100 | -1.50622800 |
| H | -5.20180000 | -0.59998200 | -0.12247800 | H | 0.62973700 | -2.97143900 | 0.52206700 |
| H | -1.67618200 | 1.28208800 | 1.51390500 | H | 0.40417800 | 0.11228200 | -1.25965800 |
| H | -3.07065800 | 2.46506000 | 3.17421100 | H | 1.45638300 | -2.33921500 | -1.68395600 |
| H | -5.54789000 | 2.11806800 | 3.19980000 | P | 2.27814000 | -0.46169000 | 0.63427400 |
| H | -6.59569500 | 0.57767700 | 1.53999400 | C | 2.59889000 | 0.32383200 | 2.29930800 |
| C | -0.00842100 | 1.02749100 | -3.59019500 | C | 1.96810300 | 1.72108700 | 2.37450300 |
| H | 1.01549000 | 1.32804600 | -3.84889200 | C | 0.43128400 | 1.79339000 | 2.43176700 |
| H | 0.01034100 | -0.04323300 | -3.33003900 | P | -0.40824000 | 1.51840000 | 0.79314000 |
| H | -0.63182000 | 1.14181800 | -4.49149600 | C | -2.17273200 | 1.80269700 | 1.21597100 |
| C | -4.15637500 | 0.30580800 | -2.63406500 | C | -2.97127200 | 0.71437600 | 1.60104800 |
| H | -4.72239300 | 0.98581400 | -1.98029300 | C | -4.30690300 | 0.90768300 | 1.95435900 |
| H | -4.29040900 | 0.65385100 | -3.67118500 | C | -4.85812600 | 2.19358500 | 1.92814800 |
| H | -4.59797600 | -0.69790600 | -2.55531900 | C | -4.06615600 | 3.28237900 | 1.55229800 |
| Co | 0.03834600 | -0.52744100 | 0.01916400 | C | -2.72700400 | 3.08996000 | 1.19665100 |
| | | | | C | 0.03786100 | 2.94041100 | -0.27135400 |
| | | | | C | -0.34002700 | 2.89430300 | -1.62529200 |
| 11 _s | | | | C | 0.74020200 | 4.05664300 | 0.20728000 |
| C | -3.82815500 | -1.92415200 | -0.69837100 | C | 1.08429500 | 5.09711600 | -0.66200200 |
| C | -4.68564400 | -1.22585300 | -1.56996200 | C | 0.72247500 | 5.03812400 | -2.00984400 |
| C | -6.05600500 | -1.13786100 | -1.31739300 | C | 0.00059200 | 3.93784600 | -2.48656100 |
| C | -6.61008400 | -1.75531200 | -0.19111800 | C | 3.00254900 | -2.14005200 | 0.80243700 |
| C | -5.77432300 | -2.46080200 | 0.67751000 | C | 3.61801400 | -2.77332600 | -0.29096600 |
| C | -4.40021600 | -2.54113300 | 0.42720400 | C | 4.05796000 | -4.09601900 | -0.19174700 |
| H | -4.27150000 | -0.72515900 | -2.44364600 | C | 3.88912800 | -4.80713100 | 0.99943700 |
| H | -6.69625500 | -0.58223000 | -2.00775400 | C | 3.27366300 | -4.18759500 | 2.09177800 |
| H | -7.68312300 | -1.68848100 | 0.00529100 | C | 2.82897300 | -2.86703700 | 1.99447600 |
| H | -6.18958800 | -2.95261900 | 1.56106300 | C | 3.41362400 | 0.41158600 | -0.51628000 |
| H | -3.77729900 | -3.09156700 | 1.13204700 | C | 4.80781000 | 0.22285500 | -0.46386100 |
| C | -2.33279400 | -1.96046300 | -0.95837900 | C | 2.89136000 | 1.32737200 | -1.44253200 |
| C | -1.71592400 | -0.51332200 | -0.90850200 | C | 3.73760000 | 2.05213500 | -2.28697800 |
| O | -2.26848200 | 0.39196800 | -1.49382400 | C | 5.11980400 | 1.86259700 | -2.22294900 |
| H | -0.46137500 | -0.24290100 | -3.30226700 | C | 5.65146800 | 0.94246200 | -1.31197200 |
| C | -1.99690300 | -2.47611600 | -2.38388000 | H | 2.06929900 | -0.33926600 | 2.99797600 |
| H | -2.58797500 | -1.92866600 | -3.12964100 | H | 2.36363100 | 2.34384600 | 1.55744500 |
| H | -2.31419700 | -3.52946700 | -2.42952600 | H | 2.33210000 | 2.18572500 | 3.30616400 |
| C | -1.54541500 | -2.80603600 | 0.04782000 | H | 0.15985800 | 2.82522400 | 2.70598500 |
| H | -1.86812400 | -3.86145400 | 0.02565000 | H | -2.55450600 | -0.29481200 | 1.61076300 |
| H | -1.71542700 | -2.45225600 | 1.07875600 | H | -4.92099200 | 0.04912000 | 2.23459800 |
| C | -0.49097100 | -2.36140300 | -2.73519300 | H | -5.90679100 | 2.34497300 | 2.19571600 |
| C | -0.15436000 | -1.21916600 | -3.70164900 | H | -4.49208500 | 4.28847400 | 1.52799900 |
| H | -0.20327300 | -3.29531900 | -3.25334000 | H | -2.11924800 | 3.94585900 | 0.89654300 |
| H | 0.92956000 | -1.17881500 | -3.89616000 | H | -0.91538700 | 2.04217900 | -1.98920900 |
| H | -0.66774700 | -1.37039100 | -4.66391700 | | | | |

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|-------------------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | 1.02652300 | 4.13413800 | 1.25566700 | H | 1.89647800 | -3.84782200 | -0.18510100 |
| H | 1.63826200 | 5.95718600 | -0.27833300 | H | 1.91759500 | -2.41351800 | -1.22144600 |
| H | 0.99676800 | 5.85055600 | -2.68715800 | C | 0.28794500 | -2.53530600 | 2.44645500 |
| H | -0.29724700 | 3.89013300 | -3.53683800 | C | -0.18572600 | -1.50612300 | 3.48021000 |
| H | 3.76051000 | -2.23328600 | -1.22846300 | H | -0.00335300 | -3.52547100 | 2.84316600 |
| H | 4.53613300 | -4.57047100 | -1.05217100 | H | -1.28344100 | -1.51206600 | 3.57124500 |
| H | 4.23494300 | -5.84071800 | 1.07681400 | H | 0.24223300 | -1.73217200 | 4.46914900 |
| H | 3.13600800 | -4.73481100 | 3.02755200 | C | 0.12995700 | -2.62152200 | -0.08234700 |
| H | 2.33849500 | -2.41085700 | 2.85639000 | C | -0.46064500 | -2.44672400 | 1.14166300 |
| H | 5.24059100 | -0.49527200 | 0.23258600 | H | -0.49266700 | -2.82019000 | -0.95908900 |
| H | 1.81702200 | 1.48112400 | -1.50854100 | H | 0.57750500 | -0.21326700 | 1.28736100 |
| H | 3.30824000 | 2.76273500 | -2.99721200 | H | -1.54855800 | -2.46686500 | 1.22460100 |
| H | 5.78377200 | 2.42517400 | -2.88402400 | P | -2.29318600 | -0.40371700 | -0.63297700 |
| H | 6.73132900 | 0.78302700 | -1.26050000 | C | -2.82710800 | 0.58880700 | -2.12025700 |
| C | -0.15937500 | 0.85171200 | 3.48743300 | C | -2.19139500 | 1.98375600 | -2.11132900 |
| H | -1.20738100 | 1.09502000 | 3.70649000 | C | -0.67042900 | 2.04862000 | -2.33518300 |
| H | -0.11636700 | -0.20371200 | 3.17465500 | P | 0.33053300 | 1.61255900 | -0.82516100 |
| H | 0.41171800 | 0.94663600 | 4.42474500 | C | 2.03804600 | 1.88927700 | -1.44542200 |
| C | 4.07126200 | 0.37262000 | 2.70501900 | C | 2.74929800 | 0.81228500 | -1.99801900 |
| H | 4.62915700 | 1.10654900 | 2.10491000 | C | 4.02659400 | 1.00594700 | -2.52438100 |
| H | 4.14705800 | 0.67924100 | 3.76100600 | C | 4.60784500 | 2.27906400 | -2.50111400 |
| H | 4.56416300 | -0.60460900 | 2.60174600 | C | 3.90311800 | 3.35523300 | -1.95418900 |
| Co | 0.00371100 | -0.49564700 | -0.05322800 | C | 2.62086200 | 3.16318200 | -1.42864000 |
| | | | | C | 0.04601600 | 2.96703800 | 0.37918400 |
| | | | | C | 0.57032400 | 2.81618500 | 1.67592300 |
| TS10 _s | | | | C | -0.68889800 | 4.12200300 | 0.07158900 |
| C | 3.83819600 | -2.05112600 | 0.79367800 | C | -0.91353400 | 5.09707600 | 1.04917600 |
| C | 4.62827100 | -1.49502400 | 1.81644100 | C | -0.40065800 | 4.93449700 | 2.33804800 |
| C | 6.02187500 | -1.50910900 | 1.74227900 | C | 0.35013200 | 3.79434900 | 2.64612300 |
| C | 6.66476500 | -2.08038500 | 0.63863100 | C | -3.06390000 | -2.03886300 | -0.95368800 |
| C | 5.89507900 | -2.63512800 | -0.38547900 | C | -3.75520300 | -2.75299100 | 0.03795800 |
| C | 4.49757200 | -2.61924600 | -0.30770100 | C | -4.25692400 | -4.03078000 | -0.22721800 |
| H | 4.15003300 | -1.03313600 | 2.68027800 | C | -4.07334800 | -4.61311300 | -1.48371600 |
| H | 6.60992700 | -1.06801300 | 2.55138700 | C | -3.37740700 | -3.91332600 | -2.47522600 |
| H | 7.75604000 | -2.09209500 | 0.57931700 | C | -2.87088600 | -2.63924200 | -2.21161900 |
| H | 6.38004500 | -3.08720100 | -1.25461000 | C | -3.19821400 | 0.31443800 | 0.79158300 |
| H | 3.92850400 | -3.05843600 | -1.12672900 | C | -4.59902800 | 0.26723500 | 0.91485100 |
| C | 2.31874700 | -1.99770500 | 0.88544000 | C | -2.44990900 | 0.96987700 | 1.78249000 |
| C | 1.83632200 | -0.52171900 | 0.77750600 | C | -3.08277500 | 1.58889300 | 2.86295800 |
| O | 2.58043000 | 0.41091100 | 1.00414300 | C | -4.47491500 | 1.54609200 | 2.97296900 |
| H | 0.12127300 | -0.48399800 | 3.20818800 | C | -5.22940800 | 0.87928300 | 2.00053500 |
| C | 1.82476100 | -2.55458700 | 2.25248400 | H | -2.41365300 | 0.01570000 | -2.96324400 |
| H | 2.29976700 | -2.00115500 | 3.07350900 | H | -2.47823100 | 2.50843900 | -1.18657700 |
| H | 2.19414300 | -3.58941200 | 2.31145700 | H | -2.65455300 | 2.55281000 | -2.93484700 |
| C | 1.61269200 | -2.78130100 | -0.23057200 | | | | |

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|-----------------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | -0.40949300 | 3.09794600 | -2.54442700 | C | -2.39562000 | -0.10031400 | -0.93430000 |
| H | 2.30719700 | -0.18634500 | -2.00435500 | O | -3.09892600 | 0.84515000 | -1.14764300 |
| H | 4.57432900 | 0.15837000 | -2.94353900 | H | -0.59494800 | -0.03270800 | -2.96236600 |
| H | 5.61185700 | 2.43005300 | -2.90547100 | C | -2.23492800 | -2.25412500 | -2.13266000 |
| H | 4.35307700 | 4.35092700 | -1.93168600 | H | -2.77319300 | -1.86571000 | -3.00794100 |
| H | 2.08007700 | 4.00903600 | -0.99922900 | H | -2.51993000 | -3.31156200 | -2.02372000 |
| H | 1.16700200 | 1.93580600 | 1.91580400 | C | -2.00194600 | -2.20171200 | 0.35245000 |
| H | -1.09242000 | 4.27952500 | -0.92813700 | H | -2.35213000 | -3.24600900 | 0.43347000 |
| H | -1.49255200 | 5.98856500 | 0.79626700 | H | -2.27561500 | -1.71708200 | 1.29959200 |
| H | -0.58058000 | 5.69629400 | 3.10050600 | C | -0.71309400 | -2.15756000 | -2.37496700 |
| H | 0.76451300 | 3.66383900 | 3.64877200 | C | -0.30863800 | -1.02879500 | -3.33482600 |
| H | -3.90682100 | -2.31618500 | 1.02581500 | H | -0.43725300 | -3.09579200 | -2.88804800 |
| H | -4.79458300 | -4.57075500 | 0.55596600 | H | 0.78290500 | -1.02092800 | -3.48357900 |
| H | -4.46799200 | -5.61087900 | -1.69022500 | H | -0.78556800 | -1.16445200 | -4.31890300 |
| H | -3.22376000 | -4.36243400 | -3.45944500 | C | -0.50192900 | -2.22033100 | 0.18796500 |
| H | -2.31702800 | -2.11520700 | -2.99409800 | C | 0.09156200 | -2.15844000 | -1.08294200 |
| H | -5.20219200 | -0.25640400 | 0.17365600 | H | 0.03340300 | -2.68553600 | 1.02092800 |
| H | -1.36428600 | 0.99333800 | 1.70009700 | H | -1.26895800 | 0.11250300 | -0.90801000 |
| H | -2.48222300 | 2.10105600 | 3.61845700 | H | 1.10551000 | -2.54343000 | -1.20567600 |
| H | -4.97423500 | 2.02640000 | 3.81813600 | P | 2.27904000 | -0.68717500 | 0.55433700 |
| H | -6.31779900 | 0.83497400 | 2.08713300 | C | 2.84512900 | 0.06805500 | 2.16551400 |
| C | -0.21913600 | 1.20332900 | -3.53173300 | C | 2.55537500 | 1.57609300 | 2.22395900 |
| H | 0.79792700 | 1.46593200 | -3.85071600 | C | 1.09331000 | 1.99445700 | 2.45006300 |
| H | -0.23282200 | 0.12498500 | -3.30635000 | P | 0.04334900 | 1.66142700 | 0.95360200 |
| H | -0.89610100 | 1.37774100 | -4.38327500 | C | -1.66065300 | 2.06876000 | 1.49893000 |
| C | -4.34108700 | 0.68474100 | -2.30874700 | C | -2.42870300 | 1.05737500 | 2.09680900 |
| H | -4.79853600 | 1.34905400 | -1.56109600 | C | -3.73636500 | 1.31081800 | 2.51211400 |
| H | -4.55389200 | 1.10862100 | -3.30357100 | C | -4.29123000 | 2.58221700 | 2.33211100 |
| H | -4.83274400 | -0.29708500 | -2.24899900 | C | -3.52848100 | 3.59746500 | 1.74611200 |
| Co | -0.03503500 | -0.46802000 | -0.02980100 | C | -2.21744400 | 3.34480100 | 1.33146000 |
| | | | | C | 0.43652600 | 2.97205400 | -0.26945500 |
| | | | | C | -0.28483400 | 2.96122300 | -1.47965100 |
| 12 _s | | | | C | 1.45727900 | 3.91759000 | -0.09749700 |
| C | -4.28000100 | -1.69633100 | -0.71370100 | C | 1.76449500 | 4.82137700 | -1.12083200 |
| C | -5.09978600 | -1.30210300 | -1.78584100 | C | 1.05224700 | 4.79702000 | -2.32168500 |
| C | -6.49026200 | -1.39025700 | -1.70115500 | C | 0.01826500 | 3.86886700 | -2.49443100 |
| C | -7.09582100 | -1.87331000 | -0.53636500 | C | 2.80667200 | -2.43734000 | 0.71201400 |
| C | -6.29440700 | -2.26188500 | 0.53870100 | C | 3.44043600 | -3.11972900 | -0.33874700 |
| C | -4.90039400 | -2.17286800 | 0.45102000 | C | 3.76475000 | -4.47331000 | -0.20989300 |
| H | -4.64989300 | -0.91222300 | -2.70005800 | C | 3.45575500 | -5.16261300 | 0.96589300 |
| H | -7.10390800 | -1.07745000 | -2.54987000 | C | 2.81436500 | -4.49317700 | 2.01312500 |
| H | -8.18431100 | -1.94375900 | -0.46828100 | C | 2.48762700 | -3.14124600 | 1.88688200 |
| H | -6.75187100 | -2.63925000 | 1.45682900 | C | 3.33234800 | 0.04052200 | -0.75678700 |
| H | -4.30513300 | -2.47910000 | 1.31051800 | C | 4.72590200 | -0.14246100 | -0.81010100 |
| C | -2.76223200 | -1.56452500 | -0.83032700 | | | | |

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|-----------------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | 2.71047900 | 0.83023800 | -1.73817000 | C | -5.37108000 | -1.80025400 | 0.55903000 |
| C | 3.46493900 | 1.44590700 | -2.74009400 | H | -4.63822100 | -1.97639000 | -2.75949200 |
| C | 4.85074100 | 1.27056400 | -2.77725000 | H | -7.09115000 | -2.08713000 | -2.90470200 |
| C | 5.47754900 | 0.47108800 | -1.81446600 | H | -8.48579300 | -2.00837900 | -0.83158600 |
| H | 2.22116400 | -0.44719200 | 2.91135000 | H | -7.36124200 | -1.81258900 | 1.39220000 |
| H | 2.97077500 | 2.05940100 | 1.32608500 | H | -4.91436400 | -1.70648300 | 1.54398900 |
| H | 3.12960200 | 1.98082600 | 3.07374800 | C | -3.04586100 | -1.74893600 | -0.51867700 |
| H | 1.07220000 | 3.08686600 | 2.59036300 | C | -2.65128900 | -0.33623700 | -0.95442600 |
| H | -1.99990500 | 0.06292900 | 2.22926200 | O | -3.16907300 | 0.29924300 | -1.84110500 |
| H | -4.32617300 | 0.51154700 | 2.96730500 | H | -0.34055400 | -0.70709700 | -2.05750100 |
| H | -5.31882100 | 2.78121200 | 2.64621200 | C | -2.36054600 | -2.76285000 | -1.48607600 |
| H | -3.95697400 | 4.59298500 | 1.60578600 | H | -2.70248300 | -2.59222200 | -2.51531700 |
| H | -1.63410700 | 4.14260100 | 0.86826300 | H | -2.72541700 | -3.75759100 | -1.18513800 |
| H | -1.10547700 | 2.25564600 | -1.62436300 | C | -2.51222300 | -2.01178200 | 0.90565400 |
| H | 2.02758400 | 3.96450200 | 0.83005000 | H | -3.01239400 | -2.91273300 | 1.30060500 |
| H | 2.56679200 | 5.54829500 | -0.97281800 | H | -2.80423300 | -1.19604100 | 1.58190900 |
| H | 1.29666600 | 5.50157400 | -3.12026000 | C | -0.81973900 | -2.77256900 | -1.46919400 |
| H | -0.55426600 | 3.85022200 | -3.42489700 | C | -0.17225400 | -1.73894300 | -2.40460300 |
| H | 3.68190400 | -2.59798400 | -1.26579100 | H | -0.51701000 | -3.76421600 | -1.84810800 |
| H | 4.26077700 | -4.98946000 | -1.03543900 | H | 0.91682800 | -1.88815700 | -2.44817600 |
| H | 3.71092900 | -6.22042400 | 1.06554100 | H | -0.57330100 | -1.82411200 | -3.42711800 |
| H | 2.56426600 | -5.02553900 | 2.93400000 | C | -1.02618800 | -2.25799600 | 0.99413300 |
| H | 1.97910300 | -2.63787300 | 2.71186800 | C | -0.26751400 | -2.66437000 | -0.06653400 |
| H | 5.22718300 | -0.77591800 | -0.07824500 | H | -0.61491500 | -2.34483100 | 2.00809900 |
| H | 1.63015000 | 0.97418000 | -1.71998600 | H | -1.78149200 | 0.10243000 | -0.40323400 |
| H | 2.96431500 | 2.06215400 | -3.49040600 | H | 0.73809700 | -3.05513200 | 0.10069400 |
| H | 5.44366400 | 1.75070100 | -3.55963800 | P | 2.47964400 | -0.59415900 | 0.49327000 |
| H | 6.55949300 | 0.32146800 | -1.84631800 | C | 3.27782500 | 0.51363500 | 1.77934400 |
| C | 0.48782300 | 1.34423800 | 3.69833700 | C | 2.84659700 | 1.98280200 | 1.61076100 |
| H | -0.45271900 | 1.83087100 | 3.98896300 | C | 1.41763700 | 2.38875100 | 2.03082300 |
| H | 0.28035400 | 0.27262600 | 3.55248300 | P | 0.11201200 | 1.84448400 | 0.81918400 |
| H | 1.19422900 | 1.43950500 | 4.53868400 | C | -1.44609000 | 2.50851600 | 1.52730400 |
| C | 4.31537800 | -0.19647100 | 2.50029300 | C | -2.30587900 | 1.61172600 | 2.17892200 |
| H | 4.98328000 | 0.41412400 | 1.87542100 | C | -3.50391900 | 2.05870000 | 2.74207500 |
| H | 4.49811400 | 0.08413500 | 3.55009600 | C | -3.85251300 | 3.41021200 | 2.65274000 |
| H | 4.59572300 | -1.25225300 | 2.38084700 | C | -2.99961300 | 4.31065600 | 2.00311800 |
| Co | 0.19235300 | -0.37204400 | -0.05765300 | C | -1.80108800 | 3.86367400 | 1.44085600 |
| | | | | C | 0.33245100 | 2.87902500 | -0.68222100 |
| 12 _T | | | | C | -0.51012000 | 2.61094000 | -1.77787200 |
| C | -4.57265800 | -1.85655700 | -0.59537000 | C | 1.31346300 | 3.87363700 | -0.80995200 |
| C | -5.22105700 | -1.95232900 | -1.83919600 | C | 1.46992100 | 4.56421400 | -2.01698500 |
| C | -6.61425700 | -2.00832400 | -1.92425700 | C | 0.64259500 | 4.27890200 | -3.10559800 |
| C | -7.39580200 | -1.96306300 | -0.76576000 | C | -0.35694600 | 3.30732700 | -2.97769700 |
| C | -6.76635100 | -1.85525500 | 0.47613700 | C | 3.12615200 | -2.26498700 | 0.88881100 |

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|----|-------------|-------------|-------------|--------------------|-------------|-------------|-------------|
| C | 3.39704400 | -3.19509100 | -0.13005700 | | | | |
| C | 3.73831800 | -4.51388300 | 0.18241600 | cat'' _D | | | |
| C | 3.80808800 | -4.92744700 | 1.51628000 | P | 1.60335900 | -0.47096800 | 0.08940000 |
| C | 3.52701800 | -4.01326400 | 2.53682300 | C | 1.30017400 | -0.86276100 | 1.89988800 |
| C | 3.18360900 | -2.69486000 | 2.22694700 | C | -0.08080600 | -0.39065000 | 2.40259100 |
| C | 3.29538800 | -0.13569300 | -1.08505100 | C | -1.35096700 | -1.00714100 | 1.78378000 |
| C | 4.64105200 | -0.42541200 | -1.37491700 | P | -1.64608200 | -0.47738200 | 0.00777200 |
| C | 2.53028500 | 0.55749700 | -2.03612800 | C | -3.36873600 | -1.10070100 | -0.26277300 |
| C | 3.09779300 | 0.97518300 | -3.24336100 | C | -3.52699100 | -2.18976600 | -1.13127800 |
| C | 4.43798400 | 0.69119200 | -3.51847900 | C | -4.79209200 | -2.73706000 | -1.36581200 |
| C | 5.20601800 | -0.01423400 | -2.58423400 | C | -5.91539900 | -2.18729900 | -0.73947300 |
| H | 2.87655200 | 0.13138700 | 2.73011700 | C | -5.76763200 | -1.09369000 | 0.12283500 |
| H | 3.05115400 | 2.29821700 | 0.57578500 | C | -4.50081300 | -0.55318300 | 0.36089200 |
| H | 3.52644000 | 2.58111600 | 2.24069400 | C | -1.86126100 | 1.34046200 | 0.06354300 |
| H | 1.38414000 | 3.49001600 | 2.04497700 | C | -1.62091500 | 2.03632500 | -1.13942500 |
| H | -2.02675300 | 0.55778400 | 2.23383600 | C | -2.18992900 | 2.08077600 | 1.21416800 |
| H | -4.16823600 | 1.35006000 | 3.24288100 | C | -2.28546100 | 3.47408800 | 1.15902400 |
| H | -4.79191300 | 3.76324300 | 3.08543700 | C | -2.05700000 | 4.15301200 | -0.04399700 |
| H | -3.27205400 | 5.36665200 | 1.93071300 | C | -1.71955400 | 3.42682900 | -1.19262200 |
| H | -1.14423000 | 4.57023600 | 0.92823600 | C | 3.31876100 | -1.11413500 | -0.15540000 |
| H | -1.30265700 | 1.86308100 | -1.70096900 | C | 4.47990800 | -0.35373100 | 0.05077100 |
| H | 1.96690400 | 4.12376700 | 0.02564100 | C | 5.74147900 | -0.91964600 | -0.16026500 |
| H | 2.24460400 | 5.33029400 | -2.10248700 | C | 5.85511900 | -2.25363400 | -0.56850300 |
| H | 0.77089100 | 4.81475200 | -4.04924900 | C | 4.70166500 | -3.01817000 | -0.77760700 |
| H | -1.01931500 | 3.08571000 | -3.81823900 | C | 3.44158100 | -2.44445900 | -0.58518200 |
| H | 3.33829800 | -2.89166900 | -1.17712600 | C | 1.79415400 | 1.33132000 | -0.13139300 |
| H | 3.94941300 | -5.22160500 | -0.62322500 | C | 1.53801400 | 2.32786100 | 0.82951700 |
| H | 4.07636700 | -5.95834900 | 1.75979400 | C | 2.06566600 | 1.74120100 | -1.46003800 |
| H | 3.57363300 | -4.32699900 | 3.58274500 | C | 2.10051500 | 3.09532300 | -1.80058800 |
| H | 2.95473500 | -2.00130500 | 3.03914300 | C | 1.85658500 | 4.07404700 | -0.83149900 |
| H | 5.24849000 | -0.98405500 | -0.66185100 | C | 1.57094500 | 3.68022900 | 0.48414200 |
| H | 1.48190200 | 0.76958900 | -1.83242600 | H | 1.29429100 | -1.96564500 | 1.87455700 |
| H | 2.48664100 | 1.51789600 | -3.96837300 | H | -0.14233400 | 0.70455300 | 2.34454500 |
| H | 4.88454600 | 1.01180200 | -4.46307800 | H | -0.11550300 | -0.63125800 | 3.47998400 |
| H | 6.25207400 | -0.24661600 | -2.79915300 | H | -2.20452700 | -0.63378300 | 2.37443700 |
| C | 1.04732900 | 1.88110000 | 3.42804600 | H | -2.63650200 | -2.60202700 | -1.62063700 |
| H | 0.13524400 | 2.36634800 | 3.80330200 | H | -4.90252400 | -3.58884300 | -2.04243100 |
| H | 0.87502000 | 0.79251100 | 3.43593600 | H | -6.90743200 | -2.60729100 | -0.92501600 |
| H | 1.86344200 | 2.09811400 | 4.13605500 | H | -6.64482000 | -0.66002300 | 0.61047700 |
| C | 4.80370500 | 0.41617300 | 1.82739200 | H | -4.39468100 | 0.30189400 | 1.03305600 |
| H | 5.26220400 | 0.89449100 | 0.94881300 | H | -1.34406400 | 1.46986300 | -2.03327600 |
| H | 5.17979000 | 0.93800300 | 2.72272900 | H | -2.37937100 | 1.57239400 | 2.16132200 |
| H | 5.15230600 | -0.62555700 | 1.87305500 | H | -2.54427700 | 4.03351100 | 2.06204900 |
| Co | 0.15452000 | -0.43311900 | 0.50020000 | H | -2.13189200 | 5.24249900 | -0.08361000 |

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|--------------------------|-------------|-------------|-------------|------------------------|-------------|-------------|-------------|
| H | -1.52334100 | 3.94865100 | -2.13279300 | C | 3.46926400 | -2.40909700 | -0.56582500 |
| H | 4.39766000 | 0.68528200 | 0.37865700 | C | 1.74818700 | 1.33397200 | -0.15186200 |
| H | 6.64050300 | -0.31768300 | -0.00281400 | C | 1.46901000 | 2.34639500 | 0.78806900 |
| H | 6.84223600 | -2.69471100 | -0.72986000 | C | 2.01903200 | 1.72371700 | -1.48724000 |
| H | 4.78447900 | -4.05868800 | -1.10311400 | C | 2.02685800 | 3.07071900 | -1.85539800 |
| H | 2.53026200 | -3.02039200 | -0.78369400 | C | 1.76143000 | 4.06465100 | -0.90719200 |
| H | 1.30386800 | 2.05912300 | 1.85838000 | C | 1.47790100 | 3.69095200 | 0.41503700 |
| H | 2.25308000 | 0.98351500 | -2.22623900 | H | 1.35218600 | -1.93131100 | 1.92343000 |
| H | 2.31636600 | 3.38732400 | -2.83208300 | H | -0.14727100 | 0.70359000 | 2.39746800 |
| H | 1.88079800 | 5.13364700 | -1.09739900 | H | -0.09867000 | -0.65095300 | 3.50898500 |
| H | 1.36795300 | 4.43391100 | 1.24927500 | H | -2.18482100 | -0.68335500 | 2.39429700 |
| C | -1.35727000 | -2.53754100 | 1.85010700 | H | -2.55881900 | -2.58975600 | -1.64253800 |
| H | -2.33847500 | -2.94901900 | 1.57006900 | H | -4.80508500 | -3.61884300 | -2.08108300 |
| H | -0.60963300 | -2.97054500 | 1.16656100 | H | -6.82927300 | -2.70045700 | -0.94508000 |
| H | -1.12667000 | -2.87994700 | 2.87310400 | H | -6.60667700 | -0.77653800 | 0.62582000 |
| C | 2.41449200 | -0.43159800 | 2.85736500 | H | -4.37619200 | 0.22403500 | 1.06596000 |
| H | 2.51619800 | 0.66235700 | 2.91333900 | H | -1.41105800 | 1.47242200 | -2.01656300 |
| H | 2.19537500 | -0.79562900 | 3.87550500 | H | -2.34802400 | 1.54987400 | 2.20147700 |
| H | 3.38851700 | -0.84452900 | 2.55930500 | H | -2.58658000 | 4.00551900 | 2.10450700 |
| Co | 0.00629300 | -1.20633700 | -1.28243900 | H | -2.26705100 | 5.22241500 | -0.05196000 |
| | | | | H | -1.67304200 | 3.94355400 | -2.11555000 |
| cat''_Q | | | | H | 4.37200200 | 0.74018000 | 0.38440600 |
| P | 1.59649200 | -0.46419200 | 0.10749200 | H | 6.63143400 | -0.22333000 | -0.00190700 |
| C | 1.32482900 | -0.82816300 | 1.92903600 | H | 6.87346100 | -2.59948600 | -0.71927600 |
| C | -0.06558700 | -0.39134400 | 2.43579700 | H | 4.83939400 | -4.00177300 | -1.08025700 |
| C | -1.31967000 | -1.02313100 | 1.80017900 | H | 2.56814700 | -3.00088000 | -0.76325800 |
| P | -1.61136400 | -0.47841300 | 0.02980000 | H | 1.23431700 | 2.09413800 | 1.82099300 |
| C | -3.32244200 | -1.13300700 | -0.25557900 | H | 2.22493800 | 0.95465900 | -2.23736700 |
| C | -3.45850300 | -2.20825500 | -1.14411800 | H | 2.24121900 | 3.34553300 | -2.89195900 |
| C | -4.71194300 | -2.77760700 | -1.38875800 | H | 1.76701000 | 5.11898700 | -1.19401700 |
| C | -5.84613400 | -2.26322900 | -0.75201600 | H | 1.25758900 | 4.45588500 | 1.16410200 |
| C | -5.72077700 | -1.18288600 | 0.13041700 | C | -1.28450300 | -2.55476000 | 1.82917900 |
| C | -4.46525200 | -0.62073600 | 0.37827500 | H | -2.25804400 | -2.98610600 | 1.55256700 |
| C | -1.87324500 | 1.33081100 | 0.09224800 | H | -0.53524900 | -2.94792500 | 1.12341100 |
| C | -1.68476300 | 2.03153000 | -1.11713400 | H | -1.02840300 | -2.91723500 | 2.83891700 |
| C | -2.19551100 | 2.06256600 | 1.25001900 | C | 2.43166100 | -0.34643500 | 2.87055000 |
| C | -2.33396600 | 3.45255900 | 1.19572100 | H | 2.50351500 | 0.75091500 | 2.90196500 |
| C | -2.15801700 | 4.13579900 | -0.01318600 | H | 2.22792100 | -0.69351600 | 3.89795000 |
| C | -1.82871300 | 3.41775600 | -1.17002600 | H | 3.41480900 | -0.73955600 | 2.57598900 |
| C | 3.32374000 | -1.08030800 | -0.13925400 | Co | 0.02726800 | -1.21363900 | -1.30956000 |
| C | 4.47179800 | -0.29856600 | 0.06050400 | | | | |
| C | 5.74289100 | -0.84226600 | -0.15303000 | I''_D | | | |
| C | 5.87910900 | -2.17561900 | -0.55617500 | C | 4.39231300 | -1.16211000 | -0.65414600 |
| C | 4.73884200 | -2.96157900 | -0.75868500 | C | 5.20484700 | -1.51261200 | -1.74717600 |

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|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | 6.30441600 | -2.36128400 | -1.58902500 | C | -5.91539300 | -0.87040600 | -1.24851500 |
| C | 6.61853600 | -2.88143900 | -0.32951100 | C | -4.79835900 | -0.93662100 | -2.08731700 |
| C | 5.82241600 | -2.53879400 | 0.76719900 | C | 0.35193600 | 3.20556300 | 0.52392400 |
| C | 4.72503400 | -1.68705800 | 0.60653900 | C | -0.05464000 | 4.43897200 | -0.00852800 |
| H | 4.98337900 | -1.11338500 | -2.73877400 | C | 0.77264900 | 5.56222900 | 0.09581200 |
| H | 6.91901400 | -2.61698900 | -2.45651700 | C | 2.00897000 | 5.47018700 | 0.74226000 |
| H | 7.47684300 | -3.54661900 | -0.20454700 | C | 2.41806300 | 4.24477700 | 1.28010100 |
| H | 6.05648100 | -2.93542600 | 1.75898300 | C | 1.59994000 | 3.11837400 | 1.16718700 |
| H | 4.11514300 | -1.41853300 | 1.46965500 | C | -2.12416400 | 2.16957300 | -0.53473700 |
| C | 3.21328900 | -0.20543700 | -0.84257200 | C | -3.44311900 | 2.22340400 | -0.05799800 |
| C | 2.13542600 | -0.40915100 | 0.24437500 | C | -1.89720300 | 2.41057100 | -1.90389500 |
| O | 2.27371600 | -0.00786400 | 1.43651900 | C | -2.95514800 | 2.70079200 | -2.76642300 |
| H | 1.62450700 | -1.45129900 | 0.10137500 | C | -4.26632800 | 2.74448700 | -2.27938000 |
| C | 2.44806800 | -0.48363800 | -2.15203700 | C | -4.50426900 | 2.50608600 | -0.92395500 |
| H | 2.32100000 | -1.57267000 | -2.26516300 | H | -0.18610200 | 1.28434600 | 2.71852100 |
| H | 3.01983200 | -0.13661500 | -3.02830500 | H | -3.11754500 | 0.57607800 | 2.17589700 |
| C | 3.72992600 | 1.26111800 | -0.84396400 | H | -2.28095700 | 0.41736300 | 3.70390500 |
| H | 2.84684200 | 1.92137400 | -0.84030700 | H | -2.52798600 | -1.72578100 | 2.71534900 |
| H | 4.26533500 | 1.43912700 | -1.79107700 | H | 0.42220900 | -3.21679900 | -0.58270200 |
| C | 1.08527600 | 0.16958500 | -2.10678900 | H | 0.69181900 | -5.69362100 | -0.65222500 |
| C | -0.08679100 | -0.54708900 | -2.35157400 | H | -1.07066700 | -7.16540600 | 0.32605600 |
| H | 1.07406600 | 1.25931700 | -2.21532500 | H | -3.10079800 | -6.14963500 | 1.36166400 |
| H | -0.99595900 | -0.03055600 | -2.66621600 | H | -3.37221700 | -3.68622000 | 1.41623400 |
| H | -0.03273200 | -1.60849300 | -2.61949900 | H | -2.65794500 | -1.14685200 | -2.20582100 |
| C | 4.62120600 | 1.62637500 | 0.30618800 | H | -4.36973000 | -1.25735700 | 1.75912800 |
| C | 5.84646300 | 2.14832400 | 0.18508300 | H | -6.61516700 | -0.94249300 | 0.79773100 |
| H | 4.20748400 | 1.43269500 | 1.29985600 | H | -6.91326400 | -0.73010800 | -1.67140800 |
| H | 6.44922100 | 2.40439500 | 1.06254400 | H | -4.91846500 | -0.84992200 | -3.16998900 |
| H | 6.29413200 | 2.33980500 | -0.79740500 | H | -1.02263400 | 4.53239900 | -0.50279700 |
| P | -0.66554200 | 1.66898200 | 0.46189000 | H | 0.44388100 | 6.51578400 | -0.32586200 |
| C | -1.16543600 | 1.52296700 | 2.27052100 | H | 2.65265700 | 6.34969000 | 0.82492100 |
| C | -2.13140600 | 0.36872300 | 2.61099600 | H | 3.38699900 | 4.16051200 | 1.77800700 |
| C | -1.72980100 | -1.08706600 | 2.30366800 | H | 1.93246100 | 2.15382400 | 1.55877200 |
| P | -1.62538400 | -1.44615900 | 0.47282300 | H | -3.66064000 | 2.03800300 | 0.99114300 |
| C | -1.48318800 | -3.28569300 | 0.42811800 | H | -0.87939300 | 2.37514800 | -2.29769300 |
| C | -0.34755900 | -3.86453100 | -0.15643500 | H | -2.75510700 | 2.88667300 | -3.82468700 |
| C | -0.19804900 | -5.25499500 | -0.19355700 | H | -5.09763300 | 2.96037000 | -2.95498400 |
| C | -1.18537800 | -6.07881600 | 0.35380900 | H | -5.52376400 | 2.53387700 | -0.53222100 |
| C | -2.32484400 | -5.50869200 | 0.93514500 | C | -0.40589700 | -1.48947000 | 2.96053900 |
| C | -2.47503700 | -4.12070000 | 0.96911700 | H | -0.21292500 | -2.56681100 | 2.84114400 |
| C | -3.34123800 | -1.20771400 | -0.15504600 | H | 0.45053600 | -0.94485300 | 2.53161000 |
| C | -3.52260500 | -1.10118900 | -1.54434700 | H | -0.44376200 | -1.27367500 | 4.04156500 |
| C | -4.47120700 | -1.15855000 | 0.67794100 | C | -1.65737700 | 2.83075200 | 2.89900600 |
| C | -5.74771100 | -0.98573400 | 0.13420400 | H | -2.62530500 | 3.15173600 | 2.48597200 |

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|------------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | -1.79026400 | 2.69506900 | 3.98525400 | C | -0.24781500 | 6.07009400 | 0.26520800 |
| H | -0.93989200 | 3.64909200 | 2.74882000 | C | 0.93085600 | 5.78239400 | 0.96513700 |
| Co | 0.19449700 | -0.31408900 | -0.27897200 | C | 1.40666200 | 4.47089800 | 1.02980400 |
| | | | | C | 2.99544200 | 1.78125100 | -0.15246700 |
| 1"Q | | | | C | 3.24283300 | 1.48079000 | -1.50143700 |
| C | -4.54677700 | 0.59723700 | -0.59209300 | C | 4.07658600 | 2.14856700 | 0.66676300 |
| C | -5.36670500 | 0.91588000 | -1.68891600 | C | 5.37326800 | 2.20473700 | 0.14743700 |
| C | -6.59889700 | 1.55561100 | -1.51351500 | C | 5.60723500 | 1.90484200 | -1.19822600 |
| C | -7.04513600 | 1.88917000 | -0.23184100 | C | 4.53655800 | 1.54793800 | -2.02314600 |
| C | -6.24623300 | 1.56987700 | 0.87118700 | C | 0.38674000 | -3.27616300 | 0.51138900 |
| C | -5.01545200 | 0.93311300 | 0.69163200 | C | 1.05609200 | -4.45033700 | 0.13333900 |
| H | -5.05062500 | 0.65704400 | -2.70076200 | C | 0.40824300 | -5.68724600 | 0.21272100 |
| H | -7.21266900 | 1.79304900 | -2.38687100 | C | -0.90948900 | -5.76438700 | 0.67564700 |
| H | -8.00654500 | 2.39047700 | -0.09303300 | C | -1.57843100 | -4.59718100 | 1.06023000 |
| H | -6.58302100 | 1.81872900 | 1.88142800 | C | -0.93879900 | -3.35713800 | 0.97561000 |
| H | -4.40318700 | 0.68068300 | 1.55858900 | C | 2.69481900 | -1.85209500 | -0.48602700 |
| C | -3.20873500 | -0.13288700 | -0.76778000 | C | 3.99068200 | -1.64316300 | 0.01070700 |
| C | -2.26450800 | 0.17969200 | 0.42938700 | C | 2.54212700 | -2.17807800 | -1.84838100 |
| O | -2.32497600 | -0.49872700 | 1.53286600 | C | 3.65255500 | -2.30753600 | -2.68282900 |
| H | -2.13701600 | 1.29177800 | 0.52399900 | C | 4.94035900 | -2.09856300 | -2.17510600 |
| C | -2.47674000 | 0.35340300 | -2.04518800 | C | 5.10313100 | -1.76517400 | -0.82870500 |
| H | -2.37892600 | 1.45126000 | -2.00546200 | H | 0.49596600 | -1.28794100 | 2.67553700 |
| H | -3.07530500 | 0.12493700 | -2.94379400 | H | 3.19211200 | 0.07832400 | 2.15492700 |
| C | -3.48404000 | -1.66030900 | -0.89192900 | H | 2.35258500 | 0.03717500 | 3.69111800 |
| H | -2.51242600 | -2.17807500 | -0.84890100 | H | 2.06315700 | 2.16411800 | 2.68687400 |
| H | -3.91620900 | -1.86043600 | -1.88689000 | H | -1.01900300 | 2.92149000 | -0.79865800 |
| C | -1.10567000 | -0.26645800 | -2.20378100 | H | -1.86764200 | 5.25973000 | -0.92020700 |
| C | 0.02227400 | 0.42784200 | -2.58309100 | H | -0.61702800 | 7.09759600 | 0.21539200 |
| H | -1.07982800 | -1.35981400 | -2.27600300 | H | 1.48186500 | 6.58526100 | 1.46170300 |
| H | 0.91268100 | -0.09762300 | -2.93457100 | H | 2.32961400 | 4.25860100 | 1.57451900 |
| H | -0.00747200 | 1.51014700 | -2.74165400 | H | 2.41638700 | 1.17945200 | -2.14320300 |
| C | -4.37614600 | -2.24425600 | 0.16333400 | H | 3.91749600 | 2.39275300 | 1.71815200 |
| C | -5.50812500 | -2.91476600 | -0.07790400 | H | 6.20468900 | 2.48473600 | 0.79935800 |
| H | -4.03883400 | -2.08413100 | 1.19147800 | H | 6.62234800 | 1.94531100 | -1.60100600 |
| H | -6.11332400 | -3.32941600 | 0.73505600 | H | 4.70933700 | 1.30466700 | -3.07419900 |
| H | -5.87516100 | -3.07330800 | -1.09906700 | H | 2.08742200 | -4.40505000 | -0.22098500 |
| P | 1.14118800 | -1.59904400 | 0.45448500 | H | 0.93846600 | -6.59544600 | -0.08587100 |
| C | 1.52210000 | -1.31166800 | 2.27101200 | H | -1.41397700 | -6.73223900 | 0.73500700 |
| C | 2.18803300 | 0.04000100 | 2.59941300 | H | -2.61079000 | -4.64799200 | 1.41564300 |
| C | 1.43819300 | 1.34958500 | 2.28734800 | H | -1.46968700 | -2.44220800 | 1.26360800 |
| P | 1.25684800 | 1.67426900 | 0.45452800 | H | 4.15006500 | -1.37387100 | 1.05272700 |
| C | 0.70494000 | 3.43095700 | 0.39778600 | H | 1.54099500 | -2.33601800 | -2.25784900 |
| C | -0.47327700 | 3.72754800 | -0.30375500 | H | 3.51195000 | -2.56598400 | -3.73542900 |
| C | -0.94844500 | 5.04157200 | -0.37060200 | H | 5.81081100 | -2.18969500 | -2.82938200 |

| | | | | | | | |
|--------------------------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | 6.10274900 | -1.59133000 | -0.42317100 | C | 1.42812100 | -1.68273600 | 2.22761400 |
| C | 0.06551700 | 1.43391300 | 2.96292700 | C | 2.39532900 | -0.49228000 | 2.39148500 |
| H | -0.38069800 | 2.43154800 | 2.82728900 | C | 1.84002300 | 0.94879000 | 2.32036400 |
| H | -0.65072600 | 0.69284300 | 2.57302800 | P | 1.38446200 | 1.48577400 | 0.58667000 |
| H | 0.17656700 | 1.26542800 | 4.04750800 | C | 0.91722900 | 3.26098500 | 0.81628600 |
| C | 2.26367600 | -2.46540100 | 2.95240100 | C | -0.36609700 | 3.69440900 | 0.45682300 |
| H | 3.30181200 | -2.55820700 | 2.60096000 | C | -0.73902600 | 5.03184500 | 0.62968500 |
| H | 2.29737500 | -2.29358600 | 4.04103800 | C | 0.16987200 | 5.94767400 | 1.16637000 |
| H | 1.76216400 | -3.42854500 | 2.78136500 | C | 1.45619600 | 5.52366200 | 1.52431100 |
| Co | -0.22912000 | 0.08483600 | -0.32517300 | C | 1.82971000 | 4.19007200 | 1.34502700 |
| | | | | C | 2.98291800 | 1.71691000 | -0.30161200 |
| | | | | C | 2.90223700 | 2.17086600 | -1.63130900 |
| | | | | C | 4.24761300 | 1.44602300 | 0.24072300 |
| | | | | C | 5.40172100 | 1.59868000 | -0.53684000 |
| | | | | C | 5.30935300 | 2.03454700 | -1.86054300 |
| | | | | C | 4.05294100 | 2.33040200 | -2.40384000 |
| | | | | C | -0.25345400 | -3.30976700 | 0.44865100 |
| | | | | C | -0.31060300 | -4.13080100 | -0.69093600 |
| | | | | C | -1.23159600 | -5.17921300 | -0.76918400 |
| | | | | C | -2.11069600 | -5.42408000 | 0.29045100 |
| | | | | C | -2.06257000 | -4.61086600 | 1.42786000 |
| | | | | C | -1.14569400 | -3.55974100 | 1.50668600 |
| | | | | C | 2.25617600 | -2.29385200 | -0.54507100 |
| | | | | C | 2.92511100 | -3.52230300 | -0.39636100 |
| | | | | C | 2.71615300 | -1.38332700 | -1.50796900 |
| | | | | C | 3.83904000 | -1.67363200 | -2.28868100 |
| | | | | C | 4.50915800 | -2.88809200 | -2.12031600 |
| | | | | C | 4.04579700 | -3.81411000 | -1.17729700 |
| | | | | H | 0.50889200 | -1.47295000 | 2.79697400 |
| | | | | H | 3.22928200 | -0.61985300 | 1.68434500 |
| | | | | H | 2.84258800 | -0.59338200 | 3.39540200 |
| | | | | H | 2.64592900 | 1.61793200 | 2.66314200 |
| | | | | H | -1.07448800 | 2.97292700 | 0.04370200 |
| | | | | H | -1.74285600 | 5.35516100 | 0.34217500 |
| | | | | H | -0.11951000 | 6.99275100 | 1.30364600 |
| | | | | H | 2.17149900 | 6.23729800 | 1.94146900 |
| | | | | H | 2.83920700 | 3.87032500 | 1.61597000 |
| | | | | H | 1.92561800 | 2.40139900 | -2.06318000 |
| | | | | H | 4.35069100 | 1.11501400 | 1.27375200 |
| | | | | H | 6.37853200 | 1.37687100 | -0.09942900 |
| | | | | H | 6.21134600 | 2.14916400 | -2.46672800 |
| | | | | H | 3.96983500 | 2.68312200 | -3.43501300 |
| | | | | H | 0.36337700 | -3.94659700 | -1.52957400 |
| | | | | H | -1.26197000 | -5.80640700 | -1.66393200 |
| TS1''_b | | | | | | | |
| C | -3.65551400 | 0.86755500 | -1.00037000 | | | | |
| C | -3.99074300 | 1.18028200 | -2.32683800 | | | | |
| C | -4.52453000 | 2.42847900 | -2.66609100 | | | | |
| C | -4.73495200 | 3.39824900 | -1.68226200 | | | | |
| C | -4.41954300 | 3.09874900 | -0.35275700 | | | | |
| C | -3.89402100 | 1.84830600 | -0.01912000 | | | | |
| H | -3.82905900 | 0.44734800 | -3.11818000 | | | | |
| H | -4.77138400 | 2.64307400 | -3.70932700 | | | | |
| H | -5.14366700 | 4.37662300 | -1.94741000 | | | | |
| H | -4.58364400 | 3.84195100 | 0.43205700 | | | | |
| H | -3.65794500 | 1.63457200 | 1.02402300 | | | | |
| C | -3.09599100 | -0.49841000 | -0.59835200 | | | | |
| C | -2.05605500 | -0.31413300 | 0.56619200 | | | | |
| O | -2.35468800 | -0.61974600 | 1.72695700 | | | | |
| H | -1.47973800 | 0.98235900 | 0.43893100 | | | | |
| C | -2.31079000 | -1.20810400 | -1.71885800 | | | | |
| H | -2.89565700 | -1.24685300 | -2.65421100 | | | | |
| H | -2.19161200 | -2.25569400 | -1.40773400 | | | | |
| C | -4.26296800 | -1.43769900 | -0.16809400 | | | | |
| H | -3.79789400 | -2.35229300 | 0.23763900 | | | | |
| H | -4.81686600 | -1.72473200 | -1.07729300 | | | | |
| C | -0.92470800 | -0.65650700 | -1.97880400 | | | | |
| C | -0.56973800 | 0.66390400 | -2.14084000 | | | | |
| H | -0.19781800 | -1.40831100 | -2.30527300 | | | | |
| H | 0.39785500 | 0.90926800 | -2.58376900 | | | | |
| H | -1.29654900 | 1.47616100 | -2.08742500 | | | | |
| C | -5.22135800 | -0.89252600 | 0.84802000 | | | | |
| C | -6.52218000 | -0.67253000 | 0.63056100 | | | | |
| H | -4.78606200 | -0.67156000 | 1.82726100 | | | | |
| H | -7.17724800 | -0.28116700 | 1.41583300 | | | | |
| H | -6.98193300 | -0.87315000 | -0.34444700 | | | | |
| P | 0.79930500 | -1.80747800 | 0.46611100 | | | | |

