

Supporting Information

**Exploring the Nature of the Energy Barriers on
the Mechanism of the Zirconocene-Catalyzed
Ethylene Polymerization: A Quantitative Study
from Reaction Force Analysis**

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Table S1. SCF energies, enthalpies and Gibbs free energies for zirconocene methyl cation and each stationary point involved in the zirconocene ethylene polymerization reaction.

Enthalpies and free energies are in standard conditions (1 atm and 298.15 K).

| System | <i>E</i> (Hartree) | <i>E</i> + <i>ZPE</i> (Hartree) | <i>H</i> (Hartree) | <i>G</i> (Hartree) | <i>Frecuency</i> (cm ⁻¹) |
|----------------------------------|--------------------|---------------------------------|--------------------|--------------------|--------------------------------------|
| Zirconocene methyl cation | -473.116478 | -472.953896 | -472.942775 | -472.989144 | 23.4617 |
| Ethylene | -78.544777 | -78.495504 | -78.491525 | -78.517031 | 828.8 |
| I-R | -551.70492 | -551.478204 | -551.462369 | -551.519615 | 41.7190 |
| I-TS | -551.69256 | -551.463898 | -551.450629 | -551.501742 | -315.6484 |
| I-P | -551.71927 | -551.488328 | -551.474116 | -551.528141 | 35.6408 |
| P₁-R | -630.2985 | -630.010743 | -629.992288 | -630.054719 | 50.7790 |
| P₁-TS | -630.28307 | -629.992993 | -629.975793 | -630.035695 | -291.7076 |
| P₁-P | -630.31243 | -630.021109 | -630.003624 | -630.064906 | 24.8306 |
| P₂-R | -708.89055 | -708.545059 | -708.523815 | -708.593309 | 45.8005 |
| P₂-TS | -708.87486 | -708.526531 | -708.507621 | -708.57191 | -287.2242 |
| P₂-P | -708.90298 | -708.555074 | -708.536666 | -708.601038 | 13.7269 |
| P₃-R | -787.47564 | -787.072088 | -787.04923 | -787.12335 | 27.2358 |
| P₃-TS | -787.45946 | -787.053998 | -787.034099 | -787.09994 | -292.5892 |
| P₃-P | -787.48855 | -787.081153 | -787.059423 | -787.130957 | 13.4295 |
| P₄-R | -866.06565 | -865.604265 | -865.579844 | -865.65663 | 15.6436 |
| P₄-TS | -866.05087 | -865.586834 | -865.563836 | -865.637187 | -286.8437 |
| P₄-P | -866.07827 | -865.613084 | -865.588818 | -865.66576 | 19.5890 |
| P₅-R | -944.65778 | -944.138355 | -944.110537 | -944.19606 | 13.6868 |
| P₅-TS | -944.91565 | -944.120112 | -944.094048 | -944.173733 | -293.9019 |
| P₅-P | -944.67044 | -944.148121 | -944.122018 | -944.202813 | 17.8485 |
| P₆-R | -1023.2495 | -1022.671114 | -1022.6411 | -1022.729089 | 20.7927 |
| P₆-TS | -1023.2338 | -1022.654031 | -1022.625176 | -1022.712142 | -296.5040 |
| P₆-P | -1023.2616 | -1022.680669 | -1022.652119 | -1022.73817 | 21.6978 |
| P₇-R | -1101.8395 | -1101.203042 | -1101.170539 | -1101.266164 | 13.4620 |
| P₇-TS | -1101.8239 | -1101.186169 | -1101.155587 | -1101.246019 | -297.6860 |
| P₇-P | -1101.8514 | -1101.213435 | -1101.182122 | -1101.275782 | 12.4070 |
| P₈-R | -1180.4297 | -1179.735619 | -1179.700814 | -1179.800143 | 15.2301 |
| P₈-TS | -1180.4157 | -1179.71977 | -1179.686948 | -1179.782598 | -296.8743 |
| P₈-P | -1180.4437 | -1179.746148 | -1179.711463 | -1179.810748 | 19.6023 |
| P₉-R | -1259.0227 | -1258.271773 | -1258.233754 | -1258.342285 | 14.9092 |
| P₉-TS | -1259.0082 | -1258.255468 | -1258.219597 | -1258.322169 | -297.0098 |
| P₉-P | -1259.0357 | -1258.281437 | -1258.245331 | -1258.348945 | 14.2507 |
| T(P₅)-R | -944.08329 | -944.624751 | -944.601899 | -944.677134 | 10.1672 |
| T(P₅)-TS | -944.063002 | -944.606616 | -944.582745 | -944.660196 | -304.9801 |
| T(P₅)-P | -944.06517 | -944.60741 | -944.583608 | -944.660577 | 10.4087 |
| T(P₉)-R | -1259.0392 | -1258.29106 | -1258.256121 | -1258.357031 | 14.5976 |
| T(P₉)-TS | -1259.0188 | -1258.273488 | -1258.237196 | -1258.341692 | -321.8485 |
| T(P₉)-P | -1259.0201 | -1258.274052 | -1258.236587 | -1258.345534 | 14.2026 |