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|--------------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | -2.83070300 | -6.24404600 | 0.23037700 | H | -1.58382800 | 0.26159000 | -2.89878800 |
| H | -2.74832600 | -4.79144000 | 2.25969400 | C | -4.86866200 | -1.12268200 | 1.37944700 |
| H | -1.14413700 | -2.91793800 | 2.38760100 | C | -6.20216900 | -1.19523200 | 1.30841900 |
| H | 2.56205200 | -4.26075700 | 0.31932200 | H | -4.39264700 | -0.48577700 | 2.13040400 |
| H | 2.18773800 | -0.44108900 | -1.63889300 | H | -6.84482700 | -0.63530900 | 1.99576700 |
| H | 4.18649600 | -0.94756900 | -3.02755900 | H | -6.70303100 | -1.81514400 | 0.55517800 |
| H | 5.38763300 | -3.11977900 | -2.72802700 | P | 1.30316600 | -1.62092100 | 0.50522000 |
| H | 4.55956100 | -4.77061800 | -1.05152800 | C | 1.95870300 | -1.25970800 | 2.22437100 |
| C | 0.62584100 | 1.14942900 | 3.23525700 | C | 2.68932400 | 0.09417800 | 2.28521300 |
| H | 0.36037900 | 2.21365000 | 3.31766200 | C | 1.82923100 | 1.37299000 | 2.32932100 |
| H | -0.26295200 | 0.61241000 | 2.86645800 | P | 1.08965500 | 1.79969600 | 0.66801100 |
| H | 0.85184900 | 0.77823300 | 4.24864700 | C | 0.16676400 | 3.35039000 | 1.02089200 |
| C | 2.06599900 | -2.95630200 | 2.78419600 | C | -1.18322600 | 3.23513800 | 1.40149200 |
| H | 3.05154700 | -3.14066600 | 2.33053100 | C | -1.93345200 | 4.37959400 | 1.68447000 |
| H | 2.21733000 | -2.85236900 | 3.87149100 | C | -1.35191300 | 5.64801400 | 1.57709200 |
| H | 1.43911600 | -3.84355500 | 2.61494600 | C | -0.01229700 | 5.76808100 | 1.19326000 |
| Co | -0.25361400 | 0.07799500 | 0.02234100 | C | 0.74473300 | 4.62469300 | 0.91651100 |
| TS1"Q | | | | C | 2.49527100 | 2.37751000 | -0.36291600 |
| C | -3.79082000 | -0.01041500 | -1.19982800 | C | 2.22342300 | 2.56868500 | -1.73123100 |
| C | -4.19633400 | -0.19937900 | -2.53087200 | C | 3.80506500 | 2.57231200 | 0.09969900 |
| C | -4.97320900 | 0.75749600 | -3.19821200 | C | 4.82276800 | 2.93869100 | -0.78869200 |
| C | -5.37245400 | 1.92485400 | -2.54599400 | C | 4.54243900 | 3.12724500 | -2.14460500 |
| C | -4.98796900 | 2.12337400 | -1.21260300 | C | 3.23525600 | 2.94861200 | -2.61376400 |
| C | -4.21252700 | 1.17057600 | -0.55436800 | C | 0.47315600 | -3.24015400 | 0.70090700 |
| H | -3.90240300 | -1.09955400 | -3.07153000 | C | 0.60187700 | -4.27338400 | -0.24301400 |
| H | -5.26498100 | 0.58245100 | -4.23750300 | C | -0.18464300 | -5.42532700 | -0.14914600 |
| H | -5.97664800 | 2.67255400 | -3.06628200 | C | -1.11092100 | -5.56613000 | 0.88886800 |
| H | -5.28895200 | 3.03248900 | -0.68461800 | C | -1.24886400 | -4.54205300 | 1.83187600 |
| H | -3.90661000 | 1.34748100 | 0.47661400 | C | -0.47163300 | -3.38604700 | 1.73474500 |
| C | -2.97248200 | -1.04143800 | -0.43015300 | C | 2.79876100 | -1.92963600 | -0.51380300 |
| C | -1.84539400 | -0.33654300 | 0.43758900 | C | 3.65990400 | -3.03321200 | -0.37204500 |
| O | -2.11114700 | 0.00577900 | 1.59437100 | C | 3.09702200 | -0.95806000 | -1.48449500 |
| H | -1.44001700 | 1.15348600 | -0.65220600 | C | 4.23859000 | -1.06861700 | -2.28319100 |
| C | -2.23432700 | -2.06931500 | -1.31566800 | C | 5.09126600 | -2.16512800 | -2.12907400 |
| H | -2.91981000 | -2.51257200 | -2.05913800 | C | 4.79617000 | -3.14841200 | -1.17684600 |
| H | -1.94665700 | -2.90220800 | -0.66021000 | H | 1.04500400 | -1.19635300 | 2.83388200 |
| C | -3.92406800 | -1.87471100 | 0.49175400 | H | 3.42875800 | 0.15117400 | 1.46989300 |
| H | -3.27444300 | -2.50513600 | 1.12307900 | H | 3.27965200 | 0.09251700 | 3.21743400 |
| H | -4.50188800 | -2.55458800 | -0.15691400 | H | 2.50066600 | 2.20659600 | 2.59071700 |
| C | -0.97257400 | -1.59936600 | -2.00033300 | H | -1.63438500 | 2.24360100 | 1.49045100 |
| C | -0.78549300 | -0.45950600 | -2.72114400 | H | -2.98016400 | 4.27995100 | 1.98395900 |
| H | -0.15929200 | -2.33247400 | -2.01412100 | H | -1.94271000 | 6.54250300 | 1.79088400 |
| H | 0.14537400 | -0.31320600 | -3.27906600 | H | 0.44727800 | 6.75625000 | 1.10765600 |
| | | | | H | 1.78928700 | 4.72864500 | 0.61506600 |

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|------------------------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | 1.20817600 | 2.40669000 | -2.10549400 | C | -4.47643500 | -0.73814000 | -0.23139100 |
| H | 4.04771900 | 2.43791400 | 1.15467200 | H | -4.17468600 | -1.73282100 | 0.13990300 |
| H | 5.84040900 | 3.07828300 | -0.41520300 | H | -5.04349400 | -0.89486900 | -1.16419000 |
| H | 5.33981400 | 3.41167300 | -2.83563900 | C | -1.04919900 | -0.39136500 | -2.03540900 |
| H | 3.00669500 | 3.09500800 | -3.67242000 | C | -0.50678300 | 0.85215400 | -2.16461300 |
| H | 1.31198300 | -4.17978100 | -1.06605200 | H | -0.42470500 | -1.24060100 | -2.33164400 |
| H | -0.07139000 | -6.21696800 | -0.89428500 | H | 0.50793500 | 0.96049500 | -2.55463800 |
| H | -1.72489900 | -6.46721400 | 0.96071300 | H | -1.09614600 | 1.76395300 | -2.07111800 |
| H | -1.97534100 | -4.63661100 | 2.64283900 | C | -5.36688800 | -0.09067700 | 0.78619000 |
| H | -0.62012900 | -2.58296800 | 2.45872800 | C | -6.61101000 | 0.33777300 | 0.54813500 |
| H | 3.44161700 | -3.81163000 | 0.35991400 | H | -4.93201600 | 0.02099300 | 1.78386300 |
| H | 2.42744100 | -0.10489600 | -1.60688100 | H | -7.22072700 | 0.79545600 | 1.33402300 |
| H | 4.45623400 | -0.29803400 | -3.02663200 | H | -7.06635300 | 0.25072900 | -0.44555500 |
| H | 5.98344100 | -2.25894300 | -2.75336400 | P | 0.37208800 | -1.85209400 | 0.48973000 |
| H | 5.45704200 | -4.01097200 | -1.05907900 | C | 0.99689500 | -1.85580800 | 2.25541400 |
| C | 0.72388200 | 1.30193800 | 3.39031500 | C | 2.19679900 | -0.90087100 | 2.42016200 |
| H | 0.33245600 | 2.30219800 | 3.62303700 | C | 1.97311700 | 0.62381400 | 2.31032700 |
| H | -0.12529400 | 0.68260600 | 3.06132100 | P | 1.66605800 | 1.21418500 | 0.55927400 |
| H | 1.12879500 | 0.87534200 | 4.32285400 | C | 1.69389300 | 3.05659000 | 0.74113300 |
| C | 2.83953300 | -2.37124400 | 2.79745400 | C | 0.62745300 | 3.83617200 | 0.27445800 |
| H | 3.81823600 | -2.40491800 | 2.29544000 | C | 0.65656500 | 5.22967200 | 0.39860800 |
| H | 3.02332500 | -2.18320100 | 3.86840600 | C | 1.75116900 | 5.85718300 | 0.99867500 |
| H | 2.37031900 | -3.36158000 | 2.70446700 | C | 2.82364800 | 5.08640200 | 1.46477300 |
| Co | -0.13476900 | 0.13885700 | -0.55265000 | C | 2.79921800 | 3.69697500 | 1.32889900 |
| | | | | C | 3.28159900 | 1.02514700 | -0.31556900 |
| | | | | C | 3.32349200 | 1.45797400 | -1.65402600 |
| | | | | C | 4.44399400 | 0.48382100 | 0.25176100 |
| | | | | C | 5.61178100 | 0.35310500 | -0.50917200 |
| | | | | C | 5.63797000 | 0.77133200 | -1.84136500 |
| | | | | C | 4.48893900 | 1.33430300 | -2.41035600 |
| | | | | C | -0.91647300 | -3.15917200 | 0.43423900 |
| | | | | C | -1.08327400 | -3.94038500 | -0.72221100 |
| | | | | C | -2.15079300 | -4.83585400 | -0.83027500 |
| | | | | C | -3.06764400 | -4.96716400 | 0.21709800 |
| | | | | C | -2.90810900 | -4.19583300 | 1.37320600 |
| | | | | C | -1.84480800 | -3.29610000 | 1.48124700 |
| | | | | C | 1.72367100 | -2.57377700 | -0.52691900 |
| | | | | C | 2.22261700 | -3.87571100 | -0.33862500 |
| | | | | C | 2.27052100 | -1.78038400 | -1.54496200 |
| | | | | C | 3.31758400 | -2.25499900 | -2.34041200 |
| | | | | C | 3.82491000 | -3.53922200 | -2.12858300 |
| | | | | C | 3.27031300 | -4.35062500 | -1.13068900 |
| | | | | H | 0.13688200 | -1.44918700 | 2.81032600 |
| | | | | H | 2.99298100 | -1.22558700 | 1.73365500 |
| 2''_D | | | | | | | |
| C | -3.48691100 | 1.47730900 | -0.92414000 | | | | |
| C | -3.76114400 | 1.90183900 | -2.23320500 | | | | |
| C | -4.09560800 | 3.23209900 | -2.51009000 | | | | |
| C | -4.16037900 | 4.17295600 | -1.47895500 | | | | |
| C | -3.90034300 | 3.76395000 | -0.16678700 | | | | |
| C | -3.57417500 | 2.43321400 | 0.10433900 | | | | |
| H | -3.70915700 | 1.19237400 | -3.06013300 | | | | |
| H | -4.30128800 | 3.53272700 | -3.54096600 | | | | |
| H | -4.41377100 | 5.21411300 | -1.69458800 | | | | |
| H | -3.95168400 | 4.48514400 | 0.65333000 | | | | |
| H | -3.37600800 | 2.13096000 | 1.13279500 | | | | |
| C | -3.16202400 | 0.02018400 | -0.59404800 | | | | |
| C | -2.12223600 | -0.03232700 | 0.58033400 | | | | |
| O | -2.50721000 | -0.23372900 | 1.72821700 | | | | |
| H | -0.94194200 | 1.57956000 | 0.43096800 | | | | |
| C | -2.49077300 | -0.74841900 | -1.75022400 | | | | |
| H | -3.08924800 | -0.66804500 | -2.67381500 | | | | |
| H | -2.51693300 | -1.81344200 | -1.48167000 | | | | |

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|------------------------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | 2.59278300 | -1.07454700 | 3.43562800 | C | -2.84012900 | -1.96324700 | 0.14945700 |
| H | 2.90268300 | 1.10619200 | 2.65200800 | C | -1.55323200 | -1.20910600 | 0.62813800 |
| H | -0.23309000 | 3.33995000 | -0.17710100 | O | -1.27613800 | -1.32917600 | 1.82209900 |
| H | -0.18278700 | 5.82323700 | 0.02699600 | H | -0.19996600 | 0.03585200 | -2.12204300 |
| H | 1.77296600 | 6.94514000 | 1.10180600 | C | -2.45518800 | -3.46273800 | 0.05414300 |
| H | 3.68480500 | 5.57117000 | 1.93197300 | H | -3.37674500 | -4.06500200 | -0.04045500 |
| H | 3.65016300 | 3.10809100 | 1.68019700 | H | -2.04314700 | -3.74635700 | 1.03850300 |
| H | 2.43102700 | 1.89610000 | -2.10769600 | C | -3.93554500 | -1.88323600 | 1.26601800 |
| H | 4.45911800 | 0.16123100 | 1.29241700 | H | -3.51357200 | -2.38576900 | 2.15103500 |
| H | 6.50653800 | -0.07679100 | -0.05160900 | H | -4.80689900 | -2.46447600 | 0.92544200 |
| H | 6.54993700 | 0.66510800 | -2.43395300 | C | -1.48628900 | -3.92368400 | -0.99567600 |
| H | 4.50063800 | 1.67473900 | -3.44885800 | C | -0.83711000 | -3.19349600 | -1.90648500 |
| H | -0.37971300 | -3.84498600 | -1.55116300 | H | -1.30541900 | -5.00628700 | -0.97426500 |
| H | -2.26574500 | -5.43225500 | -1.73900600 | H | -0.13669900 | -3.66313400 | -2.60385600 |
| H | -3.90266700 | -5.66720100 | 0.13343200 | H | -0.95940500 | -2.11036600 | -1.98653700 |
| H | -3.62064200 | -4.28904700 | 2.19677500 | C | -4.36320100 | -0.50352200 | 1.66076300 |
| H | -1.75634500 | -2.68229100 | 2.37740900 | C | -5.54561000 | 0.04953800 | 1.37086700 |
| H | 1.78252400 | -4.52946600 | 0.41475900 | H | -3.63234700 | 0.07656100 | 2.23454400 |
| H | 1.86975500 | -0.78233400 | -1.70552800 | H | -5.80071900 | 1.06253400 | 1.69722700 |
| H | 3.73498700 | -1.61659700 | -3.12221200 | H | -6.30384600 | -0.49315800 | 0.79470100 |
| H | 4.64573000 | -3.91446900 | -2.74508100 | P | 1.83155800 | -1.07574500 | 0.43922200 |
| H | 3.65343800 | -5.36190900 | -0.97205200 | C | 2.08777700 | -0.49199200 | 2.20048300 |
| C | 0.82213700 | 1.09964500 | 3.20398700 | C | 2.24435700 | 1.04246700 | 2.26325000 |
| H | 0.76298800 | 2.19763600 | 3.23317700 | C | 0.97456000 | 1.91728900 | 2.21640800 |
| H | -0.14942000 | 0.72184500 | 2.84888600 | P | 0.19543300 | 2.00883000 | 0.52101300 |
| H | 0.97318100 | 0.74063500 | 4.23552000 | C | -1.20255400 | 3.17498700 | 0.77563500 |
| C | 1.34622100 | -3.22731400 | 2.83655900 | C | -2.47437900 | 2.64722800 | 1.04690500 |
| H | 2.29101600 | -3.60868300 | 2.42136900 | C | -3.56405500 | 3.49347500 | 1.26657800 |
| H | 1.47828000 | -3.14168600 | 3.92784000 | C | -3.39304300 | 4.88037700 | 1.21429000 |
| H | 0.56227500 | -3.97521800 | 2.65149700 | C | -2.12807100 | 5.41500800 | 0.94604000 |
| Co | -0.31205800 | 0.24022700 | 0.11726400 | C | -1.03742600 | 4.56872200 | 0.72738900 |
| | | | | C | 1.35391200 | 3.00567200 | -0.49597900 |
| | | | | C | 1.06720200 | 3.10215300 | -1.86973100 |
| 2''_Q | | | | C | 2.49589600 | 3.64775900 | 0.00595500 |
| C | -3.41022600 | -1.39028900 | -1.13877500 | C | 3.34272100 | 4.35734500 | -0.85238000 |
| C | -4.13817300 | -2.18041700 | -2.04353400 | C | 3.05318600 | 4.44355000 | -2.21658900 |
| C | -4.71627700 | -1.62368500 | -3.18806200 | C | 1.90696200 | 3.81957400 | -2.72271500 |
| C | -4.58044200 | -0.25690500 | -3.45505400 | C | 1.80382300 | -2.90360600 | 0.53963900 |
| C | -3.86604400 | 0.54455200 | -2.56087200 | C | 2.39042100 | -3.68902900 | -0.46691300 |
| C | -3.29385000 | -0.01912300 | -1.41704200 | C | 2.25308200 | -5.07963100 | -0.45282700 |
| H | -4.25689400 | -3.24963400 | -1.85999600 | C | 1.52422100 | -5.70527100 | 0.56294300 |
| H | -5.27407600 | -2.26333100 | -3.87738900 | C | 0.93194800 | -4.92973500 | 1.56524200 |
| H | -5.02975500 | 0.17828000 | -4.35152100 | C | 1.06660400 | -3.53971500 | 1.55421600 |
| H | -3.75143800 | 1.61531700 | -2.74949500 | C | 3.38233800 | -0.66829300 | -0.44648600 |
| H | -2.73705800 | 0.61827600 | -0.73125400 | | | | |

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|--------------------------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | 4.62346800 | -1.26105300 | -0.15042500 | C | 4.81000100 | -2.13167000 | -0.71392500 |
| C | 3.31367900 | 0.30539500 | -1.45513500 | C | 3.99793500 | -1.10267200 | -0.22927700 |
| C | 4.46583000 | 0.70205800 | -2.14092200 | H | 3.95790000 | 0.89311800 | -2.98212400 |
| C | 5.69710800 | 0.11849200 | -1.83130200 | H | 5.39779900 | -0.91099900 | -3.83767700 |
| C | 5.77241500 | -0.86784200 | -0.83983600 | H | 5.95109600 | -2.87938700 | -2.39862100 |
| H | 1.14233400 | -0.77880600 | 2.68413200 | H | 5.04996900 | -2.97938400 | -0.06671400 |
| H | 2.96722200 | 1.36802400 | 1.49869000 | H | 3.61766800 | -1.15904400 | 0.79030600 |
| H | 2.72176200 | 1.26828900 | 3.23152400 | C | 2.81600800 | 1.13568800 | -0.44367200 |
| H | 1.28821700 | 2.94713300 | 2.45166500 | C | 1.71830900 | 0.50341800 | 0.52309200 |
| H | -2.61176500 | 1.56740200 | 1.09011200 | O | 1.95716200 | 0.55363200 | 1.73151500 |
| H | -4.54787800 | 3.06501800 | 1.47141500 | H | 0.67416700 | -1.17707800 | -1.28263700 |
| H | -4.24472000 | 5.54491300 | 1.37971800 | C | 2.02336700 | 1.94432300 | -1.49736300 |
| H | -1.98875100 | 6.49830900 | 0.90459300 | H | 2.68590600 | 2.27253000 | -2.31802700 |
| H | -0.05551000 | 4.99722100 | 0.51687000 | H | 1.69273400 | 2.86995700 | -1.00713500 |
| H | 0.18548900 | 2.59814200 | -2.27166100 | C | 3.75928000 | 2.13597300 | 0.29404100 |
| H | 2.73863100 | 3.60528700 | 1.06795100 | H | 3.10609200 | 2.83630000 | 0.84091000 |
| H | 4.23286300 | 4.84604400 | -0.44848700 | H | 4.29935700 | 2.72257300 | -0.46913100 |
| H | 3.71823200 | 4.99591000 | -2.88505100 | C | 0.79209900 | 1.25002300 | -2.03973700 |
| H | 1.67123600 | 3.88451400 | -3.78784300 | C | 0.79467500 | -0.04493400 | -2.57832700 |
| H | 2.95087500 | -3.21476200 | -1.27444700 | H | -0.04665200 | 1.90029300 | -2.30736400 |
| H | 2.71544000 | -5.67545500 | -1.24388600 | H | -0.05821300 | -0.36109500 | -3.18833400 |
| H | 1.41485100 | -6.79253200 | 0.57214700 | H | 1.72674800 | -0.57273700 | -2.78604700 |
| H | 0.35412300 | -5.40871300 | 2.35974100 | C | 4.74901100 | 1.55244100 | 1.25656400 |
| H | 0.57182500 | -2.94849100 | 2.32483300 | C | 6.07821000 | 1.62465500 | 1.12660700 |
| H | 4.69196200 | -2.04156800 | 0.60847300 | H | 4.31140100 | 1.03897600 | 2.11788300 |
| H | 2.34954500 | 0.74875600 | -1.70403300 | H | 6.75259000 | 1.18769500 | 1.87050900 |
| H | 4.39554800 | 1.46539500 | -2.91935700 | H | 6.54406900 | 2.12159300 | 0.26715300 |
| H | 6.59946700 | 0.42435600 | -2.36686900 | P | -1.20892100 | 1.54051700 | 0.45356400 |
| H | 6.73201700 | -1.33464200 | -0.60369400 | C | -1.67740000 | 1.26168700 | 2.24228400 |
| C | -0.06732000 | 1.49107000 | 3.25649200 | C | -2.38759900 | -0.09161900 | 2.42611800 |
| H | -0.84611500 | 2.25672400 | 3.38172500 | C | -1.52505200 | -1.36441500 | 2.34642400 |
| H | -0.55652400 | 0.54605400 | 2.97844300 | P | -0.91931200 | -1.70420900 | 0.61756500 |
| H | 0.42406900 | 1.35079300 | 4.23354000 | C | 0.01534400 | -3.28007000 | 0.84805000 |
| C | 3.25007800 | -1.17056000 | 2.92757900 | C | 1.35479100 | -3.36918000 | 0.45271100 |
| H | 4.22003400 | -0.81631500 | 2.54726800 | C | 2.07313500 | -4.55546700 | 0.63751600 |
| H | 3.20579300 | -0.92307200 | 4.00108200 | C | 1.45432000 | -5.66436700 | 1.22026100 |
| H | 3.22247700 | -2.26551000 | 2.83393700 | C | 0.11218900 | -5.58494100 | 1.61406600 |
| Co | -0.20040900 | -0.15347400 | -0.46176400 | C | -0.60409800 | -4.40103900 | 1.42745600 |
| | | | | C | -2.39290600 | -2.33772100 | -0.29807200 |
| | | | | C | -2.20820200 | -2.64806100 | -1.65842100 |
| | | | | C | -3.67359400 | -2.47681000 | 0.25661100 |
| | | | | C | -4.74846900 | -2.89795400 | -0.53551900 |
| | | | | C | -4.55591600 | -3.19861800 | -1.88573900 |
| | | | | C | -3.27654600 | -3.08082200 | -2.44402300 |
| TS2''_D | | | | | | | |
| C | 3.65760700 | 0.00336800 | -1.02951000 | | | | |
| C | 4.18589700 | 0.04834600 | -2.33041000 | | | | |
| C | 5.00416700 | -0.97541200 | -2.81958600 | | | | |
| C | 5.31631800 | -2.07614300 | -2.01580400 | | | | |

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|---|-------------|-------------|-------------|--------------------------|-------------|-------------|-------------|
| C | -0.48636900 | 3.22845500 | 0.46590600 | Co | 0.04674100 | -0.05073200 | -0.43615900 |
| C | -0.74241400 | 4.13714000 | -0.57422000 | | | | |
| C | -0.08572100 | 5.37041600 | -0.62014500 | TS2''_Q | | | |
| C | 0.83368200 | 5.71604700 | 0.37490400 | C | -3.76855500 | -0.21519400 | -1.04463700 |
| C | 1.09454000 | 4.81755300 | 1.41453600 | C | -4.32293600 | -0.35260900 | -2.32697600 |
| C | 0.44602800 | 3.58104800 | 1.45727800 | C | -4.98013300 | 0.71267600 | -2.95130000 |
| C | -2.80089300 | 1.75143400 | -0.44979000 | C | -5.09959200 | 1.94629600 | -2.30368800 |
| C | -3.72806200 | 2.77811800 | -0.19477000 | C | -4.56619200 | 2.09643400 | -1.02038900 |
| C | -3.09052000 | 0.81182000 | -1.45166500 | C | -3.91376000 | 1.02615600 | -0.40131300 |
| C | -4.29230200 | 0.86861100 | -2.16327400 | H | -4.24299300 | -1.30332900 | -2.85634400 |
| C | -5.21637500 | 1.87994500 | -1.88764600 | H | -5.39955800 | 0.57621800 | -3.95177600 |
| C | -4.92791700 | 2.83801300 | -0.90786900 | H | -5.60911100 | 2.78073700 | -2.79232300 |
| H | -0.69846800 | 1.21612700 | 2.74308500 | H | -4.66008100 | 3.04948800 | -0.49412100 |
| H | -3.23487600 | -0.15229200 | 1.72439800 | H | -3.51331800 | 1.15792400 | 0.60500000 |
| H | -2.83653500 | -0.08430500 | 3.43430500 | C | -3.10409300 | -1.37368800 | -0.30778300 |
| H | -2.17073100 | -2.21088600 | 2.62919700 | C | -1.94269900 | -0.81650700 | 0.58257500 |
| H | 1.83081400 | -2.50248600 | -0.00593300 | O | -1.99244200 | -1.02335100 | 1.79699700 |
| H | 3.11779300 | -4.60930100 | 0.32121100 | H | -0.45371500 | 0.57667400 | -1.88088800 |
| H | 2.01295200 | -6.59257800 | 1.36544400 | C | -2.39834300 | -2.38408200 | -1.24930800 |
| H | -0.37830100 | -6.45135700 | 2.06529000 | H | -3.13458300 | -2.75200500 | -1.99048700 |
| H | -1.65305200 | -4.35228100 | 1.73048100 | H | -2.15248700 | -3.26365600 | -0.63442100 |
| H | -1.21714200 | -2.53588300 | -2.10529500 | C | -4.17457800 | -2.14710900 | 0.51633700 |
| H | -3.85181900 | -2.25805100 | 1.30962400 | H | -3.62578500 | -2.89146400 | 1.11814400 |
| H | -5.74179300 | -2.99210700 | -0.08920000 | H | -4.82356900 | -2.69600000 | -0.18637200 |
| H | -5.39715000 | -3.52464600 | -2.50240200 | C | -1.11852300 | -1.91501600 | -1.90128200 |
| H | -3.11375300 | -3.31880000 | -3.49831300 | C | -0.93129700 | -0.73694800 | -2.63324900 |
| H | -1.45409600 | 3.88086200 | -1.36064800 | H | -0.27696500 | -2.60767500 | -1.85033400 |
| H | -0.29463000 | 6.06330500 | -1.43924700 | H | -0.06253900 | -0.69244000 | -3.29903600 |
| H | 1.34606800 | 6.68066000 | 0.33984700 | H | -1.79845500 | -0.19179600 | -3.01745100 |
| H | 1.81582200 | 5.07511000 | 2.19413000 | C | -5.01754900 | -1.31800900 | 1.43751200 |
| H | 0.69113900 | 2.87881800 | 2.25429500 | C | -6.33665500 | -1.13401000 | 1.31716700 |
| H | -3.50896500 | 3.54536400 | 0.54826800 | H | -4.47639700 | -0.83492800 | 2.25790900 |
| H | -2.36272900 | 0.02859100 | -1.66823800 | H | -6.89760500 | -0.51580900 | 2.02573700 |
| H | -4.50207200 | 0.12180100 | -2.93281400 | H | -6.90627400 | -1.59318400 | 0.50051300 |
| H | -6.15781400 | 1.92962100 | -2.44070400 | P | 1.34617100 | -1.55977800 | 0.39767300 |
| H | -5.64120300 | 3.63974500 | -0.70027600 | C | 1.73797100 | -1.21067300 | 2.20437000 |
| C | -0.33139400 | -1.32240100 | 3.30859500 | C | 2.35013100 | 0.18769100 | 2.41951700 |
| H | 0.11059300 | -2.32136200 | 3.43629900 | C | 1.42913900 | 1.42390100 | 2.37112100 |
| H | 0.45966600 | -0.64600600 | 2.94731900 | P | 0.83436700 | 1.83317000 | 0.65520800 |
| H | -0.66460700 | -0.97567200 | 4.30134100 | C | -0.09409700 | 3.40243200 | 0.87802500 |
| C | -2.50269900 | 2.37974600 | 2.88118300 | C | -1.39977300 | 3.49037400 | 0.37749500 |
| H | -3.53918300 | 2.37144000 | 2.51244500 | C | -2.13263400 | 4.67387400 | 0.51930900 |
| H | -2.54090000 | 2.22902900 | 3.97276200 | C | -1.56306000 | 5.77494600 | 1.16410000 |
| H | -2.07824000 | 3.37658700 | 2.69498400 | C | -0.25596400 | 5.69446200 | 1.66217800 |

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|---|-------------|-------------|-------------|------------------------|-------------|-------------|-------------|
| C | 0.47791400 | 4.51599500 | 1.51601300 | H | -0.31802900 | 2.24084400 | 3.40431800 |
| C | 2.30156500 | 2.42973600 | -0.27457000 | H | -0.50612600 | 0.53948900 | 2.91389200 |
| C | 2.10545800 | 2.73853600 | -1.63395400 | H | 0.53966200 | 0.96394100 | 4.29724300 |
| C | 3.58511800 | 2.57235000 | 0.27379400 | C | 2.60983700 | -2.26325400 | 2.89512600 |
| C | 4.65347500 | 2.99289900 | -0.52599600 | H | 3.66380000 | -2.16959300 | 2.59424500 |
| C | 4.45098000 | 3.29047800 | -1.87593200 | H | 2.56733600 | -2.11442100 | 3.98677300 |
| C | 3.16910000 | 3.17090300 | -2.42619500 | H | 2.28067800 | -3.28974500 | 2.68268500 |
| C | 0.89799000 | -3.33919000 | 0.41972900 | Co | -0.33992700 | -0.02792400 | -0.33949500 |
| C | 1.44826000 | -4.26728100 | -0.47795300 | | | | |
| C | 1.00469600 | -5.59391900 | -0.48974900 | 3''_D | | | |
| C | 0.00802200 | -6.01262800 | 0.39617500 | C | 3.37569300 | -1.31216900 | 1.01773000 |
| C | -0.54902800 | -5.09261000 | 1.29140400 | C | 3.92682600 | -1.56056000 | 2.28537400 |
| C | -0.11465900 | -3.76555900 | 1.29968800 | C | 4.96752300 | -0.77482100 | 2.78845500 |
| C | 2.92938900 | -1.46696100 | -0.52144900 | C | 5.48774800 | 0.27846800 | 2.02817000 |
| C | 4.08676000 | -2.19895200 | -0.19886500 | C | 4.95501000 | 0.53351700 | 0.76200200 |
| C | 2.96653800 | -0.58217500 | -1.61118700 | C | 3.91068200 | -0.25294500 | 0.26643600 |
| C | 4.14042800 | -0.40589500 | -2.34897900 | H | 3.53954700 | -2.38015900 | 2.89257600 |
| C | 5.29163300 | -1.11979000 | -2.00625600 | H | 5.37580100 | -0.98844300 | 3.78006000 |
| C | 5.26042800 | -2.02079400 | -0.93481500 | H | 6.30286100 | 0.89278600 | 2.41933100 |
| H | 0.73516700 | -1.23654100 | 2.65885600 | H | 5.34971500 | 1.35076900 | 0.15454300 |
| H | 3.20476600 | 0.31377800 | 1.73770500 | H | 3.50736700 | -0.03968000 | -0.72496900 |
| H | 2.78317100 | 0.18375000 | 3.43427400 | C | 2.31855700 | -2.22615400 | 0.40901900 |
| H | 2.03093000 | 2.28061700 | 2.71523400 | C | 1.39334800 | -1.41230700 | -0.55293900 |
| H | -1.83882500 | 2.62864500 | -0.12754600 | O | 1.38302600 | -1.69303600 | -1.74902400 |
| H | -3.14905800 | 4.73330300 | 0.12295300 | H | 1.47546300 | -0.12607700 | 2.79041000 |
| H | -2.13423000 | 6.69997000 | 1.27655500 | C | 1.27758900 | -2.75230300 | 1.42267100 |
| H | 0.19340100 | 6.55659800 | 2.16169500 | H | 1.77100400 | -3.20369400 | 2.30437700 |
| H | 1.50193100 | 4.46371700 | 1.89466600 | H | 0.74674200 | -3.57838300 | 0.92143000 |
| H | 1.11108200 | 2.62606500 | -2.07401100 | C | 3.02465200 | -3.42029000 | -0.29660400 |
| H | 3.76791200 | 2.36153600 | 1.32760000 | H | 2.23380300 | -3.99612500 | -0.80755500 |
| H | 5.64929600 | 3.09088200 | -0.08632800 | H | 3.46025700 | -4.07106600 | 0.47988100 |
| H | 5.28805100 | 3.61582200 | -2.49853300 | C | 0.25841800 | -1.67050100 | 1.78068700 |
| H | 3.00043200 | 3.40500500 | -3.48035900 | C | 0.61824300 | -0.79348100 | 2.98413000 |
| H | 2.22419600 | -3.95697300 | -1.17956200 | H | -0.71080300 | -2.15726700 | 1.98771900 |
| H | 1.44354800 | -6.30266200 | -1.19675300 | H | -0.23097400 | -0.15153600 | 3.27701300 |
| H | -0.33606100 | -7.04981100 | 0.38757800 | H | 0.88806400 | -1.39053400 | 3.88039800 |
| H | -1.33472200 | -5.40678500 | 1.98330400 | C | 4.07852900 | -3.05465000 | -1.29758300 |
| H | -0.58171900 | -3.05369500 | 1.98188400 | C | 5.37716900 | -3.35584300 | -1.19289300 |
| H | 4.07181200 | -2.92088400 | 0.61777400 | H | 3.71994100 | -2.49089400 | -2.16508500 |
| H | 2.06463100 | -0.02641700 | -1.87222700 | H | 6.09919800 | -3.05985300 | -1.96094300 |
| H | 4.15292100 | 0.29266600 | -3.18832400 | H | 5.76875700 | -3.90788300 | -0.33021400 |
| H | 6.21326500 | -0.98131900 | -2.57719600 | P | -1.95493000 | -0.81498100 | -0.46242400 |
| H | 6.15551300 | -2.59068300 | -0.67281000 | C | -2.26083000 | -0.38376800 | -2.25909900 |
| C | 0.21232300 | 1.28338200 | 3.29382700 | C | -1.99824900 | 1.09741900 | -2.59905800 |

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|---|-------------|-------------|-------------|------------------|-------------|-------------|-------------|
| C | -0.54438500 | 1.60934400 | -2.56109700 | H | -0.49902800 | -3.05445000 | -1.51781100 |
| P | 0.14122200 | 1.63055100 | -0.82847500 | H | -4.26511100 | 1.16205300 | -0.91255600 |
| C | 1.62241900 | 2.73008100 | -0.89900600 | H | -2.52845900 | -1.12933200 | 2.31695100 |
| C | 2.39698300 | 2.80287500 | 0.27090700 | H | -4.11873800 | -0.09409800 | 3.89798400 |
| C | 3.49365100 | 3.66307500 | 0.34849600 | H | -5.77659000 | 1.59416400 | 3.08878300 |
| C | 3.84607800 | 4.44941100 | -0.75374000 | H | -5.82230400 | 2.20810200 | 0.66878400 |
| C | 3.08789000 | 4.37652800 | -1.92621400 | C | 0.38227100 | 0.82108900 | -3.49216400 |
| C | 1.97765800 | 3.52819000 | -1.99774400 | H | 1.36493700 | 1.30587600 | -3.59036300 |
| C | -1.00211400 | 2.75069800 | 0.09269800 | H | 0.55965100 | -0.19525600 | -3.11417700 |
| C | -1.27970000 | 2.43716700 | 1.43244000 | H | -0.06301600 | 0.76155400 | -4.49949600 |
| C | -1.58073300 | 3.89677200 | -0.47417200 | C | -3.60442900 | -0.86158700 | -2.81718800 |
| C | -2.43404200 | 4.70402500 | 0.28296100 | H | -4.45429000 | -0.30444800 | -2.39706900 |
| C | -2.70547400 | 4.38359000 | 1.61817500 | H | -3.62374300 | -0.71879600 | -3.91046300 |
| C | -2.12118800 | 3.25164400 | 2.19427700 | H | -3.76954800 | -1.92992300 | -2.61673800 |
| C | -2.33821800 | -2.61586100 | -0.45978000 | Co | 0.14617700 | -0.31377000 | 0.33559400 |
| C | -3.49366000 | -3.17073400 | 0.11091900 | | | | |
| C | -3.70898900 | -4.55260800 | 0.07506700 | 3'' _Q | | | |
| C | -2.77844300 | -5.39597600 | -0.53901700 | C | -3.94528500 | -0.28926200 | -0.80165000 |
| C | -1.62787100 | -4.84937300 | -1.11836300 | C | -4.71455800 | -0.28066100 | -1.97856300 |
| C | -1.40500700 | -3.47108500 | -1.07458500 | C | -5.71054600 | 0.67530300 | -2.18820200 |
| C | -3.28278700 | -0.08038200 | 0.57503700 | C | -5.96506400 | 1.65429300 | -1.22076000 |
| C | -4.21933800 | 0.86813800 | 0.13412600 | C | -5.22281500 | 1.64867900 | -0.03785600 |
| C | -3.25859200 | -0.40722100 | 1.94604500 | C | -4.23099500 | 0.68302500 | 0.17053000 |
| C | -4.15364600 | 0.17970100 | 2.84047100 | H | -4.53322700 | -1.03282500 | -2.74827900 |
| C | -5.08209600 | 1.12437200 | 2.38804100 | H | -6.29145800 | 0.65673100 | -3.11437300 |
| C | -5.10743800 | 1.46668600 | 1.03436100 | H | -6.74028500 | 2.40698300 | -1.38536300 |
| H | -1.47077400 | -0.98278300 | -2.74096000 | H | -5.41624400 | 2.39620000 | 0.73590100 |
| H | -2.62963200 | 1.74972000 | -1.97977200 | H | -3.67710500 | 0.69036400 | 1.10862800 |
| H | -2.34607400 | 1.24647700 | -3.63575700 | C | -2.89192100 | -1.37703100 | -0.57768600 |
| H | -0.58597600 | 2.65569200 | -2.90273900 | C | -1.93207700 | -0.94092600 | 0.57847400 |
| H | 2.13520400 | 2.17915200 | 1.12943900 | O | -2.19570900 | -1.23837400 | 1.74106200 |
| H | 4.08265700 | 3.70893100 | 1.26756700 | H | -2.23136800 | 1.35920000 | -2.04071700 |
| H | 4.71008700 | 5.11644600 | -0.69908900 | C | -1.97495200 | -1.57978300 | -1.82285100 |
| H | 3.35629600 | 4.98828300 | -2.79141100 | H | -2.61273100 | -1.79296200 | -2.70473000 |
| H | 1.38982700 | 3.50536500 | -2.91623000 | H | -1.40965200 | -2.51132400 | -1.64148700 |
| H | -0.83686400 | 1.54451400 | 1.88127000 | C | -3.60758800 | -2.72551000 | -0.25818500 |
| H | -1.36583200 | 4.16657500 | -1.51065700 | H | -2.82564600 | -3.43658600 | 0.06325400 |
| H | -2.88644600 | 5.58996900 | -0.17006700 | H | -4.03631200 | -3.11919300 | -1.19518700 |
| H | -3.37354100 | 5.01610100 | 2.20810500 | C | -0.97026000 | -0.44970800 | -2.09527100 |
| H | -2.33160300 | 2.99259200 | 3.23437600 | C | -1.55570600 | 0.81477600 | -2.71924200 |
| H | -4.23540100 | -2.52585300 | 0.58436500 | H | -0.18619200 | -0.84153600 | -2.76913100 |
| H | -4.61291000 | -4.96984700 | 0.52656900 | H | -0.75520200 | 1.52126800 | -3.00135500 |
| H | -2.94904900 | -6.47515600 | -0.56666100 | H | -2.14636400 | 0.61302700 | -3.63994300 |
| H | -0.89409600 | -5.50009500 | -1.60120900 | C | -4.67801500 | -2.65784300 | 0.78999900 |