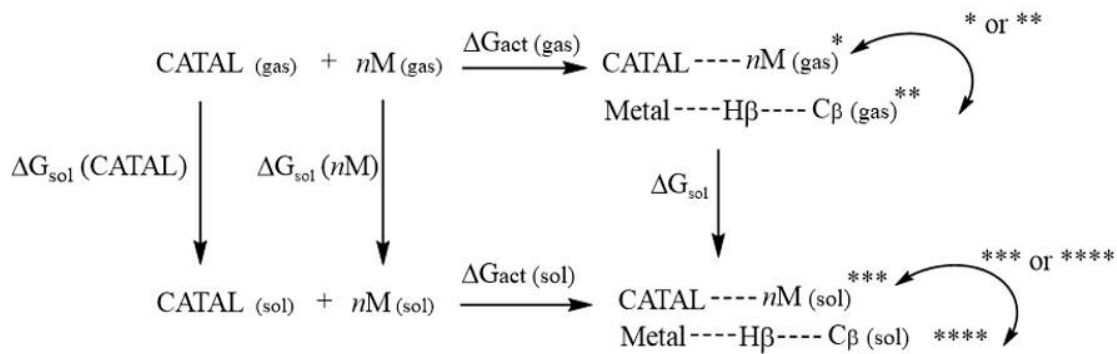


Figure S1. Thermodynamic cycle used for calculating activation free energies in gas and solution phases for an ethylene polymerization process. n denotes the number of M monomers of ethylene, CATAL corresponds to the catalyst and H β /C β the hydrogen and carbon atom in β -position.

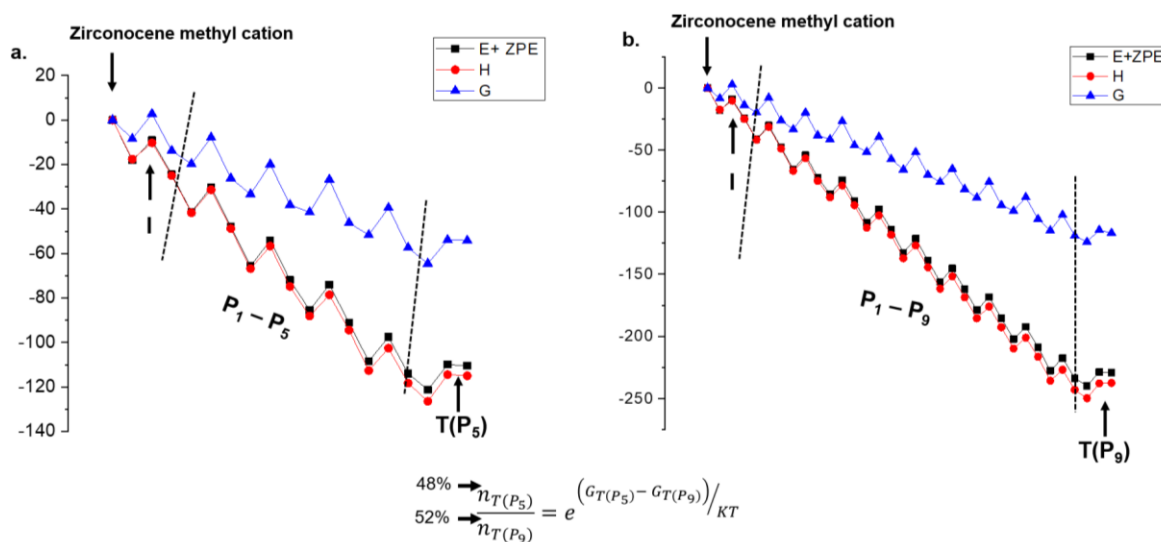


Figure S2. Relative energy data for an earlier chain termination (a) and later chain termination (b) on zirconocene ethylene polymerization reaction. Boltzmann distribution is obtained from the Gibbs free energies of the reactants and products involved in the propagation paths P_5 - P/P_9 - P and $T(P_5)$ - $R/T(P_9)$ - R reaction paths to characterize the relative preference of the zirconocene catalyst to follow an earlier or later chain termination at $T=298.15$ K.

Figure S2 shows two possible reaction paths termination, which characterizes the different chain lengths. Both chain propagation paths are kinetically and thermodynamically preferred. The Boltzmann distribution shows that the reaction path toward **T(P₉)** is highly populated in 52%, giving a larger chain than the reaction path toward **T(P₅)** (48%). However, that difference is very small, which is in agreement with the results obtained from the electronic energies in the main manuscript.

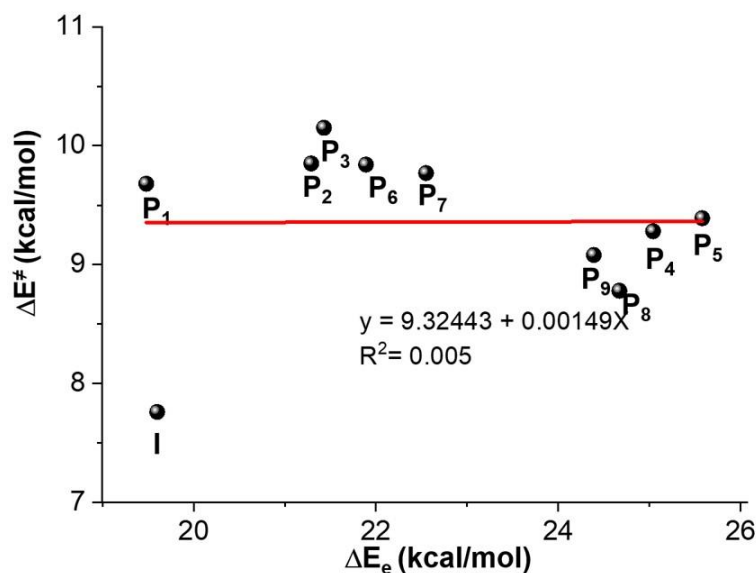


Figure S3. Correlation of the activation energy from the chain initiation to chain propagation of the ethylene polymerization reaction with the electrostatic energy difference (ΔE_e).

Optimized Cartesian coordinates

Zirconocene methyl cation

| | | | |
|----|-------------|-------------|-------------|
| C | 1.20660300 | 2.11524500 | 0.54318000 |
| H | 2.26036000 | 2.11660700 | 0.79704200 |
| C | 0.65894900 | 2.28369700 | -0.76160000 |
| H | 1.22273300 | 2.42915900 | -1.67504300 |
| C | -0.75132800 | 2.27163600 | -0.65255000 |
| C | 0.13512700 | 1.98195100 | 1.45382400 |
| H | 0.22153300 | 1.86330300 | 2.52544800 |
| C | -1.08106700 | 2.05590900 | 0.71392800 |
| H | -2.07964600 | 2.02774800 | 1.13042200 |
| C | -0.37847800 | -1.18292200 | 2.16314200 |
| C | 0.53586600 | -2.00156300 | 1.46394400 |
| H | 1.55464800 | -2.21752700 | 1.76442100 |
| C | -0.12662200 | -2.52176800 | 0.31454300 |
| C | -1.60836800 | -1.18417500 | 1.44231800 |
| H | -2.51976000 | -0.68320100 | 1.74194800 |
| C | -1.45568400 | -2.03758600 | 0.31495400 |
| H | -2.21724100 | -2.26876700 | -0.41715000 |
| H | 0.30141800 | -3.19769000 | -0.41572400 |
| Zr | 0.02628300 | -0.03670900 | -0.03094100 |
| C | -0.81150400 | -0.35721600 | -2.06941700 |
| H | -0.61971900 | -1.38710100 | -2.39250800 |
| H | -0.33891100 | 0.33266500 | -2.77837300 |
| H | -1.89414100 | -0.19745400 | -2.14548100 |
| H | -1.45346900 | 2.39577600 | -1.46555300 |
| H | -0.18575100 | -0.66215900 | 3.09134400 |

Ethylene

| | | | |
|---|-------------|------------|------------|
| C | -1.78044900 | 1.22578000 | 0.00000000 |
| H | -1.26332600 | 0.27086700 | 0.00000000 |
| H | -2.86597600 | 1.19568300 | 0.00000000 |
| C | -1.11570500 | 2.37776900 | 0.00000000 |
| H | -1.63282900 | 3.33268100 | 0.00000000 |
| H | -0.03017800 | 2.40786600 | 0.00000000 |

I-R

| | | | |
|---|-------------|-------------|-------------|
| C | 0.77192300 | 1.96476200 | 1.12064800 |
| H | 1.46753300 | 1.82363000 | 1.93759100 |
| C | 1.11072900 | 2.22218700 | -0.23051400 |
| H | 2.11523100 | 2.31438400 | -0.62614200 |
| C | -0.09237600 | 2.38552500 | -0.96493200 |
| C | -0.64740500 | 1.97772800 | 1.22092900 |
| H | -1.21954400 | 1.85258400 | 2.13071200 |
| C | -1.17776400 | 2.24500000 | -0.06856600 |
| H | -2.22585000 | 2.32734200 | -0.32401000 |
| C | 0.06078000 | -1.11785200 | 2.13538800 |
| C | 0.87067000 | -1.90574100 | 1.29245000 |
| H | 1.94039000 | -2.04346100 | 1.39184200 |
| C | 0.02692500 | -2.51919600 | 0.31853600 |
| C | -1.28358700 | -1.22543700 | 1.67864800 |
| H | -2.14895900 | -0.75991700 | 2.13284600 |
| C | -1.30322400 | -2.12027300 | 0.57576200 |

| | | | |
|----|-------------|-------------|-------------|
| H | -2.18036100 | -2.43067300 | 0.02563200 |
| H | 0.34069000 | -3.20703400 | -0.45705400 |
| Zr | -0.06807500 | -0.03094700 | -0.13966700 |
| C | -1.61733000 | -0.29920100 | -1.73339000 |
| H | -1.55042200 | -1.30393200 | -2.16766200 |
| H | -1.49331400 | 0.44135900 | -2.53094400 |
| H | -2.63921500 | -0.18692100 | -1.34922400 |
| H | -0.17245400 | 2.60244900 | -2.02226500 |
| H | 0.39947100 | -0.53570800 | 2.98220800 |
| C | 2.35423400 | -0.82081200 | -1.39565500 |
| C | 1.55974700 | -0.42294200 | -2.40423500 |
| H | 2.95828700 | -0.11155400 | -0.83022500 |
| H | 2.48979100 | -1.87355300 | -1.16845100 |
| H | 1.49015800 | 0.62228700 | -2.69736500 |
| H | 1.00890900 | -1.14091400 | -3.00650700 |