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|---|-------------|-------------|-------------|--------------------------|-------------|-------------|-------------|
| C | -5.97706300 | -2.88780600 | 0.57076500 | H | 5.24662600 | 3.92592200 | 0.18737100 |
| H | -4.33389800 | -2.37717000 | 1.79021900 | H | 5.34914600 | 3.48454900 | -2.26513500 |
| H | -6.71624400 | -2.81892900 | 1.37564500 | H | 3.45525700 | 2.31596400 | -3.39569400 |
| H | -6.35148900 | -3.15127500 | -0.42553700 | H | 3.12334100 | -3.80608000 | -0.52995000 |
| P | 1.57132300 | -1.41341600 | 0.48294000 | H | 2.65400200 | -6.23486300 | -0.41805500 |
| C | 2.06803300 | -1.05820700 | 2.25638300 | H | 0.58609600 | -7.06577500 | 0.70452300 |
| C | 2.37440300 | 0.42354500 | 2.55603500 | H | -1.01302700 | -5.43471300 | 1.71631300 |
| C | 1.24304600 | 1.46285400 | 2.43359000 | H | -0.55907800 | -3.00210900 | 1.58344400 |
| P | 0.72424200 | 1.78944300 | 0.67035700 | H | 4.44939300 | -0.38228200 | 0.78372700 |
| C | -0.31385400 | 3.29868400 | 0.80100800 | H | 1.82962400 | -1.89184200 | -2.30800500 |
| C | -1.66699500 | 3.19080800 | 0.44791500 | H | 3.60488400 | -1.51157900 | -3.98804200 |
| C | -2.51250600 | 4.30097800 | 0.53370800 | H | 5.80219300 | -0.54317000 | -3.29467800 |
| C | -2.00871800 | 5.52842400 | 0.97382300 | H | 6.19731600 | 0.02012800 | -0.89531400 |
| C | -0.65811100 | 5.64348400 | 1.32668200 | C | 0.00035000 | 1.09944600 | 3.25352300 |
| C | 0.18753400 | 4.53501800 | 1.24002600 | H | -0.71692400 | 1.93416400 | 3.27777800 |
| C | 2.23156300 | 2.36400100 | -0.20224800 | H | -0.52786200 | 0.22310000 | 2.84634200 |
| C | 2.30121800 | 2.11223600 | -1.58311200 | H | 0.29043100 | 0.87651200 | 4.29373600 |
| C | 3.30087000 | 3.02077600 | 0.42732700 | C | 3.17011800 | -1.97354200 | 2.79813100 |
| C | 4.41707000 | 3.42053500 | -0.31352200 | H | 4.14547300 | -1.77868800 | 2.32903000 |
| C | 4.47362400 | 3.17466400 | -1.68915300 | H | 3.28597300 | -1.81064100 | 3.88241200 |
| C | 3.41187400 | 2.52179400 | -2.32368100 | H | 2.92701500 | -3.03434700 | 2.64310600 |
| C | 1.31397500 | -3.23331800 | 0.51703500 | Co | -0.26884300 | -0.12603200 | -0.21227800 |
| C | 2.21179900 | -4.15541600 | -0.04241300 | | | | |
| C | 1.94752400 | -5.52721100 | 0.02343100 | | | | |
| C | 0.79014200 | -5.99327600 | 0.65446300 | TS3''_b | | | |
| C | -0.10559300 | -5.07973900 | 1.22106100 | C | -3.42460400 | -1.53601200 | -0.58610000 |
| C | 0.15003000 | -3.70823300 | 1.14845100 | C | -4.42706800 | -1.28931700 | -1.53792400 |
| C | 3.00964200 | -1.18390000 | -0.63131300 | C | -5.59513200 | -0.60171500 | -1.19150000 |
| C | 4.24773700 | -0.64165000 | -0.25353800 | C | -5.78047500 | -0.14345700 | 0.11654700 |
| C | 2.79238500 | -1.48420300 | -1.99058600 | C | -4.78634600 | -0.37606900 | 1.07235300 |
| C | 3.79162400 | -1.26688000 | -2.93940900 | C | -3.62459700 | -1.06764300 | 0.72222600 |
| C | 5.02252400 | -0.72568900 | -2.55115100 | H | -4.29980400 | -1.64861500 | -2.56232600 |
| C | 5.24374300 | -0.41175200 | -1.20843500 | H | -6.36288200 | -0.42059800 | -1.94878100 |
| H | 1.13327500 | -1.32173900 | 2.77915500 | H | -6.68839300 | 0.40170800 | 0.38621300 |
| H | 3.24174100 | 0.75497500 | 1.96858500 | H | -4.91459700 | -0.01315500 | 2.09555100 |
| H | 2.70349300 | 0.45601600 | 3.60904000 | H | -2.85373300 | -1.25255700 | 1.46739100 |
| H | 1.64795400 | 2.41265900 | 2.81955600 | C | -2.21298300 | -2.36826800 | -0.91748800 |
| H | -2.05527800 | 2.22920200 | 0.10747300 | C | -0.79896000 | -1.93111200 | -0.37195300 |
| H | -3.56391900 | 4.20322100 | 0.25299500 | O | -0.33955900 | -2.37213300 | 0.73065900 |
| H | -2.66652500 | 6.39877700 | 1.03994800 | H | 0.65617300 | -1.89087400 | -3.83013800 |
| H | -0.26221100 | 6.60313600 | 1.66877000 | C | -1.66046100 | -2.30028000 | -2.35579000 |
| H | 1.24127900 | 4.63575400 | 1.51003400 | H | -1.90703700 | -1.34476200 | -2.84435400 |
| H | 1.48293300 | 1.57954100 | -2.07363800 | H | -1.95343200 | -3.12285400 | -3.02668200 |
| H | 3.27251200 | 3.22101800 | 1.49997700 | C | -2.49942300 | -3.85752900 | -0.54855700 |
| | | | | H | -1.60584400 | -4.44232100 | -0.82997900 |

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|---|-------------|-------------|-------------|--------------|-------------|-------------|-------------|
| H | -3.33372600 | -4.21379200 | -1.17732900 | H | -2.49197500 | 1.47891900 | -1.68696300 |
| C | -0.19636000 | -2.29719000 | -1.88724600 | H | -4.73066000 | 2.51129000 | -1.99743900 |
| C | 0.77239400 | -1.52167500 | -2.79494900 | H | -5.77457300 | 3.81242300 | -0.14051200 |
| H | 0.20195300 | -3.31737100 | -1.76875200 | H | -4.55348900 | 4.08380700 | 2.01832000 |
| H | 0.54532500 | -0.43382800 | -2.85984400 | H | -2.30086100 | 3.10434300 | 2.30861800 |
| H | 1.82685700 | -1.64868000 | -2.51896500 | H | -0.03124800 | 2.68697300 | -2.16998000 |
| C | -2.80392800 | -4.12009300 | 0.89519600 | H | 0.89027600 | 3.83984100 | 1.88915300 |
| C | -3.94584600 | -4.64184900 | 1.35580400 | H | 2.03567900 | 5.85835000 | 1.05626800 |
| H | -2.00341900 | -3.83911900 | 1.58637700 | H | 2.14056400 | 6.33329400 | -1.39068400 |
| H | -4.10778300 | -4.81648100 | 2.42464300 | H | 1.07810400 | 4.74776300 | -3.00400700 |
| H | -4.76597900 | -4.91210500 | 0.67977200 | H | 4.10546400 | -1.68741500 | -1.51591800 |
| P | 2.09121800 | -0.60999500 | 0.34139500 | H | 5.00653200 | -3.95110600 | -1.91686000 |
| C | 1.85905600 | -0.38352400 | 2.18383200 | H | 4.30073900 | -5.86145100 | -0.46682900 |
| C | 1.33382500 | 1.03272400 | 2.49780800 | H | 2.66281100 | -5.46594800 | 1.37620700 |
| C | -0.15096300 | 1.35090200 | 2.21764800 | H | 1.71867400 | -3.20838700 | 1.74247200 |
| P | -0.51746800 | 1.54525900 | 0.39932700 | H | 5.05227300 | -0.53385900 | 1.06227400 |
| C | -2.23999600 | 2.21898900 | 0.32792000 | H | 2.26248000 | 1.69761600 | -1.34412800 |
| C | -2.93928800 | 2.06356800 | -0.87903400 | H | 4.05412500 | 3.30637800 | -1.94735500 |
| C | -4.19846400 | 2.64220700 | -1.05241600 | H | 6.35878500 | 3.00229700 | -1.02367100 |
| C | -4.78406000 | 3.36903000 | -0.01121000 | H | 6.84212200 | 1.06856100 | 0.47660900 |
| C | -4.10026200 | 3.51862100 | 1.19968500 | C | -1.08226600 | 0.30773400 | 2.84145300 |
| C | -2.83106100 | 2.95575900 | 1.36577500 | H | -2.13366500 | 0.62375700 | 2.79465200 |
| C | 0.34695000 | 3.11394000 | -0.08417900 | H | -0.98940000 | -0.65952600 | 2.32717600 |
| C | 0.40901800 | 3.39382700 | -1.46102400 | H | -0.82173100 | 0.16432700 | 3.90368500 |
| C | 0.93055600 | 4.01865600 | 0.81387900 | C | 3.08185500 | -0.68449700 | 3.05205100 |
| C | 1.57661300 | 5.16814600 | 0.34367200 | H | 3.83808000 | 0.11081200 | 2.97013100 |
| C | 1.63408500 | 5.43598000 | -1.02656400 | H | 2.77784200 | -0.73949400 | 4.11094300 |
| C | 1.03939100 | 4.54708500 | -1.93025200 | H | 3.55982100 | -1.63942300 | 2.79164500 |
| C | 2.85797600 | -2.27420000 | 0.15867900 | Co | 0.11248700 | -0.17400000 | -0.79872000 |
| C | 3.77904300 | -2.51103100 | -0.87783200 | | | | |
| C | 4.29227700 | -3.79150700 | -1.10478900 | | | | |
| C | 3.89737300 | -4.86029500 | -0.29464600 | TS3"Q | | | |
| C | 2.98015100 | -4.63681900 | 0.73798100 | C | -3.71855800 | -1.03679200 | -0.60465900 |
| C | 2.45797100 | -3.35950700 | 0.95862600 | C | -4.60925000 | -0.56822900 | -1.58390100 |
| C | 3.51322000 | 0.49325600 | -0.07227100 | C | -5.58416900 | 0.38591200 | -1.27421000 |
| C | 4.81889500 | 0.31809300 | 0.42294100 | C | -5.68469000 | 0.89271100 | 0.02515700 |
| C | 3.26402700 | 1.56847600 | -0.93718600 | C | -4.80450700 | 0.43392400 | 1.01037700 |
| C | 4.27599100 | 2.47170900 | -1.27791600 | C | -3.83613700 | -0.52389200 | 0.69710400 |
| C | 5.56284800 | 2.30032300 | -0.76197500 | H | -4.54344300 | -0.95739100 | -2.60316200 |
| C | 5.83313300 | 1.21613300 | 0.08270900 | H | -6.26455800 | 0.73963800 | -2.05366200 |
| H | 1.07258000 | -1.11897600 | 2.40173300 | H | -6.43756100 | 1.64702200 | 0.26621900 |
| H | 1.98622200 | 1.77664900 | 2.01280500 | H | -4.87048500 | 0.82537000 | 2.02900400 |
| H | 1.47064800 | 1.18579500 | 3.58207500 | H | -3.15595100 | -0.88211200 | 1.46945900 |
| H | -0.35145400 | 2.32449300 | 2.69224100 | C | -2.70169800 | -2.11353700 | -0.92569500 |
| | | | | C | -1.39270800 | -2.02431000 | -0.06977000 |

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|---|-------------|-------------|-------------|------------------------|-------------|-------------|-------------|
| O | -1.20029800 | -2.76519500 | 0.92746800 | C | 4.56970100 | 0.67961700 | -2.39719500 |
| H | 0.45664700 | -2.26393800 | -3.78995600 | C | 5.32102300 | 1.65050400 | -1.72605800 |
| C | -1.99122400 | -1.97978200 | -2.28991400 | C | 5.09275600 | 1.87438500 | -0.36690000 |
| H | -1.98840000 | -0.92741700 | -2.62100100 | H | 1.19779100 | -1.16252600 | 2.59701200 |
| H | -2.44866600 | -2.57653700 | -3.10070900 | H | 2.23514100 | 1.70360000 | 2.22248500 |
| C | -3.37657200 | -3.51420800 | -0.81218300 | H | 1.61701700 | 1.04619500 | 3.72398500 |
| H | -2.60135700 | -4.27033700 | -1.02703000 | H | -0.04324100 | 2.38341800 | 2.75789000 |
| H | -4.14098800 | -3.59136700 | -1.60398300 | H | -2.01655100 | 1.95268200 | -1.72436900 |
| C | -0.58480200 | -2.39127000 | -1.87639200 | H | -4.05868600 | 3.31608000 | -2.09837400 |
| C | 0.56319600 | -1.90918500 | -2.74239600 | H | -4.98207500 | 4.71709100 | -0.25054800 |
| H | -0.51151900 | -3.47905900 | -1.72252000 | H | -3.84530800 | 4.74210200 | 1.96999000 |
| H | 0.62108400 | -0.80560000 | -2.80106700 | H | -1.79348400 | 3.41518600 | 2.33642500 |
| H | 1.53363400 | -2.27700500 | -2.37682500 | H | 1.28430800 | 1.97368900 | -1.98614600 |
| C | -3.99808900 | -3.81434000 | 0.51898400 | H | 0.99180100 | 4.08759000 | 1.76799800 |
| C | -5.30597400 | -3.99846700 | 0.72921800 | H | 2.62340800 | 5.76186300 | 0.95168700 |
| H | -3.29380700 | -3.85472300 | 1.35559800 | H | 3.56811300 | 5.57761400 | -1.34946400 |
| H | -5.70334200 | -4.20948600 | 1.72754800 | H | 2.88049100 | 3.68600700 | -2.82532000 |
| H | -6.03153500 | -3.94036600 | -0.09098600 | H | 4.77494400 | -2.00324300 | -0.01493800 |
| P | 2.01592400 | -0.83624400 | 0.43001500 | H | 5.58423000 | -4.34300200 | -0.06646400 |
| C | 1.98803500 | -0.46604300 | 2.27188700 | H | 3.99615700 | -6.22969100 | 0.31884900 |
| C | 1.52975100 | 0.96487200 | 2.62669600 | H | 1.58641800 | -5.74810000 | 0.75762800 |
| C | 0.08963100 | 1.39770100 | 2.28578900 | H | 0.76094900 | -3.39835300 | 0.78816600 |
| P | -0.19197900 | 1.62782500 | 0.45285700 | H | 3.97658500 | 1.33609900 | 1.37882700 |
| C | -1.75529700 | 2.59548800 | 0.32558400 | H | 3.01825600 | -0.80143800 | -2.25098500 |
| C | -2.41144900 | 2.57513500 | -0.91676100 | H | 4.73483200 | 0.49459500 | -3.46165500 |
| C | -3.55908900 | 3.34191200 | -1.12720200 | H | 6.07534200 | 2.23199500 | -2.26180500 |
| C | -4.07763000 | 4.12492300 | -0.09082300 | H | 5.66752800 | 2.63409700 | 0.16850500 |
| C | -3.44121500 | 4.13739700 | 1.15400300 | C | -0.96127200 | 0.44166500 | 2.85936300 |
| C | -2.28269300 | 3.38188500 | 1.36126100 | H | -1.97954700 | 0.83044500 | 2.71739600 |
| C | 1.02470200 | 2.91484700 | -0.05912500 | H | -0.91334900 | -0.55138300 | 2.38809400 |
| C | 1.56460900 | 2.81663300 | -1.35043200 | H | -0.79688800 | 0.31571900 | 3.94260300 |
| C | 1.40848800 | 3.98618700 | 0.76345900 | C | 3.26335600 | -0.84735200 | 3.03043000 |
| C | 2.32420700 | 4.93558500 | 0.30158900 | H | 4.11958100 | -0.20967300 | 2.76675300 |
| C | 2.85239800 | 4.83376100 | -0.99049900 | H | 3.09389400 | -0.74090000 | 4.11484200 |
| C | 2.46603400 | 3.77559200 | -1.81860600 | H | 3.54985200 | -1.89095900 | 2.83825400 |
| C | 2.71331400 | -2.54202000 | 0.38803300 | Co | -0.14987700 | -0.51127200 | -0.38345900 |
| C | 4.06921900 | -2.81927800 | 0.14946400 | | | | |
| C | 4.52684500 | -4.14013200 | 0.12314000 | 4''_D | | | |
| C | 3.63739600 | -5.19738600 | 0.34155300 | C | 3.10868500 | -1.73178400 | 0.50056900 |
| C | 2.28713400 | -4.92605200 | 0.58725500 | C | 4.49958000 | -1.55519900 | 0.55076100 |
| C | 1.82139200 | -3.60758900 | 0.60521700 | C | 5.25360100 | -1.40671300 | -0.61797700 |
| C | 3.36520500 | 0.15639300 | -0.33932100 | C | 4.62655700 | -1.44359500 | -1.86715300 |
| C | 4.12649100 | 1.13318500 | 0.32130000 | C | 3.24320800 | -1.64192500 | -1.93386900 |
| C | 3.59924800 | -0.05223400 | -1.71210100 | C | 2.49568700 | -1.78650000 | -0.76236900 |

| | | | | | | | |
|---|-------------|-------------|-------------|----|-------------|-------------|-------------|
| H | 5.00118800 | -1.51577300 | 1.52106900 | C | -4.32174500 | -3.95171500 | -0.80808600 |
| H | 6.33422100 | -1.25416100 | -0.55128800 | C | -3.37587700 | -4.91475600 | -1.17369600 |
| H | 5.21071800 | -1.32177100 | -2.78289000 | C | -2.04737200 | -4.53472600 | -1.39611400 |
| H | 2.74271800 | -1.68270900 | -2.90375500 | C | -1.66776700 | -3.19893000 | -1.24557100 |
| H | 1.41683300 | -1.94934800 | -0.83007200 | C | -3.28751600 | 0.31345700 | 0.32934100 |
| C | 2.29417000 | -1.88355300 | 1.76200400 | C | -4.08647300 | 1.40456700 | -0.04143300 |
| C | 0.90965200 | -1.15613900 | 1.84058400 | C | -3.32866400 | -0.13328000 | 1.66597600 |
| O | -0.24732400 | -1.74967600 | 1.55780600 | C | -4.16961300 | 0.47908600 | 2.59526100 |
| H | 1.34317300 | 1.12905800 | 4.57105200 | C | -4.97165500 | 1.56180400 | 2.21233700 |
| C | 2.72727000 | -1.02628100 | 2.99008400 | C | -4.92265600 | 2.02310400 | 0.89514400 |
| H | 3.36257100 | -0.17507800 | 2.70650800 | H | -1.49670200 | -0.59731400 | -2.98746300 |
| H | 3.22373800 | -1.57616800 | 3.80394300 | H | -2.02200700 | 2.25699700 | -1.99462300 |
| C | 2.17887400 | -3.38566800 | 2.14465900 | H | -1.71718600 | 1.84774200 | -3.67654100 |
| H | 1.61626400 | -3.44139600 | 3.09365000 | H | 0.28617100 | 2.64416000 | -2.79126500 |
| H | 3.19012200 | -3.78410500 | 2.33901700 | H | 2.76406700 | 0.99424000 | 1.05372800 |
| C | 1.25724600 | -0.60016400 | 3.23792300 | H | 5.14001000 | 1.72699100 | 1.14435700 |
| C | 0.95375100 | 0.84908200 | 3.57648400 | H | 6.03674400 | 3.25432100 | -0.61896700 |
| H | 0.79402600 | -1.25547700 | 3.99992800 | H | 4.53366700 | 4.04197500 | -2.44917800 |
| H | 1.39526800 | 1.53273900 | 2.83412800 | H | 2.17475400 | 3.33238300 | -2.51926000 |
| H | -0.13458600 | 1.02655900 | 3.58526700 | H | -1.19271700 | 1.74987900 | 1.63250200 |
| C | 1.47946600 | -4.22754800 | 1.11861500 | H | 0.40346500 | 4.48036600 | -1.29680300 |
| C | 2.02910700 | -5.25078300 | 0.45598200 | H | -0.82544300 | 6.35015300 | -0.22791300 |
| H | 0.44577100 | -3.93162900 | 0.91274700 | H | -2.23599800 | 5.93537200 | 1.78678900 |
| H | 1.46223000 | -5.82460700 | -0.28469200 | H | -2.41533500 | 3.62593300 | 2.72326200 |
| H | 3.06900900 | -5.55348800 | 0.62773400 | H | -4.68975900 | -1.86666600 | -0.38315800 |
| P | -2.02245300 | -0.49146600 | -0.72868100 | H | -5.36041300 | -4.24319000 | -0.63173400 |
| C | -2.14841000 | 0.13170400 | -2.47832600 | H | -3.67227000 | -5.96125400 | -1.28092900 |
| C | -1.51179200 | 1.52562800 | -2.64082800 | H | -1.30143000 | -5.28278000 | -1.67631100 |
| C | 0.01445400 | 1.63544500 | -2.44447300 | H | -0.62520100 | -2.91170800 | -1.39905600 |
| P | 0.54067400 | 1.53433300 | -0.64785000 | H | -4.05718300 | 1.79621400 | -1.05658600 |
| C | 2.29679200 | 2.11721600 | -0.71894800 | H | -2.67413500 | -0.95163100 | 1.97812700 |
| C | 3.15368300 | 1.67674600 | 0.29952300 | H | -4.19112900 | 0.11815300 | 3.62674800 |
| C | 4.48883500 | 2.08629600 | 0.34375500 | H | -5.62412900 | 2.04809700 | 2.94179300 |
| C | 4.99077100 | 2.93824700 | -0.64384000 | H | -5.53452000 | 2.87544100 | 0.58917100 |
| C | 4.14780600 | 3.37915400 | -1.67025900 | C | 0.79154600 | 0.60852000 | -3.27040900 |
| C | 2.81046100 | 2.97435800 | -1.70776600 | H | 1.87116000 | 0.81293200 | -3.25808300 |
| C | -0.31655600 | 2.98614300 | 0.10120800 | H | 0.64578400 | -0.41070000 | -2.88331800 |
| C | -1.11145700 | 2.76209200 | 1.23403200 | H | 0.45421000 | 0.62489400 | -4.32021100 |
| C | -0.21699600 | 4.28667400 | -0.41906400 | C | -3.52420200 | 0.03392200 | -3.14129800 |
| C | -0.90689400 | 5.34107300 | 0.18439200 | H | -4.23356100 | 0.78095900 | -2.75881700 |
| C | -1.69855500 | 5.10812600 | 1.31612300 | H | -3.42334400 | 0.20344000 | -4.22621100 |
| C | -1.79833700 | 3.81691200 | 1.84222700 | H | -3.97196200 | -0.96088900 | -2.99951000 |
| C | -2.61408900 | -2.22375200 | -0.88694900 | Co | -0.07387900 | -0.31955000 | 0.35327900 |
| C | -3.94438600 | -2.61216500 | -0.66787000 | | | | |

| | | | | | | | |
|-----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 4"Q | | | | C | 0.02953200 | -3.10337900 | 1.22383200 |
| C | -1.96599300 | 2.72010100 | 0.63722200 | C | -1.64340600 | -4.22423800 | -0.11961000 |
| C | -3.33484100 | 2.99832600 | 0.76793700 | C | -1.37632400 | -5.42068700 | 0.55004200 |
| C | -4.18567800 | 2.97017400 | -0.34264400 | C | -0.40482000 | -5.46142000 | 1.55833100 |
| C | -3.67871400 | 2.66966600 | -1.61107300 | C | 0.29759300 | -4.30104300 | 1.89447500 |
| C | -2.31301500 | 2.40672900 | -1.75990000 | C | 3.04639100 | 1.16419700 | -1.20138000 |
| C | -1.46798300 | 2.43218700 | -0.64548400 | C | 4.42599200 | 1.14449100 | -0.95014200 |
| H | -3.74406300 | 3.22757100 | 1.75548100 | C | 5.22257500 | 2.24725800 | -1.27818400 |
| H | -5.25203100 | 3.17469300 | -0.21490500 | C | 4.65083900 | 3.37906100 | -1.86699300 |
| H | -4.34337600 | 2.63908200 | -2.47805400 | C | 3.27558200 | 3.40414000 | -2.12751000 |
| H | -1.90273400 | 2.18151700 | -2.74637500 | C | 2.48043200 | 2.30664700 | -1.79122000 |
| H | -0.39349400 | 2.25855600 | -0.77188900 | C | 2.88993200 | -1.26269900 | 0.36793400 |
| C | -1.04409400 | 2.72712600 | 1.83262200 | C | 3.25191400 | -2.60041200 | 0.14902800 |
| C | 0.14424600 | 1.69658700 | 1.83306800 | C | 3.14733200 | -0.68582800 | 1.62927200 |
| O | 1.35334600 | 1.96745900 | 1.42158600 | C | 3.77911200 | -1.42614100 | 2.62972300 |
| H | -0.65159100 | -0.41626300 | 4.62976500 | C | 4.14756900 | -2.75771100 | 2.39844000 |
| C | -1.56730900 | 2.00839000 | 3.11092600 | C | 3.87706700 | -3.34137900 | 1.15862700 |
| H | -2.40320800 | 1.32708700 | 2.88945800 | H | 1.41799600 | -0.24912300 | -3.06931300 |
| H | -1.86144300 | 2.66853500 | 3.94108600 | H | 1.00083500 | -2.99475400 | -1.76618000 |
| C | -0.56595400 | 4.17279900 | 2.13633800 | H | 0.88707300 | -2.70899300 | -3.49483700 |
| H | 0.07181000 | 4.12781100 | 3.03724900 | H | -1.29849800 | -2.74598100 | -2.69408800 |
| H | -1.43857500 | 4.80370700 | 2.38242100 | H | -3.00517800 | -0.09293400 | 1.10042700 |
| C | -0.22646000 | 1.24870000 | 3.27173600 | H | -5.47200700 | 0.15122800 | 1.24841400 |
| C | -0.27551400 | -0.23342300 | 3.60734000 | H | -6.93684400 | -0.90533000 | -0.47760100 |
| H | 0.43419500 | 1.77057900 | 3.99261100 | H | -5.91076200 | -2.21975800 | -2.33327600 |
| H | -0.93374100 | -0.76782200 | 2.90258000 | H | -3.45985000 | -2.49421300 | -2.46212800 |
| H | 0.72593600 | -0.69037300 | 3.53581200 | H | 0.58040200 | -2.19922400 | 1.48311000 |
| C | 0.21740000 | 4.78437900 | 1.01279600 | H | -2.40804300 | -4.20195100 | -0.89934500 |
| C | -0.15015300 | 5.86083700 | 0.30955300 | H | -1.92922900 | -6.32595500 | 0.28611500 |
| H | 1.13969900 | 4.24947600 | 0.76253100 | H | -0.19847900 | -6.39868000 | 2.08146500 |
| H | 0.46493500 | 6.24674600 | -0.51026300 | H | 1.05818000 | -4.32335300 | 2.67851400 |
| H | -1.08180000 | 6.39772400 | 0.52543300 | H | 4.88467400 | 0.26574100 | -0.49272700 |
| P | 1.91326300 | -0.22690200 | -0.79389900 | H | 6.29600400 | 2.21939200 | -1.07305100 |
| C | 1.80110200 | -1.08253000 | -2.45805700 | H | 5.27362100 | 4.24080600 | -2.12025900 |
| C | 0.76103400 | -2.22143700 | -2.51276100 | H | 2.81857300 | 4.28620200 | -2.58359300 |
| C | -0.73362500 | -1.84413700 | -2.40695900 | H | 1.40478100 | 2.34282000 | -1.97930400 |
| P | -1.22064800 | -1.44700200 | -0.64606100 | H | 3.03542500 | -3.08684800 | -0.80041300 |
| C | -3.05705000 | -1.32295700 | -0.67628300 | H | 2.81065100 | 0.33967800 | 1.81649700 |
| C | -3.64528900 | -0.57845000 | 0.35966200 | H | 3.97397000 | -0.96542500 | 3.60193600 |
| C | -5.03249100 | -0.43532800 | 0.43806800 | H | 4.63551500 | -3.33861700 | 3.18524900 |
| C | -5.85166800 | -1.02415200 | -0.53010000 | H | 4.14708400 | -4.38394000 | 0.97215300 |
| C | -5.27581600 | -1.76002500 | -1.57150800 | C | -1.12220000 | -0.69711100 | -3.34100000 |
| C | -3.88793700 | -1.91276500 | -1.64347200 | H | -2.20976700 | -0.54106900 | -3.36419400 |
| C | -0.93934700 | -3.05430200 | 0.21049800 | H | -0.66036400 | 0.24960900 | -3.02635800 |

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|--------------------------------------|-------------|-------------|-------------|--------------------------------------|-------------|-------------|-------------|
| H | -0.78812900 | -0.91237900 | -4.36967900 | H | -6.56728700 | -0.83135000 | 0.15373800 |
| C | 3.13575200 | -1.50231100 | -3.08174200 | H | -4.44917700 | 0.27329200 | 0.83238200 |
| H | 3.56633000 | -2.39207300 | -2.60168000 | H | -0.88878700 | 1.40166100 | -1.89521100 |
| H | 2.98605300 | -1.74543100 | -4.14696600 | H | -2.66331500 | 1.78344400 | 2.01850100 |
| H | 3.88087600 | -0.69536900 | -3.02495600 | H | -2.86259700 | 4.22888400 | 1.69278800 |
| Co | -0.05339600 | 0.27661600 | 0.29226500 | H | -2.10672500 | 5.27956800 | -0.43710800 |
| | | | | H | -1.12646400 | 3.86356400 | -2.24329100 |
| | | | | H | 4.43160800 | 0.34079200 | 0.19719900 |
| cat_S^{DCE} | | | | H | 6.41659100 | -1.07140300 | -0.27956900 |
| P | 1.46579500 | -0.34529900 | 0.21608400 | H | 6.13273300 | -3.46990000 | -0.89218300 |
| C | 1.24653500 | -0.56418100 | 2.05931600 | H | 3.84629200 | -4.45920500 | -1.02796700 |
| C | -0.12632600 | -0.11138200 | 2.59157100 | H | 1.84747500 | -3.03640700 | -0.54701100 |
| C | -1.37430300 | -0.78051700 | 1.98993800 | H | 1.08754700 | 2.30999200 | 1.65591500 |
| P | -1.56835000 | -0.38795500 | 0.18041400 | H | 2.60837400 | 0.85427600 | -2.12204000 |
| C | -3.19180500 | -1.10270300 | -0.27598100 | H | 2.96035100 | 3.18796600 | -2.86831400 |
| C | -3.17204200 | -2.21874200 | -1.12765100 | H | 2.37660300 | 5.08964800 | -1.35777600 |
| C | -4.36414300 | -2.83593000 | -1.51455200 | H | 1.44098000 | 4.62257900 | 0.90840400 |
| C | -5.58540400 | -2.33734200 | -1.05059600 | C | -1.38473600 | -2.30207200 | 2.16074400 |
| C | -5.61186100 | -1.22185200 | -0.20515900 | H | -2.36580200 | -2.72699200 | 1.90220000 |
| C | -4.42044300 | -0.60217800 | 0.17982600 | H | -0.63449200 | -2.77907600 | 1.51030300 |
| C | -1.78295100 | 1.42732800 | 0.06431600 | H | -1.16094400 | -2.57181600 | 3.20557400 |
| C | -1.34898800 | 2.02915000 | -1.12791500 | C | 2.39921900 | -0.00639700 | 2.89693600 |
| C | -2.32792500 | 2.22856700 | 1.07983800 | H | 2.42210200 | 1.09246100 | 2.89872800 |
| C | -2.44143900 | 3.61003700 | 0.89668200 | H | 2.28793300 | -0.33867500 | 3.94195700 |
| C | -2.01861000 | 4.19915400 | -0.29925500 | H | 3.37339900 | -0.36570200 | 2.53537900 |
| C | -1.47333000 | 3.40582700 | -1.31410000 | Co | -0.03132400 | -1.20088600 | -1.00916300 |
| C | 3.01124700 | -1.26357800 | -0.13418000 | | | | |
| C | 4.29918300 | -0.71046900 | -0.06582800 | | | | |
| C | 5.41551600 | -1.50578800 | -0.33702700 | cat_T^{DCE} | | | |
| C | 5.25593900 | -2.85331000 | -0.67974500 | P | 1.61093500 | -0.46521600 | 0.10840600 |
| C | 3.97481100 | -3.40889000 | -0.75536300 | C | 1.23434100 | -0.80837200 | 1.91041500 |
| C | 2.85701000 | -2.61554100 | -0.48659500 | C | -0.15709600 | -0.32765200 | 2.37510500 |
| C | 1.84913100 | 1.40557000 | -0.16593600 | C | -1.41758800 | -0.97023600 | 1.76388700 |
| C | 1.51706800 | 2.48089400 | 0.67109000 | P | -1.74576400 | -0.45776000 | -0.00369500 |
| C | 2.36204200 | 1.67879600 | -1.44815400 | C | -3.46684300 | -1.04313400 | -0.27610800 |
| C | 2.55682900 | 2.99359800 | -1.87153800 | C | -3.65515600 | -2.11116800 | -1.16645800 |
| C | 2.23061900 | 4.05934100 | -1.02464900 | C | -4.93410500 | -2.62539900 | -1.39957400 |
| C | 1.71019100 | 3.79803500 | 0.24435000 | C | -6.03808000 | -2.06715400 | -0.74886800 |
| H | 1.28958200 | -1.66391600 | 2.12698400 | C | -5.85950100 | -0.99718800 | 0.13600100 |
| H | -0.22093300 | 0.98147800 | 2.51622600 | C | -4.58097600 | -0.48728600 | 0.37260000 |
| H | -0.13284200 | -0.33507300 | 3.67225700 | C | -1.86847000 | 1.37225900 | 0.02854400 |
| H | -2.25398700 | -0.36327200 | 2.50579000 | C | -1.45359300 | 2.05028100 | -1.13012500 |
| H | -2.20920400 | -2.60488300 | -1.47895600 | C | -2.30163400 | 2.11846500 | 1.13599400 |
| H | -4.34081700 | -3.70452300 | -2.17712500 | C | -2.31990500 | 3.51517400 | 1.08048100 |
| H | -6.52033200 | -2.81725000 | -1.35013600 | C | -1.91126500 | 4.17957900 | -0.08023900 |

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|---|-------------|-------------|-------------|--------------------------------------|-------------|-------------|-------------|
| C | -1.48121300 | 3.44431700 | -1.18928800 | H | 3.30964900 | -0.77491400 | 2.61261900 |
| C | 3.26055200 | -1.23735100 | -0.12273600 | Co | -0.03220800 | -1.10188000 | -1.28046100 |
| C | 4.47447500 | -0.58728400 | 0.15113900 | | | | |
| C | 5.68725200 | -1.25309800 | -0.04389100 | TS4_T^{DCE} | | | |
| C | 5.69996000 | -2.57285100 | -0.50895800 | C | -3.41386100 | -1.48632700 | -0.66063500 |
| C | 4.49511800 | -3.22575100 | -0.78770000 | C | -4.41855300 | -1.19139900 | -1.59428600 |
| C | 3.28236000 | -2.55645800 | -0.60357000 | C | -5.55599600 | -0.47480100 | -1.21270600 |
| C | 1.92687100 | 1.32610500 | -0.13807900 | C | -5.70099700 | -0.03460900 | 0.10682800 |
| C | 1.59015200 | 2.33942600 | 0.77164900 | C | -4.70279500 | -0.31805500 | 1.04141000 |
| C | 2.42332400 | 1.69411100 | -1.40383200 | C | -3.57094400 | -1.04375400 | 0.66144800 |
| C | 2.59550200 | 3.03629400 | -1.74177200 | H | -4.31834700 | -1.53531700 | -2.62665900 |
| C | 2.26035000 | 4.03907000 | -0.82435100 | H | -6.33140300 | -0.25607900 | -1.95119700 |
| C | 1.75646200 | 3.68528000 | 0.42861500 | H | -6.58471700 | 0.53564500 | 0.40193100 |
| H | 1.22844200 | -1.91143200 | 1.90398300 | H | -4.80119500 | 0.03085100 | 2.07207900 |
| H | -0.22707300 | 0.76508400 | 2.28993700 | H | -2.80333600 | -1.27070700 | 1.40136300 |
| H | -0.20290900 | -0.54124600 | 3.45675200 | C | -2.23246000 | -2.35127000 | -1.05385700 |
| H | -2.27385400 | -0.60391500 | 2.35408700 | C | -0.93361900 | -1.99349900 | -0.32486700 |
| H | -2.78801500 | -2.54106800 | -1.67599300 | O | -0.53961900 | -2.38588000 | 0.75754800 |
| H | -5.06876500 | -3.45902500 | -2.09329800 | H | 0.52285100 | -1.06826500 | -3.81309100 |
| H | -7.03989900 | -2.46339400 | -0.93209500 | C | -1.59332200 | -2.07097200 | -2.43476500 |
| H | -6.72178800 | -0.55712100 | 0.64313600 | H | -1.95342400 | -1.12954000 | -2.87290400 |
| H | -4.45352700 | 0.34923600 | 1.06279600 | H | -1.73277400 | -2.87631700 | -3.16938100 |
| H | -1.09745600 | 1.47331000 | -1.98876000 | C | -2.57480400 | -3.86125400 | -0.87496900 |
| H | -2.62247000 | 1.61486900 | 2.04967400 | H | -1.68744800 | -4.44007900 | -1.18643400 |
| H | -2.65335700 | 4.08716500 | 1.94988200 | H | -3.38557500 | -4.09068200 | -1.58445700 |
| H | -1.92131900 | 5.27157900 | -0.11775400 | C | -0.14244300 | -1.91905100 | -1.95252200 |
| H | -1.15080200 | 3.95799900 | -2.09496500 | C | 0.72575500 | -0.93314000 | -2.73661800 |
| H | 4.47303500 | 0.44278700 | 0.51332900 | H | 0.38301500 | -2.88072800 | -1.86810900 |
| H | 6.62791900 | -0.73929500 | 0.16961000 | H | 0.47864300 | 0.14406900 | -2.56204500 |
| H | 6.65057400 | -3.09025100 | -0.66001500 | H | 1.79942900 | -1.07502400 | -2.56946900 |
| H | 4.50019900 | -4.25357900 | -1.15881600 | C | -2.97643900 | -4.26372500 | 0.51278800 |
| H | 2.33742600 | -3.05461700 | -0.84061500 | C | -4.20345700 | -4.66341800 | 0.85907500 |
| H | 1.18169200 | 2.09845200 | 1.75110800 | H | -2.19256000 | -4.20056100 | 1.27455400 |
| H | 2.67637000 | 0.91838600 | -2.13222900 | H | -4.44444600 | -4.94411000 | 1.88907800 |
| H | 2.98748700 | 3.30169900 | -2.72678800 | H | -5.01476000 | -4.72195400 | 0.12469000 |
| H | 2.38692000 | 5.09135600 | -1.08976000 | P | 2.10014000 | -0.70128800 | 0.42533700 |
| H | 1.48186800 | 4.45967500 | 1.14852800 | C | 2.01372600 | -0.27630200 | 2.24470600 |
| C | -1.40797900 | -2.49914000 | 1.83080700 | C | 1.54347400 | 1.17722600 | 2.47058700 |
| H | -2.38620000 | -2.92028100 | 1.55534800 | C | 0.04953500 | 1.53395200 | 2.27235200 |
| H | -0.65575000 | -2.92641600 | 1.14811000 | P | -0.42342200 | 1.75356900 | 0.48851700 |
| H | -1.16920500 | -2.83786000 | 2.85214200 | C | -2.13323100 | 2.41949600 | 0.46804600 |
| C | 2.32865700 | -0.36073000 | 2.88402300 | C | -2.88978900 | 2.24021100 | -0.70057800 |
| H | 2.42383300 | 0.73381300 | 2.93040900 | C | -4.15917900 | 2.80961200 | -0.81534500 |
| H | 2.08718300 | -0.71621900 | 3.89914000 | C | -4.69271200 | 3.54805300 | 0.24455900 |

| | | | | | | | |
|---|-------------|-------------|-------------|--------------------------------------|-------------|-------------|-------------|
| C | -1.96362500 | -0.31364800 | 2.61065500 | H | 1.85582600 | 5.04849500 | 2.44085100 |
| C | -1.00020300 | -1.48819100 | 2.36803600 | H | 0.91907000 | 2.77434100 | 2.30508000 |
| P | -0.78835300 | -1.74288900 | 0.52569600 | H | -4.09352700 | 1.36687000 | 1.33564200 |
| C | 0.38178700 | -3.14731800 | 0.33976700 | H | -1.63295700 | 1.88615700 | -2.18727500 |
| C | 1.72873600 | -2.95576900 | 0.70057100 | H | -3.66038700 | 1.83201800 | -3.60195600 |
| C | 2.66468500 | -3.97444600 | 0.51304200 | H | -5.90923000 | 1.52844700 | -2.55685700 |
| C | 2.27680800 | -5.19213800 | -0.05423800 | H | -6.09841800 | 1.30438300 | -0.07984600 |
| C | 0.94697400 | -5.38178600 | -0.43776200 | C | 0.28723700 | -1.39147600 | 3.18689600 |
| C | 0.00415800 | -4.36750000 | -0.24401900 | H | 0.83380900 | -2.34395000 | 3.18414800 |
| C | -2.44816100 | -2.40474900 | 0.09535400 | H | 0.96417000 | -0.60672800 | 2.82702800 |
| C | -3.23624100 | -1.76628400 | -0.87330900 | H | 0.02440100 | -1.16481700 | 4.23342600 |
| C | -2.97687400 | -3.51858900 | 0.77451200 | C | -2.20069000 | 2.15201200 | 3.17013200 |
| C | -4.25643800 | -3.98850400 | 0.47671800 | H | -3.27762600 | 2.10135500 | 2.95896000 |
| C | -5.03113100 | -3.34877400 | -0.49766700 | H | -2.06805300 | 1.96514500 | 4.24764500 |
| C | -4.51987500 | -2.23621200 | -1.16816500 | H | -1.86306200 | 3.17629200 | 2.96321200 |
| C | -0.47150300 | 3.24813300 | 0.70130000 | Co | -0.17121900 | 0.01767000 | -0.74032700 |
| C | -0.92602600 | 4.26089200 | -0.15673600 | | | | |
| C | -0.38032500 | 5.54555700 | -0.08397500 | | | | |
| C | 0.61936300 | 5.83586900 | 0.84800800 | TS8_s^{DCE} | | | |
| C | 1.07317300 | 4.83264400 | 1.70985000 | C | -3.98572100 | -2.03057300 | -0.92007200 |
| C | 0.53563900 | 3.54638200 | 1.63764700 | C | -4.27545000 | -1.70761700 | -2.25825700 |
| C | -2.70740200 | 1.63620600 | -0.31727900 | C | -5.57360300 | -1.80602500 | -2.75988900 |
| C | -3.97736200 | 1.47347000 | 0.25954100 | C | -6.61707700 | -2.23710700 | -1.93304600 |
| C | -2.61144900 | 1.76311500 | -1.71853600 | C | -6.34454700 | -2.56461900 | -0.60362700 |
| C | -3.75510500 | 1.73022400 | -2.51837500 | C | -5.04215600 | -2.45931400 | -0.10205500 |
| C | -5.01308900 | 1.56218500 | -1.93285700 | H | -3.47408700 | -1.36698900 | -2.91613200 |
| C | -5.11886800 | 1.43711600 | -0.54473800 | H | -5.77263500 | -1.54347800 | -3.80214600 |
| H | -0.37296500 | 1.11889400 | 2.76438500 | H | -7.63438300 | -2.31671000 | -2.32433000 |
| H | -2.88897800 | -0.46214000 | 2.03373100 | H | -7.14880800 | -2.90587600 | 0.05330600 |
| H | -2.26231900 | -0.36579600 | 3.67061000 | H | -4.85966600 | -2.72197200 | 0.94029800 |
| H | -1.52892200 | -2.39769200 | 2.69095000 | C | -2.56448800 | -1.90684200 | -0.40785700 |
| H | 2.06340000 | -2.00839100 | 1.12075100 | C | -1.93594200 | -0.50883700 | -0.61708200 |
| H | 3.70382200 | -3.80580400 | 0.80191000 | O | -2.48848200 | 0.41340300 | -1.15785900 |
| H | 3.01111100 | -5.98733000 | -0.20360400 | H | 0.32708500 | -0.21336600 | -1.65026700 |
| H | 0.63549700 | -6.32476300 | -0.89362600 | C | -1.58940000 | -2.85790200 | -1.16806800 |
| H | -1.02574200 | -4.53305000 | -0.55995600 | H | -1.87083000 | -2.88705500 | -2.23076300 |
| H | -2.86651700 | -0.88637200 | -1.39561500 | H | -1.70257500 | -3.88058900 | -0.77937800 |
| H | -2.38693100 | -4.03097200 | 1.53696000 | C | -2.42372700 | -2.02121000 | 1.12903900 |
| H | -4.65057700 | -4.85780800 | 1.00839600 | H | -2.65093400 | -3.04726300 | 1.46455900 |
| H | -6.03371100 | -3.71668400 | -0.72890700 | H | -3.15267900 | -1.34826900 | 1.59786700 |
| H | -5.11985800 | -1.72184200 | -1.92184400 | C | -0.13440000 | -2.38462900 | -1.04897500 |
| H | -1.71241100 | 4.05679600 | -0.88395600 | C | 0.29180000 | -1.29492000 | -2.02611500 |
| H | -0.74462800 | 6.32370600 | -0.75894100 | H | 0.59052000 | -3.20008800 | -1.09545300 |
| H | 1.04357100 | 6.84109500 | 0.90350400 | H | 1.30500700 | -1.45989100 | -2.41059900 |
| | | | | H | -0.41850000 | -1.20674000 | -2.86115700 |