I-TS

| | | | |
|----|-------------|-------------|-------------|
| C | 1.06919800 | 2.06394500 | 0.79952700 |
| H | 2.02544000 | 1.99381200 | 1.30299900 |
| C | 0.86832700 | 2.31061700 | -0.58455800 |
| H | 1.64644800 | 2.46028400 | -1.32215000 |
| C | -0.52206600 | 2.35635000 | -0.82798600 |
| C | -0.20600900 | 1.97397500 | 1.41314700 |
| H | -0.39586500 | 1.82183600 | 2.46738700 |
| C | -1.19314000 | 2.13437700 | 0.40673900 |
| H | -2.26484900 | 2.14005800 | 0.56123800 |
| C | -0.11710100 | -1.18160600 | 2.13236400 |
| C | 0.68551900 | -2.00774600 | 1.31099600 |
| H | 1.73529100 | -2.22053300 | 1.46229200 |
| C | -0.13976800 | -2.53419600 | 0.28003000 |
| C | -1.44279900 | -1.19780400 | 1.61424300 |
| H | -2.29869200 | -0.68889800 | 2.03891700 |
| C | -1.45469400 | -2.05323700 | 0.48328400 |
| H | -2.32119900 | -2.29309600 | -0.12037500 |
| H | 0.17417900 | -3.21641800 | -0.50028500 |
| Zr | -0.03377500 | -0.02874000 | -0.10189900 |
| C | -0.82592800 | -0.43717300 | -2.22637400 |
| H | -1.05153600 | -1.46508600 | -2.50601400 |
| H | -0.87696700 | 0.21028800 | -3.09906900 |
| H | -1.67824100 | -0.09745200 | -1.56496200 |
| H | -0.99618000 | 2.54795500 | -1.78199200 |
| H | 0.21421800 | -0.65489300 | 3.01769800 |
| C | 2.06511600 | -0.54194700 | -1.10683100 |
| C | 1.33388000 | -0.52453100 | -2.30808800 |
| H | 2.70091400 | 0.30769600 | -0.88168900 |
| H | 2.41155400 | -1.50123600 | -0.74139300 |
| H | 1.36141600 | 0.36541900 | -2.92771200 |
| H | 1.16844800 | -1.45229500 | -2.84462900 |

I-P

| | | | |
|---|-------------|------------|-------------|
| C | 0.97374100 | 2.01544200 | 0.99519400 |
| H | 1.83251600 | 1.91085200 | 1.64632700 |
| C | 1.01347800 | 2.25520300 | -0.40047500 |
| H | 1.90737000 | 2.36482800 | -0.99877800 |
| C | -0.32139500 | 2.33444900 | -0.86822700 |
| C | -0.39085700 | 1.98170100 | 1.39624400 |

| | | | |
|----|-------------|-------------|-------------|
| H | -0.75229300 | 1.84384900 | 2.40671800 |
| C | -1.19256000 | 2.16846700 | 0.24670700 |
| H | -2.27466500 | 2.20851500 | 0.22427600 |
| C | 0.00343900 | -1.14376900 | 2.16848200 |
| C | 0.73545000 | -2.00992100 | 1.31465700 |
| H | 1.79123700 | -2.23300000 | 1.38708000 |
| C | -0.16409000 | -2.52993900 | 0.35334100 |
| C | -1.35627000 | -1.14868600 | 1.74451600 |
| H | -2.17168900 | -0.61026000 | 2.20968700 |
| C | -1.45653900 | -2.00774600 | 0.62460500 |
| H | -2.36503700 | -2.23822600 | 0.08084200 |
| H | 0.08897200 | -3.22593800 | -0.43647300 |
| Zr | -0.02677200 | -0.03397600 | -0.06257200 |
| C | -0.53456500 | -0.68458300 | -2.58714200 |
| H | -0.69617400 | -1.74740100 | -2.39390700 |
| H | -0.91034200 | -0.47260300 | -3.58997300 |
| H | -1.26842000 | -0.09927000 | -1.97261400 |
| H | -0.62876000 | 2.53748900 | -1.88700300 |
| H | 0.40115100 | -0.60980800 | 3.02181700 |
| C | 1.78326800 | -0.53225900 | -1.22377300 |
| C | 0.97700900 | -0.28590500 | -2.53598300 |
| H | 2.67831000 | 0.08689100 | -1.21294800 |
| H | 2.08118000 | -1.57921100 | -1.14863000 |
| H | 1.07029100 | 0.75420800 | -2.85791900 |
| H | 1.43148600 | -0.89631600 | -3.32255800 |

Pi-R

| | | | |
|----|-------------|-------------|-------------|
| C | -0.43842900 | -2.54212700 | 0.56658200 |
| H | 0.18803000 | -3.05801800 | 1.28313900 |
| C | -1.65405700 | -1.84909200 | 0.85008200 |
| H | -2.13956100 | -1.77266700 | 1.81431800 |
| C | -2.16476200 | -1.35664800 | -0.37304900 |
| C | -0.19475500 | -2.45319700 | -0.81442700 |
| H | 0.64592300 | -2.88879000 | -1.33788300 |
| C | -1.25176400 | -1.69520200 | -1.40279000 |
| H | -1.37153300 | -1.48161500 | -2.45744000 |
| C | -1.56450300 | 1.78575500 | -0.71901700 |
| C | -0.26357700 | 2.16739000 | -1.12580500 |
| H | 0.07520000 | 2.26922500 | -2.14919800 |
| C | 0.51035400 | 2.42054200 | 0.03934000 |
| C | -1.60745900 | 1.81680500 | 0.70195100 |
| H | -2.47252400 | 1.60408400 | 1.31749200 |
| C | -0.33268800 | 2.22595800 | 1.16228900 |
| H | -0.05384900 | 2.38924800 | 2.19555200 |
| H | 1.53460900 | 2.76728600 | 0.06618800 |
| Zr | -0.03013400 | -0.06350400 | 0.06619000 |
| C | 2.62052000 | 0.92276700 | -2.47602900 |
| H | 2.50338000 | 1.86901700 | -1.94018600 |
| H | 2.26304400 | 1.05725900 | -3.50002800 |
| H | 3.68830300 | 0.69563900 | -2.51396400 |
| H | -3.08964800 | -0.80946200 | -0.49758800 |
| H | -2.38831400 | 1.54732300 | -1.37850900 |
| C | 2.19382900 | -0.34812800 | -0.28813300 |
| C | 1.88992800 | -0.21384200 | -1.76253900 |
| H | 2.86714500 | 0.42991800 | 0.07238400 |

| | | | |
|---|-------------|-------------|-------------|
| H | 2.56744400 | -1.33334400 | -0.01013700 |
| H | 2.02801800 | -1.16184200 | -2.28969300 |
| H | 0.77806700 | -0.02339300 | -1.96312200 |
| C | 1.50473300 | -0.13713500 | 2.47191200 |
| C | 0.25901800 | -0.44427900 | 2.87960900 |
| H | 1.83659500 | 0.89105700 | 2.36019300 |
| H | 2.25825700 | -0.90671200 | 2.34388200 |
| H | -0.47329000 | 0.31841300 | 3.12977500 |
| H | -0.01584500 | -1.46990600 | 3.09994900 |