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|---|-------------|-------------|-------------|---------------------|-------------|-------------|-------------|
| C | -1.00276500 | -1.64455700 | 1.50898200 | H | 0.97572600 | 4.20558300 | 0.97109300 |
| C | -0.02590600 | -2.53699500 | 0.98428700 | H | 1.44766500 | 5.90263200 | -0.73547000 |
| H | -0.82754100 | -1.19605600 | 2.48790200 | H | 0.73535700 | 5.55137600 | -3.10214200 |
| H | 0.97850800 | -2.52348700 | 1.39754900 | H | -0.47949200 | 3.45817400 | -3.72420300 |
| H | -0.34334600 | -3.55817300 | 0.76733200 | H | 3.11512600 | -2.46755600 | -1.56513600 |
| P | 2.34207300 | -0.45402000 | 0.39867300 | H | 3.96603100 | -4.78155800 | -1.38720200 |
| C | 2.89725100 | 0.48300300 | 1.91370900 | H | 4.47114100 | -5.76605800 | 0.85172700 |
| C | 2.24759000 | 1.87492100 | 1.95694200 | H | 4.10888600 | -4.40108300 | 2.90956700 |
| C | 0.74469500 | 1.94580600 | 2.28556600 | H | 3.24455500 | -2.10036200 | 2.74330100 |
| P | -0.35533400 | 1.49522800 | 0.83683900 | H | 5.17131000 | -0.74525500 | -0.52537200 |
| C | -2.03344700 | 1.98280000 | 1.43216700 | H | 1.66774600 | 1.49993600 | -1.67040900 |
| C | -2.68860700 | 1.20193200 | 2.39915600 | H | 2.95703500 | 2.62494700 | -3.44514100 |
| C | -3.96331700 | 1.54640600 | 2.85271600 | H | 5.37452900 | 2.07168700 | -3.77700900 |
| C | -4.60904800 | 2.67611900 | 2.34210400 | H | 6.46493200 | 0.37872900 | -2.30319500 |
| C | -3.96689600 | 3.45856700 | 1.37954000 | C | 0.40662300 | 1.18554200 | 3.56949100 |
| C | -2.68945800 | 3.11612200 | 0.92671900 | H | -0.59492700 | 1.43463300 | 3.94144400 |
| C | 0.00853700 | 2.81955900 | -0.39917400 | H | 0.46425300 | 0.09584600 | 3.44268000 |
| C | -0.40445500 | 2.64008400 | -1.73095600 | H | 1.12883000 | 1.46721100 | 4.35283700 |
| C | 0.66417400 | 4.01249400 | -0.05450600 | C | 4.41561200 | 0.60349300 | 2.05442200 |
| C | 0.92757700 | 4.98567500 | -1.02275300 | H | 4.83202800 | 1.28638400 | 1.29924500 |
| C | 0.52716600 | 4.79008700 | -2.34655600 | H | 4.65656400 | 1.01604600 | 3.04752200 |
| C | -0.14920800 | 3.61710500 | -2.69488100 | H | 4.92777900 | -0.36390500 | 1.95933700 |
| C | 3.12458900 | -2.10705600 | 0.57259200 | Co | -0.11241700 | -0.58714600 | 0.03063400 |
| C | 3.32630800 | -2.88700600 | -0.58023700 | | | | |
| C | 3.80928100 | -4.19281900 | -0.48016100 | cat _{LIRh} | | | |
| C | 4.09278600 | -4.74409100 | 0.77375200 | P | 1.47124900 | -0.27898400 | 0.30743200 |
| C | 3.88987600 | -3.97988900 | 1.92548300 | C | 1.24514500 | -0.44585900 | 2.15133700 |
| C | 3.40604200 | -2.67167400 | 1.82807500 | C | -0.12329500 | 0.04078500 | 2.67359200 |
| C | 3.32003100 | 0.30161000 | -0.96418000 | C | -1.38480400 | -0.62853000 | 2.09360900 |
| C | 4.67940700 | -0.00624700 | -1.15790400 | P | -1.55221100 | -0.32867100 | 0.26711600 |
| C | 2.71653300 | 1.24915300 | -1.80244000 | C | -3.18184300 | -1.03866600 | -0.17869900 |
| C | 3.44918800 | 1.88741000 | -2.80697200 | C | -3.20090100 | -2.19703600 | -0.97076800 |
| C | 4.79858100 | 1.57782600 | -2.99056300 | C | -4.41546200 | -2.78505300 | -1.32869200 |
| C | 5.41000200 | 0.62768300 | -2.16452400 | C | -5.61648100 | -2.21949500 | -0.89439600 |
| H | 2.51313600 | -0.11704400 | 2.75215900 | C | -5.60271600 | -1.06483200 | -0.10612200 |
| H | 2.47337500 | 2.40815000 | 1.02043400 | C | -4.39071000 | -0.47225900 | 0.24897300 |
| H | 2.76204200 | 2.44219600 | 2.75058000 | C | -1.77008600 | 1.48348800 | 0.07747700 |
| H | 0.50509000 | 3.00443400 | 2.46763300 | C | -1.44273500 | 2.04306200 | -1.16796600 |
| H | -2.20808700 | 0.31438400 | 2.80274100 | C | -2.22573600 | 2.32165200 | 1.10482100 |
| H | -4.45445500 | 0.92382500 | 3.60445000 | C | -2.34207300 | 3.69688800 | 0.88980000 |
| H | -5.60953500 | 2.94303400 | 2.69096500 | C | -2.01393200 | 4.24446300 | -0.35163600 |
| H | -4.46288600 | 4.34188900 | 0.96984600 | C | -1.56993500 | 3.41354500 | -1.38435400 |
| H | -2.21373500 | 3.73605600 | 0.16727200 | C | 3.05114200 | -1.14543500 | -0.02716600 |
| H | -0.94728800 | 1.73846100 | -2.00839300 | C | 4.30329300 | -0.51625400 | 0.02947200 |

| | | | | | | | |
|----|-------------|-------------|-------------|-------------------|-------------|-------------|-------------|
| C | 5.46306000 | -1.24404700 | -0.23939300 | 3_{LIRh} | | | |
| C | 5.38287900 | -2.59971500 | -0.57030600 | C | -3.36095000 | -0.94012200 | -0.91791100 |
| C | 4.13893100 | -3.23222800 | -0.63142900 | C | -4.09277600 | -1.29111700 | -2.06166900 |
| C | 2.97630800 | -2.50830900 | -0.36189700 | C | -4.98368800 | -0.39133800 | -2.64569100 |
| C | 1.79898400 | 1.47086200 | -0.13350200 | C | -5.16930500 | 0.87854800 | -2.09122600 |
| C | 1.48876000 | 2.56259100 | 0.68763900 | C | -4.46224800 | 1.23256700 | -0.94299500 |
| C | 2.26450800 | 1.71473100 | -1.43882600 | C | -3.56793200 | 0.32939900 | -0.36106300 |
| C | 2.42448600 | 3.01784700 | -1.90370200 | H | -3.97030200 | -2.27499700 | -2.50178300 |
| C | 2.11176800 | 4.10069000 | -1.07573100 | H | -5.53746000 | -0.68423000 | -3.53316500 |
| C | 1.64509100 | 3.86868900 | 0.21760100 | H | -5.86537800 | 1.57824500 | -2.54423200 |
| H | 1.27921100 | -1.53683400 | 2.25779600 | H | -4.60081400 | 2.21036400 | -0.49397300 |
| H | -0.20292100 | 1.12466600 | 2.56477600 | H | -3.04095800 | 0.62099600 | 0.54187900 |
| H | -0.13006800 | -0.15497600 | 3.75313700 | C | -2.44776700 | -1.96526500 | -0.24473100 |
| H | -2.25266200 | -0.16228000 | 2.57365700 | C | -1.42239900 | -1.24303500 | 0.67634900 |
| H | -2.26116600 | -2.63902100 | -1.29801800 | O | -1.42145600 | -1.36995500 | 1.88418000 |
| H | -4.42370800 | -3.68085900 | -1.94255600 | H | -1.42818000 | -0.12866900 | -2.78934900 |
| H | -6.56229700 | -2.67600600 | -1.17060800 | C | -1.52862800 | -2.71586200 | -1.24118400 |
| H | -6.53692600 | -0.62496300 | 0.23020600 | H | -2.12488100 | -3.17178300 | -2.04112100 |
| H | -4.38578100 | 0.42961800 | 0.85343100 | H | -1.06710400 | -3.53913500 | -0.68722300 |
| H | -1.06541400 | 1.39439300 | -1.95411700 | C | -3.31254800 | -2.98919700 | 0.54811300 |
| H | -2.48694800 | 1.91293000 | 2.07490000 | H | -2.62425200 | -3.65842400 | 1.07828400 |
| H | -2.68758300 | 4.33881400 | 1.69470000 | H | -3.85080400 | -3.58853900 | -0.19480900 |
| H | -2.09942000 | 5.31483400 | -0.51352900 | C | -0.42691600 | -1.80470600 | -1.78466900 |
| H | -1.30501100 | 3.83569000 | -2.34900400 | C | -0.77611700 | -0.98396300 | -3.02139100 |
| H | 4.37188500 | 0.53701700 | 0.28031500 | H | 0.47338700 | -2.39451800 | -1.96800400 |
| H | 6.43008900 | -0.75247300 | -0.18990300 | H | 0.12664000 | -0.58800100 | -3.49942900 |
| H | 6.28835600 | -3.16071600 | -0.78161600 | H | -1.31880100 | -1.58020100 | -3.77017400 |
| H | 4.07316700 | -4.28475900 | -0.89060300 | C | -4.29212900 | -2.38991900 | 1.51454800 |
| H | 2.00163400 | -2.99205900 | -0.40781500 | C | -5.61620900 | -2.40423800 | 1.34938400 |
| H | 1.10769300 | 2.41473000 | 1.68820000 | H | -3.86511100 | -1.91005100 | 2.39284400 |
| H | 2.49807600 | 0.87947600 | -2.09278100 | H | -6.28771600 | -1.95438000 | 2.07635200 |
| H | 2.78778300 | 3.18882300 | -2.91275200 | H | -6.07641500 | -2.86957600 | 0.47970900 |
| H | 2.22800300 | 5.11688000 | -1.44017800 | P | 1.58853700 | -1.14627400 | 0.52225200 |
| H | 1.39214900 | 4.70251900 | 0.86528700 | C | 1.79969300 | -0.69618700 | 2.32070400 |
| C | -1.43657400 | -2.13667600 | 2.36765400 | C | 1.97926500 | 0.81127300 | 2.62253400 |
| H | -2.40924000 | -2.55482300 | 2.09373300 | C | 0.74637200 | 1.73404600 | 2.53400400 |
| H | -0.66933800 | -2.67412400 | 1.80068700 | P | 0.17184000 | 1.88922800 | 0.78157300 |
| H | -1.27326100 | -2.32509000 | 3.43431000 | C | -1.05933500 | 3.25030100 | 0.75732200 |
| C | 2.40215200 | 0.13382000 | 2.97537000 | C | -1.86127000 | 3.37251700 | -0.38713200 |
| H | 2.44487100 | 1.22403400 | 2.92390100 | C | -2.76101200 | 4.43147600 | -0.51256800 |
| H | 2.27120600 | -0.14665100 | 4.02612500 | C | -2.87838000 | 5.37303000 | 0.51228000 |
| H | 3.36552400 | -0.25914500 | 2.64101300 | C | -2.08295400 | 5.25853600 | 1.65484200 |
| Rh | -0.00997400 | -1.24327000 | -0.95438800 | C | -1.17152900 | 4.20836800 | 1.77587000 |
| | | | | C | 1.57587400 | 2.66802000 | -0.11545200 |

| | | | | | | | |
|---|-------------|-------------|-------------|---------------------------------|-------------|-------------|-------------|
| C | 1.71358700 | 2.35271300 | -1.47584200 | H | -0.02056000 | 1.19056100 | 4.47964400 |
| C | 2.48386700 | 3.55830000 | 0.47472400 | C | 2.89412100 | -1.51706300 | 3.02501700 |
| C | 3.51950200 | 4.10848600 | -0.28180600 | H | 3.89933300 | -1.21234200 | 2.72386100 |
| C | 3.65018800 | 3.78779900 | -1.63543200 | H | 2.80809300 | -1.35779000 | 4.10470600 |
| C | 2.74082800 | 2.91383800 | -2.23477900 | H | 2.79394000 | -2.58667300 | 2.83419700 |
| C | 1.61140500 | -2.98193200 | 0.52170400 | Rh | -0.19384000 | -0.21874200 | -0.44243400 |
| C | 2.42155800 | -3.70658900 | -0.36274900 | | | | |
| C | 2.36674100 | -5.10209200 | -0.38868400 | TS ₄ _{LIRh} | | | |
| C | 1.51243800 | -5.78978800 | 0.47308300 | C | -3.59784600 | -0.91733500 | -0.53447800 |
| C | 0.71365200 | -5.07454800 | 1.36929700 | C | -4.46240900 | -0.54491100 | -1.57344200 |
| C | 0.75794900 | -3.68187800 | 1.39286700 | C | -5.46309700 | 0.40571900 | -1.36413600 |
| C | 3.03759300 | -0.62832800 | -0.46976000 | C | -5.61166200 | 1.00446700 | -0.11105500 |
| C | 4.18978400 | -0.05656200 | 0.08810900 | C | -4.75098900 | 0.64676800 | 0.92829500 |
| C | 2.96504300 | -0.78142500 | -1.86680600 | C | -3.75762800 | -0.30993600 | 0.71753700 |
| C | 4.02508100 | -0.38766300 | -2.68007600 | H | -4.36675200 | -1.01637500 | -2.54730900 |
| C | 5.16397900 | 0.19049900 | -2.11543600 | H | -6.12694900 | 0.67781400 | -2.17994000 |
| C | 5.24029500 | 0.35744800 | -0.73255800 | H | -6.38603200 | 1.74813700 | 0.05116200 |
| H | 0.83168600 | -1.00868100 | 2.72559600 | H | -4.85256300 | 1.11165200 | 1.90463100 |
| H | 2.78514900 | 1.23182300 | 2.01831300 | H | -3.10823200 | -0.60120700 | 1.53169800 |
| H | 2.32399400 | 0.86753400 | 3.66162700 | C | -2.63267400 | -2.05724500 | -0.72071800 |
| H | 1.08674600 | 2.72361400 | 2.85695000 | C | -1.16749700 | -2.02160900 | -0.13317700 |
| H | -1.78152000 | 2.63707000 | -1.18164200 | O | -0.88519300 | -2.40355800 | 1.02014100 |
| H | -3.37567200 | 4.51288000 | -1.40396900 | H | 0.29021600 | -2.67931500 | -3.51561400 |
| H | -3.58442300 | 6.19290800 | 0.42054800 | C | -2.04347600 | -2.29114000 | -2.12770000 |
| H | -2.16568500 | 5.99130700 | 2.45215300 | H | -2.01008000 | -1.36602100 | -2.71434500 |
| H | -0.54819900 | 4.14845700 | 2.66120000 | H | -2.52641700 | -3.07041500 | -2.72365700 |
| H | 1.01814300 | 1.65337000 | -1.93540600 | C | -3.32185000 | -3.38001200 | -0.23696600 |
| H | 2.39279100 | 3.82495400 | 1.52259600 | H | -2.62634300 | -4.20753000 | -0.42746300 |
| H | 4.22412300 | 4.78961800 | 0.18624300 | H | -4.19432200 | -3.53200800 | -0.88339000 |
| H | 4.45910500 | 4.21561300 | -2.21995600 | C | -0.64474700 | -2.63539600 | -1.59043100 |
| H | 2.84218500 | 2.65372400 | -3.28375000 | C | 0.52088600 | -2.26315600 | -2.52691900 |
| H | 3.09817000 | -3.19254500 | -1.03462500 | H | -0.54291900 | -3.69893100 | -1.35323800 |
| H | 2.99894000 | -5.64793600 | -1.08261100 | H | 0.65759200 | -1.18033300 | -2.69198500 |
| H | 1.47216300 | -6.87461500 | 0.45204500 | H | 1.47266400 | -2.67508200 | -2.19904800 |
| H | 0.05089000 | -5.59940400 | 2.05075800 | C | -3.74593100 | -3.41584700 | 1.20087600 |
| H | 0.12309000 | -3.14644400 | 2.08784700 | C | -5.01221200 | -3.52506500 | 1.60753000 |
| H | 4.28462700 | 0.07215500 | 1.15673200 | H | -2.94246900 | -3.34800600 | 1.93030600 |
| H | 2.08056900 | -1.21020100 | -2.32045900 | H | -5.27314200 | -3.56014700 | 2.66235600 |
| H | 3.95386100 | -0.52110500 | -3.75520800 | H | -5.83518300 | -3.58439600 | 0.89727600 |
| H | 5.98482200 | 0.51132500 | -2.74943700 | P | 1.84236200 | -0.86815000 | 0.44370700 |
| H | 6.12097900 | 0.80660800 | -0.28404200 | C | 1.58290400 | -0.82726300 | 2.28486400 |
| C | -0.39853400 | 1.29665800 | 3.45652300 | C | 1.38918900 | 0.61416700 | 2.79130400 |
| H | -1.20269500 | 2.03644000 | 3.47211900 | C | 0.07511500 | 1.32402500 | 2.40062600 |
| H | -0.82484500 | 0.34336700 | 3.14291600 | P | -0.09736400 | 1.54828000 | 0.56738700 |

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|---|-------------|-------------|-------------|------------|-------------|-------------|-------------|
| C | -1.65925300 | 2.44505100 | 0.24505300 | H | 2.32975700 | 0.59752000 | -1.94305200 |
| C | -2.22599800 | 2.32403500 | -1.03250200 | H | 4.18812000 | 2.03639400 | -2.75178400 |
| C | -3.31479400 | 3.11573800 | -1.39464900 | H | 6.11497300 | 2.52460600 | -1.25720700 |
| C | -3.85222000 | 4.02379200 | -0.47938600 | H | 6.18946200 | 1.54134300 | 1.02463800 |
| C | -3.30078800 | 4.13629500 | 0.79858600 | C | -1.14137400 | 0.58674900 | 2.97446300 |
| C | -2.20198400 | 3.35610000 | 1.16101200 | H | -2.06726900 | 1.14043400 | 2.81025000 |
| C | 1.09336600 | 2.86862900 | 0.08097600 | H | -1.25045900 | -0.40518700 | 2.53185900 |
| C | 1.07332100 | 3.28285000 | -1.26172500 | H | -1.00534900 | 0.46690400 | 4.05471300 |
| C | 1.97651500 | 3.49067800 | 0.97055800 | C | 2.63346300 | -1.56263400 | 3.12921900 |
| C | 2.83745200 | 4.49543100 | 0.52005000 | H | 3.56566800 | -1.00045500 | 3.22040100 |
| C | 2.81073700 | 4.90172000 | -0.81357400 | H | 2.23192100 | -1.69352900 | 4.13974500 |
| C | 1.91807700 | 4.29716500 | -1.70361400 | H | 2.86698600 | -2.55118200 | 2.73013800 |
| C | 2.50113600 | -2.53951800 | 0.06294000 | Rh | 0.01488700 | -0.28887000 | -0.71946700 |
| C | 3.68611900 | -2.68440400 | -0.67564300 | | | | |
| C | 4.16412100 | -3.95591000 | -0.99623100 | 4_{LIRh} | | | |
| C | 3.47105900 | -5.09349600 | -0.57967500 | C | 3.11686400 | 1.77507100 | 0.50308700 |
| C | 2.29741700 | -4.95470500 | 0.16547100 | C | 3.18544100 | 3.07821100 | 1.01773800 |
| C | 1.81062600 | -3.68796100 | 0.48546400 | C | 2.68987700 | 4.15950000 | 0.28816800 |
| C | 3.22250800 | 0.23762500 | -0.02090600 | C | 2.11072400 | 3.95963500 | -0.96743900 |
| C | 4.31789100 | 0.50568100 | 0.81203600 | C | 2.03207200 | 2.67062700 | -1.48937500 |
| C | 3.18926500 | 0.79419000 | -1.30811400 | C | 2.53135200 | 1.58198700 | -0.76312000 |
| C | 4.22987200 | 1.60584200 | -1.75634400 | H | 3.64817500 | 3.25267200 | 1.98362400 |
| C | 5.30973800 | 1.88153300 | -0.91508000 | H | 2.75399500 | 5.16084100 | 0.70297100 |
| C | 5.35103400 | 1.33106100 | 0.36762500 | H | 1.71080400 | 4.80042900 | -1.52482700 |
| H | 0.64131900 | -1.37655700 | 2.36904100 | H | 1.58377100 | 2.50036100 | -2.46184300 |
| H | 2.25670200 | 1.21419500 | 2.50733000 | H | 2.51978100 | 0.59506600 | -1.20925300 |
| H | 1.39396800 | 0.57179000 | 3.88667600 | C | 3.73897000 | 0.61648500 | 1.24547400 |
| H | 0.11088000 | 2.33256600 | 2.82774000 | C | 2.82335600 | -0.54057100 | 1.63821400 |
| H | -1.80784700 | 1.61623900 | -1.74366300 | O | 1.74609100 | -0.94055000 | 1.20905900 |
| H | -3.74956000 | 3.01515600 | -2.38381700 | H | 3.10637300 | -1.01652900 | 5.10173400 |
| H | -4.70377200 | 4.63654500 | -0.75913700 | C | 4.00660300 | 0.72471200 | 2.79185200 |
| H | -3.71982000 | 4.83820300 | 1.51334200 | H | 3.34582000 | 1.44782900 | 3.27304400 |
| H | -1.76664700 | 3.47174100 | 2.14784800 | H | 5.04335600 | 0.90588500 | 3.07754300 |
| H | 0.39582900 | 2.80791600 | -1.96459600 | C | 5.03964700 | 0.10384900 | 0.53206200 |
| H | 2.00450300 | 3.20966800 | 2.01571200 | H | 5.58360300 | -0.52872900 | 1.24304000 |
| H | 3.52425300 | 4.96222500 | 1.21970000 | H | 5.66144800 | 0.98261500 | 0.33488000 |
| H | 3.47934100 | 5.68438800 | -1.15891900 | C | 3.46739900 | -0.73518600 | 2.99144700 |
| H | 1.88880100 | 4.60761000 | -2.74378300 | C | 2.55346900 | -1.06718200 | 4.15884000 |
| H | 4.23611500 | -1.81214600 | -1.00726300 | H | 4.29467000 | -1.45038700 | 2.91834100 |
| H | 5.08058900 | -4.05363000 | -1.57043100 | H | 1.71624900 | -0.36359800 | 4.21414500 |
| H | 3.84450500 | -6.08182300 | -0.83065900 | H | 2.14577900 | -2.07791000 | 4.05857700 |
| H | 1.75514100 | -5.83546800 | 0.49690100 | C | 4.80652000 | -0.68114200 | -0.72384800 |
| H | 0.88337100 | -3.57921300 | 1.03469100 | C | 5.21975800 | -0.31908200 | -1.93903300 |
| H | 4.37582700 | 0.07500600 | 1.80250100 | H | 4.26932000 | -1.62100900 | -0.60257200 |

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|---|-------------|-------------|-------------|---------------------|-------------|-------------|-------------|
| H | 5.04051800 | -0.94275500 | -2.81099800 | H | -3.91620300 | -0.24775400 | 3.44195300 |
| H | 5.75542500 | 0.61354000 | -2.10400700 | H | -0.26133700 | -4.61176500 | -0.04349300 |
| P | -0.66322300 | -1.70714300 | -0.73963300 | H | 1.56313600 | -6.18857200 | -0.57283000 |
| C | -1.47691600 | -1.61978400 | -2.42000200 | H | 3.51910100 | -5.43700700 | -1.90948000 |
| C | -2.55042400 | -0.52532100 | -2.57771800 | H | 3.63829100 | -3.08476000 | -2.71110000 |
| C | -2.08183700 | 0.93603700 | -2.40748200 | H | 1.83069100 | -1.49059000 | -2.14581100 |
| P | -1.57098900 | 1.23289700 | -0.65105900 | H | -3.61099300 | -2.45226200 | -0.69271200 |
| C | -1.36895700 | 3.03951900 | -0.40991500 | H | -0.18397200 | -2.63912500 | 1.91182500 |
| C | -0.80211400 | 3.44557100 | 0.80923600 | H | -1.60826500 | -3.56695200 | 3.70546400 |
| C | -0.64097700 | 4.79911900 | 1.09826400 | H | -4.04039700 | -3.92208600 | 3.30932700 |
| C | -1.03676900 | 5.76284400 | 0.16759400 | H | -5.02323200 | -3.35568200 | 1.09682100 |
| C | -1.60260700 | 5.36633600 | -1.04582500 | C | -0.94424800 | 1.29687500 | -3.37103600 |
| C | -1.77640400 | 4.01067400 | -1.33361300 | H | -0.70432300 | 2.36160900 | -3.33345500 |
| C | -3.08201900 | 0.91762900 | 0.34913200 | H | -0.03192100 | 0.74355000 | -3.13235300 |
| C | -2.93195300 | 0.37721200 | 1.63379100 | H | -1.23737400 | 1.05127800 | -4.39778500 |
| C | -4.36315900 | 1.26358700 | -0.10479300 | C | -1.97274100 | -2.97700900 | -2.93870100 |
| C | -5.47633900 | 1.05098900 | 0.70880000 | H | -2.86681300 | -3.32273700 | -2.41638100 |
| C | -5.31896100 | 0.50862500 | 1.98721800 | H | -2.22248300 | -2.88407800 | -4.00109200 |
| C | -4.04415100 | 0.17948000 | 2.45214200 | H | -1.20521300 | -3.74847900 | -2.84039200 |
| C | 0.65918100 | -2.94084000 | -1.05688900 | Rh | 0.22296700 | 0.14057600 | 0.02660400 |
| C | 0.59176500 | -4.26965300 | -0.61826300 | | | | |
| C | 1.62317500 | -5.16166700 | -0.92094100 | TS5 _{LIRh} | | | |
| C | 2.72037700 | -4.74025200 | -1.67374000 | C | 3.81824000 | 0.84372000 | -0.66400900 |
| C | 2.78767500 | -3.41907600 | -2.12476100 | C | 4.55798800 | 0.47638000 | -1.79713700 |
| C | 1.76685500 | -2.52247200 | -1.81208000 | C | 5.86857800 | 0.01482600 | -1.67475300 |
| C | -1.78569500 | -2.50634500 | 0.46700100 | C | 6.46180700 | -0.08941600 | -0.41423800 |
| C | -3.15468900 | -2.70661800 | 0.25431000 | C | 5.73678100 | 0.28532100 | 0.71771300 |
| C | -1.23968700 | -2.81382500 | 1.72699000 | C | 4.42688200 | 0.75531300 | 0.59410100 |
| C | -2.04445300 | -3.32864200 | 2.73981700 | H | 4.10760600 | 0.54687500 | -2.78246800 |
| C | -3.41092900 | -3.52912600 | 2.51665900 | H | 6.42378700 | -0.26685400 | -2.56474600 |
| C | -3.96154700 | -3.21470000 | 1.27511800 | H | 7.47935300 | -0.45595700 | -0.31691800 |
| H | -0.61658200 | -1.33406500 | -3.03672800 | H | 6.18812900 | 0.21526000 | 1.70317700 |
| H | -3.39340700 | -0.72068600 | -1.90963700 | H | 3.87575300 | 1.04652100 | 1.47943700 |
| H | -2.94109300 | -0.61588900 | -3.59862200 | C | 2.40354000 | 1.38255900 | -0.84176800 |
| H | -2.94493500 | 1.57412600 | -2.62295500 | C | 1.45066600 | 1.04911100 | 0.32924100 |
| H | -0.48211600 | 2.69623600 | 1.52983500 | O | 1.59422100 | 1.34786900 | 1.49549600 |
| H | -0.19795800 | 5.10065800 | 2.04250200 | H | 0.19299900 | -1.01580900 | -3.60633000 |
| H | -0.90614400 | 6.81803500 | 0.38776100 | C | 1.63314200 | 0.69431600 | -1.99567100 |
| H | -1.91847500 | 6.11259700 | -1.76874000 | H | 1.58522900 | 1.19750000 | -2.96057700 |
| H | -2.23702900 | 3.72223100 | -2.27205900 | H | 0.25080400 | 1.35285300 | -1.69627200 |
| H | -1.93963800 | 0.09492100 | 1.97254700 | C | 2.43055000 | 2.92455800 | -1.07683900 |
| H | -4.49686200 | 1.70615100 | -1.08712600 | H | 1.39692400 | 3.25205000 | -1.24560700 |
| H | -6.46594200 | 1.31414100 | 0.34697000 | H | 2.98827600 | 3.08823000 | -2.00519800 |
| H | -6.18765600 | 0.34431900 | 2.61779600 | C | 1.51576400 | -0.72093600 | -1.91489700 |

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|---|-------------|-------------|-------------|------------|-------------|-------------|-------------|
| C | 1.00030900 | -1.53209500 | -3.07589700 | H | 4.48157800 | -5.02004400 | 0.81156300 |
| H | 2.20675800 | -1.23026900 | -1.25194600 | H | 2.28253900 | -6.05933800 | 0.29870600 |
| H | 1.80587900 | -1.72030700 | -3.79950400 | H | 0.22866600 | -4.69182700 | 0.30088900 |
| H | 0.62612600 | -2.50454000 | -2.74389400 | H | -1.50071300 | -1.67102300 | -1.80900600 |
| C | 3.04085700 | 3.72134200 | 0.03697700 | H | -1.93005700 | -4.05305000 | 1.75767300 |
| C | 4.17001100 | 4.42192200 | -0.07802400 | H | -3.78504600 | -5.28544800 | 0.70401200 |
| H | 2.51306400 | 3.70807000 | 0.98819000 | H | -4.50783400 | -4.72839300 | -1.60750700 |
| H | 4.57290500 | 4.99407300 | 0.75353100 | H | -3.35323000 | -2.91679400 | -2.86254200 |
| H | 4.73015700 | 4.44923400 | -1.01067600 | H | -3.96347700 | 3.11799700 | -0.14264300 |
| P | -1.78535500 | 1.19523500 | 0.50300300 | H | -4.02485600 | 5.58488800 | -0.24730600 |
| C | -1.95084200 | 0.81810500 | 2.32039600 | H | -1.98554100 | 6.91047500 | 0.26722600 |
| C | -2.04037400 | -0.69318000 | 2.64328900 | H | 0.12116300 | 5.74213500 | 0.89770800 |
| C | -0.75030900 | -1.53347700 | 2.54537400 | H | 0.18802500 | 3.28086000 | 0.99235500 |
| P | -0.22862500 | -1.77191800 | 0.77326800 | H | -4.46372400 | -0.13726800 | 1.18752700 |
| C | 1.24393500 | -2.85935900 | 0.83049800 | H | -2.31015300 | 1.25791100 | -2.27741500 |
| C | 2.49149600 | -2.27818800 | 1.11611500 | H | -4.12986900 | 0.43513700 | -3.73028800 |
| C | 3.64982400 | -3.05240500 | 1.11529700 | H | -6.10177900 | -0.71075300 | -2.73048400 |
| C | 3.57860600 | -4.41699700 | 0.82044700 | H | -6.24767200 | -0.98309300 | -0.26403800 |
| C | 2.34408400 | -5.00034400 | 0.53132700 | C | 0.37956500 | -1.00379000 | 3.43385600 |
| C | 1.18000800 | -4.22734300 | 0.53463800 | H | 1.20164600 | -1.72091900 | 3.49373700 |
| C | -1.57796500 | -2.77294300 | 0.04683400 | H | 0.78053300 | -0.05742500 | 3.06926800 |
| C | -1.99074200 | -2.46847300 | -1.26011500 | H | -0.00667200 | -0.85097200 | 4.44783100 |
| C | -2.23404800 | -3.79630700 | 0.74846100 | C | -3.06661200 | 1.60437700 | 3.02310400 |
| C | -3.28324600 | -4.49651600 | 0.15194800 | H | -4.06341400 | 1.27470400 | 2.71905700 |
| C | -3.68755900 | -4.18479100 | -1.14849500 | H | -2.98203100 | 1.45344200 | 4.10447900 |
| C | -3.03801800 | -3.17117100 | -1.85573200 | H | -2.99070100 | 2.67592000 | 2.82550100 |
| C | -1.87937300 | 3.02412700 | 0.42105100 | Rh | 0.00513800 | 0.14846300 | -0.58694200 |
| C | -3.06701100 | 3.68678700 | 0.07945600 | | | | |
| C | -3.10116300 | 5.08152600 | 0.02260000 | 5_{LiRh} | | | |
| C | -1.95644200 | 5.82602200 | 0.31459200 | C | 3.74010700 | 1.05449700 | -0.58704600 |
| C | -0.77394100 | 5.17134400 | 0.66873800 | C | 4.57256400 | 0.47957600 | -1.55708000 |
| C | -0.73407800 | 3.77832400 | 0.71998400 | C | 5.88533300 | 0.12122600 | -1.24985200 |
| C | -3.24795800 | 0.62022400 | -0.43611400 | C | 6.38871800 | 0.32997800 | 0.03562100 |
| C | -4.36947600 | -0.00996600 | 0.11795800 | C | 5.57109800 | 0.91357200 | 1.00459700 |
| C | -3.17539300 | 0.77301700 | -1.83440700 | C | 4.26013000 | 1.28056400 | 0.69438700 |
| C | -4.20021900 | 0.30659500 | -2.65429000 | H | 4.19483700 | 0.30619800 | -2.55934900 |
| C | -5.30779000 | -0.33500600 | -2.09235700 | H | 6.51256600 | -0.32494500 | -2.01603400 |
| C | -5.38836800 | -0.49026200 | -0.70853100 | H | 7.40823500 | 0.04510200 | 0.27764800 |
| H | -0.99315000 | 1.19460600 | 2.69966700 | H | 5.95164600 | 1.08883800 | 2.00663200 |
| H | -2.82608500 | -1.16730600 | 2.05043000 | H | 3.63706300 | 1.73467600 | 1.45412100 |
| H | -2.36712600 | -0.76589400 | 3.68742200 | C | 2.32362200 | 1.48345600 | -0.96353800 |
| H | -1.00787300 | -2.53765100 | 2.89961600 | C | 1.29917100 | 1.31667800 | 0.17425900 |
| H | 2.56161400 | -1.21807900 | 1.32745900 | O | 1.35583100 | 1.76413000 | 1.29776400 |
| H | 4.60594600 | -2.58434600 | 1.32892300 | H | 0.46534600 | -1.09157800 | -3.77971100 |

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|---|-------------|-------------|-------------|---------------|-------------|-------------|-------------|
| C | 1.67926500 | 0.62499200 | -2.06746900 | C | -5.30071200 | -1.15390600 | -0.50915500 |
| H | 1.36982600 | 1.12885500 | -2.97783100 | H | -1.05003100 | 1.18124100 | 2.67729700 |
| H | -0.44985500 | 1.57156500 | -1.53550300 | H | -2.57165700 | -1.42567900 | 2.16137700 |
| C | 2.30630400 | 2.97861300 | -1.42913900 | H | -2.07276700 | -0.92079000 | 3.75610900 |
| H | 1.27751500 | 3.20792000 | -1.73444900 | H | -0.53454500 | -2.51416600 | 2.90513500 |
| H | 2.93862600 | 3.03036600 | -2.32197500 | H | 2.75503300 | -0.92386300 | 1.33919300 |
| C | 1.63335900 | -0.74393700 | -1.99177700 | H | 4.90147000 | -2.11427700 | 1.35577500 |
| C | 1.14761300 | -1.62180700 | -3.10847800 | H | 4.99301900 | -4.53660100 | 0.76940000 |
| H | 2.20513000 | -1.23633400 | -1.21385100 | H | 2.90026500 | -5.73791100 | 0.17449900 |
| H | 2.00803500 | -1.96452700 | -3.69832200 | H | 0.74040000 | -4.54866700 | 0.16855800 |
| H | 0.64707900 | -2.51514000 | -2.72694000 | H | -1.36999800 | -1.74532600 | -1.78853900 |
| C | 2.77228700 | 3.97250700 | -0.40880600 | H | -1.38069200 | -4.13552700 | 1.79814500 |
| C | 3.88953600 | 4.69130900 | -0.52414300 | H | -3.12465800 | -5.57767900 | 0.82313300 |
| H | 2.14520500 | 4.09535500 | 0.47188500 | H | -3.98914100 | -5.12897000 | -1.46260500 |
| H | 4.18651600 | 5.40942900 | 0.23541600 | H | -3.10074000 | -3.20647600 | -2.76700400 |
| H | 4.54705200 | 4.58637500 | -1.38466800 | H | -4.34049800 | 2.63324100 | -0.04805300 |
| P | -1.91744100 | 1.02813500 | 0.51449000 | H | -4.74666700 | 5.06380700 | -0.14636900 |
| C | -1.95415700 | 0.66278500 | 2.33672600 | H | -2.88995000 | 6.66167100 | 0.27954800 |
| C | -1.82313300 | -0.83442100 | 2.69194700 | H | -0.61869500 | 5.79929300 | 0.81956800 |
| C | -0.43974700 | -1.49060700 | 2.52593300 | H | -0.20688200 | 3.36979500 | 0.91303700 |
| P | 0.02229100 | -1.69393000 | 0.72879100 | H | -4.27630600 | -0.74547800 | 1.32146400 |
| C | 1.58487000 | -2.65429800 | 0.77643200 | H | -2.68986700 | 1.13745800 | -2.21959000 |
| C | 2.77450700 | -1.98081200 | 1.10448000 | H | -4.47430700 | 0.08995500 | -3.56487000 |
| C | 3.99361200 | -2.65505300 | 1.10826600 | H | -6.14693800 | -1.39883500 | -2.47572500 |
| C | 4.04301300 | -4.01093800 | 0.77401900 | H | -6.03028100 | -1.79580900 | -0.02529900 |
| C | 2.86813000 | -4.68515200 | 0.43881200 | C | 0.64758500 | -0.78923100 | 3.34882000 |
| C | 1.64351100 | -4.01259000 | 0.43716300 | H | 1.55070000 | -1.39931900 | 3.41212900 |
| C | -1.24454400 | -2.83678800 | 0.07093000 | H | 0.92130500 | 0.18240800 | 2.93526100 |
| C | -1.74087500 | -2.59079700 | -1.21822300 | H | 0.27712200 | -0.63632000 | 4.36854700 |
| C | -1.75297900 | -3.92180300 | 0.80178400 | C | -3.15335300 | 1.30596600 | 3.05052900 |
| C | -2.73731500 | -4.74134400 | 0.24930100 | H | -4.10540500 | 0.86200400 | 2.74851900 |
| C | -3.22167400 | -4.48980000 | -1.03686400 | H | -3.04331800 | 1.15953900 | 4.12982300 |
| C | -2.72079900 | -3.41430900 | -1.77219500 | H | -3.20623000 | 2.37967700 | 2.86040300 |
| C | -2.23987400 | 2.83005500 | 0.42381000 | Rh | -0.08680400 | 0.27745600 | -0.67344700 |
| C | -3.52189500 | 3.31954400 | 0.13648200 | | | | |
| C | -3.75118400 | 4.69558700 | 0.08276400 | ϕ_{L1Rh} | | | |
| C | -2.70915200 | 5.59199700 | 0.32421900 | C | 3.74969200 | 0.99524700 | -0.60537300 |
| C | -1.43376800 | 5.10827500 | 0.62636700 | C | 4.57302800 | 0.41529100 | -1.58040400 |
| C | -1.19783800 | 3.73500900 | 0.67584900 | C | 5.88353400 | 0.04408500 | -1.27938600 |
| C | -3.34187100 | 0.26856500 | -0.34972800 | C | 6.39367300 | 0.24484300 | 0.00480000 |
| C | -4.29794900 | -0.55658300 | 0.25720600 | C | 5.58505100 | 0.83291600 | 0.97852300 |
| C | -3.41929600 | 0.49400100 | -1.73727700 | C | 4.27612700 | 1.21259700 | 0.67452300 |
| C | -4.42653400 | -0.09687600 | -2.49631900 | H | 4.18959200 | 0.24831500 | -2.58158100 |
| C | -5.36698200 | -0.92973400 | -1.88397900 | H | 6.50376600 | -0.40545700 | -2.04919600 |

| | | | | | | | |
|---|-------------|-------------|-------------|---------------------|-------------|-------------|-------------|
| H | 7.41153200 | -0.04958100 | 0.24198200 | C | -1.30954700 | 5.11420900 | 0.85898000 |
| H | 5.97109300 | 1.00196000 | 1.97945100 | C | -1.13843300 | 3.73145100 | 0.90054700 |
| H | 3.65995100 | 1.67047300 | 1.43761800 | C | -3.34149500 | 0.34782600 | -0.36027600 |
| C | 2.33631800 | 1.43804000 | -0.97850200 | C | -4.34693200 | -0.40603300 | 0.25958600 |
| C | 1.31368900 | 1.29089600 | 0.16195400 | C | -3.38011600 | 0.51588000 | -1.75751100 |
| O | 1.38069100 | 1.73707400 | 1.28526400 | C | -4.40023200 | -0.05780100 | -2.51267900 |
| H | 0.44353000 | -1.14470300 | -3.76529200 | C | -5.38942900 | -0.82110800 | -1.88682100 |
| C | 1.67865300 | 0.57717000 | -2.07262300 | C | -5.36021100 | -0.99045300 | -0.50268400 |
| H | 1.37963600 | 1.07355400 | -2.99058700 | H | -1.02905700 | 1.18443700 | 2.66854700 |
| H | -0.42262900 | 1.55902900 | -1.54692300 | H | -2.62001200 | -1.37193400 | 2.12255800 |
| C | 2.33637600 | 2.92986200 | -1.45443500 | H | -2.13924800 | -0.89415900 | 3.73203300 |
| H | 1.31186100 | 3.16844600 | -1.76661800 | H | -0.61426100 | -2.51057100 | 2.90764300 |
| H | 2.97443500 | 2.96940700 | -2.34373600 | H | 2.70316900 | -0.95765600 | 1.36584100 |
| C | 1.61298500 | -0.79051500 | -1.97906600 | H | 4.84419600 | -2.15759800 | 1.38591900 |
| C | 1.11754600 | -1.67554700 | -3.08625500 | H | 4.92795000 | -4.57703300 | 0.78835200 |
| H | 2.18039800 | -1.28095900 | -1.19699800 | H | 2.83270000 | -5.76698100 | 0.17974500 |
| H | 1.97382200 | -2.03723100 | -3.67054500 | H | 0.67788700 | -4.56838300 | 0.17077400 |
| H | 0.60354400 | -2.55678900 | -2.69445600 | H | -1.43548400 | -1.74393000 | -1.77306700 |
| C | 2.80634400 | 3.92406400 | -0.43617800 | H | -1.43597000 | -4.14385100 | 1.80478500 |
| C | 3.93587900 | 4.62461600 | -0.54414500 | H | -3.20355500 | -5.56607300 | 0.84389100 |
| H | 2.17047600 | 4.06300300 | 0.43556100 | H | -4.09238700 | -5.09749500 | -1.42881500 |
| H | 4.23575800 | 5.34366100 | 0.21329600 | H | -3.19805800 | -3.17986400 | -2.73640000 |
| H | 4.60094300 | 4.50310500 | -1.39654500 | H | -4.14142700 | 2.79067100 | -0.40842700 |
| P | -1.90013800 | 1.06644300 | 0.50761100 | H | -4.42952400 | 5.23691200 | -0.49069900 |
| C | -1.95043700 | 0.69742900 | 2.32806300 | H | -2.62012400 | 6.73970800 | 0.31604500 |
| C | -1.86667100 | -0.80490800 | 2.67390800 | H | -0.51800700 | 5.76297200 | 1.22176300 |
| C | -0.49535600 | -1.49069300 | 2.52552900 | H | -0.21969100 | 3.31612800 | 1.29640600 |
| P | -0.02553100 | -1.70788700 | 0.73249800 | H | -4.35351700 | -0.55053100 | 1.33091900 |
| C | 1.52794400 | -2.68074700 | 0.79127000 | H | -2.60929500 | 1.10022900 | -2.25053900 |
| C | 2.71878700 | -2.01383100 | 1.12756100 | H | -4.41848300 | 0.08615800 | -3.58863700 |
| C | 3.93485800 | -2.69339500 | 1.13316600 | H | -6.17829200 | -1.27921900 | -2.47521400 |
| C | 3.97996800 | -4.04785300 | 0.79247900 | H | -6.12763400 | -1.57800900 | -0.00859700 |
| C | 2.80375700 | -4.71560200 | 0.44952900 | C | 0.59966400 | -0.80908500 | 3.35436600 |
| C | 1.58195300 | -4.03778000 | 0.44629800 | H | 1.48700900 | -1.44043300 | 3.43081300 |
| C | -1.30566100 | -2.84002600 | 0.08078700 | H | 0.90182300 | 0.15268300 | 2.93697200 |
| C | -1.81297100 | -2.58589200 | -1.20164400 | H | 0.22290500 | -0.63957800 | 4.36913000 |
| C | -1.81684100 | -3.92298400 | 0.81330600 | C | -3.12431700 | 1.37668100 | 3.04995600 |
| C | -2.81516100 | -4.73099100 | 0.26911700 | H | -4.08925100 | 0.93892700 | 2.78274900 |
| C | -3.31300500 | -4.46853300 | -1.00977600 | H | -2.99109200 | 1.25628200 | 4.12985700 |
| C | -2.80911700 | -3.39560500 | -1.74680200 | H | -3.16669200 | 2.44583100 | 2.83329300 |
| C | -2.15222600 | 2.88015500 | 0.43284200 | Rh | -0.08885400 | 0.26302100 | -0.67668800 |
| C | -3.34170700 | 3.43333500 | -0.05968500 | | | | |
| C | -3.50484100 | 4.81958500 | -0.10371300 | TS6 _{LIRh} | | | |
| C | -2.49051200 | 5.66241000 | 0.35155900 | C | -3.65612800 | 1.33181200 | -0.80541700 |

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|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | -4.58381700 | 1.93570800 | 0.05061200 | C | 5.44238900 | -1.60642400 | 0.17010400 |
| C | -5.82294800 | 1.33973200 | 0.29812800 | C | 5.28830000 | -2.15185200 | -1.10609200 |
| C | -6.15189400 | 0.12318100 | -0.30060600 | C | 4.18025300 | -1.80383800 | -1.88102200 |
| C | -5.22182600 | -0.50335900 | -1.13213800 | C | -2.04434500 | -2.24099400 | 0.75564300 |
| C | -3.98333900 | 0.08949400 | -1.37259800 | C | -2.47438100 | -3.42497800 | 0.14259800 |
| H | -4.34252700 | 2.88609600 | 0.51293600 | C | -3.78607300 | -3.87256000 | 0.31825700 |
| H | -6.53320300 | 1.83432400 | 0.95462900 | C | -4.67363800 | -3.15401400 | 1.11930400 |
| H | -7.11695000 | -0.33811700 | -0.11304200 | C | -4.25105900 | -1.97120000 | 1.73080700 |
| H | -5.45138800 | -1.46416000 | -1.58230500 | C | -2.95060300 | -1.50884400 | 1.54297400 |
| H | -3.27044200 | -0.42986000 | -2.00353200 | C | 0.62776200 | -2.96915900 | -0.21405000 |
| C | -2.28406200 | 1.98402200 | -1.08312400 | C | 1.61496500 | -3.74746800 | 0.40593800 |
| C | -1.29844500 | 1.29332100 | -0.05061100 | C | 0.40969900 | -3.12795300 | -1.59614900 |
| O | -1.51068500 | 1.42527900 | 1.13598500 | C | 1.15120400 | -4.04974700 | -2.33286600 |
| H | -2.46746200 | 6.12293700 | -0.58499800 | C | 2.14127000 | -4.81093400 | -1.70638600 |
| C | -2.32858200 | 3.48710700 | -0.83312000 | C | 2.37046600 | -4.65532500 | -0.33904500 |
| H | -2.84888600 | 4.01959900 | -1.62982600 | H | -0.48357000 | -0.69535400 | 2.75431000 |
| H | -0.94300200 | -0.21959600 | -1.90932600 | H | 2.32887100 | -1.72842200 | 2.15777400 |
| C | -1.86910900 | 1.75921300 | -2.57182500 | H | 1.80797800 | -1.20388500 | 3.73983900 |
| H | -1.79433700 | 2.72720600 | -3.07462800 | H | 3.03573000 | 0.54163400 | 2.71640800 |
| H | -2.64091000 | 1.19907400 | -3.09656600 | H | 0.74177600 | 3.31981900 | 0.52674900 |
| C | -1.84158800 | 4.20295500 | 0.18358100 | H | 1.54559300 | 5.64989400 | 0.43226200 |
| C | -1.94734300 | 5.69631000 | 0.27825400 | H | 3.98281400 | 6.11911100 | 0.22958500 |
| H | -1.34555000 | 3.70540100 | 1.01133500 | H | 5.59930200 | 4.23312300 | 0.14096100 |
| H | -2.48607200 | 5.99301900 | 1.18724900 | H | 4.79962400 | 1.90161000 | 0.26367700 |
| H | -0.95280000 | 6.15621800 | 0.34278200 | H | 2.36500200 | -0.66549900 | -1.98880600 |
| C | -0.54030500 | 1.04897300 | -2.74170600 | H | 4.62703000 | -0.30844900 | 1.66871400 |
| C | 0.64242200 | 1.67728900 | -2.25808100 | H | 6.30322700 | -1.87153600 | 0.77646700 |
| H | -0.45060000 | 0.41293200 | -3.62074500 | H | 6.02691600 | -2.84687200 | -1.49378000 |
| H | 1.59799000 | 1.42740200 | -2.71145500 | H | 4.04891800 | -2.23005400 | -2.87044900 |
| H | 0.57318900 | 2.67721700 | -1.84175100 | H | -1.78966000 | -4.01057600 | -0.46002400 |
| P | -0.31770000 | -1.63618900 | 0.61369200 | H | -4.10517800 | -4.79308400 | -0.16170000 |
| C | 0.17338500 | -1.50194000 | 2.41191300 | H | -5.68974200 | -3.50896600 | 1.26234900 |
| C | 1.63059900 | -1.06071900 | 2.66718300 | H | -4.93931700 | -1.39742100 | 2.34317500 |
| C | 2.00618100 | 0.40388600 | 2.36830700 | H | -2.64457200 | -0.57913600 | 2.00843100 |
| P | 2.05301400 | 0.74262400 | 0.54056400 | H | 1.81467700 | -3.65165100 | 1.46384900 |
| C | 2.71266800 | 2.44634300 | 0.41621700 | H | -0.34046400 | -2.52058100 | -2.09360700 |
| C | 1.80441000 | 3.51598400 | 0.45605900 | H | 0.96443100 | -4.16303300 | -3.39655800 |
| C | 2.25957500 | 4.83229000 | 0.39712500 | H | 2.73212700 | -5.51726900 | -2.28149800 |
| C | 3.62745000 | 5.09442300 | 0.28317000 | H | 3.13980800 | -5.24067700 | 0.15519700 |
| C | 4.53554000 | 4.03506500 | 0.23323500 | C | 1.12646400 | 1.41783000 | 3.10888900 |
| C | 4.08347300 | 2.71527100 | 0.30249600 | H | 1.53777700 | 2.42699200 | 3.02692500 |
| C | 3.37069500 | -0.36541700 | -0.09381000 | H | 0.10736100 | 1.43477600 | 2.72063000 |
| C | 3.22717700 | -0.91798700 | -1.37855800 | H | 1.09171600 | 1.15430000 | 4.17187400 |
| C | 4.49067400 | -0.71961300 | 0.67484400 | C | -0.16896200 | -2.75253100 | 3.23754900 |

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|------------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | 0.47375500 | -3.60130700 | 2.99314500 | C | 0.96080400 | 5.21516700 | 0.33496900 |
| H | -0.02831400 | -2.52449200 | 4.29934800 | C | 2.23233000 | 5.76961200 | 0.16945300 |
| H | -1.20583600 | -3.06205500 | 3.09503900 | C | 3.35024800 | 4.93675800 | 0.11225900 |
| Rh | 0.14332200 | 0.21223300 | -0.77730400 | C | 3.20204600 | 3.55300700 | 0.22218900 |
| | | | | C | 3.26701800 | 0.44226700 | -0.02654900 |
| 7_{LIRh} | | | | C | 3.31509800 | -0.13058700 | -1.30645600 |
| C | -4.02921200 | 0.82128900 | -0.65190100 | C | 4.42055900 | 0.41231600 | 0.77302000 |
| C | -5.14528600 | 1.58977800 | -0.31083400 | C | 5.59310500 | -0.17446600 | 0.29722000 |
| C | -6.37628100 | 0.98161200 | -0.04426700 | C | 5.63000200 | -0.73798500 | -0.97985400 |
| C | -6.50934300 | -0.40408000 | -0.11228900 | C | 4.48842200 | -0.71478900 | -1.78232600 |
| C | -5.39919600 | -1.18169700 | -0.45344900 | C | -1.28444200 | -2.92965200 | 0.57029900 |
| C | -4.17670700 | -0.57263100 | -0.72326300 | C | -1.27849400 | -4.17859400 | -0.06750900 |
| H | -5.06256400 | 2.66800900 | -0.25787700 | C | -2.39480000 | -5.01404600 | 0.00463900 |
| H | -7.23139100 | 1.59971400 | 0.21415500 | C | -3.52220200 | -4.62245100 | 0.72791800 |
| H | -7.46505100 | -0.87566800 | 0.09656000 | C | -3.53326000 | -3.38213800 | 1.36959400 |
| H | -5.48147100 | -2.26274600 | -0.50324900 | C | -2.42917400 | -2.53524800 | 1.28402500 |
| H | -3.32165000 | -1.18881800 | -0.98481900 | C | 1.51503300 | -2.79247600 | -0.21016200 |
| C | -2.66382500 | 1.42833800 | -1.02323200 | C | 2.63396500 | -3.27345500 | 0.48250300 |
| C | -1.57696200 | 0.80321600 | -0.02608600 | C | 1.43699300 | -3.00936000 | -1.59957100 |
| O | -1.85240200 | 0.71316100 | 1.14904900 | C | 2.44020800 | -3.70404600 | -2.27179600 |
| H | -2.48228200 | 5.55870400 | -0.34128400 | C | 3.55627100 | -4.16881400 | -1.57166700 |
| C | -2.58308600 | 2.93456300 | -0.78203800 | C | 3.65039600 | -3.94760900 | -0.19781800 |
| H | -2.41149400 | 3.54042000 | -1.66928400 | H | -0.42041300 | -0.92106900 | 2.62034100 |
| H | -0.82629500 | -0.31821400 | -2.32633400 | H | 2.59996000 | -1.09628700 | 2.21090200 |
| C | -2.39038000 | 1.10830400 | -2.51964000 | H | 1.87020900 | -0.74101400 | 3.75812400 |
| H | -2.69453800 | 1.96800300 | -3.12447300 | H | 2.62355900 | 1.26588400 | 2.72465600 |
| H | -3.01300200 | 0.26855500 | -2.83088800 | H | -0.18601200 | 3.41011400 | 0.54452200 |
| C | -2.73209300 | 3.54633000 | 0.39697000 | H | 0.08783600 | 5.85776900 | 0.37348500 |
| C | -2.70716800 | 5.03108000 | 0.59046500 | H | 2.34947300 | 6.84549400 | 0.08113000 |
| H | -2.89688300 | 2.94593600 | 1.28958600 | H | 4.34125100 | 5.36042200 | -0.02018100 |
| H | -3.67630900 | 5.38801800 | 0.96239300 | H | 4.07880000 | 2.91808600 | 0.17096000 |
| H | -1.96361800 | 5.31589900 | 1.34434800 | H | 2.42922300 | -0.13764800 | -1.93336600 |
| C | -0.93904600 | 0.75927400 | -2.81834100 | H | 4.41424100 | 0.84737100 | 1.76620400 |
| C | 0.09080300 | 1.67548700 | -2.26675900 | H | 6.47791400 | -0.19042500 | 0.92620000 |
| H | -0.77828500 | 0.45338300 | -3.85761400 | H | 6.54287300 | -1.19763800 | -1.34582900 |
| H | 1.03742500 | 1.71503700 | -2.80778100 | H | 4.50419900 | -1.16301000 | -2.77016000 |
| H | -0.24032400 | 2.65569300 | -1.93740100 | H | -0.40187800 | -4.51066600 | -0.61089200 |
| P | 0.16394400 | -1.79595300 | 0.53005000 | H | -2.37355100 | -5.97853200 | -0.49410800 |
| C | 0.46492600 | -1.50855600 | 2.35396600 | H | -4.38494900 | -5.27854600 | 0.79264200 |
| C | 1.71362400 | -0.65855200 | 2.67586800 | H | -4.40721200 | -3.06370500 | 1.92881000 |
| C | 1.67278500 | 0.85137400 | 2.37036600 | H | -2.46391100 | -1.56753000 | 1.77095300 |
| P | 1.68818100 | 1.18243300 | 0.54310900 | H | 2.73246100 | -3.12497300 | 1.54911400 |
| C | 1.92788800 | 2.99139000 | 0.38908400 | H | 0.58045800 | -2.63880500 | -2.15592400 |
| C | 0.80609800 | 3.83311700 | 0.43963000 | H | 2.35598800 | -3.87178100 | -3.34135100 |

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|---------------------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | 4.34794700 | -4.69612900 | -2.09490000 | P | 1.23986400 | -1.50565000 | 0.40547300 |
| H | 4.51613600 | -4.30247300 | 0.35292800 | C | 0.95549900 | -1.35974700 | 2.24020300 |
| C | 0.55215100 | 1.60140600 | 3.09851300 | C | 1.12905500 | 0.05919900 | 2.81986800 |
| H | 0.66885900 | 2.68254100 | 2.98813600 | C | 0.19920700 | 1.18045600 | 2.31039100 |
| H | -0.43521100 | 1.32594700 | 2.72963700 | P | 0.56469600 | 1.56625700 | 0.53695100 |
| H | 0.60372300 | 1.36802900 | 4.16765600 | C | -0.23554800 | 3.16934100 | 0.12994600 |
| C | 0.45385500 | -2.78968500 | 3.20159600 | C | -0.02546300 | 3.67728500 | -1.16277600 |
| H | 1.34552000 | -3.39914600 | 3.03750100 | C | -0.48205400 | 4.94840500 | -1.50482000 |
| H | 0.43012700 | -2.51565200 | 4.26174400 | C | -1.18008400 | 5.71735900 | -0.56996500 |
| H | -0.42083700 | -3.40880600 | 2.99497100 | C | -1.40618300 | 5.21211400 | 0.71102000 |
| Rh | 0.10925000 | 0.19687000 | -0.80560400 | C | -0.92725900 | 3.94885100 | 1.06683800 |
| | | | | C | 2.31822000 | 2.12375300 | 0.50952100 |
| | | | | C | 3.00575100 | 2.09796000 | -0.71130300 |
| TS7 _{LIRh} | | | | C | 2.94808900 | 2.66917200 | 1.63753300 |
| C | -4.15492400 | -0.46915600 | 0.23418800 | C | 4.25222700 | 3.15778200 | 1.54678700 |
| C | -4.70134500 | 0.71890300 | 0.74150300 | C | 4.93313800 | 3.12218600 | 0.32846900 |
| C | -5.66391200 | 0.70142100 | 1.75543200 | C | 4.30428300 | 2.59731300 | -0.80254100 |
| C | -6.10770400 | -0.50933200 | 2.28436600 | C | 1.04667500 | -3.29980600 | 0.04313100 |
| C | -5.58083800 | -1.70293900 | 1.78336200 | C | 1.77668500 | -3.89420900 | -0.99796100 |
| C | -4.61893500 | -1.68163500 | 0.77498100 | C | 1.58451200 | -5.23677700 | -1.32472100 |
| H | -4.38720200 | 1.67612600 | 0.34325400 | C | 0.66738600 | -6.00938800 | -0.61076500 |
| H | -6.06683300 | 1.64048200 | 2.12448200 | C | -0.05357600 | -5.43035400 | 0.43528300 |
| H | -6.85652600 | -0.52609300 | 3.07102900 | C | 0.12838400 | -4.08610300 | 0.75907400 |
| H | -5.91928200 | -2.65649800 | 2.17938500 | C | 2.97349300 | -1.15104600 | -0.05665400 |
| H | -4.21886600 | -2.62035000 | 0.41359200 | C | 4.02222600 | -1.01979800 | 0.86215800 |
| C | -3.09337100 | -0.46815500 | -0.87001000 | C | 3.24595800 | -1.00940900 | -1.42928700 |
| C | -1.76423000 | -1.18087600 | -0.35265100 | C | 4.54608200 | -0.78316700 | -1.87464200 |
| O | -1.80651000 | -1.92081900 | 0.63336500 | C | 5.58684800 | -0.65772900 | -0.95166300 |
| H | -2.66323000 | 3.54288100 | -1.98989500 | C | 5.31964300 | -0.76425300 | 0.41389400 |
| C | -2.79683200 | 0.95509300 | -1.31099100 | H | -0.10579900 | -1.62215000 | 2.28681200 |
| H | -2.41573000 | 1.61213100 | -0.53220900 | H | 2.17394900 | 0.36307700 | 2.72238400 |
| H | -2.00948700 | -0.81755500 | -3.53731900 | H | 0.93846000 | -0.03268000 | 3.89586800 |
| C | -3.49980400 | -1.37879500 | -2.05196500 | H | 0.44453000 | 2.07852500 | 2.88699100 |
| H | -4.30742800 | -0.93015900 | -2.63788200 | H | 0.50442200 | 3.08316000 | -1.90122800 |
| H | -3.88075000 | -2.32158000 | -1.65117100 | H | -0.30795300 | 5.33079500 | -2.50590500 |
| C | -3.05831100 | 1.48807900 | -2.51271800 | H | -1.54398500 | 6.70432200 | -0.83880600 |
| C | -2.92220900 | 2.93832800 | -2.85942500 | H | -1.94282700 | 5.80564600 | 1.44516700 |
| H | -3.45137900 | 0.85829500 | -3.30715800 | H | -1.08170400 | 3.59542600 | 2.07893400 |
| H | -2.16150300 | 3.10023800 | -3.63405800 | H | 2.52776300 | 1.67796600 | -1.58943100 |
| H | -3.86825700 | 3.31081100 | -3.27259200 | H | 2.43055500 | 2.72412600 | 2.58871800 |
| C | -2.24536600 | -1.66441800 | -2.88854800 | H | 4.73248200 | 3.57029200 | 2.42908900 |
| C | -1.08867800 | -1.92750600 | -1.93191600 | H | 5.94823000 | 3.50164000 | 0.26030500 |
| H | -2.40913200 | -2.53189300 | -3.53870300 | H | 4.82853200 | 2.56210800 | -1.75228400 |
| H | -0.11833200 | -1.73711300 | -2.41972500 | H | 2.50204300 | -3.31910200 | -1.55898000 |
| H | -1.04849900 | -2.94664400 | -1.55495200 | | | | |

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|-----------------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | 2.15929400 | -5.67712700 | -2.13392700 | C | -1.99581900 | -3.55484000 | 2.62084600 |
| H | 0.52032700 | -7.05532800 | -0.86278000 | C | -0.87444600 | -2.76479200 | 2.37367600 |
| H | -0.76363900 | -6.02391900 | 1.00336500 | C | 2.13526800 | -2.55939000 | -0.51775200 |
| H | -0.45797500 | -3.65287200 | 1.55579600 | C | 2.52792900 | -3.89939600 | -0.35442700 |
| H | 3.84002200 | -1.10548500 | 1.92440100 | C | 2.48905700 | -1.88613800 | -1.69427300 |
| H | 2.43327500 | -1.07085100 | -2.14766000 | C | 3.25558500 | -2.51871300 | -2.67427800 |
| H | 4.74246100 | -0.68545700 | -2.93801800 | C | 3.66290700 | -3.84077900 | -2.49298700 |
| H | 6.59898600 | -0.46603900 | -1.29459900 | C | 3.28919800 | -4.53163800 | -1.33647200 |
| H | 6.12180900 | -0.65223300 | 1.13692200 | H | 1.50374700 | -1.21289700 | 3.04784600 |
| C | -1.28383700 | 0.85022900 | 2.53012700 | H | 3.97353200 | -0.95995200 | 1.27282100 |
| H | -1.93967500 | 1.66530800 | 2.21866400 | H | 4.02156900 | -0.78790300 | 3.01547300 |
| H | -1.58623600 | -0.04378500 | 1.98699600 | H | 3.99103700 | 1.40400800 | 2.06863500 |
| H | -1.45343200 | 0.67580800 | 3.59863100 | H | -0.23469000 | 2.83105700 | -0.02114000 |
| C | 1.74090400 | -2.36445500 | 3.10184600 | H | -0.76307100 | 5.24885700 | 0.11008400 |
| H | 2.75115300 | -2.00962200 | 3.31745000 | H | 0.99242600 | 6.86547200 | 0.80862100 |
| H | 1.22397000 | -2.47956700 | 4.06017600 | H | 3.27784900 | 6.05890300 | 1.35239200 |
| H | 1.81787900 | -3.35097400 | 2.64258700 | H | 3.81468600 | 3.64557300 | 1.20111300 |
| Rh | -0.08119100 | -0.17759300 | -0.82761300 | H | 1.99776200 | 1.74141900 | -2.33621200 |
| | | | | H | 5.16877200 | 0.73416100 | 0.40549600 |
| | | | | H | 6.75409100 | 0.63978400 | -1.46640200 |
| δ_{L1Rh} | | | | H | 5.99226300 | 1.10216200 | -3.78585200 |
| C | -2.65493400 | -0.12371500 | -0.51759600 | H | 3.60853400 | 1.67963400 | -4.21105100 |
| O | -2.22320100 | -0.28262800 | 0.62261800 | H | -0.25365300 | -3.71545300 | -0.83819000 |
| H | -4.72828500 | 4.96424000 | 1.01313000 | H | -2.24764300 | -5.10218100 | -0.39983600 |
| P | 1.14939400 | -1.67554000 | 0.75350800 | H | -3.37295200 | -5.00685400 | 1.81633500 |
| C | 2.19081100 | -1.61998700 | 2.29996400 | H | -2.48280100 | -3.50894900 | 3.59023700 |
| C | 3.37735300 | -0.65186100 | 2.13854100 | H | -0.51202300 | -2.09934800 | 3.15002700 |
| C | 3.04417600 | 0.85328300 | 2.06494000 | H | 2.22302500 | -4.45636200 | 0.52333700 |
| P | 2.17799000 | 1.28093400 | 0.48283900 | H | 2.15719500 | -0.86624700 | -1.83647600 |
| C | 1.82082500 | 3.07664500 | 0.59436000 | H | 3.52972900 | -1.97668200 | -3.57419100 |
| C | 0.53507100 | 3.53814500 | 0.28184600 | H | 4.25853100 | -4.33719400 | -3.25324200 |
| C | 0.23550400 | 4.89968900 | 0.35518600 | H | 3.58637700 | -5.56719000 | -1.20085000 |
| C | 1.22272200 | 5.80629500 | 0.74597400 | C | 2.20770000 | 1.32860500 | 3.26077300 |
| C | 2.50957200 | 5.35265200 | 1.05254900 | H | 2.17402900 | 2.41929900 | 3.31008600 |
| C | 2.81154900 | 3.99384300 | 0.97207300 | H | 1.17652000 | 0.96532100 | 3.20396100 |
| C | 3.46189600 | 1.23601700 | -0.83083000 | H | 2.65022900 | 0.95852300 | 4.19186400 |
| C | 3.04201300 | 1.50901300 | -2.14380600 | C | 2.68367900 | -2.98644900 | 2.78787900 |
| C | 4.80865700 | 0.93312500 | -0.59678700 | H | 3.47070400 | -3.38053400 | 2.13984900 |
| C | 5.71373400 | 0.88286100 | -1.66052200 | H | 3.10422900 | -2.87469600 | 3.79300600 |
| C | 5.28671900 | 1.14487900 | -2.96173000 | H | 1.87639500 | -3.72129900 | 2.84084300 |
| C | 3.94696000 | 1.46762300 | -3.20127100 | C | -5.06007900 | 0.37330700 | -0.79975100 |
| C | -0.22916200 | -2.82043100 | 1.12869100 | C | -5.40786200 | -0.30980700 | 0.37592700 |
| C | -0.73696000 | -3.66638000 | 0.13153200 | C | -6.68634100 | -0.84107400 | 0.54336800 |
| C | -1.86473700 | -4.44981800 | 0.37931100 | C | -7.64377500 | -0.69591800 | -0.46253800 |
| C | -2.49593600 | -4.39639000 | 1.62365200 | | | | |

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|------------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | -7.31033100 | -0.01300800 | -1.63260100 | H | -1.65570600 | -3.78070400 | -0.77372500 |
| C | -6.02876200 | 0.51547000 | -1.80051700 | C | -2.53012300 | -2.20998100 | 1.08437800 |
| H | -4.67549300 | -0.41919500 | 1.16882800 | H | -2.84885600 | -3.24482900 | 1.24046500 |
| H | -6.93303500 | -1.36730200 | 1.46080700 | H | -3.21363000 | -1.56221900 | 1.64376700 |
| H | -8.63971500 | -1.10947900 | -0.33527500 | C | -0.23226800 | -2.23379700 | -1.25274500 |
| H | -8.04672900 | 0.11049200 | -2.42132200 | C | 0.13586600 | -1.20410500 | -2.20193800 |
| H | -5.79635200 | 1.04290400 | -2.71821600 | H | 0.54938700 | -2.92058700 | -0.94886800 |
| C | -3.65265400 | 0.97677800 | -0.93360400 | H | 1.15825100 | -1.22519700 | -2.57690300 |
| C | -3.20591500 | 1.18240500 | -2.40609000 | H | -0.60091300 | -0.95171100 | -2.96731800 |
| H | -2.28393400 | 1.77770500 | -2.39604700 | C | -1.13920800 | -2.04022700 | 1.62725400 |
| H | -3.93442600 | 1.73360100 | -3.00206500 | C | -0.36480800 | -3.02512800 | 2.09510900 |
| C | -3.45848800 | 2.22527300 | -0.10691000 | H | -0.77304200 | -0.99604800 | 1.79891700 |
| H | -2.25969600 | -0.21170800 | -3.81975500 | H | 0.63251700 | -2.83647000 | 2.47326300 |
| H | -2.44278500 | 2.62072100 | -0.13605300 | H | -0.71786400 | -4.05363300 | 2.11953100 |
| C | -2.89790100 | -0.23097500 | -2.93312500 | P | 2.30722700 | -0.55073600 | 0.39658600 |
| C | -2.22332800 | -0.92276100 | -1.73783800 | C | 2.92495400 | 0.37719900 | 1.89414100 |
| H | -3.82469000 | -0.74662700 | -3.19899300 | C | 2.44038100 | 1.83945700 | 1.89673300 |
| H | -1.12444300 | -0.87493300 | -1.79281100 | C | 0.95473200 | 2.11170800 | 2.21725700 |
| H | -2.48565200 | -1.97604200 | -1.60173400 | P | -0.20966700 | 1.77130500 | 0.79936900 |
| C | -4.37937200 | 2.87985200 | 0.60344100 | C | -1.81223500 | 2.37741600 | 1.46090100 |
| C | -4.10958200 | 4.13458800 | 1.37851500 | C | -2.66823200 | 1.48811100 | 2.12511500 |
| H | -5.39875900 | 2.49974500 | 0.63788700 | C | -3.87053000 | 1.93482300 | 2.67111400 |
| H | -3.05863400 | 4.43450900 | 1.31312000 | C | -4.23447400 | 3.27844800 | 2.55330300 |
| H | -4.36266100 | 4.00168100 | 2.43804800 | C | -3.38732700 | 4.17112300 | 1.89431700 |
| Rh | 0.27508300 | 0.24050800 | 0.16537100 | C | -2.18112800 | 3.72500600 | 1.35143200 |
| | | | | C | 0.19636400 | 3.00531700 | -0.49536400 |
| | | | | C | -0.38526800 | 2.82626900 | -1.76245600 |
| 9_{L1Rh} | | | | C | 1.06420700 | 4.08541100 | -0.28916600 |
| C | -4.06915300 | -1.99608300 | -0.95096700 | C | 1.37505400 | 4.94999400 | -1.34199200 |
| C | -4.32790200 | -1.69468700 | -2.29878500 | C | 0.80887100 | 4.75564600 | -2.60186400 |
| C | -5.61797800 | -1.75963300 | -2.81891200 | C | -0.08259300 | 3.69779300 | -2.80673000 |
| C | -6.68776800 | -2.12982700 | -1.99920400 | C | 2.90405200 | -2.26791200 | 0.63234300 |
| C | -6.44750400 | -2.43190600 | -0.66012600 | C | 3.01109900 | -3.10773300 | -0.48994900 |
| C | -5.15122900 | -2.36289900 | -0.14057700 | C | 3.33227600 | -4.45643100 | -0.34124300 |
| H | -3.50975400 | -1.40010800 | -2.94823700 | C | 3.55036800 | -4.99008800 | 0.93150000 |
| H | -5.78930900 | -1.51822300 | -3.86403900 | C | 3.45248900 | -4.16376300 | 2.05165600 |
| H | -7.69498300 | -2.18174500 | -2.40184000 | C | 3.13038400 | -2.81290900 | 1.90507900 |
| H | -7.26790300 | -2.72391600 | -0.01084400 | C | 3.35689600 | 0.08654900 | -0.97086000 |
| H | -5.00013500 | -2.60437700 | 0.90493200 | C | 4.65089200 | -0.40679000 | -1.20683800 |
| C | -2.64624500 | -1.87900700 | -0.42638500 | C | 2.87732800 | 1.13615400 | -1.76892200 |
| C | -2.09130800 | -0.42056800 | -0.58486300 | C | 3.67069400 | 1.68225500 | -2.77951200 |
| O | -2.73303100 | 0.49519000 | -1.04759800 | C | 4.95202600 | 1.18029600 | -3.01049900 |
| H | 0.17813200 | -0.03265400 | -1.66740400 | C | 5.43907800 | 0.13473500 | -2.22167100 |
| C | -1.65216400 | -2.78453100 | -1.22489100 | H | 2.47596700 | -0.14502900 | 2.74415100 |
| H | -2.01208800 | -2.89470200 | -2.25154100 | | | | |

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|---------------------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | 2.72951400 | 2.31644000 | 0.95502400 | H | 4.88010100 | -2.62581300 | -1.06099800 |
| H | 3.01542500 | 2.35217300 | 2.67758300 | C | 2.62280900 | -1.90722400 | 0.39913600 |
| H | 0.86142300 | 3.18447800 | 2.42135700 | C | 1.99320500 | -0.50817800 | 0.63397300 |
| H | -2.39569000 | 0.44394700 | 2.21428800 | O | 2.53908300 | 0.39053900 | 1.24078000 |
| H | -4.52544700 | 1.23320300 | 3.17915800 | H | 0.02474700 | -0.55917000 | 2.33575000 |
| H | -5.17455500 | 3.62667900 | 2.97039500 | C | 1.70318200 | -2.86269000 | 1.22853500 |
| H | -3.66465600 | 5.21671400 | 1.79857200 | H | 2.02953400 | -2.84280000 | 2.27220400 |
| H | -1.53360000 | 4.42681800 | 0.83698200 | H | 1.85496000 | -3.88447000 | 0.86658400 |
| H | -1.07808900 | 2.00573600 | -1.91921900 | C | 2.41875300 | -2.08140500 | -1.12525000 |
| H | 1.50939200 | 4.26053100 | 0.68294100 | H | 2.65727200 | -3.10899000 | -1.42588000 |
| H | 2.05988900 | 5.77546300 | -1.17287600 | H | 3.10413300 | -1.41460400 | -1.65136200 |
| H | 1.05498900 | 5.42690800 | -3.41898900 | C | 0.21008700 | -2.48866200 | 1.18012500 |
| H | -0.53801200 | 3.54924400 | -3.78135600 | C | -0.29947200 | -1.61179300 | 2.33444400 |
| H | 2.85502000 | -2.70253900 | -1.48477800 | H | -0.42701100 | -3.36865400 | 1.17421800 |
| H | 3.41407700 | -5.08890600 | -1.22015800 | H | -1.38714300 | -1.63370700 | 2.39741200 |
| H | 3.80038300 | -6.04020900 | 1.04741600 | H | 0.10849000 | -2.03391600 | 3.26439900 |
| H | 3.62799500 | -4.56718200 | 3.04443400 | C | 0.97660100 | -1.76236300 | -1.48499000 |
| H | 3.05788200 | -2.19255900 | 2.79147500 | C | 0.02895000 | -2.67093000 | -0.91031900 |
| H | 5.04344400 | -1.21604600 | -0.60196900 | H | 0.77989700 | -1.36403400 | -2.47607500 |
| H | 1.88505400 | 1.53347500 | -1.60359700 | H | -0.98464600 | -2.69618600 | -1.28291300 |
| H | 3.28100600 | 2.49587100 | -3.38352500 | H | 0.39067300 | -3.65961300 | -0.65387800 |
| H | 5.56865800 | 1.59945800 | -3.79990600 | P | -2.39813500 | -0.45253900 | -0.44775100 |
| H | 6.43649000 | -0.25893400 | -2.39325700 | C | -2.95127300 | 0.53165700 | -1.93229700 |
| C | 0.48384100 | 1.35712000 | 3.46791000 | C | -2.31907200 | 1.93605500 | -1.93039100 |
| H | -0.47771100 | 1.73390800 | 3.82200200 | C | -0.81597300 | 2.05458200 | -2.26569900 |
| H | 0.37561200 | 0.28383900 | 3.28180000 | P | 0.30993100 | 1.63835900 | -0.83567800 |
| H | 1.21460700 | 1.48517000 | 4.27363900 | C | 1.96914300 | 2.13641800 | -1.45164300 |
| C | 4.45099100 | 0.33936100 | 2.04102100 | C | 2.67530200 | 1.27362100 | -2.30417300 |
| H | 4.93307500 | 0.93951200 | 1.26436000 | C | 3.93531800 | 1.62550100 | -2.78610400 |
| H | 4.73314200 | 0.75668600 | 3.01355200 | C | 4.51046600 | 2.84475600 | -2.41884300 |
| H | 4.84998400 | -0.67566500 | 1.98058200 | C | 3.81194100 | 3.71221700 | -1.57796500 |
| Rh | -0.13175400 | -0.44611700 | -0.06829800 | C | 2.54738000 | 3.36333800 | -1.09826400 |
| | | | | C | -0.05746900 | 2.91979800 | 0.43338200 |
| | | | | C | 0.43713800 | 2.72873000 | 1.73479900 |
| | | | | C | -0.80840300 | 4.07118300 | 0.15702500 |
| | | | | C | -1.08519000 | 4.99457300 | 1.16774600 |
| | | | | C | -0.60614900 | 4.78735400 | 2.46157100 |
| | | | | C | 0.16570200 | 3.65615400 | 2.73975400 |
| | | | | C | -3.20595500 | -2.08525300 | -0.64711100 |
| | | | | C | -3.44157700 | -2.87303700 | 0.49266500 |
| | | | | C | -3.92428200 | -4.17493800 | 0.36692700 |
| | | | | C | -4.17439700 | -4.71354600 | -0.89822000 |
| | | | | C | -3.93954200 | -3.94058100 | -2.03609900 |
| | | | | C | -3.45488300 | -2.63624800 | -1.91404800 |
| TS8 _{L1Rh} | | | | | | | |
| C | 4.06845100 | -2.01612500 | 0.84789800 | | | | |
| C | 4.40767900 | -1.72784600 | 2.18124100 | | | | |
| C | 5.72729900 | -1.80485200 | 2.62251400 | | | | |
| C | 6.74421900 | -2.17844400 | 1.73946200 | | | | |
| C | 6.42290800 | -2.47172200 | 0.41468600 | | | | |
| C | 5.09892400 | -2.38886600 | -0.02626000 | | | | |
| H | 3.63221200 | -1.43652600 | 2.88134200 | | | | |
| H | 5.96187900 | -1.57275200 | 3.65760200 | | | | |
| H | 7.77278200 | -2.24166700 | 2.08246900 | | | | |
| H | 7.20097400 | -2.76887000 | -0.28277300 | | | | |

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|--------------------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | -3.28709700 | 0.28945300 | 0.97334000 | C | -6.68283000 | -1.45696700 | -1.12654800 |
| C | -4.66882000 | 0.12887900 | 1.17072900 | C | -6.17733900 | -1.54621700 | 0.17052000 |
| C | -2.55691800 | 1.06507500 | 1.88343700 | C | -4.80593500 | -1.69916500 | 0.38356900 |
| C | -3.19159800 | 1.69564500 | 2.95472000 | H | -3.76544400 | -1.76011700 | -2.84308400 |
| C | -4.56691400 | 1.54130200 | 3.13603800 | H | -6.18171700 | -1.47517100 | -3.22467500 |
| C | -5.30165800 | 0.75164700 | 2.24613800 | H | -7.74855100 | -1.33116000 | -1.29404500 |
| H | -2.56404000 | -0.03241300 | -2.78595200 | H | -6.84794500 | -1.48914400 | 1.02321500 |
| H | -2.54647400 | 2.42811800 | -0.97960600 | H | -4.43979100 | -1.74972400 | 1.40194900 |
| H | -2.84369400 | 2.51449700 | -2.70039300 | C | -2.41355800 | -1.92409500 | -0.46696100 |
| H | -0.61678200 | 3.11159800 | -2.47388300 | C | -1.57783100 | -0.81647100 | -1.17149600 |
| H | 2.24153100 | 0.32611900 | -2.59482600 | O | -1.84398500 | -0.37162200 | -2.27695800 |
| H | 4.46814700 | 0.94463800 | -3.44335200 | H | 0.63318700 | -1.85114700 | -1.78640000 |
| H | 5.49528700 | 3.11621300 | -2.78705900 | C | -1.91875000 | -3.28478600 | -1.06219000 |
| H | 4.24961700 | 4.66360200 | -1.29026600 | H | -2.18554600 | -3.33954200 | -2.12177400 |
| H | 2.01982200 | 4.04815900 | -0.44416700 | H | -2.49457800 | -4.06031300 | -0.54523200 |
| H | 1.04351600 | 1.85613200 | 1.94905000 | C | -1.97252300 | -1.87505900 | 1.00220900 |
| H | -1.18140500 | 4.26540700 | -0.84075800 | H | -2.35520000 | -2.75276800 | 1.54038300 |
| H | -1.67462300 | 5.87722500 | 0.93816100 | H | -2.37413900 | -0.98988400 | 1.49853100 |
| H | -0.82613400 | 5.50507800 | 3.24611300 | C | -0.41176500 | -3.58671700 | -0.88878500 |
| H | 0.55353400 | 3.49248700 | 3.74091800 | C | 0.48071500 | -2.94057400 | -1.94936400 |
| H | -3.25441800 | -2.46664000 | 1.48086600 | H | -0.29800700 | -4.66953100 | -1.01747000 |
| H | -4.10696600 | -4.76779500 | 1.25834100 | H | 1.48528200 | -3.37104500 | -1.92840200 |
| H | -4.55053100 | -5.72748400 | -0.99475100 | H | 0.06992800 | -3.02786000 | -2.95980000 |
| H | -4.13334300 | -4.34915900 | -3.02339500 | C | -0.45158500 | -1.87289900 | 1.02193000 |
| H | -3.26961000 | -2.05662000 | -2.81188500 | C | 0.08974900 | -3.21670300 | 0.51898400 |
| H | -5.24734500 | -0.48791100 | 0.49249300 | H | -0.05391100 | -1.65938400 | 2.01347200 |
| H | -1.48861700 | 1.17273600 | 1.75559000 | H | 1.18140300 | -3.24689800 | 0.54364400 |
| H | -2.60850400 | 2.30000800 | 3.64285600 | H | -0.25747300 | -3.97146800 | 1.24157500 |
| H | -5.06524200 | 2.02708300 | 3.96972200 | P | 2.50172500 | -0.17763700 | 0.46912300 |
| H | -6.37030600 | 0.62135600 | 2.38911600 | C | 2.77156700 | 0.63970800 | 2.11978600 |
| C | -0.44040400 | 1.26175100 | -3.52233300 | C | 1.87837300 | 1.88531100 | 2.26561000 |
| H | 0.55065800 | 1.53745200 | -3.88678300 | C | 0.35821300 | 1.66204200 | 2.45896200 |
| H | -0.44896800 | 0.18380700 | -3.34442900 | P | -0.55768400 | 1.34744000 | 0.86860200 |
| H | -1.16255500 | 1.47869900 | -4.31695800 | C | -2.34405700 | 1.58992700 | 1.24944300 |
| C | -4.47277300 | 0.65019900 | -2.07425400 | C | -2.80742300 | 1.96873400 | 2.51881600 |
| H | -4.89162500 | 1.29017700 | -1.29268000 | C | -4.16809200 | 2.19414500 | 2.73609700 |
| H | -4.70989600 | 1.10385500 | -3.04275900 | C | -5.08137200 | 2.05942500 | 1.69091400 |
| H | -4.97265100 | -0.31993400 | -2.02524700 | C | -4.62519800 | 1.71238500 | 0.41813200 |
| Rh | 0.08643000 | -0.53438700 | -0.02518100 | C | -3.26979300 | 1.48082500 | 0.19828100 |
| | | | | C | -0.23226800 | 2.79404900 | -0.21207800 |
| | | | | C | -0.46309800 | 2.64761100 | -1.58992300 |
| 10 _{LIRh} | | | | C | 0.19207100 | 4.03403400 | 0.28628800 |
| C | -3.90974300 | -1.77216400 | -0.69194500 | C | 0.41171300 | 5.10049400 | -0.58626300 |
| C | -4.43441300 | -1.70241500 | -1.99368900 | C | 0.19786400 | 4.94524100 | -1.95719800 |
| C | -5.80274200 | -1.53754300 | -2.20834800 | | | | |

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|---|-------------|-------------|-------------|---------------------|-------------|-------------|-------------|
| C | -0.24979100 | 3.72016700 | -2.45582300 | H | 4.88735800 | 0.11688700 | 2.29263000 |
| C | 3.39756700 | -1.77069000 | 0.56747500 | Rh | 0.18916700 | -0.42437000 | -0.30185900 |
| C | 3.90561500 | -2.34108900 | -0.61174100 | | | | |
| C | 4.46751700 | -3.61729100 | -0.59563500 | TS9 _{LIRh} | | | |
| C | 4.52831400 | -4.34329500 | 0.59628500 | C | 4.02091400 | -1.87962000 | 0.53214400 |
| C | 4.02720900 | -3.78339600 | 1.77283700 | C | 4.75000300 | -1.45631300 | 1.65712200 |
| C | 3.46144400 | -2.50729100 | 1.76039000 | C | 6.12728400 | -1.24830800 | 1.58586600 |
| C | 3.43758100 | 0.79047800 | -0.76810700 | C | 6.81464700 | -1.46929800 | 0.39027400 |
| C | 4.83735700 | 0.90359500 | -0.78532700 | C | 6.10724600 | -1.90436400 | -0.73067800 |
| C | 2.68827800 | 1.44029000 | -1.75867400 | C | 4.72615300 | -2.10412500 | -0.65993200 |
| C | 3.31275700 | 2.22653000 | -2.72779500 | H | 4.23528800 | -1.27300500 | 2.59187900 |
| C | 4.70269800 | 2.35273500 | -2.72261300 | H | 6.66439600 | -0.91399200 | 2.46913200 |
| C | 5.46237200 | 1.68334000 | -1.75761900 | H | 7.88739600 | -1.30883000 | 0.33548200 |
| H | 2.44334900 | -0.11314500 | 2.84029900 | H | 6.62652500 | -2.08935600 | -1.66681500 |
| H | 2.06803400 | 2.56687800 | 1.43154200 | H | 4.20573000 | -2.43547700 | -1.55084500 |
| H | 2.21692700 | 2.41177000 | 3.16605000 | C | 2.51420200 | -2.04923200 | 0.61508700 |
| H | -0.04847200 | 2.61822800 | 2.80515500 | C | 1.78416800 | -0.71226100 | 0.97562800 |
| H | -2.12460600 | 2.10718900 | 3.34591800 | O | 2.24921800 | 0.08310200 | 1.77302500 |
| H | -4.50781600 | 2.48090900 | 3.72670400 | H | 0.27966100 | -1.55146900 | 3.31078100 |
| H | -6.13940700 | 2.23001200 | 1.86433700 | C | 2.11500700 | -3.03460300 | 1.75295300 |
| H | -5.32375800 | 1.60532700 | -0.40512500 | H | 2.55459400 | -2.70098500 | 2.69562800 |
| H | -2.94383600 | 1.21517600 | -0.79795800 | H | 2.57453100 | -3.99695100 | 1.50735400 |
| H | -0.80818700 | 1.69786100 | -1.98650400 | C | 1.86159800 | -2.55343800 | -0.67965000 |
| H | 0.34755100 | 4.18577700 | 1.34803100 | H | 2.19325600 | -3.57793900 | -0.89787500 |
| H | 0.74636800 | 6.05451800 | -0.19050900 | H | 2.13963900 | -1.93931100 | -1.54168800 |
| H | 0.37166300 | 5.77778300 | -2.63194500 | C | 0.58234600 | -3.21183300 | 1.93258600 |
| H | -0.42939500 | 3.59502500 | -3.51932000 | C | 0.06739800 | -2.62444000 | 3.25118700 |
| H | 3.86589300 | -1.78724200 | -1.54393600 | H | 0.37890700 | -4.29091500 | 1.96639500 |
| H | 4.85845300 | -4.04302300 | -1.51493400 | H | -1.01562400 | -2.76342700 | 3.34442600 |
| H | 4.96495600 | -5.33720000 | 0.60766700 | H | 0.54820800 | -3.11335000 | 4.10472700 |
| H | 4.07404100 | -4.33945700 | 2.70431200 | C | 0.36865800 | -2.51901100 | -0.52444400 |
| H | 3.06735400 | -2.09708700 | 2.68380600 | C | -0.22154000 | -2.73066800 | 0.73752900 |
| H | 5.43626500 | 0.37586000 | -0.05206900 | H | -0.23046400 | -2.65792300 | -1.42033000 |
| H | 1.60949000 | 1.32639100 | -1.76024400 | H | -0.77529900 | -1.02976500 | 1.45700600 |
| H | 2.71575600 | 2.73444600 | -3.47896300 | H | -1.27116200 | -3.00548800 | 0.76219800 |
| H | 5.19633400 | 2.96268600 | -3.47317900 | P | -2.37287200 | -0.37365400 | -0.61180600 |
| H | 6.54479800 | 1.76932200 | -1.76339600 | C | -2.56046300 | 0.43877000 | -2.28313400 |
| C | 0.07228700 | 0.61473400 | 3.54575000 | C | -1.96957600 | 1.86250000 | -2.28990400 |
| H | -0.99291900 | 0.44862100 | 3.70781200 | C | -0.43398500 | 2.01670300 | -2.35850900 |
| H | 0.51775300 | -0.35123000 | 3.31106800 | P | 0.44279900 | 1.66609800 | -0.75823400 |
| H | 0.50765600 | 0.95855300 | 4.48996200 | C | 2.18353500 | 2.11420400 | -1.10886500 |
| C | 4.23200300 | 0.98148400 | 2.42697800 | C | 3.11640800 | 1.11370200 | -1.40903000 |
| H | 4.59469600 | 1.79177700 | 1.78900700 | C | 4.43965100 | 1.44656700 | -1.69896500 |
| H | 4.31601400 | 1.31035200 | 3.46854100 | C | 4.83939300 | 2.78455900 | -1.69237100 |