P₁-TS

| | | | |
|----|-------------|-------------|-------------|
| C | -0.65796200 | -2.49583800 | 0.71213200 |
| H | -0.35020700 | -2.97051900 | 1.63459000 |
| C | -1.86377200 | -1.78024600 | 0.50565400 |
| H | -2.64178300 | -1.61639900 | 1.24058900 |
| C | -1.89780700 | -1.37313400 | -0.85591800 |
| C | 0.07336100 | -2.48994800 | -0.49586500 |
| H | 1.02833300 | -2.97273400 | -0.65981500 |
| C | -0.70126800 | -1.80007200 | -1.47292800 |
| H | -0.43774100 | -1.65623900 | -2.51319700 |
| C | -1.89038100 | 1.64224700 | 0.15296600 |
| C | -1.06763700 | 1.88183200 | -0.98209500 |
| H | -1.36003900 | 1.76959700 | -2.01836600 |
| C | 0.17692300 | 2.38024200 | -0.51194300 |
| C | -1.14402700 | 1.95076600 | 1.31224200 |
| H | -1.50104700 | 1.88702400 | 2.33104200 |
| C | 0.14202200 | 2.39945900 | 0.89818400 |
| H | 0.94182100 | 2.72707700 | 1.55042300 |
| H | 1.00866400 | 2.68928200 | -1.13210400 |
| Zr | -0.02979800 | -0.05611200 | 0.23120500 |
| C | 3.06080500 | 0.79479100 | -2.13592500 |
| H | 3.00095100 | 1.82082700 | -1.76345000 |
| H | 2.82949500 | 0.79690100 | -3.20370300 |
| H | 4.09088200 | 0.45429500 | -2.00807300 |
| H | -2.70300100 | -0.83785100 | -1.34142500 |
| H | -2.91570200 | 1.29712600 | 0.13508800 |
| C | 2.41815500 | -0.11314500 | 0.13621900 |
| C | 2.11132700 | -0.13528700 | -1.36828900 |
| H | 2.76502600 | 0.88041600 | 0.42720200 |
| H | 3.20763800 | -0.83522200 | 0.32261700 |
| H | 2.18793700 | -1.15391000 | -1.75350000 |
| H | 1.08717700 | 0.20076500 | -1.67252400 |
| C | 1.75427300 | -0.72204600 | 2.05057800 |
| C | 0.47333200 | -0.33341500 | 2.51489100 |
| H | 2.61636100 | -0.14489600 | 2.36412200 |
| H | 1.95436600 | -1.78072700 | 1.91254200 |
| H | 0.41925500 | 0.60347500 | 3.05717500 |
| H | -0.19525700 | -1.10393300 | 2.88056900 |

P₁-P

| | | | |
|---|-------------|-------------|-------------|
| C | -0.85505100 | -2.43133700 | 0.63758700 |
| H | -0.52973500 | -2.88112400 | 1.56489000 |
| C | -2.06044800 | -1.71037700 | 0.43800300 |
| H | -2.81676800 | -1.51765300 | 1.18839000 |
| C | -2.12833100 | -1.33850500 | -0.93360100 |

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|----|-------------|-------------|-------------|
| C | -0.16110100 | -2.46454500 | -0.59478000 |
| H | 0.78322700 | -2.96084000 | -0.77941700 |
| C | -0.95152500 | -1.79024100 | -1.56973200 |
| H | -0.70675100 | -1.66917000 | -2.61786100 |
| C | -2.05976700 | 1.64843100 | 0.19823500 |
| C | -1.39706900 | 1.86140300 | -1.04329100 |
| H | -1.81984100 | 1.70675100 | -2.02738800 |
| C | -0.10107600 | 2.35925400 | -0.75986000 |
| C | -1.16950200 | 2.01049500 | 1.24274900 |
| H | -1.38048400 | 1.97157200 | 2.30294300 |
| C | 0.04155500 | 2.44007300 | 0.64893900 |
| H | 0.91481000 | 2.79189800 | 1.18237200 |
| H | 0.64235700 | 2.64669200 | -1.49379900 |
| Zr | -0.23080900 | -0.03519500 | 0.09132300 |
| C | 3.28154700 | 0.76077600 | -1.96715500 |
| H | 3.15543900 | 1.82026600 | -1.72502600 |
| H | 3.04416400 | 0.61407000 | -3.02254900 |
| H | 4.33433200 | 0.50754600 | -1.81737800 |
| H | -2.93970200 | -0.80162300 | -1.40684900 |
| H | -3.07935300 | 1.30857400 | 0.32427800 |
| C | 2.73258400 | 0.11170700 | 0.42523500 |
| C | 2.41071200 | -0.11417200 | -1.06575900 |
| H | 2.58295300 | 1.16759300 | 0.68503300 |
| H | 3.81346400 | -0.04629600 | 0.49239900 |
| H | 2.54150100 | -1.17159000 | -1.31756100 |
| H | 1.36721800 | 0.13206600 | -1.39832300 |
| C | 2.06102600 | -0.80784800 | 1.48699100 |
| C | 0.70951300 | -0.32766900 | 2.08261600 |
| H | 2.76430600 | -0.88423500 | 2.32283000 |
| H | 1.98552000 | -1.82758000 | 1.08721100 |
| H | 0.86497500 | 0.60408600 | 2.63166100 |
| H | 0.31859200 | -1.06711000 | 2.78102700 |