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|---|-------------|-------------|-------------|--------------------|-------------|-------------|-------------|
| C | 3.91210700 | 3.78852200 | -1.40041100 | C | 0.19232600 | 1.16371400 | -3.47188200 |
| C | 2.58870200 | 3.45721000 | -1.10875300 | H | 1.23050000 | 1.45097000 | -3.65341700 |
| C | -0.09237000 | 2.93212400 | 0.45015200 | H | 0.17649500 | 0.09533100 | -3.23146300 |
| C | 0.29655800 | 2.74760700 | 1.78868600 | H | -0.36690600 | 1.30764600 | -4.40247600 |
| C | -0.87588800 | 4.04187400 | 0.10725000 | C | -4.00422600 | 0.47144900 | -2.79760000 |
| C | -1.28901000 | 4.93921200 | 1.09489400 | H | -4.61022900 | 1.17787100 | -2.22367600 |
| C | -0.91592500 | 4.74319400 | 2.42519700 | H | -4.00694100 | 0.80017400 | -3.84251700 |
| C | -0.11329700 | 3.65096600 | 2.76816300 | H | -4.48305400 | -0.50969900 | -2.75078100 |
| C | -3.13337500 | -2.02632600 | -0.81021200 | Rh | -0.07578600 | -0.55582900 | 0.19218500 |
| C | -3.79304600 | -2.63428400 | 0.27056800 | | | | |
| C | -4.24738000 | -3.95005500 | 0.17334100 | | | | |
| C | -4.04425800 | -4.67914800 | -1.00060700 | 11 _{LIRh} | | | |
| C | -3.38478300 | -4.08428300 | -2.07829400 | C | 3.94667900 | -1.94813700 | 0.72542200 |
| C | -2.92772900 | -2.76886800 | -1.98446800 | C | 4.83557700 | -1.29142400 | 1.59426200 |
| C | -3.49340100 | 0.52394800 | 0.52065400 | C | 6.20125400 | -1.23473000 | 1.32018300 |
| C | -4.89265300 | 0.48050500 | 0.39949100 | C | 6.71795900 | -1.83596700 | 0.17048500 |
| C | -2.92037300 | 1.29275300 | 1.54385200 | C | 5.85069800 | -2.49682300 | -0.69883800 |
| C | -3.72534100 | 2.02628100 | 2.41751900 | C | 4.48178700 | -2.54975100 | -0.42433300 |
| C | -5.11381300 | 1.98789600 | 2.28188300 | H | 4.45730300 | -0.80435400 | 2.48389300 |
| C | -5.69524500 | 1.20963100 | 1.27604200 | H | 6.86354500 | -0.71728000 | 2.00847800 |
| H | -1.96851100 | -0.19448400 | -2.95012100 | H | 7.78213000 | -1.79261400 | -0.04176800 |
| H | -2.38145700 | 2.42798400 | -1.44873700 | H | 6.23498700 | -2.97642000 | -1.59467400 |
| H | -2.35257000 | 2.35167900 | -3.19352000 | H | 3.83774900 | -3.07254500 | -1.12172900 |
| H | -0.22482300 | 3.06919100 | -2.58294600 | C | 2.45196300 | -1.93434800 | 0.99928100 |
| H | 2.81143400 | 0.07446500 | -1.41007300 | C | 1.88488900 | -0.47054200 | 0.85144800 |
| H | 5.15585800 | 0.65966200 | -1.91260900 | O | 2.49940500 | 0.46252800 | 1.33668800 |
| H | 5.87102500 | 3.04471900 | -1.90980500 | H | 0.60122500 | -0.06368300 | 3.22131200 |
| H | 4.21955000 | 4.83001000 | -1.39437000 | C | 2.11272300 | -2.35007600 | 2.45859200 |
| H | 1.87526400 | 4.24107300 | -0.87521500 | H | 2.69939900 | -1.75707600 | 3.16198100 |
| H | 0.91578500 | 1.89547100 | 2.05385700 | H | 2.42722300 | -3.39261400 | 2.57385400 |
| H | -1.16846200 | 4.22023300 | -0.92059600 | C | 1.64547600 | -2.84844500 | 0.06236700 |
| H | -1.90156200 | 5.79258700 | 0.81992100 | H | 1.97770400 | -3.89029800 | 0.16181400 |
| H | -1.24415900 | 5.43994300 | 3.19054300 | H | 1.80164600 | -2.57635900 | -0.98840700 |
| H | 0.18783100 | 3.49820600 | 3.80037400 | C | 0.60709800 | -2.21415000 | 2.81435100 |
| H | -3.95212400 | -2.08027000 | 1.18987000 | C | 0.28262100 | -0.99663300 | 3.69172400 |
| H | -4.75924600 | -4.40434200 | 1.01649900 | H | 0.33412100 | -3.09809800 | 3.40901700 |
| H | -4.39789900 | -5.70297600 | -1.07532300 | H | -0.79461700 | -0.93131600 | 3.88123300 |
| H | -3.22460300 | -4.64278800 | -2.99576700 | H | 0.79292700 | -1.08071300 | 4.65648800 |
| H | -2.41148400 | -2.32775100 | -2.83077400 | C | 0.17840200 | -2.73061700 | 0.37350300 |
| H | -5.35455000 | -0.13237500 | -0.36599000 | C | -0.27859000 | -2.32492800 | 1.59793000 |
| H | -1.84309600 | 1.31920800 | 1.65271900 | H | -0.53026000 | -3.08306600 | -0.37023600 |
| H | -3.26454500 | 2.62251100 | 3.19892700 | H | -0.35441200 | 0.24522000 | 1.31546700 |
| H | -5.74341500 | 2.55537000 | 2.96080600 | H | -1.34982200 | -2.31002700 | 1.78115200 |
| H | -6.77570800 | 1.16894800 | 1.17513800 | P | -2.33070100 | -0.49031500 | -0.66685800 |
| | | | | C | -2.74261200 | 0.41211100 | -2.24767300 |

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|---|-------------|-------------|-------------|----------------------|-------------|-------------|-------------|
| C | -2.18586300 | 1.84608800 | -2.21179500 | H | -2.76752800 | -4.62336400 | -3.36637100 |
| C | -0.65712000 | 2.01123900 | -2.36265300 | H | -2.28660900 | -2.23494700 | -3.03939500 |
| P | 0.31162500 | 1.68132600 | -0.80533500 | H | -5.23580600 | -0.89997000 | -0.09476500 |
| C | 2.02897600 | 2.06129000 | -1.31924900 | H | -1.99158500 | 1.46541700 | 1.46182200 |
| C | 2.86462600 | 1.02911900 | -1.76927300 | H | -3.52449900 | 2.51323900 | 3.07682300 |
| C | 4.15973300 | 1.30668600 | -2.20113000 | H | -5.92623200 | 1.84998700 | 3.12835700 |
| C | 4.63174200 | 2.62194900 | -2.18855100 | H | -6.76593400 | 0.13965000 | 1.53134500 |
| C | 3.80289200 | 3.65531700 | -1.74823800 | C | -0.08938000 | 1.17927500 | -3.52249000 |
| C | 2.50500500 | 3.37840700 | -1.31429100 | H | 0.93064200 | 1.48123700 | -3.76558800 |
| C | -0.13149400 | 3.00631000 | 0.37645900 | H | -0.07874100 | 0.10690300 | -3.29898700 |
| C | 0.32118100 | 2.88065000 | 1.70132000 | H | -0.70803600 | 1.32590900 | -4.41405600 |
| C | -0.90907100 | 4.11553300 | 0.01851100 | C | -4.23604300 | 0.41667800 | -2.58452200 |
| C | -1.25533200 | 5.06878300 | 0.97937100 | H | -4.80207800 | 1.02456600 | -1.87349000 |
| C | -0.82057500 | 4.92898600 | 2.29716700 | H | -4.38265200 | 0.84176400 | -3.58336600 |
| C | -0.02262800 | 3.83757500 | 2.65358000 | H | -4.65545200 | -0.59275400 | -2.58268600 |
| C | -2.89639800 | -2.20792300 | -0.95970100 | Rh | 0.02103900 | -0.43877500 | 0.03460400 |
| C | -3.38508900 | -2.99471300 | 0.09631800 | | | | |
| C | -3.64875700 | -4.35160700 | -0.09340300 | TS10 _{LIRh} | | | |
| C | -3.42570800 | -4.94500800 | -1.33730500 | C | 4.04577800 | -2.04611300 | 0.70266500 |
| C | -2.93827400 | -4.17201800 | -2.39357700 | C | 4.89665300 | -1.35699800 | 1.58349800 |
| C | -2.67086700 | -2.81545800 | -2.20684700 | C | 6.28150800 | -1.48381300 | 1.49431800 |
| C | -3.49619200 | 0.20442700 | 0.56665000 | C | 6.85242300 | -2.30431600 | 0.51764800 |
| C | -4.85410400 | -0.15689200 | 0.59599200 | C | 6.02098600 | -2.99274400 | -0.36443600 |
| C | -3.03251500 | 1.17066300 | 1.47232500 | C | 4.63189500 | -2.86327700 | -0.27277200 |
| C | -3.90341400 | 1.76527100 | 2.38699600 | H | 4.47633700 | -0.70903200 | 2.34455700 |
| C | -5.24800900 | 1.39398100 | 2.41344300 | H | 6.91580700 | -0.93930300 | 2.18810500 |
| C | -5.72016200 | 0.43141100 | 1.51681600 | H | 7.93157700 | -2.40467900 | 0.44753300 |
| H | -2.21613100 | -0.14649400 | -3.02599700 | H | 6.44803900 | -3.63695100 | -1.12776000 |
| H | -2.54613600 | 2.35549000 | -1.31237500 | H | 4.01365400 | -3.41443900 | -0.97134600 |
| H | -2.63362400 | 2.38020100 | -3.05838600 | C | 2.53344600 | -1.89054200 | 0.82658100 |
| H | -0.46370300 | 3.06605500 | -2.58828900 | C | 2.11307200 | -0.43062500 | 0.51905900 |
| H | 2.51170300 | 0.00240900 | -1.76369200 | O | 2.90236200 | 0.48482200 | 0.42064800 |
| H | 4.80340300 | 0.49593300 | -2.52827200 | H | 0.32917400 | -0.16356700 | 3.20117500 |
| H | 5.64417200 | 2.83870000 | -2.51549300 | C | 2.08553300 | -2.20228000 | 2.29029600 |
| H | 4.16679100 | 4.67821700 | -1.73444100 | H | 2.54546700 | -1.47845100 | 2.96789400 |
| H | 1.87113300 | 4.18592600 | -0.96246800 | H | 2.51927200 | -3.17660900 | 2.53139700 |
| H | 0.95196100 | 2.04071900 | 1.97185800 | C | 1.74370400 | -2.79981600 | -0.12824900 |
| H | -1.25439400 | 4.25003500 | -0.99933800 | H | 1.98070400 | -3.85037800 | 0.08679300 |
| H | -1.86553600 | 5.91982200 | 0.69273700 | H | 2.02577800 | -2.61050900 | -1.16801000 |
| H | -1.09544600 | 5.66924100 | 3.04229800 | C | 0.55344500 | -2.23857200 | 2.54518500 |
| H | 0.33145300 | 3.73046800 | 3.67449000 | C | 0.09362600 | -1.17433800 | 3.55063500 |
| H | -3.56399900 | -2.54878200 | 1.06866300 | H | 0.32783300 | -3.21249500 | 3.00316500 |
| H | -4.02996400 | -4.94352100 | 0.73329500 | H | -0.98770700 | -1.23041500 | 3.71378500 |
| H | -3.63238300 | -6.00067600 | -1.48367300 | H | 0.59248800 | -1.32228200 | 4.51407600 |

| | | | | | | | | |
|---|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
| C | 0.27120900 | -2.56050500 | 0.04235600 | H | -1.81168200 | 4.09984900 | -0.05654000 | |
| C | -0.26509400 | -2.23417800 | 1.27483500 | H | -2.07465200 | 5.42345600 | 1.99178300 | |
| H | -0.37841600 | -2.89804500 | -0.75903500 | H | -0.51329000 | 5.11231700 | 3.90154200 | |
| H | 0.93689100 | 0.01816600 | 1.22824300 | H | 1.34728300 | 3.46761600 | 3.71771900 | |
| H | -1.33744000 | -2.30835300 | 1.42732100 | H | -3.53668800 | -2.79658500 | 0.82803700 | |
| P | -2.29934700 | -0.53207700 | -0.66869700 | H | -3.99560700 | -5.13370700 | 0.19694500 | |
| C | -2.94075900 | 0.54675200 | -2.04097100 | H | -3.54476100 | -5.91834500 | -2.11951200 | |
| C | -2.58210000 | 2.02041700 | -1.77589000 | H | -2.62554000 | -4.33278900 | -3.80220000 | |
| C | -1.12540500 | 2.43555800 | -2.05618600 | H | -2.13976500 | -2.00211800 | -3.17566700 | |
| P | 0.10478400 | 1.86550000 | -0.77019200 | H | -5.15190100 | -0.93166600 | 0.17320700 | |
| C | 1.68088100 | 2.36012300 | -1.55542400 | H | -1.57758900 | 0.89246900 | 1.72990500 | |
| C | 2.38144500 | 1.42585300 | -2.33160600 | H | -2.84681400 | 1.70369800 | 3.69647100 | |
| C | 3.53045200 | 1.80761100 | -3.02111100 | H | -5.27339100 | 1.17907600 | 3.90984000 | |
| C | 3.99321500 | 3.12424000 | -2.93466700 | H | -6.40999900 | -0.14602100 | 2.14086900 | |
| C | 3.29813600 | 4.05802000 | -2.16368400 | C | -0.68129600 | 2.02100000 | -3.46736900 | |
| C | 2.14130000 | 3.67982400 | -1.47834900 | H | 0.20829300 | 2.56876300 | -3.78065500 | |
| C | -0.09130500 | 2.99490300 | 0.66073700 | H | -0.45911100 | 0.95198300 | -3.53932700 | |
| C | 0.79859600 | 2.83593700 | 1.73884100 | H | -1.48655400 | 2.24413700 | -4.17544100 | |
| C | -1.11877300 | 3.94158600 | 0.76051500 | C | -4.44534200 | 0.39266600 | -2.28733600 | |
| C | -1.26929700 | 4.69799000 | 1.92629400 | H | -5.02815200 | 0.82201600 | -1.46811200 | |
| C | -0.39178700 | 4.52538800 | 2.99619100 | H | -4.71225900 | 0.92792200 | -3.20477800 | |
| C | 0.65061200 | 3.59845000 | 2.89498300 | H | -4.73665000 | -0.65383600 | -2.40829600 | |
| C | -2.81503400 | -2.22451100 | -1.12824600 | Rh | -0.00086500 | -0.36250600 | 0.00730900 | |
| C | -3.33197100 | -3.12436200 | -0.18472400 | | | | | |
| C | -3.59280000 | -4.44871300 | -0.54306700 | | | | | |
| C | -3.34027700 | -4.88852600 | -1.84290800 | 12_{LIRh} | C | -4.51842600 | -1.55811500 | -0.69691600 |
| C | -2.82340000 | -3.99830600 | -2.78829800 | C | -5.34195400 | -1.15495600 | -1.75957700 | |
| C | -2.55602300 | -2.67680000 | -2.43406400 | C | -6.72946700 | -1.25572500 | -1.67242300 | |
| C | -3.27551500 | -0.05644200 | 0.80647900 | C | -7.32750400 | -1.75668300 | -0.51433700 | |
| C | -4.64307300 | -0.35170900 | 0.93429700 | C | -6.52212300 | -2.14826100 | 0.55409800 | |
| C | -2.63822500 | 0.68146800 | 1.81705200 | C | -5.13157900 | -2.04674900 | 0.46442700 | |
| C | -3.35452600 | 1.12951200 | 2.92729600 | H | -4.90192600 | -0.75181600 | -2.66436100 | |
| C | -4.71417000 | 0.83487500 | 3.04494300 | H | -7.34307800 | -0.93995100 | -2.51111100 | |
| C | -5.35415400 | 0.09054100 | 2.05015200 | H | -8.40822400 | -1.83785100 | -0.44603000 | |
| H | -2.40804200 | 0.19900900 | -2.93050800 | H | -6.97149800 | -2.53605700 | 1.46366300 | |
| H | -2.88274500 | 2.29198000 | -0.75911900 | H | -4.53509400 | -2.35614500 | 1.31423100 | |
| H | -3.20538900 | 2.62491800 | -2.44545400 | C | -2.99780500 | -1.41772800 | -0.80958100 | |
| H | -1.08218300 | 3.52929100 | -2.00624400 | C | -2.63891900 | 0.06139300 | -0.79143500 | |
| H | 2.02968700 | 0.40002200 | -2.38479100 | O | -3.35352900 | 1.00018000 | -1.03680200 | |
| H | 4.06937100 | 1.07778300 | -3.61817700 | H | -0.71490600 | 0.23766700 | -2.68626200 | |
| H | 4.89266800 | 3.41996300 | -3.46653700 | C | -2.48791000 | -2.00245500 | -2.16827500 | |
| H | 3.65320100 | 5.08207100 | -2.09565500 | H | -3.00517500 | -1.52055500 | -2.99998900 | |
| H | 1.60187600 | 4.41191600 | -0.88557600 | H | -2.80241900 | -3.05094900 | -2.15799500 | |
| H | 1.61387800 | 2.12365100 | 1.66464000 | C | -2.24702200 | -2.16104100 | 0.32086500 | |

| | | | | | | | |
|---|-------------|-------------|-------------|---------------------|-------------|-------------|-------------|
| H | -2.67652900 | -3.16835400 | 0.38990500 | H | 1.78085400 | 3.32354100 | 2.21765100 |
| H | -2.43275400 | -1.68361100 | 1.28926000 | H | -1.73092900 | 0.39798900 | 2.22759300 |
| C | -0.96457300 | -1.93236800 | -2.40911900 | H | -3.91990200 | 1.04827000 | 3.20946600 |
| C | -0.51727200 | -0.70072900 | -3.21173700 | H | -4.64081400 | 3.42788000 | 3.15639600 |
| H | -0.72586100 | -2.79913500 | -3.04052400 | H | -3.16808700 | 5.14768200 | 2.13673300 |
| H | 0.55760200 | -0.74315600 | -3.41085300 | H | -0.99043200 | 4.49819500 | 1.15478200 |
| H | -1.04040900 | -0.66712300 | -4.17354200 | H | -1.16393900 | 2.41098100 | -1.44235100 |
| C | -0.75942000 | -2.31410900 | 0.10527700 | H | 2.54477300 | 3.85699000 | 0.22270000 |
| C | -0.16842700 | -2.15460800 | -1.13667100 | H | 2.92310200 | 5.19971600 | -1.79883500 |
| H | -0.22736900 | -2.84122900 | 0.89163900 | H | 1.28308100 | 5.15178400 | -3.66570300 |
| H | -1.54636700 | 0.30529700 | -0.58485000 | H | -0.77445400 | 3.76377700 | -3.46655500 |
| H | 0.83651800 | -2.53179200 | -1.28904300 | H | 3.18882700 | -3.12308000 | -1.08236500 |
| P | 2.25887800 | -0.77917700 | 0.53319100 | H | 3.34178000 | -5.52701900 | -0.56297800 |
| C | 3.10867600 | 0.06654400 | 1.96646600 | H | 2.75518200 | -6.35869800 | 1.70605700 |
| C | 3.01402800 | 1.60057100 | 1.87152000 | H | 2.00043600 | -4.75404700 | 3.45116400 |
| C | 1.65143400 | 2.23556900 | 2.21538200 | H | 1.81804100 | -2.35388800 | 2.93319400 |
| P | 0.37865300 | 1.86435400 | 0.91992900 | H | 5.01921200 | -1.55177300 | -0.38073700 |
| C | -1.21755600 | 2.40373000 | 1.63205400 | H | 1.73007100 | 0.83959200 | -1.78411600 |
| C | -2.05034800 | 1.43688500 | 2.21644600 | H | 3.07401400 | 1.54123800 | -3.74295000 |
| C | -3.27738800 | 1.80394200 | 2.76745300 | H | 5.39424700 | 0.68064400 | -4.02728200 |
| C | -3.68182900 | 3.14072800 | 2.73593100 | H | 6.35068900 | -0.87118700 | -2.33794900 |
| C | -2.85441000 | 4.10846000 | 2.16056400 | C | 1.14022500 | 1.81126800 | 3.59907800 |
| C | -1.62527500 | 3.74416500 | 1.60927500 | H | 0.32332400 | 2.45519700 | 3.93084500 |
| C | 0.67419600 | 3.01456100 | -0.47080500 | H | 0.77452700 | 0.77940300 | 3.60625600 |
| C | -0.25993500 | 3.00621500 | -1.52292500 | H | 1.95366600 | 1.88627000 | 4.32854000 |
| C | 1.81583100 | 3.81836900 | -0.57760400 | C | 4.57234500 | -0.35976500 | 2.13675200 |
| C | 2.03209500 | 4.58343400 | -1.72684600 | H | 5.20391400 | 0.06354900 | 1.35150400 |
| C | 1.11012100 | 4.55880900 | -2.77286000 | H | 4.94070400 | 0.01347200 | 3.09824500 |
| C | -0.04366900 | 3.77580800 | -2.66342400 | H | 4.69072300 | -1.44597600 | 2.12953500 |
| C | 2.51105000 | -2.55903800 | 0.89087700 | Rh | 0.11798800 | -0.29214300 | 0.15216200 |
| C | 2.92717200 | -3.47084000 | -0.08944800 | | | | |
| C | 3.01409500 | -4.83321500 | 0.20521000 | cat _{L2Rh} | | | |
| C | 2.68499300 | -5.29952600 | 1.47818300 | C | -0.24365800 | 1.54747800 | 0.91202200 |
| C | 2.26135600 | -4.39827900 | 2.45901200 | C | -1.15398500 | 0.52785500 | 1.24793000 |
| C | 2.16763800 | -3.03888800 | 2.16684300 | C | -1.62760900 | 0.39759000 | 2.56110700 |
| C | 3.28280100 | -0.38357900 | -0.93496200 | C | -1.18657900 | 1.27989400 | 3.54271000 |
| C | 4.59073400 | -0.86885200 | -1.10430400 | C | 0.26470000 | 1.73733500 | -0.48073200 |
| C | 2.74583700 | 0.48013400 | -1.90215300 | C | 1.12675700 | 0.82208200 | -1.11156400 |
| C | 3.50329100 | 0.86679400 | -3.00836800 | C | 1.51416800 | 1.01286600 | -2.44683500 |
| C | 4.80358500 | 0.38438100 | -3.16560400 | C | 1.06209800 | 2.12717400 | -3.14525900 |
| C | 5.34259100 | -0.48699500 | -2.21538100 | H | -2.32980400 | -0.38802600 | 2.81309600 |
| H | 2.55113800 | -0.27550400 | 2.84315500 | H | -1.55325200 | 1.18364700 | 4.56024800 |
| H | 3.35496500 | 1.92116200 | 0.88149000 | H | 2.15949500 | 0.29383300 | -2.93644200 |
| H | 3.73686900 | 2.01039900 | 2.58694400 | H | 1.36463300 | 2.27794800 | -4.17714000 |

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|---|-------------|-------------|-------------|------------|-------------|-------------|-------------|
| C | -0.27114400 | 2.28673400 | 3.23874800 | C | -5.02919700 | -3.31196000 | 1.70801300 |
| C | 0.19927100 | 2.42178600 | 1.92811900 | H | -3.45545900 | -4.44522200 | 2.65604400 |
| C | -0.18665000 | 2.85867400 | -1.21331300 | H | -6.36885800 | -2.00112200 | 0.64239800 |
| C | 0.21475900 | 3.05360100 | -2.53851600 | H | -5.82666100 | -3.93061500 | 2.10828900 |
| C | 2.14783300 | -0.25939400 | 1.38696700 | P | 1.53982900 | -0.75176500 | -0.27298000 |
| C | 3.02540400 | 0.82267000 | 1.54566800 | P | -1.56127500 | -0.75450900 | 0.00467700 |
| C | 1.75089100 | -0.99899400 | 2.50793800 | Rh | -0.02659500 | -2.26445100 | -0.36300300 |
| C | 3.49820900 | 1.15716300 | 2.81313800 | H | -0.13733700 | 3.90928700 | -3.10001800 |
| H | 3.31601600 | 1.42148300 | 0.68995100 | H | 0.07099100 | 2.95466800 | 4.01882800 |
| C | 2.21998900 | -0.65701000 | 3.77680900 | O | -1.04262100 | 3.68051100 | -0.55786600 |
| H | 1.05983900 | -1.82728500 | 2.37615000 | O | 1.11113200 | 3.34862300 | 1.54492200 |
| C | 3.09421800 | 0.42080500 | 3.93044000 | C | -1.56030900 | 4.81317500 | -1.25192200 |
| H | 4.17476100 | 1.99828600 | 2.92970500 | H | -2.11891200 | 4.51360500 | -2.14517900 |
| H | 1.89897100 | -1.22718500 | 4.64347900 | H | -2.23538400 | 5.30615000 | -0.55105500 |
| H | 3.45795800 | 0.68917400 | 4.91778200 | H | -0.76022100 | 5.50669700 | -1.53498500 |
| C | 3.03603800 | -1.40948900 | -1.10781800 | C | 1.62665500 | 4.24039100 | 2.53033900 |
| C | 3.05328100 | -2.77497800 | -1.43144400 | H | 2.12228100 | 3.69618400 | 3.34125500 |
| C | 4.16386700 | -0.62364500 | -1.38955100 | H | 2.35742100 | 4.86351800 | 2.01279000 |
| C | 4.17777100 | -3.34681700 | -2.02958800 | H | 0.83566700 | 4.87616800 | 2.94461900 |
| H | 2.18958700 | -3.40180700 | -1.21677400 | | | | |
| C | 5.28297500 | -1.19550100 | -1.99276800 | $3L_{2Rh}$ | | | |
| H | 4.16479100 | 0.43437400 | -1.15134700 | C | -2.71430100 | -0.79951700 | 0.63168000 |
| C | 5.29233500 | -2.55605900 | -2.31279600 | C | -1.65622200 | -1.46562300 | 1.27882400 |
| H | 4.18081000 | -4.40457000 | -2.27446800 | C | -1.81101600 | -1.92303100 | 2.59415100 |
| H | 6.14853400 | -0.57850000 | -2.21425200 | C | -3.00994700 | -1.70591900 | 3.26713600 |
| H | 6.16635200 | -2.99751100 | -2.78189000 | C | -2.65355800 | -0.41311100 | -0.81169300 |
| C | -2.22061200 | 0.18283300 | -1.41788000 | C | -1.93660400 | 0.68899700 | -1.31505000 |
| C | -1.88854100 | -0.21926300 | -2.71748700 | C | -1.82481800 | 0.89346200 | -2.70563400 |
| C | -3.06191400 | 1.28854400 | -1.22304400 | C | -2.47745900 | 0.03834800 | -3.58608400 |
| C | -2.38988800 | 0.48082600 | -3.81525000 | H | -1.00008500 | -2.43929700 | 3.09187700 |
| H | -1.22148000 | -1.06617800 | -2.85500200 | H | -3.12986200 | -2.06539800 | 4.28473100 |
| C | -3.56991600 | 1.97823300 | -2.32268600 | H | -1.23091300 | 1.71339900 | -3.09105600 |
| H | -3.30237000 | 1.61852500 | -0.21807300 | H | -2.39587600 | 0.20000400 | -4.65646400 |
| C | -3.23088300 | 1.57830900 | -3.61842400 | C | -4.05645200 | -1.01621900 | 2.65817100 |
| H | -2.11887000 | 0.17518500 | -4.82131100 | C | -3.90829800 | -0.56314400 | 1.34305800 |
| H | -4.22213200 | 2.83218800 | -2.16818900 | C | -3.32529100 | -1.25513100 | -1.73068300 |
| H | -3.61932100 | 2.12418300 | -4.47297200 | C | -3.23693000 | -1.02905000 | -3.10815600 |
| C | -2.97742600 | -1.70783800 | 0.67270200 | C | -1.65440500 | 1.89288200 | 1.39509400 |
| C | -2.67604600 | -2.80702000 | 1.49797600 | C | -2.86785200 | 2.59968500 | 1.43393000 |
| C | -4.31567900 | -1.42744300 | 0.36304500 | C | -1.08092000 | 1.42341900 | 2.58011500 |
| C | -3.69801300 | -3.60246900 | 2.01577900 | C | -3.50559400 | 2.81637400 | 2.65229800 |
| H | -1.63630800 | -3.02242700 | 1.73549400 | H | -3.31515900 | 2.97269800 | 0.51933400 |
| C | -5.33437200 | -2.22679600 | 0.88289600 | C | -1.72226400 | 1.65081900 | 3.79824700 |
| H | -4.56413500 | -0.59137100 | -0.28061600 | H | -0.14021600 | 0.89344900 | 2.54803200 |

| | | | | | | | |
|----|-------------|-------------|-------------|---------------------|-------------|-------------|-------------|
| C | -2.93348100 | 2.34260000 | 3.83673800 | C | -4.70747800 | -3.17861100 | -2.05115300 |
| H | -4.44556500 | 3.35882400 | 2.67772100 | H | -4.01944600 | -3.67422100 | -2.74334500 |
| H | -1.27537200 | 1.28034500 | 4.71573700 | H | -5.16607100 | -3.92433100 | -1.40064800 |
| H | -3.43099500 | 2.51541800 | 4.78632800 | H | -5.48882400 | -2.65780300 | -2.61605400 |
| C | -0.84614800 | 3.41496800 | -0.82476400 | C | -6.06798200 | 0.45614700 | 1.35405600 |
| C | 0.13407600 | 4.26137700 | -0.28244000 | H | -5.87341200 | 1.05135200 | 2.25273500 |
| C | -1.81186300 | 3.94307900 | -1.69122300 | H | -6.65978800 | 1.04346800 | 0.65066700 |
| C | 0.16401500 | 5.61097000 | -0.62572700 | H | -6.62139800 | -0.44991100 | 1.62640200 |
| H | 0.86688400 | 3.86632700 | 0.41370000 | C | 4.17985100 | 0.28321500 | -0.47776200 |
| C | -1.77522400 | 5.29665200 | -2.03386900 | C | 5.21738600 | 0.33858900 | -1.41848600 |
| H | -2.59503200 | 3.31177700 | -2.09366700 | C | 5.82237200 | -0.82946100 | -1.88087400 |
| C | -0.78681200 | 6.12979200 | -1.50919000 | C | 5.40487300 | -2.07827100 | -1.40936300 |
| H | 0.92796300 | 6.25659600 | -0.20351900 | C | 4.39833200 | -2.14370300 | -0.44681600 |
| H | -2.52570300 | 5.69740500 | -2.70843900 | C | 3.80291900 | -0.96865200 | 0.02275600 |
| H | -0.76124600 | 7.18090800 | -1.77960000 | H | 5.54795500 | 1.29749200 | -1.80402400 |
| C | -0.37769200 | -2.72715500 | -0.97111700 | H | 6.62072900 | -0.76546300 | -2.61464300 |
| C | 0.20810300 | -2.44696100 | -2.21400700 | H | 5.87331000 | -2.98609500 | -1.77739300 |
| C | -1.23196900 | -3.83138600 | -0.84196800 | H | 4.07721600 | -3.10009700 | -0.04570300 |
| C | -0.05361100 | -3.26124400 | -3.31662000 | H | 3.05071300 | -1.04214300 | 0.79692200 |
| H | 0.85787000 | -1.58178500 | -2.32079900 | C | 3.50237600 | 1.56793700 | -0.00138400 |
| C | -1.48381400 | -4.64988900 | -1.94220200 | C | 2.15399600 | 1.23201700 | 0.70708500 |
| H | -1.70346800 | -4.04227400 | 0.11212600 | O | 1.94580100 | 1.46652000 | 1.87523300 |
| C | -0.89936500 | -4.36391100 | -3.17987300 | H | 2.65201800 | -0.18254400 | -2.58433100 |
| H | 0.39649800 | -3.03207200 | -4.27778800 | C | 3.02843300 | 2.43900800 | -1.19137700 |
| H | -2.14336200 | -5.50578100 | -1.83704700 | H | 3.86902500 | 2.65336600 | -1.86294100 |
| H | -1.10695200 | -4.99817400 | -4.03636000 | H | 2.69868300 | 3.40035500 | -0.78680200 |
| C | 1.04147700 | -2.52277300 | 1.57587900 | C | 4.45597600 | 2.36773200 | 0.92832700 |
| C | 1.56071400 | -1.83456300 | 2.68711100 | H | 3.90752200 | 3.24518300 | 1.29121200 |
| C | 1.43257000 | -3.84809600 | 1.34604800 | H | 5.28214400 | 2.72883100 | 0.30572000 |
| C | 2.44293700 | -2.46928700 | 3.55873200 | C | 1.86709000 | 1.76416900 | -1.92278800 |
| H | 1.29052300 | -0.79817600 | 2.85904800 | C | 2.26764300 | 0.75804300 | -3.00094200 |
| C | 2.32549400 | -4.47682900 | 2.21780500 | H | 1.19004300 | 2.51361800 | -2.33832900 |
| H | 1.04722700 | -4.39086400 | 0.49027500 | H | 1.42074200 | 0.51615200 | -3.65183600 |
| C | 2.83055900 | -3.79165200 | 3.32337800 | H | 3.07518000 | 1.15300300 | -3.63470900 |
| H | 2.83674600 | -1.92789600 | 4.41354900 | C | 5.00338100 | 1.58576600 | 2.08756400 |
| H | 2.62398200 | -5.50378300 | 2.02976600 | C | 6.27405400 | 1.19447900 | 2.19692200 |
| H | 3.52601900 | -4.28246100 | 3.99730000 | H | 4.29011500 | 1.32384800 | 2.86621600 |
| P | -0.84975500 | 1.68602100 | -0.23291800 | H | 6.62394600 | 0.62324200 | 3.05286300 |
| P | -0.03454900 | -1.59691500 | 0.42386600 | H | 7.01193400 | 1.43466000 | 1.43387600 |
| Rh | 0.93878800 | 0.42991900 | -0.60965300 | | | | |
| H | -3.73834500 | -1.68685500 | -3.80629000 | TS4 _{L2Rh} | | | |
| H | -4.97328600 | -0.83644300 | 3.20463300 | C | -2.73751200 | -0.85144100 | 0.63275900 |
| O | -4.01591900 | -2.28284600 | -1.18226900 | C | -1.60586600 | -1.35360300 | 1.30044900 |
| O | -4.85650800 | 0.13822200 | 0.67178800 | C | -1.68434800 | -1.71225900 | 2.65330900 |

| | | | | | | | |
|---|-------------|-------------|-------------|----|-------------|-------------|-------------|
| C | -2.88279300 | -1.54976800 | 3.34187900 | H | -1.97337500 | -5.43231700 | -1.75034800 |
| C | -2.71131400 | -0.53661300 | -0.82460300 | H | -1.01389200 | -4.91198700 | -3.98271300 |
| C | -1.96534700 | 0.52352700 | -1.36410800 | C | 1.10918400 | -2.31256200 | 1.58572100 |
| C | -1.84017000 | 0.65911200 | -2.75945500 | C | 1.68482400 | -1.57781800 | 2.63688900 |
| C | -2.51647000 | -0.21171900 | -3.60492200 | C | 1.41686700 | -3.67117300 | 1.44447200 |
| H | -0.82069100 | -2.11048900 | 3.16891600 | C | 2.54631300 | -2.19904800 | 3.53788300 |
| H | -2.94421500 | -1.83011800 | 4.38897100 | H | 1.46349300 | -0.52017100 | 2.74076900 |
| H | -1.20907900 | 1.42985200 | -3.18339600 | C | 2.29152500 | -4.28590800 | 2.34332000 |
| H | -2.42614400 | -0.09644300 | -4.68071100 | H | 0.98496800 | -4.24901000 | 0.63563400 |
| C | -4.00294800 | -1.01245300 | 2.71147400 | C | 2.85509800 | -3.55434600 | 3.38903800 |
| C | -3.93062300 | -0.66239000 | 1.35895200 | H | 2.98344200 | -1.62417300 | 4.34819500 |
| C | -3.38705700 | -1.41527800 | -1.70554700 | H | 2.53070600 | -5.33803200 | 2.22258600 |
| C | -3.30220000 | -1.24268700 | -3.08928600 | H | 3.53535700 | -4.03577600 | 4.08482400 |
| C | -1.74528600 | 1.85978300 | 1.30082700 | P | -0.89030900 | 1.54809500 | -0.29010200 |
| C | -3.01227400 | 2.46330800 | 1.29374200 | P | 0.00660400 | -1.42805100 | 0.42153000 |
| C | -1.09582500 | 1.61557400 | 2.51391700 | Rh | 1.06946100 | 0.45699100 | -0.29820400 |
| C | -3.63005900 | 2.79411400 | 2.49673800 | H | -3.81525400 | -1.91704400 | -3.76263300 |
| H | -3.51331900 | 2.66978100 | 0.35392100 | H | -4.91813500 | -0.86794300 | 3.27122000 |
| C | -1.71785200 | 1.95256900 | 3.71765800 | O | -4.06749900 | -2.42606100 | -1.11303100 |
| H | -0.11076300 | 1.16213300 | 2.50874500 | O | -4.95027500 | -0.09908300 | 0.66602800 |
| C | -2.98447700 | 2.53761700 | 3.71083500 | C | -4.75694100 | -3.35676800 | -1.94513800 |
| H | -4.61254000 | 3.25619800 | 2.48805400 | H | -4.06882000 | -3.87039400 | -2.62434500 |
| H | -1.21192000 | 1.75492900 | 4.65793200 | H | -5.20656700 | -4.08301800 | -1.26688000 |
| H | -3.46771100 | 2.79840400 | 4.64760800 | H | -5.54539400 | -2.86273800 | -2.52431000 |
| C | -0.92328800 | 3.26965000 | -0.93692600 | C | -6.16408200 | 0.18297000 | 1.35973400 |
| C | -0.12492900 | 4.20148900 | -0.24924900 | H | -5.99323200 | 0.87157000 | 2.19435300 |
| C | -1.79423900 | 3.72221100 | -1.93699400 | H | -6.82074100 | 0.65576900 | 0.62820500 |
| C | -0.16862900 | 5.55217700 | -0.58879600 | H | -6.63496000 | -0.73458700 | 1.73044300 |
| H | 0.52781300 | 3.86676600 | 0.55101500 | C | 4.27128800 | 0.17845700 | -0.70541700 |
| C | -1.83198800 | 5.07769200 | -2.27286900 | C | 5.30063200 | -0.05234200 | -1.62567600 |
| H | -2.46255600 | 3.03707200 | -2.44187000 | C | 5.41575300 | -1.29012400 | -2.25961600 |
| C | -1.01589500 | 5.99313700 | -1.60868400 | C | 4.50507700 | -2.31799000 | -1.98946300 |
| H | 0.45704200 | 6.25963500 | -0.05291500 | C | 3.48814700 | -2.10675200 | -1.06056500 |
| H | -2.51194000 | 5.41511400 | -3.04926600 | C | 3.38728700 | -0.86621200 | -0.42209900 |
| H | -1.04982100 | 7.04579800 | -1.87255100 | H | 6.00945700 | 0.73743400 | -1.85489500 |
| C | -0.31748600 | -2.56203300 | -0.97414800 | H | 6.21801200 | -1.45309700 | -2.97323700 |
| C | 0.22228600 | -2.27044100 | -2.23384300 | H | 4.59687100 | -3.27564800 | -2.49214700 |
| C | -1.11670300 | -3.70259300 | -0.80444200 | H | 2.78433300 | -2.89499300 | -0.82077400 |
| C | -0.02847200 | -3.11537600 | -3.31481800 | H | 2.68866500 | -0.74247900 | 0.41518300 |
| H | 0.81687600 | -1.36985300 | -2.35648600 | C | 4.10616800 | 1.51708700 | -0.02170500 |
| C | -1.35649300 | -4.54939000 | -1.88550200 | C | 2.63417900 | 1.91614400 | 0.25647700 |
| H | -1.55953900 | -3.91842700 | 0.16191600 | O | 2.25794000 | 2.50216200 | 1.27418000 |
| C | -0.81555200 | -4.25569700 | -3.14070600 | H | 2.56788000 | 0.89890700 | -2.71372600 |
| H | 0.38195700 | -2.87823400 | -4.29163800 | C | 4.01906600 | 2.66686100 | -1.07877300 |

| | | | | | | | |
|------------|-------------|-------------|-------------|----|-------------|-------------|-------------|
| H | 4.58322400 | 2.49764300 | -1.99741300 | C | -1.21454600 | 3.29100500 | -0.52767800 |
| H | 4.29242300 | 3.62227300 | -0.62622400 | C | -0.41282000 | 4.24274000 | 0.12069600 |
| C | 5.07306600 | 1.69731300 | 1.15776400 | C | -2.22089400 | 3.72670200 | -1.40566600 |
| H | 4.93337600 | 2.70960600 | 1.55415600 | C | -0.59449800 | 5.60332000 | -0.12946900 |
| H | 6.09989800 | 1.61820700 | 0.78382100 | H | 0.35624800 | 3.91675100 | 0.81012500 |
| C | 2.47589800 | 2.55207100 | -1.25610400 | C | -2.39464400 | 5.08821600 | -1.65350400 |
| C | 2.09004400 | 1.87125900 | -2.57807600 | H | -2.87603800 | 3.01402600 | -1.89109900 |
| H | 1.93510600 | 3.48953600 | -1.16313400 | C | -1.57983500 | 6.02932300 | -1.02149900 |
| H | 1.00966900 | 1.75759400 | -2.69529700 | H | 0.03711800 | 6.32891500 | 0.37438900 |
| H | 2.43889700 | 2.52312500 | -3.38890700 | H | -3.17342600 | 5.41112800 | -2.33764700 |
| C | 4.83314600 | 0.68377100 | 2.24229500 | H | -1.71810200 | 7.08834600 | -1.21739200 |
| C | 5.66277900 | -0.31648600 | 2.54155400 | C | 0.31142200 | -2.19240600 | -1.14738500 |
| H | 3.89315900 | 0.78440000 | 2.78258300 | C | 0.99993000 | -1.51713600 | -2.16233800 |
| H | 5.43276200 | -1.03527600 | 3.32302300 | C | -0.24698200 | -3.45485600 | -1.39712100 |
| H | 6.60468100 | -0.45064700 | 2.01315500 | C | 1.13634600 | -2.10205900 | -3.42027700 |
| | | | | H | 1.41579700 | -0.53774000 | -1.95763400 |
| | | | | C | -0.09638400 | -4.04089100 | -2.65308700 |
| 4_{L2Rh} | | | | H | -0.81030400 | -3.96472000 | -0.62302100 |
| C | -2.62925800 | -1.25488800 | 0.23387600 | C | 0.59155600 | -3.36443500 | -3.66496300 |
| C | -1.57102800 | -1.74752600 | 1.01472700 | H | 1.66656100 | -1.57245100 | -4.20569500 |
| C | -1.81988200 | -2.35731300 | 2.25150600 | H | -0.52373600 | -5.02019800 | -2.84486900 |
| C | -3.12886800 | -2.46585300 | 2.71241400 | H | 0.69881500 | -3.82067500 | -4.64450300 |
| C | -2.40616200 | -0.69437000 | -1.13157400 | C | 1.18514100 | -2.31090900 | 1.67805700 |
| C | -1.78944000 | 0.54372800 | -1.38682700 | C | 1.60120400 | -1.60589600 | 2.82107600 |
| C | -1.56563000 | 0.95363500 | -2.71267900 | C | 1.58585700 | -3.64137500 | 1.50361300 |
| C | -1.95947000 | 0.14688200 | -3.77276400 | C | 2.41112600 | -2.22346600 | 3.77383500 |
| H | -1.00123900 | -2.73886700 | 2.84874200 | H | 1.28948500 | -0.57075100 | 2.96144100 |
| H | -3.32734300 | -2.94471500 | 3.66649400 | C | 2.39604000 | -4.25573900 | 2.45967400 |
| H | -1.09616500 | 1.90449600 | -2.92030300 | H | 1.27775600 | -4.19329800 | 0.62272500 |
| H | -1.78522200 | 0.47516900 | -4.79276200 | C | 2.81151100 | -3.54938400 | 3.59088700 |
| C | -4.19203800 | -1.95335500 | 1.97094000 | H | 2.72924300 | -1.67122400 | 4.65264800 |
| C | -3.94408700 | -1.34620000 | 0.73467000 | H | 2.70623700 | -5.28640900 | 2.31771400 |
| C | -2.78940200 | -1.50420700 | -2.22796600 | H | 3.44613800 | -4.03098600 | 4.32839900 |
| C | -2.56874400 | -1.08478300 | -3.54186500 | P | -1.06954600 | 1.53374200 | -0.01775600 |
| C | -2.27461100 | 1.48832100 | 1.36742300 | P | 0.14521700 | -1.40032100 | 0.48167500 |
| C | -3.59406500 | 1.92372200 | 1.18104200 | Rh | 0.88311600 | 0.77189200 | 0.72878900 |
| C | -1.85114000 | 1.07436000 | 2.63627400 | H | -2.85557100 | -1.71043200 | -4.37722100 |
| C | -4.48250600 | 1.92532800 | 2.25445300 | H | -5.20125800 | -2.02914000 | 2.35514400 |
| H | -3.93049200 | 2.25199300 | 0.20378200 | O | -3.33985900 | -2.70024500 | -1.90512400 |
| C | -2.74310100 | 1.07721400 | 3.70855100 | O | -4.90577800 | -0.79438500 | -0.04488300 |
| H | -0.82710200 | 0.73133900 | 2.76462100 | C | -3.70937200 | -3.58190200 | -2.96324600 |
| C | -4.05993700 | 1.50031700 | 3.51754200 | H | -2.84304300 | -3.85323400 | -3.57572100 |
| H | -5.50478600 | 2.25913700 | 2.10560300 | H | -4.10523900 | -4.47538500 | -2.47882300 |
| H | -2.41215800 | 0.74322900 | 4.68726700 | H | -4.48490800 | -3.13889000 | -3.59844500 |
| H | -4.75596300 | 1.50058800 | 4.35096700 | | | | |

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|---------------------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | -6.24798400 | -0.79399800 | 0.43744500 | H | 7.35868700 | -1.53293300 | -1.18229800 |
| H | -6.32641300 | -0.26462200 | 1.39317200 | H | 7.86254800 | -1.62271200 | 1.25514000 |
| H | -6.83407300 | -0.26884800 | -0.31785900 | H | 6.33449800 | -0.49577300 | 2.86390700 |
| H | -6.63213700 | -1.81419000 | 0.55006400 | H | 4.32530100 | 0.68438500 | 2.05112000 |
| C | 4.18148000 | 0.38030600 | -0.78760700 | C | 3.47658100 | 1.00028400 | -0.56366100 |
| C | 4.94165100 | 0.17488400 | -1.94592800 | C | 2.22308300 | 0.88352000 | 0.32669700 |
| C | 5.18051400 | -1.11363000 | -2.42987100 | O | 2.14405800 | 1.12185600 | 1.50730700 |
| C | 4.67349700 | -2.22507500 | -1.75569000 | H | 1.76720800 | -1.19745900 | -3.80877100 |
| C | 3.92758200 | -2.03655000 | -0.59172500 | C | 2.90808900 | 0.38883200 | -1.86074800 |
| C | 3.68626700 | -0.74847300 | -0.11630700 | H | 3.20176500 | 0.81822000 | -2.81733100 |
| H | 5.36239900 | 1.01927300 | -2.48006600 | H | 1.62837200 | 1.31854700 | -1.94928500 |
| H | 5.76890900 | -1.24478800 | -3.33343100 | C | 3.85012000 | 2.49879600 | -0.79908200 |
| H | 4.85751300 | -3.22694200 | -2.13185500 | H | 3.03651800 | 2.96038000 | -1.36899200 |
| H | 3.52674600 | -2.88762600 | -0.05354700 | H | 4.73717300 | 2.49333100 | -1.44122600 |
| H | 3.11976900 | -0.62093500 | 0.79984200 | C | 2.50947000 | -0.97158400 | -1.78183600 |
| C | 3.94111700 | 1.75924700 | -0.20382100 | C | 2.27434800 | -1.77864300 | -3.03188000 |
| C | 2.44685000 | 2.16448300 | -0.00720700 | H | 2.87217200 | -1.53513600 | -0.92802000 |
| O | 1.95526400 | 2.49876500 | 1.13494900 | H | 3.23887200 | -2.10912800 | -3.44160700 |
| H | 2.27056000 | 1.36092300 | -2.71019400 | H | 1.68345600 | -2.67404600 | -2.82991900 |
| C | 3.96688400 | 2.94324800 | -1.23080000 | C | 4.11635000 | 3.28910400 | 0.44639600 |
| H | 4.44779300 | 2.75031500 | -2.18963300 | C | 5.32525700 | 3.71373900 | 0.81571900 |
| H | 4.40025600 | 3.83621600 | -0.77673400 | H | 3.25425800 | 3.50960300 | 1.07319900 |
| C | 4.82455400 | 2.01152800 | 1.04724200 | H | 5.47482600 | 4.28741200 | 1.72634200 |
| H | 4.66487800 | 3.05425200 | 1.34784500 | H | 6.20920600 | 3.50132000 | 0.21791600 |
| H | 5.87056500 | 1.91565100 | 0.73368400 | C | -2.53328500 | -0.65035100 | 1.12327000 |
| C | 2.41284900 | 3.00277900 | -1.28996900 | C | -1.32747600 | -1.28440900 | 1.48517300 |
| C | 1.83590300 | 2.34845400 | -2.53597800 | C | -1.06775800 | -1.60047500 | 2.82558300 |
| H | 1.96891900 | 3.98778500 | -1.13187400 | C | -2.00138100 | -1.28147200 | 3.80733600 |
| H | 0.75737100 | 2.23530400 | -2.44663300 | C | -2.91935200 | -0.36122700 | -0.29405900 |
| H | 2.04430900 | 2.97008100 | -3.41344000 | C | -2.35047100 | 0.66124100 | -1.07781600 |
| C | 4.56057600 | 1.12340200 | 2.22871800 | C | -2.72592800 | 0.81356000 | -2.42381100 |
| C | 5.41604200 | 0.21784300 | 2.70597500 | C | -3.70951800 | -0.00552000 | -2.96829300 |
| H | 3.59470700 | 1.25762400 | 2.71279600 | H | -0.14905800 | -2.10051000 | 3.10278200 |
| H | 5.17573500 | -0.39457000 | 3.57098000 | H | -1.79869500 | -1.52950900 | 4.84480000 |
| H | 6.38714200 | 0.05368100 | 2.24318300 | H | -2.26254200 | 1.57656800 | -3.03761300 |
| | | | | H | -4.00893900 | 0.12549300 | -4.00376700 |
| | | | | C | -3.19469900 | -0.64364700 | 3.47632000 |
| TS5 _{L2Rh} | | | | C | -3.46135200 | -0.33231400 | 2.13918800 |
| C | 4.68391700 | 0.23869400 | -0.02388200 | C | -3.91487500 | -1.18337500 | -0.87349600 |
| C | 5.55764900 | -0.38842400 | -0.92421700 | C | -4.31744900 | -0.99605400 | -2.19914800 |
| C | 6.69650400 | -1.05166200 | -0.46859600 | C | -1.49701200 | 2.15330000 | 1.27220200 |
| C | 6.98019600 | -1.10015100 | 0.89803300 | C | -2.71613900 | 2.83201800 | 1.42686200 |
| C | 6.12218300 | -0.46941700 | 1.79908700 | C | -0.69896100 | 1.90174300 | 2.39317900 |
| C | 4.98491800 | 0.20066200 | 1.34292000 | C | -3.12524400 | 3.25521900 | 2.68906400 |
| H | 5.34856000 | -0.36395200 | -1.98895300 | | | | |

| | | | | | | | |
|----|-------------|-------------|-------------|------------|-------------|-------------|-------------|
| H | -3.35432600 | 3.01695700 | 0.57092200 | H | -3.90542200 | -0.39266700 | 4.25320100 |
| C | -1.11525100 | 2.32595400 | 3.65633100 | O | -4.41282300 | -2.15254700 | -0.06777200 |
| H | 0.23538900 | 1.37076800 | 2.27935100 | O | -4.58855800 | 0.29591000 | 1.72273800 |
| C | -2.32539900 | 3.00340500 | 3.80757600 | C | -5.40958100 | -3.02693700 | -0.59100400 |
| H | -4.07096000 | 3.77684700 | 2.80022700 | H | -5.04023900 | -3.57801100 | -1.46208600 |
| H | -0.49355500 | 2.11815500 | 4.52221900 | H | -5.63613200 | -3.72982600 | 0.21178600 |
| H | -2.64756500 | 3.33245800 | 4.79110700 | H | -6.31884600 | -2.47739700 | -0.86053400 |
| C | -0.99579900 | 3.27297100 | -1.28765000 | C | -5.56497800 | 0.65112100 | 2.69810800 |
| C | 0.21774400 | 3.96534800 | -1.39732800 | H | -5.15118300 | 1.33398400 | 3.44755800 |
| C | -2.17519600 | 3.88806400 | -1.73566600 | H | -6.36150200 | 1.15603200 | 2.14992400 |
| C | 0.25952300 | 5.24493700 | -1.95140500 | H | -5.97225500 | -0.23675000 | 3.19510000 |
| H | 1.12781700 | 3.49877500 | -1.03933500 | | | | |
| C | -2.12976400 | 5.16212700 | -2.30184700 | 5_{L2Rh} | | | |
| H | -3.12678300 | 3.37614200 | -1.65390300 | C | 4.53544500 | 0.05042900 | 0.08573500 |
| C | -0.91499300 | 5.84307100 | -2.41132200 | C | 5.38491300 | -0.88818100 | -0.51593800 |
| H | 1.20740600 | 5.76952900 | -2.02520400 | C | 6.36094000 | -1.55005200 | 0.22918100 |
| H | -3.04703900 | 5.62422200 | -2.65404600 | C | 6.50919000 | -1.28060200 | 1.59099400 |
| H | -0.88556900 | 6.83575000 | -2.85013700 | C | 5.67876600 | -0.33610600 | 2.19534800 |
| C | -0.95912500 | -2.64011800 | -1.02348100 | C | 4.70277400 | 0.32690800 | 1.44909900 |
| C | -0.95021500 | -2.25986500 | -2.37058600 | H | 5.28528200 | -1.10723500 | -1.57369700 |
| C | -1.67232300 | -3.78078400 | -0.62750200 | H | 7.00535600 | -2.27642100 | -0.25732600 |
| C | -1.62926800 | -3.02122700 | -3.32090200 | H | 7.26654600 | -1.79766000 | 2.17251800 |
| H | -0.43081100 | -1.35237900 | -2.66580700 | H | 5.78826500 | -0.10958300 | 3.25198000 |
| C | -2.34483500 | -4.54476500 | -1.57958000 | H | 4.06997300 | 1.06201000 | 1.92984000 |
| H | -1.70261300 | -4.06579300 | 0.41921400 | C | 3.52042500 | 0.81382100 | -0.76455400 |
| C | -2.32222000 | -4.16727800 | -2.92592700 | C | 2.24392500 | 1.19708600 | 0.00475100 |
| H | -1.62814800 | -2.71407300 | -4.36209300 | O | 2.17495900 | 1.91157100 | 0.97699400 |
| H | -2.89286800 | -5.42966400 | -1.27122900 | H | 1.93400600 | -1.55996800 | -3.90330300 |
| H | -2.85253500 | -4.76155500 | -3.66392500 | C | 2.95727000 | 0.01396200 | -1.95080500 |
| C | 1.22502700 | -2.67639200 | 0.91295200 | H | 3.02490700 | 0.47622100 | -2.93148400 |
| C | 2.07343900 | -2.14470600 | 1.90013100 | H | 1.16233000 | 1.63128000 | -1.97478700 |
| C | 1.50093300 | -3.94679100 | 0.38806000 | C | 4.16416200 | 2.12175900 | -1.33756300 |
| C | 3.16585900 | -2.87738400 | 2.35969900 | H | 3.39402600 | 2.62056300 | -1.94087700 |
| H | 1.89007500 | -1.15470000 | 2.29927000 | H | 4.95887700 | 1.79801100 | -2.01837600 |
| C | 2.60229500 | -4.67295000 | 0.84714400 | C | 2.56259800 | -1.28853000 | -1.85178100 |
| H | 0.86840200 | -4.37099500 | -0.38242000 | C | 2.22237600 | -2.15031300 | -3.02916900 |
| C | 3.43652100 | -4.14197300 | 1.83102600 | H | 2.71336300 | -1.80199900 | -0.90890900 |
| H | 3.81433900 | -2.45198400 | 3.11873000 | H | 3.10899100 | -2.74216000 | -3.29422600 |
| H | 2.80560600 | -5.65471500 | 0.43014200 | H | 1.42474100 | -2.85766900 | -2.79696200 |
| H | 4.29479000 | -4.70666200 | 2.18199400 | C | 4.71664400 | 3.07163200 | -0.31867600 |
| P | -0.95816900 | 1.65691000 | -0.41548900 | C | 6.01465200 | 3.34821700 | -0.18765800 |
| P | -0.06938700 | -1.60655200 | 0.18728500 | H | 3.99619200 | 3.54900400 | 0.34190900 |
| Rh | 0.88424900 | 0.25280500 | -0.94388100 | H | 6.37514900 | 4.05189600 | 0.55780100 |
| H | -5.07989300 | -1.62678600 | -2.63792400 | H | 6.76368700 | 2.88049800 | -0.82350500 |

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|---|-------------|-------------|-------------|------------|-------------|-------------|-------------|
| C | -2.54522400 | -0.64375200 | 1.12327900 | H | -1.87431700 | -3.96712700 | 0.17989200 |
| C | -1.35617800 | -1.34450000 | 1.39999100 | C | -2.51461200 | -3.87144600 | -3.16045300 |
| C | -1.08114800 | -1.78169100 | 2.70310600 | H | -1.75582000 | -2.38513800 | -4.52799100 |
| C | -1.98010400 | -1.51059000 | 3.73044000 | H | -3.13755100 | -5.18621700 | -1.56647200 |
| C | -2.95336000 | -0.24369200 | -0.25829000 | H | -3.08104400 | -4.39811800 | -3.92252800 |
| C | -2.35776900 | 0.80000800 | -0.98852700 | C | 1.13509800 | -2.71617000 | 0.76790200 |
| C | -2.74589000 | 1.05114100 | -2.31705500 | C | 2.08865600 | -2.15678800 | 1.63625500 |
| C | -3.76824000 | 0.30611700 | -2.89299700 | C | 1.25143000 | -4.06036900 | 0.39378700 |
| H | -0.17228200 | -2.32938900 | 2.91614900 | C | 3.12770600 | -2.93684400 | 2.13735700 |
| H | -1.76628500 | -1.85354600 | 4.73822800 | H | 2.02773000 | -1.10731000 | 1.90606800 |
| H | -2.25975100 | 1.83145400 | -2.88993000 | C | 2.30283600 | -4.83555500 | 0.88963400 |
| H | -4.07689300 | 0.51072000 | -3.91360000 | H | 0.53560200 | -4.50289800 | -0.28884800 |
| C | -3.14759100 | -0.79081800 | 3.48615900 | C | 3.23920000 | -4.27809800 | 1.76072100 |
| C | -3.42909100 | -0.35858600 | 2.18625800 | H | 3.86272900 | -2.49035900 | 2.79783600 |
| C | -3.98888200 | -0.99075000 | -0.87003600 | H | 2.38789500 | -5.87578600 | 0.59014900 |
| C | -4.40199200 | -0.70723600 | -2.17487000 | H | 4.05804500 | -4.88180200 | 2.13987900 |
| C | -1.23917700 | 2.01594600 | 1.44799700 | P | -0.90259000 | 1.69335100 | -0.32702900 |
| C | -2.36015500 | 2.79131400 | 1.78390700 | P | -0.11807400 | -1.58719200 | 0.06328900 |
| C | -0.40124100 | 1.53779000 | 2.46069200 | Rh | 0.83833500 | 0.38485300 | -1.05832200 |
| C | -2.63428500 | 3.08379600 | 3.11799100 | H | -5.19347800 | -1.28101900 | -2.63925900 |
| H | -3.02453000 | 3.16041800 | 1.01139500 | H | -3.82570600 | -0.56993400 | 4.30038000 |
| C | -0.67826300 | 1.83550900 | 3.79460000 | O | -4.51124900 | -1.98840400 | -0.11638000 |
| H | 0.45873400 | 0.93562100 | 2.20911900 | O | -4.52657900 | 0.36431100 | 1.85173700 |
| C | -1.79168800 | 2.60893800 | 4.12627300 | C | -5.54627500 | -2.79416700 | -0.67556300 |
| H | -3.50461100 | 3.68255000 | 3.36838500 | H | -5.20788500 | -3.30410700 | -1.58352000 |
| H | -0.02612300 | 1.45413500 | 4.57442200 | H | -5.78722400 | -3.53561300 | 0.08736900 |
| H | -2.00426200 | 2.83911500 | 5.16594900 | H | -6.43836600 | -2.19763000 | -0.89811800 |
| C | -0.95361400 | 3.38805700 | -1.03018600 | C | -5.44905400 | 0.70678600 | 2.88327600 |
| C | 0.25017800 | 4.09889600 | -1.14511100 | H | -4.97033900 | 1.31207000 | 3.66048200 |
| C | -2.16005000 | 4.02654700 | -1.35531800 | H | -6.23181700 | 1.29212200 | 2.39904700 |
| C | 0.24868700 | 5.42013800 | -1.59093700 | H | -5.89171000 | -0.18822300 | 3.33531500 |
| H | 1.18664700 | 3.62247900 | -0.88133500 | | | | |
| C | -2.15562400 | 5.34498800 | -1.81202700 | 6_{L2Rh} | | | |
| H | -3.10218000 | 3.49777400 | -1.26705800 | C | -4.92253700 | 0.03539100 | -0.39896600 |
| C | -0.95332600 | 6.04373000 | -1.93241000 | C | -5.77133400 | 0.25310000 | 0.69444400 |
| H | 1.18759800 | 5.95898100 | -1.67470500 | C | -6.76789300 | -0.66478100 | 1.02738000 |
| H | -3.09448100 | 5.82398700 | -2.07277700 | C | -6.93503500 | -1.82812300 | 0.27507700 |
| H | -0.95311800 | 7.06923600 | -2.28888900 | C | -6.09037800 | -2.06355500 | -0.81010300 |
| C | -1.05510100 | -2.51869500 | -1.19648200 | C | -5.09302000 | -1.14397800 | -1.14036500 |
| C | -1.03718700 | -2.06938400 | -2.52446000 | H | -5.65451400 | 1.15199200 | 1.28698000 |
| C | -1.82830800 | -3.63716900 | -0.85281300 | H | -7.41547000 | -0.46580900 | 1.87642800 |
| C | -1.76552900 | -2.74381500 | -3.50346400 | H | -7.71294000 | -2.54130400 | 0.53056200 |
| H | -0.46579800 | -1.18185300 | -2.78563200 | H | -6.20298700 | -2.96452400 | -1.40586400 |
| C | -2.54612200 | -4.31661400 | -1.83562600 | H | -4.44271600 | -1.37133600 | -1.97597400 |

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|---|-------------|-------------|-------------|----|-------------|-------------|-------------|
| C | -3.77792000 | 1.02191000 | -0.71320900 | H | 1.54223100 | -4.47570900 | 3.55751300 |
| C | -2.49495700 | 0.47724800 | 0.03744600 | H | -0.25930600 | -0.73576900 | 4.69196800 |
| O | -2.55580500 | 0.18915000 | 1.20815100 | H | 0.81267400 | -2.88660200 | 5.32729600 |
| H | -4.83739800 | 4.83026700 | 0.59653200 | C | -0.89274800 | -3.16950200 | -0.71904200 |
| C | -4.10666000 | 2.41912200 | -0.19289300 | C | -2.29257400 | -3.16850100 | -0.63711000 |
| H | -4.72111600 | 2.99106700 | -0.88801000 | C | -0.22573400 | -4.34948100 | -1.07815700 |
| H | -1.70477900 | -0.64534500 | -1.86534600 | C | -3.01606500 | -4.32598600 | -0.91961200 |
| C | -3.49776000 | 1.12542800 | -2.22842700 | H | -2.82120700 | -2.26849000 | -0.34824700 |
| H | -4.18836000 | 1.85524900 | -2.66837600 | C | -0.95474100 | -5.50298100 | -1.37199500 |
| H | -3.69100700 | 0.17979600 | -2.72936400 | H | 0.85656700 | -4.37317400 | -1.13578700 |
| C | -3.77458500 | 2.98952700 | 0.96759900 | C | -2.34866800 | -5.49454500 | -1.29333400 |
| C | -4.19095200 | 4.37707800 | 1.35438100 | H | -4.09899600 | -4.30832200 | -0.84755300 |
| H | -3.17249200 | 2.44474200 | 1.68828800 | H | -0.42954900 | -6.40915300 | -1.65825800 |
| H | -4.72974800 | 4.37307000 | 2.31010500 | H | -2.91160500 | -6.39497900 | -1.51985200 |
| H | -3.31550300 | 5.02299500 | 1.49058400 | C | 2.18158800 | 1.99813300 | -1.31194400 |
| C | -2.07365500 | 1.51963000 | -2.53327100 | C | 1.84674800 | 1.66964400 | -2.63371200 |
| C | -1.35301100 | 2.45111300 | -1.80936400 | C | 3.43984500 | 2.55366500 | -1.03740100 |
| H | -1.70752600 | 1.23916500 | -3.51844300 | C | 2.75094600 | 1.90244900 | -3.66932900 |
| H | -0.45818800 | 2.89061200 | -2.23318100 | H | 0.88458700 | 1.21200000 | -2.84612400 |
| H | -1.78767500 | 2.97852800 | -0.96956400 | C | 4.33630500 | 2.80039400 | -2.07617900 |
| C | 2.71902400 | -0.42602500 | 0.94213000 | H | 3.72000700 | 2.78193800 | -0.01439500 |
| C | 2.08993600 | 0.78916500 | 1.27436500 | C | 3.99465000 | 2.47361000 | -3.39153700 |
| C | 2.23565700 | 1.32828300 | 2.56003300 | H | 2.48858700 | 1.63064500 | -4.68712900 |
| C | 2.98507300 | 0.65182000 | 3.51748200 | H | 5.30652000 | 3.23554800 | -1.85753800 |
| C | 2.71733500 | -0.99911300 | -0.43930900 | H | 4.70007700 | 2.65612100 | -4.19649700 |
| C | 1.61166700 | -1.63381300 | -1.03188900 | C | 0.53038700 | 3.19999100 | 0.80641600 |
| C | 1.67371900 | -2.08138600 | -2.36453800 | C | -0.40559300 | 3.16005000 | 1.85317900 |
| C | 2.85527000 | -1.94588500 | -3.08479100 | C | 1.02092700 | 4.43517000 | 0.36582600 |
| H | 1.76883500 | 2.26976400 | 2.81660000 | C | -0.81331100 | 4.33872900 | 2.47434500 |
| H | 3.09897000 | 1.07589300 | 4.51053300 | H | -0.80746000 | 2.20736100 | 2.18308600 |
| H | 0.80893800 | -2.54185700 | -2.82735500 | C | 0.59146700 | 5.61546600 | 0.97712800 |
| H | 2.90794000 | -2.30336500 | -4.10861700 | H | 1.73555000 | 4.48103800 | -0.44789500 |
| C | 3.57939100 | -0.57292900 | 3.22404700 | C | -0.31686000 | 5.56978500 | 2.03535500 |
| C | 3.44631200 | -1.11009400 | 1.93983000 | H | -1.52679600 | 4.29748100 | 3.29119800 |
| C | 3.90981500 | -0.87928600 | -1.19261000 | H | 0.97510400 | 6.56938800 | 0.62818500 |
| C | 3.97837700 | -1.35679000 | -2.50519100 | H | -0.64137100 | 6.48830300 | 2.51464700 |
| C | 0.27404800 | -2.00827200 | 1.58443300 | P | -0.01291600 | -1.65319900 | -0.19072100 |
| C | 0.87828700 | -3.22366800 | 1.94323400 | P | 1.00449000 | 1.61456800 | 0.03808400 |
| C | -0.13769300 | -1.11666500 | 2.58023300 | Rh | -0.84165300 | 0.36093600 | -1.02494100 |
| C | 1.07230200 | -3.53522200 | 3.28678400 | H | 4.89090000 | -1.26102700 | -3.07931200 |
| H | 1.20581300 | -3.92180400 | 1.18142900 | H | 4.13928000 | -1.09786800 | 3.98727800 |
| C | 0.05753500 | -1.43530200 | 3.92431700 | O | 4.94043600 | -0.26766700 | -0.56102400 |
| H | -0.61099900 | -0.18566200 | 2.30151000 | O | 3.97016700 | -2.30329400 | 1.56360500 |
| C | 0.66167400 | -2.64172100 | 4.28021300 | C | 6.17279700 | -0.11475500 | -1.26203700 |

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|---------------------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | 6.04282300 | 0.47761700 | -2.17339400 | C | 2.68007700 | -0.92496400 | -0.51112600 |
| H | 6.83769300 | 0.41423100 | -0.57809800 | C | 1.62161500 | -1.63529700 | -1.10637100 |
| H | 6.60908600 | -1.08820100 | -1.51348800 | C | 1.69389900 | -2.02192700 | -2.45863900 |
| C | 4.66580500 | -3.07365500 | 2.54119000 | C | 2.84138400 | -1.74644800 | -3.19573600 |
| H | 4.01876700 | -3.31346200 | 3.39180900 | H | 1.67435600 | 2.05536900 | 3.00152700 |
| H | 4.95948800 | -3.99575000 | 2.03778100 | H | 3.06906600 | 0.78237700 | 4.57319200 |
| H | 5.56242900 | -2.55280100 | 2.89609600 | H | 0.86617100 | -2.54537200 | -2.92167700 |
| | | | | H | 2.90461500 | -2.05974800 | -4.23349500 |
| | | | | C | 3.59061700 | -0.74053400 | 3.15407700 |
| TS6 _{L2Rh} | | | | C | 3.45890800 | -1.17372200 | 1.83217000 |
| C | -4.78627900 | 0.02960100 | -0.23085200 | C | 3.83198500 | -0.65186800 | -1.28466300 |
| C | -5.38268700 | 0.44978500 | 0.96831700 | C | 3.91539600 | -1.07150300 | -2.61668500 |
| C | -6.34901700 | -0.32700700 | 1.60463700 | C | 0.32863300 | -2.26035500 | 1.49665900 |
| C | -6.74576300 | -1.54805000 | 1.05487200 | C | 1.05694400 | -3.42466000 | 1.78401000 |
| C | -6.16388500 | -1.97795900 | -0.13659400 | C | -0.21044000 | -1.49613900 | 2.53792100 |
| C | -5.19291700 | -1.19839500 | -0.77093800 | C | 1.25767000 | -3.80700600 | 3.10813000 |
| H | -5.08545100 | 1.39612600 | 1.40354700 | H | 1.47558100 | -4.02178500 | 0.98159700 |
| H | -6.79433800 | 0.02488300 | 2.53074900 | C | -0.00305800 | -1.88370800 | 3.86275700 |
| H | -7.50092400 | -2.15330400 | 1.54736200 | H | -0.78708500 | -0.60902000 | 2.30549000 |
| H | -6.46281800 | -2.92256100 | -0.58155200 | C | 0.73252400 | -3.03470500 | 4.14900000 |
| H | -4.75996400 | -1.57547200 | -1.68871100 | H | 1.82404700 | -4.70665800 | 3.32871300 |
| C | -3.66652400 | 0.89060200 | -0.85306000 | H | -0.41478000 | -1.28400000 | 4.66889600 |
| C | -2.33740100 | 0.55537100 | -0.04967300 | H | 0.89441600 | -3.33375700 | 5.18025600 |
| O | -2.35597300 | 0.51573700 | 1.15591100 | C | -0.85178700 | -3.23990600 | -0.90781600 |
| H | -4.76548800 | 4.88293400 | -0.40206000 | C | -2.25185000 | -3.18808500 | -0.95920600 |
| C | -4.00822500 | 2.36566000 | -0.66102600 | C | -0.19068600 | -4.41847600 | -1.28303700 |
| H | -4.86876100 | 2.66489700 | -1.26014100 | C | -2.98345000 | -4.29610100 | -1.38565700 |
| H | -1.58502700 | -0.55413000 | -2.12769000 | H | -2.76918200 | -2.28402200 | -0.65875700 |
| C | -3.47504900 | 0.63897100 | -2.36669200 | C | -0.92515600 | -5.51978200 | -1.72437100 |
| H | -4.12161200 | 1.31856900 | -2.93198900 | H | 0.89166000 | -4.47478600 | -1.24395400 |
| H | -3.77224200 | -0.37175000 | -2.63950200 | C | -2.32013700 | -5.46149600 | -1.77596200 |
| C | -3.42356300 | 3.27511000 | 0.12025300 | H | -4.06771200 | -4.24567000 | -1.41288100 |
| C | -3.88048600 | 4.70024500 | 0.21548000 | H | -0.40614700 | -6.42492200 | -2.02497100 |
| H | -2.57081200 | 3.00221000 | 0.73267900 | H | -2.88703800 | -6.32260600 | -2.11663900 |
| H | -4.12116500 | 4.96440800 | 1.25242700 | C | 2.15135100 | 2.37088200 | -0.93803100 |
| H | -3.08738700 | 5.38757500 | -0.10193400 | C | 2.22344600 | 2.01958800 | -2.29083700 |
| C | -2.03978500 | 0.81984900 | -2.81703400 | C | 3.11116700 | 3.24451600 | -0.40244900 |
| C | -1.24087500 | 1.92382500 | -2.41274500 | C | 3.21905400 | 2.55843500 | -3.10808900 |
| H | -1.80505000 | 0.36386700 | -3.77784100 | H | 1.51797200 | 1.30792300 | -2.70423300 |
| H | -0.40019800 | 2.20646100 | -3.03760700 | C | 4.10037700 | 3.78632700 | -1.21975500 |
| H | -1.68433100 | 2.72813300 | -1.83828700 | H | 3.08248900 | 3.50025700 | 0.65210400 |
| C | 2.67443500 | -0.45019800 | 0.90725400 | C | 4.15214300 | 3.44880700 | -2.57595400 |
| C | 1.99648900 | 0.70374900 | 1.34436500 | H | 3.26908100 | 2.27321200 | -4.15439900 |
| C | 2.15923100 | 1.15035900 | 2.66361200 | H | 4.83353900 | 4.46771900 | -0.79907100 |
| C | 2.95185800 | 0.43110300 | 3.55247700 | | | | |

| | | | | | | | |
|------------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | 4.92491900 | 3.87112700 | -3.21114400 | C | -4.22088100 | 2.16044800 | -0.44389800 |
| C | 0.15185400 | 2.97051000 | 1.10422300 | H | -5.22982900 | 2.29024100 | -0.83666900 |
| C | -0.55558300 | 2.69872400 | 2.28771000 | H | -1.69096900 | -0.24700000 | -2.52393700 |
| C | 0.17730700 | 4.28237800 | 0.60882900 | C | -3.64152300 | 0.54045900 | -2.22558700 |
| C | -1.18671800 | 3.72965100 | 2.98228300 | H | -4.34707600 | 1.22882700 | -2.69960200 |
| H | -0.61573200 | 1.68628300 | 2.66611800 | H | -3.95726300 | -0.46413000 | -2.50242100 |
| C | -0.46554900 | 5.30850900 | 1.30310000 | C | -3.61520300 | 3.19541400 | 0.13776000 |
| H | 0.70471500 | 4.50844800 | -0.31090600 | C | -4.23376000 | 4.55192200 | 0.29540300 |
| C | -1.14030300 | 5.03737700 | 2.49449700 | H | -2.61163500 | 3.08278400 | 0.53103900 |
| H | -1.72123400 | 3.50705200 | 3.90071600 | H | -4.28370400 | 4.83803100 | 1.35318900 |
| H | -0.43340300 | 6.32091200 | 0.91234400 | H | -3.62807100 | 5.31823700 | -0.20401200 |
| H | -1.63433700 | 5.83853100 | 3.03538700 | C | -2.25193700 | 0.75162900 | -2.81610500 |
| P | 0.01412700 | -1.77610100 | -0.23682200 | C | -1.45571600 | 1.92324700 | -2.35077400 |
| P | 0.89876500 | 1.59789900 | 0.15802700 | H | -2.22961900 | 0.59311700 | -3.89982600 |
| Rh | -0.70360300 | 0.29130900 | -1.09183600 | H | -0.71757900 | 2.29905700 | -3.05871500 |
| H | 4.79861900 | -0.86135400 | -3.20607900 | H | -2.00016800 | 2.72286100 | -1.85991500 |
| H | 4.18817200 | -1.29871100 | 3.86341500 | C | 2.51275500 | -0.35736000 | 1.10654700 |
| O | 4.80551300 | 0.04849300 | -0.65439400 | C | 1.74031600 | 0.76975400 | 1.45865400 |
| O | 4.03895700 | -2.30011500 | 1.34517400 | C | 1.69242700 | 1.19111400 | 2.79569000 |
| C | 5.98144300 | 0.39044500 | -1.38632100 | C | 2.37114000 | 0.48073000 | 3.78069900 |
| H | 5.74189200 | 0.99487500 | -2.26666600 | C | 2.73540400 | -0.82212200 | -0.29834800 |
| H | 6.59460200 | 0.97768400 | -0.70172500 | C | 1.78257800 | -1.53988100 | -1.04457600 |
| H | 6.53367500 | -0.50590500 | -1.69125800 | C | 2.05987700 | -1.91994800 | -2.36959400 |
| C | 4.78997900 | -3.11622000 | 2.24114000 | C | 3.30146800 | -1.63154700 | -2.92836600 |
| H | 4.17279400 | -3.45987400 | 3.07812200 | H | 1.14392700 | 2.07792600 | 3.07491700 |
| H | 5.11725100 | -3.97617700 | 1.65513100 | H | 2.32354500 | 0.81491600 | 4.81257200 |
| H | 5.66768300 | -2.58426900 | 2.62569700 | H | 1.31593200 | -2.45055900 | -2.95187800 |
| | | | | H | 3.51904500 | -1.93742800 | -3.94736900 |
| | | | | C | 3.11040600 | -0.65392500 | 3.46000100 |
| 7_{L2Rh} | | | | C | 3.19126400 | -1.06216100 | 2.12598700 |
| C | -4.63748900 | -0.24602700 | 0.03318100 | C | 3.99235900 | -0.54840000 | -0.88556000 |
| C | -5.09049400 | 0.07912500 | 1.32311100 | C | 4.27528000 | -0.95772900 | -2.19288200 |
| C | -5.89327200 | -0.79683800 | 2.04991900 | C | 0.26470900 | -2.36883800 | 1.32351900 |
| C | -6.27022800 | -2.02552400 | 1.50202800 | C | 1.05087000 | -3.50372800 | 1.57419100 |
| C | -5.83918700 | -2.35753900 | 0.21932100 | C | -0.41814400 | -1.74814500 | 2.37691300 |
| C | -5.03245100 | -1.47655600 | -0.50692900 | C | 1.15665600 | -4.00533700 | 2.86939000 |
| H | -4.80742800 | 1.03018900 | 1.75710700 | H | 1.59273400 | -3.98433700 | 0.76814300 |
| H | -6.22696300 | -0.51723400 | 3.04508800 | C | -0.30231600 | -2.25188200 | 3.67370700 |
| H | -6.89659100 | -2.71025900 | 2.06599200 | H | -1.01851500 | -0.86827500 | 2.18322800 |
| H | -6.12760500 | -3.30471400 | -0.22707700 | C | 0.48402900 | -3.37765700 | 3.92211000 |
| H | -4.72676200 | -1.77612900 | -1.50075700 | H | 1.76853100 | -4.88208000 | 3.05869800 |
| C | -3.69835200 | 0.74462800 | -0.68839400 | H | -0.82434900 | -1.75980900 | 4.48893900 |
| C | -2.27401300 | 0.60271800 | 0.02061300 | H | 0.57382500 | -3.76688300 | 4.93192700 |
| O | -2.21377300 | 0.64110100 | 1.22651700 | C | -0.68945800 | -3.12111800 | -1.27476300 |
| H | -5.24632200 | 4.58733100 | -0.11866700 | | | | |

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|----|-------------|-------------|-------------|---------------------|-------------|-------------|-------------|
| C | -2.05037900 | -2.99917700 | -1.58578400 | H | 3.92213200 | -3.31062000 | 3.45063000 |
| C | -0.01938200 | -4.31502000 | -1.58409900 | H | 5.07385500 | -3.72300800 | 2.15204200 |
| C | -2.73733600 | -4.05192600 | -2.19134100 | H | 5.37398300 | -2.29775700 | 3.18357900 |
| H | -2.57238500 | -2.08119100 | -1.34208700 | | | | |
| C | -0.70383600 | -5.36022200 | -2.20338100 | TS7 _{L2Rh} | | | |
| H | 1.03560200 | -4.42509200 | -1.36007100 | C | 2.68743900 | 0.40019800 | -0.04502400 |
| C | -2.06292700 | -5.23289900 | -2.50511100 | O | 2.71694000 | 1.10662800 | 0.95918700 |
| H | -3.79486000 | -3.94829200 | -2.41548800 | H | 5.53782800 | -3.32422400 | 2.94871800 |
| H | -0.17577400 | -6.27693100 | -2.44812100 | C | 5.20282000 | 0.02174400 | -0.35839600 |
| H | -2.59180100 | -6.05231500 | -2.98232100 | C | 6.30347600 | -0.77395600 | -0.72292400 |
| C | 2.11149500 | 2.20939200 | -0.98544300 | C | 7.58420400 | -0.23640700 | -0.82108100 |
| C | 2.05755600 | 1.87402200 | -2.34385100 | C | 7.79973200 | 1.11879400 | -0.55462400 |
| C | 3.20742300 | 2.93351400 | -0.49390800 | C | 6.72014800 | 1.91733000 | -0.18491000 |
| C | 3.07549900 | 2.27508100 | -3.20888600 | C | 5.43438900 | 1.37443600 | -0.08642000 |
| H | 1.23362800 | 1.27417100 | -2.71772400 | H | 6.15601300 | -1.83117300 | -0.91856800 |
| C | 4.21896800 | 3.34118300 | -1.36090800 | H | 8.41495100 | -0.87674800 | -1.10368000 |
| H | 3.26713300 | 3.17614100 | 0.56236500 | H | 8.79720400 | 1.54142300 | -0.63063900 |
| C | 4.15301000 | 3.01536300 | -2.71917500 | H | 6.86993900 | 2.97105000 | 0.03286100 |
| H | 3.03162300 | 2.00082500 | -4.25838200 | H | 4.61829600 | 2.01511800 | 0.21968800 |
| H | 5.06267700 | 3.90605600 | -0.97666900 | C | 3.81837000 | -0.65956300 | -0.32507800 |
| H | 4.94534100 | 3.33073000 | -3.39129800 | C | 3.49279500 | -1.18381700 | -1.73532800 |
| C | 0.10853700 | 3.18373000 | 0.88339700 | H | 2.56587400 | -1.78143200 | -1.67123600 |
| C | -0.68821900 | 3.15574300 | 2.04101600 | H | 4.26639500 | -1.84214100 | -2.13400500 |
| C | 0.28735300 | 4.40304500 | 0.21044500 | C | 3.76626500 | -1.76128000 | 0.71060100 |
| C | -1.24682300 | 4.33221900 | 2.54030300 | H | 2.72120700 | -0.20488700 | -3.52671600 |
| H | -0.89383500 | 2.21930100 | 2.54114300 | H | 3.04953400 | -2.55632300 | 0.51218000 |
| C | -0.29419900 | 5.57222700 | 0.70206600 | C | 3.25876000 | 0.05911500 | -2.61165200 |
| H | 0.88330300 | 4.44541700 | -0.69370800 | C | 2.46893200 | 1.06181100 | -1.76887900 |
| C | -1.05200200 | 5.54307000 | 1.87405000 | H | 4.22273500 | 0.48631400 | -2.90387600 |
| H | -1.85092300 | 4.29468800 | 3.44148700 | H | 1.54209600 | 1.39191600 | -2.25778000 |
| H | -0.14570900 | 6.50712400 | 0.17033600 | H | 2.99936200 | 1.97921200 | -1.52232400 |
| H | -1.49538200 | 6.45560400 | 2.26022700 | C | 4.52501600 | -1.81697300 | 1.80986300 |
| P | 0.08348000 | -1.72247900 | -0.38089200 | C | 4.52183400 | -2.93412200 | 2.80778800 |
| P | 0.78725500 | 1.65167800 | 0.14925100 | H | 5.23294700 | -1.01176200 | 1.99948900 |
| Rh | -0.69866100 | 0.42051200 | -1.12038500 | H | 3.87943900 | -3.75896100 | 2.49272800 |
| H | 5.23613300 | -0.74179100 | -2.64202500 | H | 4.18372400 | -2.58751500 | 3.79334700 |
| H | 3.62347000 | -1.20352500 | 4.23847100 | C | -2.99390100 | -0.04444100 | 0.81479400 |
| O | 4.86440500 | 0.13796800 | -0.10771200 | C | -2.14846600 | -1.11821200 | 1.14846500 |
| O | 3.89583100 | -2.14595400 | 1.71492700 | C | -2.26178800 | -1.74261300 | 2.39782800 |
| C | 6.15775500 | 0.43134900 | -0.63056500 | C | -3.19128800 | -1.27502100 | 3.32228200 |
| H | 6.09566900 | 1.05472700 | -1.52835500 | C | -2.99840900 | 0.55589400 | -0.55073700 |
| H | 6.67615700 | 0.98213400 | 0.15536900 | C | -1.95224400 | 1.34271500 | -1.05666800 |
| H | 6.71154900 | -0.48717500 | -0.85679500 | C | -1.95041800 | 1.73707200 | -2.40886600 |
| C | 4.60178800 | -2.90293400 | 2.69478600 | C | -3.01859700 | 1.40050000 | -3.23041900 |

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|---|-------------|-------------|-------------|-----------------|-------------|-------------|-------------|
| H | -1.63410300 | -2.58528900 | 2.65264200 | C | 1.21451300 | -4.09566700 | 2.48730000 |
| H | -3.28006200 | -1.76214100 | 4.28846300 | H | 0.77173800 | -1.99680900 | 2.35739300 |
| H | -1.12116200 | 2.30553500 | -2.81195500 | C | 0.43573800 | -5.46421900 | 0.65254900 |
| H | -3.02061600 | 1.71530200 | -4.26935500 | H | -0.70362900 | -4.45305000 | -0.86478000 |
| C | -3.99958800 | -0.17825800 | 3.03253200 | C | 1.10746000 | -5.34502200 | 1.86979800 |
| C | -3.90133300 | 0.43593800 | 1.77970600 | H | 1.73524800 | -3.99720800 | 3.43334600 |
| C | -4.07724100 | 0.22607600 | -1.40746400 | H | 0.35354000 | -6.43132100 | 0.16605000 |
| C | -4.09020600 | 0.65557400 | -2.73720400 | H | 1.54829700 | -6.22052900 | 2.33647200 |
| C | -0.80823100 | 1.82523500 | 1.67470600 | P | -0.41886200 | 1.62972700 | -0.09826900 |
| C | -1.69975900 | 2.83254600 | 2.07468200 | P | -0.83121000 | -1.60176400 | -0.03540600 |
| C | -0.16591600 | 1.03591500 | 2.63356200 | Rh | 0.80921800 | -0.10655600 | -0.77415200 |
| C | -1.96338700 | 3.02504400 | 3.42831000 | H | -4.91245900 | 0.39814400 | -3.39224600 |
| H | -2.19356800 | 3.45245300 | 1.33403500 | H | -4.69722700 | 0.18881900 | 3.77443500 |
| C | -0.43278800 | 1.23548300 | 3.98867500 | O | -5.04504100 | -0.54477000 | -0.85632500 |
| H | 0.53845100 | 0.27660200 | 2.31529500 | O | -4.62193500 | 1.52321800 | 1.41030900 |
| C | -1.33286300 | 2.22508200 | 4.38648700 | C | -6.14272600 | -0.94364000 | -1.67549500 |
| H | -2.65842700 | 3.80009400 | 3.73624900 | H | -5.80371800 | -1.52515900 | -2.53904200 |
| H | 0.06242900 | 0.61665100 | 4.73081600 | H | -6.77246700 | -1.56885600 | -1.04133100 |
| H | -1.54032800 | 2.37765800 | 5.44135000 | H | -6.71832800 | -0.07620400 | -2.01773700 |
| C | 0.13118600 | 3.33192300 | -0.51467700 | C | -5.52640000 | 2.08462800 | 2.35985300 |
| C | 1.42615800 | 3.72273500 | -0.13636300 | H | -5.00236300 | 2.40536700 | 3.26686600 |
| C | -0.74065000 | 4.28694100 | -1.06103300 | H | -5.96976300 | 2.95275800 | 1.87045800 |
| C | 1.85158900 | 5.03454800 | -0.34103200 | H | -6.31721700 | 1.37376400 | 2.62503600 |
| H | 2.08441400 | 3.00442400 | 0.33762900 | | | | |
| C | -0.30891400 | 5.59939400 | -1.25799700 | δ_{L2Rh} | | | |
| H | -1.75679600 | 4.02018100 | -1.32336100 | C | 3.60425600 | 0.90049900 | -1.11227400 |
| C | 0.98894100 | 5.97460400 | -0.90852500 | O | 3.53570400 | 2.11763000 | -1.11926300 |
| H | 2.85705200 | 5.32207600 | -0.04834100 | H | 4.59359700 | 0.53309800 | 4.52289400 |
| H | -0.99411200 | 6.32822600 | -1.68017900 | C | 5.77835800 | 0.02860700 | -0.29530000 |
| H | 1.32167100 | 6.99622200 | -1.06529500 | C | 6.50612000 | -1.15987000 | -0.42385000 |
| C | -1.74192900 | -2.17941200 | -1.51014400 | C | 7.88429700 | -1.13183600 | -0.65495000 |
| C | -1.23774100 | -1.85346200 | -2.77714200 | C | 8.55609700 | 0.08491900 | -0.76562000 |
| C | -2.92357300 | -2.92609500 | -1.40115200 | C | 7.83850700 | 1.27772600 | -0.64345900 |
| C | -1.91048800 | -2.26433400 | -3.92800100 | C | 6.46500000 | 1.24812600 | -0.41159000 |
| H | -0.33079100 | -1.25545700 | -2.84508600 | H | 6.01092600 | -2.12009600 | -0.34187400 |
| C | -3.58889000 | -3.34203400 | -2.55336900 | H | 8.42916900 | -2.06676900 | -0.74807100 |
| H | -3.32522300 | -3.16974600 | -0.42328900 | H | 9.62675400 | 0.10540600 | -0.94600900 |
| C | -3.08690000 | -3.00821200 | -3.81514500 | H | 8.34863000 | 2.23285800 | -0.72821000 |
| H | -1.52325400 | -1.99762900 | -4.90660800 | H | 5.91384800 | 2.17711600 | -0.31477700 |
| H | -4.50371300 | -3.92006600 | -2.46758400 | C | 4.27073700 | 0.05086600 | -0.00022600 |
| H | -3.61504300 | -3.32581700 | -4.70909300 | C | 3.56670200 | -1.31095100 | -0.22787000 |
| C | -0.05336300 | -3.09012500 | 0.68187400 | H | 2.57762000 | -1.26001700 | 0.23791900 |
| C | 0.66316400 | -2.96719500 | 1.88464900 | H | 4.07925200 | -2.14999000 | 0.24411500 |
| C | -0.15483900 | -4.34450800 | 0.06364000 | C | 3.95336300 | 0.61435400 | 1.36499700 |