P₂-R

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|----|-------------|-------------|-------------|
| C | -0.41935200 | -2.78415100 | 0.69558300 |
| H | 0.27834000 | -3.23658000 | 1.38880100 |
| C | -1.72420700 | -2.29547000 | 1.00618400 |
| H | -2.21441600 | -2.34163300 | 1.96998200 |
| C | -2.30403600 | -1.82249800 | -0.19389200 |
| C | -0.19272700 | -2.58835200 | -0.67729700 |
| H | 0.70349800 | -2.86538000 | -1.21623100 |
| C | -1.35184700 | -1.96797300 | -1.23335200 |
| H | -1.50276000 | -1.71998500 | -2.27638900 |
| C | -2.18761600 | 1.38954700 | -0.35507300 |
| C | -0.96195900 | 1.98804800 | -0.73362100 |
| H | -0.64588700 | 2.19929600 | -1.74747500 |
| C | -0.22906200 | 2.28541700 | 0.44720300 |
| C | -2.22784500 | 1.33087000 | 1.06524300 |
| H | -3.04736300 | 0.95332000 | 1.66384700 |
| C | -1.02720900 | 1.90005600 | 1.55364800 |
| H | -0.77086400 | 2.04244900 | 2.59577500 |
| H | 0.73206100 | 2.77914100 | 0.49686700 |
| Zr | -0.38732300 | -0.24959800 | 0.32615000 |
| C | 2.05931400 | 1.25677500 | -2.17221000 |
| H | 1.83766500 | 2.12993800 | -1.54394700 |
| H | 1.55591800 | 1.41963900 | -3.13356600 |

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|---|-------------|-------------|-------------|
| H | -3.30033300 | -1.41373800 | -0.29670600 |
| H | -2.96922300 | 1.06839000 | -1.03063100 |
| C | 1.85196100 | -0.17297200 | -0.04202100 |
| C | 1.51096800 | -0.00783200 | -1.50331800 |
| H | 2.39276800 | 0.68323600 | 0.36293600 |
| H | 2.37995000 | -1.09895600 | 0.18426100 |
| H | 1.77664300 | -0.89752400 | -2.08361200 |
| H | 0.37916300 | 0.03087700 | -1.68522000 |
| C | 1.15837100 | -0.22582700 | 2.72771800 |
| C | -0.02261400 | -0.74076900 | 3.11784900 |
| H | 1.32866200 | 0.84567200 | 2.67435100 |
| H | 2.01918300 | -0.86311400 | 2.55628000 |
| H | -0.85980600 | -0.11296700 | 3.41004200 |
| H | -0.13793700 | -1.80685500 | 3.27979000 |
| C | 3.56895400 | 1.16986300 | -2.40276100 |
| H | 3.78384500 | 0.30013900 | -3.03574000 |
| H | 4.07398100 | 0.99144400 | -1.44596600 |
| C | 4.12195700 | 2.43419300 | -3.05619800 |
| H | 5.19893200 | 2.35401700 | -3.21935800 |
| H | 3.64946100 | 2.61452400 | -4.02660700 |
| H | 3.94343900 | 3.31230500 | -2.42750400 |

P₂-TS

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|----|-------------|-------------|-------------|
| C | -0.31866200 | -2.51591000 | 0.57417500 |
| H | 0.10674800 | -2.98163800 | 1.45313200 |
| C | -1.63730900 | -2.01058900 | 0.45500300 |
| H | -2.39763300 | -2.02319800 | 1.22560500 |
| C | -1.80160600 | -1.54017400 | -0.87665400 |
| C | 0.34651000 | -2.31453600 | -0.65554700 |
| H | 1.36209100 | -2.61258600 | -0.88277700 |
| C | -0.57864300 | -1.71783700 | -1.56017800 |
| H | -0.38952800 | -1.47169300 | -2.59734200 |
| C | -2.28344400 | 1.34388500 | 0.37015300 |
| C | -1.58976400 | 1.80361400 | -0.78300000 |
| H | -1.92061300 | 1.70603200 | -1.80905800 |
| C | -0.42956800 | 2.49329200 | -0.33918700 |
| C | -1.53470600 | 1.70975600 | 1.51101200 |
| H | -1.80964600 | 1.51488900 | 2.53846400 |
| C | -0.37952600 | 2.41511600 | 1.06866200 |
| H | 0.38708500 | 2.84187600 | 1.70300000 |
| H | 0.29208900 | 2.98982200 | -0.97507100 |
| Zr | -0.14413300 | 0.01804300 | 0.23155000 |
| C | 2.58270800 | 1.56901100 | -2.22289500 |
| H | 2.34998600 | 2.53075800 | -1.74811600 |
| H | 2.17940000 | 1.60967000 | -3.24202300 |
| H | -2.70730300 | -1.12545900 | -1.29874200 |
| H | -3.22727800 | 0.81498200 | 0.37690900 |
| C | 2.27137900 | 0.41268300 | 0.02464600 |
| C | 1.87860700 | 0.43158400 | -1.45791100 |
| H | 2.45739100 | 1.43219300 | 0.37010200 |
| H | 3.18235700 | -0.16910900 | 0.12320600 |
| H | 2.11725100 | -0.52831100 | -1.92308500 |
| H | 0.79224000 | 0.58895400 | -1.68527600 |
| C | 1.83510400 | -0.42320800 | 1.90860900 |
| C | 0.53336400 | -0.30493600 | 2.46034500 |
| H | 2.59759800 | 0.27628500 | 2.23082300 |

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|---|------------|-------------|-------------|
| H | 2.21158100 | -1.41805900 | 1.68825100 |
| H | 0.34724900 | 0.56952100 | 3.07311100 |
| H | 0.03948600 | -1.20659800 | 2.80311100 |
| C | 4.09993100 | 1.38898800 | -2.28666000 |
| H | 4.32741300 | 0.39805900 | -2.70001300 |
| H | 4.51932400 | 1.41212100 | -1.27399900 |
| C | 4.76264000 | 2.46881800 | -3.13943600 |
| H | 5.84570500 | 2.33283500 | -3.17301900 |
| H | 4.38941700 | 2.44164700 | -4.16753500 |
| H | 4.56299100 | 3.46604700 | -2.73521000 |

P₂-P

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|----|-------------|-------------|-------------|
| C | -0.75609100 | -2.76210500 | 0.73692800 |
| H | -0.24503600 | -3.19838500 | 1.58364900 |
| C | -2.08669700 | -2.27198300 | 0.72903300 |
| H | -2.76934700 | -2.27422500 | 1.56946900 |
| C | -2.38337900 | -1.82799700 | -0.58915600 |
| C | -0.21922700 | -2.58185500 | -0.55967500 |
| H | 0.77142800 | -2.87449100 | -0.88433300 |
| C | -1.22841700 | -2.00482100 | -1.38307400 |
| H | -1.13655700 | -1.76914500 | -2.43618100 |
| C | -2.70333900 | 1.08034700 | 0.69129600 |
| C | -2.21739100 | 1.44068600 | -0.59784500 |
| H | -2.70622700 | 1.24241700 | -1.54271900 |
| C | -1.00167000 | 2.14400000 | -0.41910900 |
| C | -1.78509000 | 1.56213900 | 1.66025100 |
| H | -1.87780500 | 1.45880000 | 2.73284400 |
| C | -0.72925200 | 2.20675100 | 0.97220600 |
| H | 0.12297500 | 2.68814900 | 1.43367300 |
| H | -0.39476400 | 2.57200300 | -1.20798800 |
| Zr | -0.63926200 | -0.25991000 | 0.33360500 |
| C | 2.49670800 | 1.29650100 | -1.86502800 |
| H | 2.15517400 | 2.27823600 | -1.50914400 |
| H | 2.09189000 | 1.16862500 | -2.87596000 |
| H | -3.32914400 | -1.42449500 | -0.92559400 |
| H | -3.63323100 | 0.56768900 | 0.89987200 |
| C | 2.29586800 | 0.37608000 | 0.52262600 |
| C | 1.91683000 | 0.20070300 | -0.96025900 |
| H | 2.00071200 | 1.37492500 | 0.86940700 |
| H | 3.38868700 | 0.38154700 | 0.52787500 |
| H | 2.24296400 | -0.78641600 | -1.30896100 |
| H | 0.82111700 | 0.23245600 | -1.20474400 |
| C | 1.84019300 | -0.70799400 | 1.54225400 |
| C | 0.47228700 | -0.48546200 | 2.24319200 |
| H | 2.59779900 | -0.73407300 | 2.33255200 |
| H | 1.89529300 | -1.69675100 | 1.06728600 |
| H | 0.51482300 | 0.43179400 | 2.83558000 |
| H | 0.25180200 | -1.31195900 | 2.91873200 |
| C | 4.02616300 | 1.28722500 | -1.94415400 |
| H | 4.37000100 | 0.27319000 | -2.18524600 |
| H | 4.45859900 | 1.54579600 | -0.97176600 |
| C | 4.53760300 | 2.26982000 | -2.99642100 |
| H | 5.62892000 | 2.26898600 | -3.03555700 |
| H | 4.16541000 | 2.00917600 | -3.99165500 |
| H | 4.21182300 | 3.28997900 | -2.77103900 |