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|---|-------------|-------------|-------------|----|-------------|-------------|-------------|
| H | 2.63330200 | -2.17579500 | -2.01832600 | C | -1.19839300 | 5.49896200 | -1.63387500 |
| H | 2.89639600 | 0.85978300 | 1.51699700 | H | -2.60451400 | 4.24212500 | -0.60744700 |
| C | 3.38911100 | -1.43365100 | -1.74938800 | C | 0.09391000 | 5.61674400 | -2.15487700 |
| C | 2.99239600 | -0.01157900 | -2.15929100 | H | 1.99419500 | 4.63209400 | -2.44722500 |
| H | 4.33125000 | -1.72170500 | -2.22470000 | H | -1.89274800 | 6.33049600 | -1.70829900 |
| H | 1.90378300 | 0.12834400 | -2.05200900 | H | 0.40348600 | 6.54108600 | -2.63327700 |
| H | 3.26728800 | 0.29668900 | -3.17157300 | C | -0.84959600 | -2.28293500 | -1.16274500 |
| C | 4.78678700 | 0.77636800 | 2.39475300 | C | -0.34342700 | -1.84291000 | -2.39076600 |
| C | 4.37118000 | 1.27546200 | 3.74587100 | C | -1.65398200 | -3.43173100 | -1.11499500 |
| H | 5.84140000 | 0.53662400 | 2.26945600 | C | -0.63556000 | -2.54155300 | -3.56206700 |
| H | 3.29973800 | 1.49918500 | 3.78198400 | H | 0.25112400 | -0.93787000 | -2.42477800 |
| H | 4.92207500 | 2.18496200 | 4.01686700 | C | -1.93634700 | -4.13387700 | -2.28544300 |
| C | -3.19061200 | -0.70211500 | 0.54397500 | H | -2.06401400 | -3.76993100 | -0.16914700 |
| C | -2.10488000 | -1.29285100 | 1.21624100 | C | -1.43043200 | -3.68832800 | -3.51020400 |
| C | -2.24176300 | -1.73424900 | 2.54019100 | H | -0.25128900 | -2.18506500 | -4.51290700 |
| C | -3.45778400 | -1.57799500 | 3.19820500 | H | -2.55895400 | -5.02220200 | -2.24328400 |
| C | -3.11729200 | -0.25275000 | -0.87934800 | H | -1.66013600 | -4.23183900 | -4.42179100 |
| C | -2.33679500 | 0.83840900 | -1.30157400 | C | 0.58206800 | -2.48453400 | 1.36915600 |
| C | -2.30140400 | 1.21175300 | -2.65359200 | C | 1.07911400 | -1.99849100 | 2.59225200 |
| C | -3.04752000 | 0.49871200 | -3.58645500 | C | 1.01801800 | -3.72997800 | 0.89838100 |
| H | -1.41210700 | -2.20520600 | 3.05072600 | C | 1.98557200 | -2.75181800 | 3.33513800 |
| H | -3.56725800 | -1.92793900 | 4.22024400 | H | 0.76356500 | -1.02331100 | 2.95123700 |
| H | -1.69367300 | 2.05118800 | -2.97043300 | C | 1.93270200 | -4.47787400 | 1.64238700 |
| H | -3.02461200 | 0.78807600 | -4.63278800 | H | 0.65558700 | -4.11462300 | -0.04759100 |
| C | -4.54029300 | -0.97279000 | 2.56230300 | C | 2.41763900 | -3.99271700 | 2.85813200 |
| C | -4.40715600 | -0.53232800 | 1.24170700 | H | 2.36011100 | -2.36763300 | 4.27899100 |
| C | -3.85732800 | -0.96908500 | -1.84805600 | H | 2.26701100 | -5.44071300 | 1.26813400 |
| C | -3.82267200 | -0.59196300 | -3.19468100 | H | 3.13159800 | -4.57646700 | 3.43099500 |
| C | -2.19036500 | 2.10741900 | 1.31124000 | P | -1.17101200 | 1.63853800 | -0.13574000 |
| C | -3.51173100 | 2.55376200 | 1.16126400 | P | -0.47357900 | -1.36484100 | 0.37616900 |
| C | -1.62160500 | 2.04461500 | 2.58987700 | Rh | 0.67271900 | 0.49182800 | 0.22203200 |
| C | -4.24893600 | 2.93891600 | 2.27988100 | H | -4.38617600 | -1.14428400 | -3.93558400 |
| H | -3.97539200 | 2.56953700 | 0.18141400 | H | -5.47468600 | -0.84721800 | 3.09419000 |
| C | -2.36538000 | 2.42248500 | 3.70835400 | O | -4.55615400 | -2.03325100 | -1.38343100 |
| H | -0.60339900 | 1.68014200 | 2.69847300 | O | -5.39219900 | 0.09935100 | 0.55644600 |
| C | -3.67908400 | 2.87099400 | 3.55378500 | C | -5.28579500 | -2.82423000 | -2.31822100 |
| H | -5.27185500 | 3.28131300 | 2.15714200 | H | -4.62629800 | -3.24673000 | -3.08381600 |
| H | -1.92291900 | 2.36079200 | 4.69810700 | H | -5.73141500 | -3.63304800 | -1.73763000 |
| H | -4.25931000 | 3.16175800 | 4.42436200 | H | -6.08017000 | -2.24137100 | -2.79831800 |
| C | -0.71458000 | 3.23551800 | -0.91926900 | C | -6.63523200 | 0.32962500 | 1.21540800 |
| C | 0.58083200 | 3.36093300 | -1.44239700 | H | -6.50251100 | 0.93594800 | 2.11797400 |
| C | -1.60258700 | 4.31752400 | -1.01375800 | H | -7.25316900 | 0.87429800 | 0.50021900 |
| C | 0.98559100 | 4.54809200 | -2.05450400 | H | -7.12811400 | -0.61384200 | 1.47677300 |
| H | 1.28176500 | 2.53480300 | -1.36433500 | | | | |

| | | | | | | | |
|-----------------------------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| ${}^9\text{L}_{2\text{Rh}}$ | | | | H | -2.42919400 | -0.07364900 | -4.73528900 |
| C | 5.29905500 | 0.82883100 | -0.18904300 | C | -3.91318400 | -1.71821200 | 2.51742200 |
| C | 5.73521700 | 0.52626600 | -1.48987600 | C | -3.83881800 | -1.25836000 | 1.19942900 |
| C | 7.05521200 | 0.15993400 | -1.74077000 | C | -3.06220600 | -1.76615700 | -1.86445500 |
| C | 7.97553200 | 0.08657800 | -0.69144600 | C | -3.00498300 | -1.49821600 | -3.23439100 |
| C | 7.55695700 | 0.38133800 | 0.60474300 | C | -2.35345000 | 1.66404000 | 1.31759300 |
| C | 6.23045800 | 0.74577500 | 0.85367500 | C | -3.69165500 | 2.08334500 | 1.29386300 |
| H | 5.03349300 | 0.57386800 | -2.31707100 | C | -1.75113100 | 1.34714100 | 2.54104200 |
| H | 7.36548800 | -0.07071000 | -2.75583600 | C | -4.41672800 | 2.17282100 | 2.48042600 |
| H | 9.00585600 | -0.19694100 | -0.88466800 | H | -4.16657800 | 2.33658800 | 0.35230700 |
| H | 8.26056900 | 0.33069000 | 1.43073300 | C | -2.47851600 | 1.43878600 | 3.72813000 |
| H | 5.93689600 | 0.96853100 | 1.87250900 | H | -0.72275200 | 1.00461800 | 2.56163500 |
| C | 3.84376800 | 1.20469300 | 0.03827900 | C | -3.81163600 | 1.85100500 | 3.69924100 |
| C | 2.86902100 | 0.05667400 | -0.39127900 | H | -5.45297700 | 2.49601400 | 2.45490900 |
| O | 3.22997300 | -1.01713600 | -0.80917600 | H | -2.00580300 | 1.18138300 | 4.67110900 |
| H | 0.85466700 | 0.62935400 | -1.92840500 | H | -4.37874200 | 1.92188000 | 4.62246200 |
| C | 3.41592100 | 2.44362800 | -0.81178600 | C | -1.70766600 | 3.29043900 | -0.89355100 |
| H | 3.99346000 | 2.46146300 | -1.74046400 | C | -0.90940800 | 4.34606300 | -0.42374800 |
| H | 3.67465800 | 3.34928300 | -0.25584600 | C | -2.78069100 | 3.58054200 | -1.75001700 |
| C | 3.50890000 | 1.46967100 | 1.52958000 | C | -1.16028400 | 5.65901500 | -0.82260300 |
| H | 4.11857900 | 2.30409100 | 1.88793800 | H | -0.10417700 | 4.14344000 | 0.27423800 |
| H | 3.76639700 | 0.58061500 | 2.11568700 | C | -3.02661800 | 4.89427100 | -2.15110600 |
| C | 1.92861400 | 2.44326900 | -1.14480700 | H | -3.42903600 | 2.78659000 | -2.10106900 |
| C | 1.42646200 | 1.67878500 | -2.27954000 | C | -2.21450600 | 5.93476100 | -1.69554800 |
| H | 1.40148700 | 3.36358700 | -0.92663100 | H | -0.53286500 | 6.46366600 | -0.45108300 |
| H | 0.59871700 | 2.13040900 | -2.82555600 | H | -3.85919000 | 5.10377700 | -2.81603800 |
| H | 2.17524100 | 1.22517900 | -2.93215300 | H | -2.40773400 | 6.95532400 | -2.01168200 |
| C | 2.05933700 | 1.78981800 | 1.74406400 | C | 0.07011300 | -2.61651300 | -1.04359600 |
| C | 1.56633100 | 2.94683100 | 2.20066700 | C | 0.58510600 | -2.29570900 | -2.30505700 |
| H | 1.33148800 | 0.93013900 | 1.68626700 | C | -0.54844400 | -3.86133300 | -0.84933900 |
| H | 0.50022700 | 3.09835600 | 2.32830600 | C | 0.47926700 | -3.20201500 | -3.36031600 |
| H | 2.22542600 | 3.76709200 | 2.47549400 | H | 1.07147700 | -1.34207800 | -2.46392500 |
| Rh | 0.97903100 | 0.77442600 | -0.21911800 | C | -0.64284200 | -4.76995400 | -1.90188500 |
| C | -2.60454600 | -1.22047500 | 0.51716700 | H | -0.96073400 | -4.11639100 | 0.12105200 |
| C | -1.43591800 | -1.62598400 | 1.18891100 | C | -0.13351100 | -4.44036000 | -3.16076800 |
| C | -1.51998000 | -2.09745900 | 2.50763100 | H | 0.87616000 | -2.93983100 | -4.33646200 |
| C | -2.75088500 | -2.14638000 | 3.15523000 | H | -1.12228100 | -5.73071200 | -1.74138900 |
| C | -2.60162500 | -0.81686000 | -0.92025500 | H | -0.21417900 | -5.14656600 | -3.98173600 |
| C | -2.13805600 | 0.42708000 | -1.37705800 | C | 1.39638300 | -2.22029700 | 1.51389900 |
| C | -2.05869600 | 0.68020600 | -2.75934600 | C | 1.68773600 | -1.56992900 | 2.72566700 |
| C | -2.48870900 | -0.27785600 | -3.67032900 | C | 2.10362700 | -3.38124800 | 1.18186200 |
| H | -0.63281300 | -2.43110900 | 3.02855100 | C | 2.65944500 | -2.07513800 | 3.58733700 |
| H | -2.80784800 | -2.51685700 | 4.17441800 | H | 1.14800900 | -0.67160100 | 3.00778500 |
| H | -1.66351000 | 1.62112600 | -3.12088900 | C | 3.08451900 | -3.88062500 | 2.04181800 |

| | | | | | | | |
|---------------------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | 1.90283500 | -3.89194500 | 0.24784600 | H | 1.67028600 | 3.95444000 | -0.50260600 |
| C | 3.36629600 | -3.23086100 | 3.24341700 | H | 0.44842300 | 3.08889900 | -2.24025000 |
| H | 2.86634300 | -1.56438500 | 4.52307400 | H | 2.12399200 | 2.89491700 | -2.79783500 |
| H | 3.62932100 | -4.77883900 | 1.76696900 | C | 1.84706600 | 1.42940200 | 1.77358700 |
| H | 4.12988200 | -3.62073400 | 3.90958500 | C | 1.37553000 | 2.71978300 | 1.36392500 |
| P | -1.35255000 | 1.61844900 | -0.21938500 | H | 1.33325600 | 0.93396000 | 2.59083700 |
| P | 0.20295700 | -1.44016400 | 0.35414200 | H | 0.35990400 | 3.00099500 | 1.61305600 |
| H | -3.34285800 | -2.23013000 | -3.95674200 | H | 2.06563800 | 3.55211400 | 1.43720900 |
| H | -4.85919000 | -1.74632000 | 3.04265600 | C | -2.41198700 | -1.40841300 | 0.58789500 |
| O | -3.52817500 | -2.92810300 | -1.34293800 | C | -1.16341600 | -1.70087900 | 1.17388000 |
| O | -4.90615000 | -0.80477500 | 0.49471600 | C | -1.11368500 | -2.22418800 | 2.47459200 |
| C | -4.01155000 | -3.92627600 | -2.23795200 | C | -2.28713900 | -2.43323500 | 3.19267800 |
| H | -3.22864000 | -4.25818000 | -2.92730400 | C | -2.55582200 | -0.95328200 | -0.82635600 |
| H | -4.31850500 | -4.76372200 | -1.60987100 | C | -2.21415500 | 0.33691600 | -1.25933800 |
| H | -4.87515300 | -3.56345400 | -2.80733300 | C | -2.25010100 | 0.65286300 | -2.62993800 |
| C | -6.17842900 | -0.78349400 | 1.13641200 | C | -2.69746100 | -0.28928700 | -3.54879200 |
| H | -6.16286800 | -0.15186200 | 2.03113300 | H | -0.16807700 | -2.49030200 | 2.92405600 |
| H | -6.87178000 | -0.36157000 | 0.40742700 | H | -2.23622700 | -2.84244400 | 4.19719700 |
| H | -6.50659700 | -1.79419200 | 1.40569300 | H | -1.94655000 | 1.63506100 | -2.97193600 |
| | | | | H | -2.73311900 | -0.03911800 | -4.60483900 |
| | | | | C | -3.52751300 | -2.12183200 | 2.64196900 |
| TS8 _{L2Rh} | | | | C | -3.58846000 | -1.61605200 | 1.34070400 |
| C | 5.25827300 | 0.95813200 | -0.01753600 | C | -3.03500100 | -1.88784100 | -1.77579600 |
| C | 5.75555000 | 0.85297000 | -1.32774600 | C | -3.11142400 | -1.55382400 | -3.13014400 |
| C | 7.08327400 | 0.50544400 | -1.56772900 | C | -2.49537600 | 1.46436300 | 1.46075400 |
| C | 7.94972300 | 0.25662900 | -0.50008600 | C | -3.88386100 | 1.66284400 | 1.46462700 |
| C | 7.47096900 | 0.35825900 | 0.80532900 | C | -1.82900100 | 1.24850600 | 2.67379300 |
| C | 6.13774600 | 0.70302400 | 1.04313600 | C | -4.59107100 | 1.63597900 | 2.66473100 |
| H | 5.09651100 | 1.03675900 | -2.16973600 | H | -4.41547200 | 1.82688600 | 0.53486300 |
| H | 7.44167400 | 0.42704100 | -2.59019900 | C | -2.53921100 | 1.22081700 | 3.87449400 |
| H | 8.98540900 | -0.01218900 | -0.68589400 | H | -0.75971600 | 1.07816600 | 2.67513300 |
| H | 8.13284100 | 0.17014800 | 1.64584300 | C | -3.92128400 | 1.41420900 | 3.87161200 |
| H | 5.79315800 | 0.77372400 | 2.06812300 | H | -5.66599000 | 1.78880300 | 2.65850000 |
| C | 3.80133700 | 1.31832400 | 0.20824200 | H | -2.01351600 | 1.04248400 | 4.80774500 |
| C | 2.80730500 | 0.34388300 | -0.47270100 | H | -4.47603500 | 1.39348600 | 4.80481500 |
| O | 3.11716800 | -0.53215200 | -1.24790500 | C | -2.08240700 | 3.18565000 | -0.75683500 |
| H | 1.22516700 | 1.49688200 | -2.28726900 | C | -1.32356200 | 4.33393300 | -0.48680000 |
| C | 3.44668000 | 2.69799300 | -0.43400000 | C | -3.30154900 | 3.33008700 | -1.44071300 |
| H | 3.95866300 | 2.78181100 | -1.39657400 | C | -1.76196200 | 5.59332100 | -0.89976700 |
| H | 3.84853200 | 3.48804200 | 0.20853600 | H | -0.38973500 | 4.25279700 | 0.05273000 |
| C | 3.35141500 | 1.24475200 | 1.68676900 | C | -3.73684400 | 4.58804700 | -1.85512000 |
| H | 3.85862100 | 2.01808100 | 2.27660000 | H | -3.91111700 | 2.46119200 | -1.65887700 |
| H | 3.63246600 | 0.27259500 | 2.09444200 | C | -2.96795800 | 5.72326000 | -1.58859900 |
| C | 1.93969700 | 2.91570000 | -0.66468600 | H | -1.15855700 | 6.46957800 | -0.68242200 |
| C | 1.38522200 | 2.56315000 | -2.05495400 | | | | |

| | | | | | | | |
|--------------------|-------------|-------------|-------------|----|-------------|-------------|-------------|
| H | -4.68042400 | 4.68019000 | -2.38455900 | C | 7.54156700 | -0.30935900 | -0.20607800 |
| H | -3.30893400 | 6.70146500 | -1.91379600 | C | 6.85010200 | -0.37970600 | 1.00245000 |
| C | 0.18498800 | -2.27989500 | -1.29425800 | C | 5.59312800 | 0.21640500 | 1.13204500 |
| C | 0.51349900 | -1.71187900 | -2.52948600 | H | 5.28066400 | 1.48616800 | -1.99678500 |
| C | -0.27957000 | -3.60276100 | -1.24080900 | H | 7.49342400 | 0.43594800 | -2.23030100 |
| C | 0.37443200 | -2.45412900 | -3.70249400 | H | 8.51807100 | -0.77356800 | -0.30902700 |
| H | 0.88298600 | -0.69536200 | -2.56975400 | H | 7.28399500 | -0.90121600 | 1.85083500 |
| C | -0.40527500 | -4.34648300 | -2.41232600 | H | 5.07718500 | 0.13915700 | 2.08051200 |
| H | -0.54381900 | -4.04707400 | -0.28697900 | C | 3.63216200 | 1.54846000 | 0.18745400 |
| C | -0.08263400 | -3.77188600 | -3.64530000 | C | 2.61111500 | 0.93581500 | -0.82539200 |
| H | 0.62130500 | -2.00233100 | -4.65849300 | O | 2.92963800 | 0.58993100 | -1.94568500 |
| H | -0.76134800 | -5.37085800 | -2.36370500 | H | 1.35117200 | 3.06337500 | -1.73340400 |
| H | -0.18768600 | -4.35080800 | -4.55799500 | C | 3.74978900 | 3.07899900 | -0.09364800 |
| C | 1.73064000 | -2.22981100 | 1.14419200 | H | 4.19498300 | 3.24683300 | -1.07841200 |
| C | 2.08806000 | -1.85127500 | 2.44932300 | H | 4.46830700 | 3.44963300 | 0.64571400 |
| C | 2.48569400 | -3.21929200 | 0.50033500 | C | 2.96745900 | 1.39284700 | 1.55426400 |
| C | 3.15889900 | -2.46192400 | 3.10031500 | H | 3.49756500 | 1.99430900 | 2.30556300 |
| H | 1.53106500 | -1.08006400 | 2.96713500 | H | 3.00516600 | 0.36223700 | 1.88540500 |
| C | 3.56640300 | -3.81972400 | 1.14877200 | C | 2.43741100 | 3.89172800 | 0.01852100 |
| H | 2.24456700 | -3.51715600 | -0.51190900 | C | 1.71806600 | 4.01954200 | -1.33146500 |
| C | 3.90574600 | -3.44607400 | 2.44900100 | H | 2.73277900 | 4.91314400 | 0.28504900 |
| H | 3.41306300 | -2.16095700 | 4.11214600 | H | 0.85987000 | 4.69300800 | -1.25845500 |
| H | 4.14299700 | -4.58043200 | 0.63122500 | H | 2.40023100 | 4.42257800 | -2.08778300 |
| H | 4.74596600 | -3.91557800 | 2.95136900 | C | 1.53381800 | 1.87104500 | 1.42265300 |
| P | -1.51120400 | 1.56395500 | -0.08878900 | C | 1.52447600 | 3.38739400 | 1.16765500 |
| P | 0.39745900 | -1.32600300 | 0.25385500 | H | 0.93319900 | 1.62513500 | 2.30081100 |
| Rh | 0.93144200 | 0.92806800 | -0.04377500 | H | 0.50702300 | 3.76741600 | 1.04077200 |
| H | -3.46810600 | -2.27160900 | -3.85737600 | H | 1.88108000 | 3.82887800 | 2.11097900 |
| H | -4.42966000 | -2.27758600 | 3.21921100 | Rh | 0.67399300 | 1.06236200 | -0.26134500 |
| O | -3.37841600 | -3.10183500 | -1.27997600 | C | -2.14317700 | -1.64106300 | 0.61247000 |
| O | -4.74429700 | -1.27346600 | 0.71923600 | C | -0.85611500 | -1.71525700 | 1.18866700 |
| C | -3.90053600 | -4.07739700 | -2.17805000 | C | -0.71525600 | -2.22366400 | 2.49068900 |
| H | -3.17488800 | -4.33407100 | -2.95639300 | C | -1.83008700 | -2.61854400 | 3.22163000 |
| H | -4.10608200 | -4.95961300 | -1.57024300 | C | -2.40984200 | -1.22080400 | -0.79459700 |
| H | -4.83058000 | -3.73045500 | -2.64299600 | C | -2.35834600 | 0.11471100 | -1.22217400 |
| C | -5.97093300 | -1.47404100 | 1.41650800 | C | -2.55162800 | 0.42790400 | -2.57962500 |
| H | -6.00376100 | -0.89140100 | 2.34325400 | C | -2.86813300 | -0.57838900 | -3.48562100 |
| H | -6.75530700 | -1.12630900 | 0.74282700 | H | 0.25795100 | -2.34717300 | 2.93601100 |
| H | -6.12982900 | -2.53447900 | 1.64398600 | H | -1.69997100 | -3.00947900 | 4.22603900 |
| | | | | H | -2.47531100 | 1.45292000 | -2.92119600 |
| | | | | H | -3.02832500 | -0.33217800 | -4.53100700 |
| 10 _{L2Rh} | | | | C | -3.10885600 | -2.52305600 | 2.68187400 |
| C | 5.00071600 | 0.89534600 | 0.05931500 | C | -3.26084800 | -2.04705400 | 1.37790000 |
| C | 5.71357900 | 0.96789600 | -1.15007300 | C | -2.76226400 | -2.22493600 | -1.72743200 |
| C | 6.96542300 | 0.36925400 | -1.28313200 | | | | |

| | | | | | | | |
|---|-------------|-------------|-------------|--------------------|-------------|-------------|-------------|
| C | -2.99377900 | -1.90264600 | -3.06724300 | H | 5.31487800 | -3.39584500 | 2.64618100 |
| C | -2.74652300 | 1.17676000 | 1.50809500 | P | -1.82233800 | 1.42976900 | -0.05805400 |
| C | -4.14483100 | 1.06992600 | 1.53451300 | P | 0.62779100 | -1.13930400 | 0.23999100 |
| C | -2.03237100 | 1.15903000 | 2.71267000 | H | -3.24938600 | -2.67258800 | -3.78324700 |
| C | -4.81276900 | 0.93839900 | 2.75005600 | H | -3.96842800 | -2.82390000 | 3.26686200 |
| H | -4.71151100 | 1.07126800 | 0.61128000 | O | -2.83449400 | -3.48484700 | -1.23265300 |
| C | -2.70316100 | 1.02175700 | 3.92879700 | O | -4.46153300 | -1.91859600 | 0.76241000 |
| H | -0.95217900 | 1.23985600 | 2.69718000 | C | -3.23786500 | -4.53492800 | -2.10815600 |
| C | -4.09393500 | 0.91035600 | 3.94893800 | H | -2.53640600 | -4.65400000 | -2.93997900 |
| H | -5.89520100 | 0.85504700 | 2.76198400 | H | -3.23700400 | -5.44218300 | -1.50252100 |
| H | -2.13863400 | 0.99998400 | 4.85612600 | H | -4.24646400 | -4.35847600 | -2.49925200 |
| H | -4.61776500 | 0.80365400 | 4.89404300 | C | -5.63046900 | -2.33533800 | 1.46369900 |
| C | -2.61188100 | 2.95808200 | -0.71065900 | H | -5.76929600 | -1.76190300 | 2.38628400 |
| C | -1.94257700 | 4.17647300 | -0.53812600 | H | -6.46504800 | -2.14181700 | 0.78858400 |
| C | -3.89350500 | 2.96413400 | -1.28786400 | H | -5.59235100 | -3.40528600 | 1.69810700 |
| C | -2.53122000 | 5.37807500 | -0.93757800 | | | | |
| H | -0.96013100 | 4.18936300 | -0.08468000 | 11 _{L2Rh} | | | |
| C | -4.47874200 | 4.16335700 | -1.68946700 | C | -5.14565500 | 0.82050300 | -0.17484500 |
| H | -4.43110600 | 2.03482600 | -1.43609900 | C | -5.89991700 | 0.06768000 | 0.74155600 |
| C | -3.79983000 | 5.37308700 | -1.51668300 | C | -7.08049300 | -0.56481500 | 0.35505700 |
| H | -1.99638300 | 6.31244000 | -0.79631700 | C | -7.54136900 | -0.45958200 | -0.95914800 |
| H | -5.46850600 | 4.15315700 | -2.13599000 | C | -6.80748200 | 0.28851800 | -1.87883600 |
| H | -4.26015100 | 6.30473100 | -1.83133500 | C | -5.62344100 | 0.91935300 | -1.49001700 |
| C | 0.48766500 | -2.05457300 | -1.33651000 | H | -5.55603900 | -0.03923200 | 1.76255000 |
| C | 0.59565600 | -1.38467500 | -2.56067600 | H | -7.64111000 | -1.14261400 | 1.08447800 |
| C | 0.28649300 | -3.44329800 | -1.31471400 | H | -8.46126700 | -0.95230600 | -1.25995600 |
| C | 0.50564700 | -2.09839300 | -3.75600700 | H | -7.15263600 | 0.38507200 | -2.90435800 |
| H | 0.77048900 | -0.31605100 | -2.58167200 | H | -5.07669700 | 1.49010500 | -2.23119500 |
| C | 0.21079000 | -4.15257700 | -2.51063300 | C | -3.82795200 | 1.45066800 | 0.24858800 |
| H | 0.19071800 | -3.96517300 | -0.36841200 | C | -2.76307700 | 0.33304500 | 0.55754200 |
| C | 0.31711500 | -3.48101800 | -3.73242900 | O | -3.09867200 | -0.68387300 | 1.13170100 |
| H | 0.58260100 | -1.57325400 | -4.70302300 | H | -1.98011000 | 1.05740300 | 3.15683100 |
| H | 0.06078000 | -5.22741300 | -2.48961700 | C | -3.97153600 | 2.26554600 | 1.56511700 |
| H | 0.25194900 | -4.03620300 | -4.66331000 | H | -4.41968700 | 1.64325200 | 2.34180100 |
| C | 2.10076000 | -1.88203700 | 1.04400100 | H | -4.67558300 | 3.07793100 | 1.35782200 |
| C | 2.38947700 | -1.67639300 | 2.40517700 | C | -3.22780300 | 2.39191200 | -0.80624600 |
| C | 3.01808000 | -2.60207100 | 0.26256300 | H | -3.91010800 | 3.23054600 | -0.99793400 |
| C | 3.53014000 | -2.23299700 | 2.98071700 | H | -3.08824300 | 1.87998000 | -1.76365800 |
| H | 1.74068900 | -1.06212500 | 3.01845300 | C | -2.63392200 | 2.85091200 | 2.09307100 |
| C | 4.17009000 | -3.13874600 | 0.83827300 | C | -2.10209800 | 2.12793700 | 3.33783400 |
| H | 2.84001400 | -2.74702400 | -0.79548800 | H | -2.83033700 | 3.88805000 | 2.40150500 |
| C | 4.42155100 | -2.97078800 | 2.19943300 | H | -1.13144500 | 2.53460700 | 3.64249200 |
| H | 3.72854600 | -2.07287500 | 4.03586300 | H | -2.80011100 | 2.25120400 | 4.17190600 |
| H | 4.87025900 | -3.68736300 | 0.21634600 | C | -1.89505100 | 2.89762000 | -0.32819500 |

| | | | | | | | |
|----|-------------|-------------|-------------|----------------------|-------------|-------------|-------------|
| C | -1.59790100 | 3.00147200 | 1.00593900 | C | -0.58214400 | -1.95117300 | 2.54551400 |
| H | -1.21613300 | 3.30550200 | -1.07233400 | C | 0.31416500 | -3.71993800 | 1.15016300 |
| H | -0.58429900 | 0.71339500 | 1.53967900 | C | -0.46860100 | -2.77786400 | 3.66203400 |
| H | -0.65477200 | 3.44616100 | 1.30772600 | H | -0.97740000 | -0.94940800 | 2.64791200 |
| Rh | -0.86415700 | 0.88657700 | 0.07113600 | C | 0.41285700 | -4.54744100 | 2.26770400 |
| C | 2.47128000 | -1.43785900 | -0.59439400 | H | 0.63633800 | -4.08304800 | 0.18029500 |
| C | 1.21059200 | -1.73275000 | -1.14474200 | C | 0.02702200 | -4.07633900 | 3.52497000 |
| C | 1.11286500 | -2.27047600 | -2.43690400 | H | -0.76678300 | -2.40698700 | 4.63792400 |
| C | 2.26811200 | -2.50578600 | -3.17664600 | H | 0.80082600 | -5.55520900 | 2.15725400 |
| C | 2.61213500 | -0.92693400 | 0.79942900 | H | 0.11343800 | -4.71980400 | 4.39537500 |
| C | 2.25119600 | 0.37713800 | 1.17169200 | C | -1.67714200 | -1.99995600 | -1.22506000 |
| C | 2.23970900 | 0.74106300 | 2.53070500 | C | -2.09329800 | -1.20029500 | -2.30334700 |
| C | 2.65533100 | -0.16782500 | 3.49739800 | C | -2.38868900 | -3.16039400 | -0.91331900 |
| H | 0.14644700 | -2.51274300 | -2.85859900 | C | -3.20978800 | -1.55741100 | -3.05584700 |
| H | 2.19179900 | -2.92604300 | -4.17490800 | H | -1.54402300 | -0.29543200 | -2.55379000 |
| H | 1.91402900 | 1.73045500 | 2.82899300 | C | -3.51143900 | -3.51324700 | -1.66636500 |
| H | 2.65253800 | 0.12003600 | 4.54438600 | H | -2.08799500 | -3.77512100 | -0.07260200 |
| C | 3.52513000 | -2.20415100 | -2.65647900 | C | -3.92643300 | -2.71338600 | -2.73126400 |
| C | 3.62719100 | -1.67221600 | -1.36690600 | H | -3.52797100 | -0.93082800 | -3.88330000 |
| C | 3.05614100 | -1.82835500 | 1.79653000 | H | -4.06699400 | -4.41046500 | -1.41104900 |
| C | 3.08294800 | -1.44699700 | 3.14036900 | H | -4.80751600 | -2.98418100 | -3.30463000 |
| C | 2.46187700 | 1.38198100 | -1.61887900 | P | 1.52445500 | 1.54460900 | -0.04852500 |
| C | 3.85182900 | 1.56421700 | -1.66632900 | P | -0.31542400 | -1.35280300 | -0.18750900 |
| C | 1.75298700 | 1.16622300 | -2.80731900 | H | 3.41122500 | -2.13880200 | 3.90533700 |
| C | 4.52109300 | 1.51110900 | -2.88659500 | H | 4.41087200 | -2.38215400 | -3.25270600 |
| H | 4.40823200 | 1.73990100 | -0.75233900 | O | 3.41085700 | -3.05947300 | 1.35385800 |
| C | 2.42567700 | 1.11305300 | -4.02937700 | O | 4.79926800 | -1.32372100 | -0.78214000 |
| H | 0.67642600 | 1.02535400 | -2.77582900 | C | 3.87312700 | -4.01384200 | 2.30681100 |
| C | 3.81015800 | 1.28271400 | -4.06928700 | H | 3.10757700 | -4.23131400 | 3.05830600 |
| H | 5.59731100 | 1.65124200 | -2.91704100 | H | 4.08932200 | -4.91929100 | 1.73820700 |
| H | 1.86998800 | 0.93531300 | -4.94516100 | H | 4.78779100 | -3.66770400 | 2.80177300 |
| H | 4.33548400 | 1.24142500 | -5.01862700 | C | 6.00608300 | -1.53371300 | -1.51202000 |
| C | 2.11063100 | 3.20725900 | 0.48322500 | H | 6.00999800 | -0.96539900 | -2.44813300 |
| C | 1.42272300 | 4.32975600 | -0.00310400 | H | 6.80914600 | -1.17474000 | -0.86694500 |
| C | 3.27696800 | 3.40507000 | 1.23915300 | H | 6.15983400 | -2.59732700 | -1.72755500 |
| C | 1.87210600 | 5.61988900 | 0.28051000 | | | | |
| H | 0.54076300 | 4.20195500 | -0.62021900 | TS10 _{L2Rh} | | | |
| C | 3.72275500 | 4.69572400 | 1.52468100 | C | -5.21640000 | 0.39509900 | -0.39447200 |
| H | 3.84178500 | 2.55558500 | 1.60411000 | C | -6.05617100 | -0.08256200 | 0.62502500 |
| C | 3.01990200 | 5.80599600 | 1.05225700 | C | -7.23383700 | -0.76560600 | 0.32720000 |
| H | 1.32491100 | 6.47602200 | -0.10242000 | C | -7.60228900 | -0.99007700 | -1.00122800 |
| H | 4.62566100 | 4.83171100 | 2.11241800 | C | -6.78003800 | -0.52068200 | -2.02425000 |
| H | 3.36911100 | 6.80903000 | 1.27762000 | C | -5.59928500 | 0.16312900 | -1.72278800 |
| C | -0.18829000 | -2.41655100 | 1.28539100 | H | -5.78577700 | 0.06850300 | 1.66348000 |

| | | | | | | | |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | -7.86304400 | -1.12591000 | 1.13598400 | C | 1.53498500 | -3.90071400 | 3.02636000 |
| H | -8.51928800 | -1.52334700 | -1.23393500 | H | 1.22378800 | -3.98195000 | 0.89847500 |
| H | -7.05246600 | -0.68349700 | -3.06309400 | C | 0.77750200 | -1.88697500 | 4.13772400 |
| H | -4.98384400 | 0.51312200 | -2.54271000 | H | -0.15583800 | -0.41189000 | 2.86347300 |
| C | -3.91603800 | 1.11109600 | -0.04282900 | C | 1.38837000 | -3.14185800 | 4.19093000 |
| C | -2.94716800 | 0.12405400 | 0.66174000 | H | 2.01289400 | -4.87445100 | 3.06693400 |
| O | -3.31311200 | -0.88543700 | 1.22004800 | H | 0.67166200 | -1.29235400 | 5.03995000 |
| H | -2.24606500 | 1.80920400 | 3.02274800 | H | 1.75407700 | -3.52709400 | 5.13792800 |
| C | -4.17870700 | 2.27499300 | 0.96386300 | C | -1.51290800 | -2.53490900 | -0.39858100 |
| H | -4.66674900 | 1.88464100 | 1.85955700 | C | -2.29051000 | -2.08048900 | -1.47655400 |
| H | -4.90015200 | 2.93358900 | 0.47131800 | C | -1.83264000 | -3.75038400 | 0.21214300 |
| C | -3.20562700 | 1.70781700 | -1.27165300 | C | -3.36452800 | -2.83410800 | -1.94089400 |
| H | -3.87484500 | 2.43041200 | -1.75750100 | H | -2.06471500 | -1.12153900 | -1.93435600 |
| H | -2.98219300 | 0.93253700 | -2.00976100 | C | -2.91753500 | -4.50066100 | -0.24902900 |
| C | -2.92361100 | 3.08842300 | 1.37311500 | H | -1.25643400 | -4.10892400 | 1.05670600 |
| C | -2.49388800 | 2.85867600 | 2.82900500 | C | -3.68363400 | -4.04665500 | -1.32234000 |
| H | -3.19873100 | 4.15080000 | 1.30594700 | H | -3.96534300 | -2.46714200 | -2.76673200 |
| H | -1.61425000 | 3.46259700 | 3.07388800 | H | -3.16482500 | -5.43843500 | 0.23939600 |
| H | -3.30161900 | 3.14146200 | 3.51168000 | H | -4.53055900 | -4.62882600 | -1.67241600 |
| C | -1.93054500 | 2.38796400 | -0.86072500 | C | 2.02826500 | 1.55695800 | -1.79487500 |
| C | -1.78259600 | 2.94749900 | 0.39104000 | C | 1.16269100 | 1.26259300 | -2.85654400 |
| H | -1.21904400 | 2.63579400 | -1.64514900 | C | 3.37860100 | 1.83544500 | -2.05329200 |
| H | -1.83777200 | 0.61558000 | 1.45725000 | C | 1.64173000 | 1.24645400 | -4.16667100 |
| H | -0.93407300 | 3.59163600 | 0.57575600 | H | 0.12334700 | 1.02659600 | -2.65147500 |
| Rh | -0.86376800 | 0.78904100 | 0.23466100 | C | 3.85094000 | 1.82858800 | -3.36422000 |
| C | 2.90850100 | -0.70284500 | 0.50769800 | H | 4.05603000 | 2.04475600 | -1.23252200 |
| C | 2.56955900 | 0.60213800 | 0.90804600 | C | 2.98490000 | 1.53136200 | -4.42066100 |
| C | 3.06203900 | 1.10987400 | 2.12014400 | H | 0.97051000 | 1.00405600 | -4.98484300 |
| C | 3.86298500 | 0.31700000 | 2.93597300 | H | 4.89579700 | 2.04720200 | -3.56122500 |
| C | 2.48790200 | -1.29521800 | -0.79543600 | H | 3.35858700 | 1.51749800 | -5.43997400 |
| C | 1.18324800 | -1.75019100 | -1.05105200 | C | 1.55204000 | 3.30504700 | 0.47763900 |
| C | 0.87562300 | -2.33827400 | -2.28853700 | C | 1.12782200 | 3.63824700 | 1.77814000 |
| C | 1.85903700 | -2.46288000 | -3.26475000 | C | 2.01353300 | 4.32353600 | -0.36600700 |
| H | 2.83859600 | 2.12144300 | 2.42632100 | C | 1.20173300 | 4.95258700 | 2.23255300 |
| H | 4.23900600 | 0.71864200 | 3.87211100 | H | 0.72088400 | 2.87103500 | 2.42908200 |
| H | -0.12078600 | -2.70730400 | -2.48824600 | C | 2.07036100 | 5.64405300 | 0.08834800 |
| H | 1.61514200 | -2.92194100 | -4.21808500 | H | 2.32954100 | 4.09674300 | -1.37697000 |
| C | 4.19387600 | -0.98446500 | 2.56693500 | C | 1.67298000 | 5.96098000 | 1.38652600 |
| C | 3.72713600 | -1.48864000 | 1.34981300 | H | 0.87859500 | 5.19110400 | 3.24120800 |
| C | 3.47032800 | -1.43033400 | -1.80210400 | H | 2.42962700 | 6.42230000 | -0.57810500 |
| C | 3.15554400 | -2.00858100 | -3.03514100 | H | 1.72235400 | 6.98715700 | 1.73739100 |
| C | 0.45668100 | -2.14981600 | 1.75079000 | P | -0.15168500 | -1.45422700 | 0.18354100 |
| C | 1.08039600 | -3.40484900 | 1.80554700 | P | 1.36396800 | 1.57224900 | -0.09713500 |
| C | 0.30857500 | -1.39236600 | 2.92109100 | H | 3.90784300 | -2.10783200 | -3.80691200 |

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|--------------------|-------------|-------------|-------------|----|-------------|-------------|-------------|
| H | 4.81394700 | -1.58971000 | 3.21560300 | Rh | -0.75626000 | 0.68085700 | 0.31391900 |
| O | 4.69866700 | -0.94963900 | -1.48828400 | C | 2.81819500 | -1.09429000 | -0.74673400 |
| O | 3.99836300 | -2.73862600 | 0.89954800 | C | 1.60945700 | -1.58301100 | -1.27528600 |
| C | 5.74366100 | -1.08474800 | -2.44865900 | C | 1.54751800 | -2.05611600 | -2.59187900 |
| H | 5.50684100 | -0.55354700 | -3.37668400 | C | 2.69108300 | -2.02813300 | -3.38608500 |
| H | 6.62634500 | -0.63624900 | -1.99087200 | C | 2.91896300 | -0.68055200 | 0.68519700 |
| H | 5.94402400 | -2.13932900 | -2.67011100 | C | 2.30333200 | 0.47142200 | 1.20274400 |
| C | 4.82270800 | -3.58181000 | 1.70029200 | C | 2.25895900 | 0.68710400 | 2.59317800 |
| H | 4.37839400 | -3.75542100 | 2.68603300 | C | 2.89106800 | -0.20204700 | 3.45386900 |
| H | 4.88994400 | -4.52805900 | 1.16178300 | H | 0.61610400 | -2.43698500 | -2.99295900 |
| H | 5.82683700 | -3.15874100 | 1.81899600 | H | 2.64925200 | -2.39787000 | -4.40615000 |
| | | | | H | 1.72961500 | 1.54170600 | 2.99748300 |
| | | | | H | 2.86394000 | -0.02788400 | 4.52516600 |
| 12 _{L2Rh} | | | | C | 3.89053100 | -1.51594000 | -2.89454500 |
| C | -5.58220200 | 0.54126800 | -0.14479800 | C | 3.95446100 | -1.04771200 | -1.57686200 |
| C | -6.51063300 | 0.03335700 | 0.77678600 | C | 3.55740000 | -1.57095200 | 1.58243000 |
| C | -7.79611800 | -0.32838600 | 0.37724800 | C | 3.55640300 | -1.32328600 | 2.95798400 |
| C | -8.18155300 | -0.19614200 | -0.95840200 | C | 2.03939800 | 1.68575200 | -1.52091700 |
| C | -7.26577400 | 0.29697300 | -1.88663000 | C | 3.34760200 | 2.17178900 | -1.66712500 |
| C | -5.97815900 | 0.65924400 | -1.48350100 | C | 1.27684100 | 1.38865900 | -2.65508000 |
| H | -6.23057900 | -0.09124400 | 1.81645000 | C | 3.89093200 | 2.33142600 | -2.93922200 |
| H | -8.49562600 | -0.71767500 | 1.11124800 | H | 3.93756800 | 2.42056300 | -0.79170400 |
| H | -9.18289800 | -0.47735900 | -1.27068000 | C | 1.82374000 | 1.55369600 | -3.92883100 |
| H | -7.54794000 | 0.40216100 | -2.93018600 | H | 0.26504700 | 1.01702500 | -2.52997300 |
| H | -5.28897500 | 1.03501000 | -2.22980900 | C | 3.13096300 | 2.02091700 | -4.07157300 |
| C | -4.16608700 | 0.89996900 | 0.31356600 | H | 4.90517400 | 2.70305600 | -3.04839500 |
| C | -3.43370900 | -0.38525500 | 0.66671700 | H | 1.23051400 | 1.31313200 | -4.80595000 |
| O | -3.89824600 | -1.47291100 | 0.88904800 | H | 3.55686400 | 2.14801800 | -5.06226500 |
| H | -2.12714800 | 0.35285900 | 2.96238300 | C | 1.62646300 | 3.29308900 | 0.71391100 |
| C | -4.20525300 | 1.79444300 | 1.59799300 | C | 0.87565300 | 4.32210900 | 0.12009800 |
| H | -4.75852300 | 1.28710200 | 2.39114300 | C | 2.66961500 | 3.63415900 | 1.58657700 |
| H | -4.79352500 | 2.67049800 | 1.30729500 | C | 1.13309800 | 5.65703900 | 0.42465800 |
| C | -3.37568700 | 1.67895800 | -0.76257000 | H | 0.10233300 | 4.08519700 | -0.60177900 |
| H | -4.02072500 | 2.49942500 | -1.10290700 | C | 2.92607200 | 4.97364200 | 1.88819700 |
| H | -3.18756100 | 1.05037900 | -1.63743000 | H | 3.29668800 | 2.86662300 | 2.02131600 |
| C | -2.84087900 | 2.26454900 | 2.15259800 | C | 2.15493700 | 5.98648300 | 1.31833800 |
| C | -2.29945600 | 1.38243500 | 3.28708700 | H | 0.53970400 | 6.43803700 | -0.04088600 |
| H | -3.03056600 | 3.24826800 | 2.60335000 | H | 3.73826300 | 5.22103100 | 2.56502100 |
| H | -1.34699900 | 1.77447300 | 3.65983800 | H | 2.35640600 | 7.02632400 | 1.55682700 |
| H | -3.00676300 | 1.35725300 | 4.12318500 | C | 0.38268500 | -2.53283800 | 1.16209200 |
| C | -2.07904100 | 2.29290700 | -0.28639400 | C | -0.09568100 | -2.14386400 | 2.42060100 |
| C | -1.81785500 | 2.52353700 | 1.06085700 | C | 1.08089800 | -3.74174100 | 1.02645000 |
| H | -1.53853700 | 2.84464900 | -1.05080200 | C | 0.11894100 | -2.95608900 | 3.53427900 |
| H | -2.30626100 | -0.29303600 | 0.80323400 | H | -0.61544200 | -1.19629500 | 2.52500400 |
| H | -1.02941300 | 3.21608800 | 1.33321000 | | | | |

| | | | |
|---|-------------|-------------|-------------|
| C | 1.28649400 | -4.55463500 | 2.14029000 |
| H | 1.47188200 | -4.03776000 | 0.05895700 |
| C | 0.80952700 | -4.16160300 | 3.39443500 |
| H | -0.24468700 | -2.64382300 | 4.50855800 |
| H | 1.82521300 | -5.49079700 | 2.03108000 |
| H | 0.98035400 | -4.79291100 | 4.26119800 |
| C | -1.25342800 | -2.21189500 | -1.23857800 |
| C | -1.89185600 | -1.43032600 | -2.21802000 |
| C | -1.73401900 | -3.49798000 | -0.96596300 |
| C | -2.99229700 | -1.93006500 | -2.91103300 |
| H | -1.52947400 | -0.42907200 | -2.42827500 |
| C | -2.84067300 | -3.99307700 | -1.65938900 |
| H | -1.25989800 | -4.10784200 | -0.20532400 |
| C | -3.47351000 | -3.21158100 | -2.62647800 |
| H | -3.48107300 | -1.31721800 | -3.66235000 |
| H | -3.21139000 | -4.98868300 | -1.43535500 |
| H | -4.33992000 | -3.59631300 | -3.15560900 |
| P | 1.28728500 | 1.57396900 | 0.14771000 |
| P | 0.08879800 | -1.43605900 | -0.26564700 |
| H | 4.03982900 | -2.00808300 | 3.64264200 |
| H | 4.76330100 | -1.48292100 | -3.53417400 |
| O | 4.11603600 | -2.66866700 | 1.01654400 |
| O | 5.06335700 | -0.50356600 | -1.01770200 |
| C | 4.75438900 | -3.61852500 | 1.86754300 |
| H | 4.05446700 | -4.02876500 | 2.60279400 |
| H | 5.10054100 | -4.41782400 | 1.21093100 |
| H | 5.61323900 | -3.17476000 | 2.38399300 |
| C | 6.23107200 | -0.37054100 | -1.82576200 |
| H | 6.03604600 | 0.24836200 | -2.70828800 |
| H | 6.97365200 | 0.12060100 | -1.19546200 |
| H | 6.61230000 | -1.34884900 | -2.14043100 |