P₃-R

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|----|-------------|-------------|-------------|
| C | 0.12112600 | 2.77905400 | 1.44264200 |
| H | -0.24071400 | 2.71583200 | 2.46103300 |
| C | 1.48534300 | 2.87547200 | 1.03367300 |
| H | 2.34804400 | 2.93731500 | 1.68421400 |
| C | 1.50626600 | 2.97159400 | -0.37729500 |
| C | -0.68411600 | 2.78966300 | 0.29107700 |
| H | -1.76468600 | 2.73838700 | 0.27411300 |
| C | 0.17220800 | 2.88549200 | -0.84719600 |
| H | -0.14641400 | 2.95295100 | -1.87970200 |
| C | 2.30671600 | 0.15319500 | -1.71722700 |
| C | 1.29720300 | -0.83350200 | -1.82214700 |
| H | 0.60351800 | -0.94572600 | -2.64551100 |
| C | 1.36924700 | -1.66790900 | -0.67358200 |
| C | 3.02097600 | -0.07559100 | -0.50912700 |
| H | 3.87302400 | 0.49170600 | -0.15607300 |
| C | 2.45080300 | -1.20899700 | 0.11950900 |
| H | 2.79745200 | -1.66665500 | 1.03739600 |
| H | 0.75504400 | -2.53620400 | -0.47329600 |
| Zr | 0.67993200 | 0.63638600 | 0.15448300 |
| C | -2.03573800 | -1.26036900 | -1.68201100 |
| H | -1.36890400 | -2.09260000 | -1.43518200 |
| H | -1.83318000 | -0.98903400 | -2.72526200 |
| H | 2.39043900 | 3.08410100 | -0.99037300 |
| H | 2.51675300 | 0.92273300 | -2.44805800 |
| C | -1.29632900 | -0.37128400 | 0.64449000 |
| C | -1.69753200 | -0.06516500 | -0.77696000 |
| H | -1.25469000 | -1.43933200 | 0.85276000 |
| H | -1.89681200 | 0.14438100 | 1.39381200 |
| H | -2.48670400 | 0.69342900 | -0.82088300 |
| H | -0.86094100 | 0.48415000 | -1.34339500 |
| C | 0.61649600 | -0.56211400 | 2.74655400 |
| C | 1.62416200 | 0.32585000 | 2.83582800 |
| H | 0.76466400 | -1.56227900 | 2.34934800 |
| H | -0.35921900 | -0.34769300 | 3.16909900 |
| H | 2.63752300 | 0.08464500 | 2.52732600 |
| H | 1.48553900 | 1.27471700 | 3.34225900 |
| C | -3.50895100 | -1.69059800 | -1.59644300 |
| H | -3.68886500 | -2.43433300 | -2.38337200 |
| H | -4.11721500 | -0.81886200 | -1.86799900 |
| C | -4.00635800 | -2.25716500 | -0.25688700 |
| H | -5.08049100 | -2.05638400 | -0.18303800 |
| H | -3.54618000 | -1.71824100 | 0.58057300 |
| C | -3.80679400 | -3.76648400 | -0.07530200 |
| H | -4.38104900 | -4.29264600 | -0.84766800 |
| H | -4.24908900 | -4.05805500 | 0.88353500 |
| C | -2.35701000 | -4.25087600 | -0.12142500 |
| H | -2.29322600 | -5.30993600 | 0.14114000 |
| H | -1.92297700 | -4.13976800 | -1.12019400 |
| H | -1.73078700 | -3.69755200 | 0.59046100 |

P₃-TS

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|---|-------------|-------------|-------------|
| C | -0.29091100 | -0.01532000 | -0.32701200 |
| H | -0.32555200 | 0.12129300 | 0.74560200 |
| C | 0.87265500 | 0.02497900 | -1.13489900 |
| H | 1.88383200 | 0.19904300 | -0.78946200 |

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|----|-------------|-------------|-------------|
| C | 0.46608600 | -0.14182700 | -2.48727000 |
| C | -1.40354100 | -0.25738000 | -1.16281000 |
| H | -2.43500800 | -0.32308000 | -0.84108500 |
| C | -0.93404900 | -0.32457500 | -2.50646600 |
| H | -1.54410100 | -0.46129500 | -3.39029200 |
| C | 2.20605800 | -2.79826200 | -2.52724800 |
| C | 1.17103000 | -3.31942800 | -3.35102200 |
| H | 0.90158300 | -2.96687100 | -4.33840700 |
| C | 0.61464400 | -4.44320900 | -2.68186900 |
| C | 2.25666200 | -3.56629400 | -1.34230700 |
| H | 2.95008000 | -3.42539300 | -0.52451900 |
| C | 1.26379400 | -4.58245500 | -1.43745800 |
| H | 1.05946700 | -5.34376900 | -0.69523900 |
| H | -0.17555800 | -5.07854400 | -3.06192500 |
| Zr | 0.03053800 | -2.35210300 | -1.33303400 |
| C | -3.08216900 | -4.36685200 | -2.82810000 |
| H | -2.43466300 | -5.25031500 | -2.82089700 |
| H | -3.19268500 | -4.06086600 | -3.87427500 |
| H | 1.11302600 | -0.12382200 | -3.35419600 |
| H | 2.85160800 | -1.96379700 | -2.76692400 |
| C | -1.96837700 | -3.59816200 | -0.65284600 |
| C | -2.38093500 | -3.21536000 | -2.07621600 |
| H | -1.65124200 | -4.64189700 | -0.62078500 |
| H | -2.82733400 | -3.46505700 | -0.00157800 |
| H | -3.03842600 | -2.34241900 | -2.05588500 |
| H | -1.54720100 | -2.92247900 | -2.76678000 |
| C | -0.89994000 | -2.94586900 | 1.05717800 |
| C | 0.48185200 | -2.64589400 | 0.96088300 |
| H | -1.19196200 | -3.92400100 | 1.42111400 |
| H | -1.58512100 | -2.14779900 | 1.32870700 |
| H | 1.16848000 | -3.46611700 | 1.13582600 |
| H | 0.82595900 | -1.68572400 | 1.32654700 |
| C | -4.46217300 | -4.71295400 | -2.23586400 |
| H | -5.13664000 | -4.98346200 | -3.05669800 |
| H | -4.88863800 | -3.80144300 | -1.79802400 |
| C | -4.47991600 | -5.85267800 | -1.20098300 |
| H | -5.27327600 | -5.66114800 | -0.47061300 |
| H | -3.53968900 | -5.86539500 | -0.63364100 |
| C | -4.71418700 | -7.23846600 | -1.81237200 |
| H | -5.70377900 | -7.25017800 | -2.28533700 |
| H | -4.75254500 | -7.97584500 | -1.00338700 |
| C | -3.66276500 | -7.66680400 | -2.83513200 |
| H | -3.85221300 | -8.68415500 | -3.18566000 |
| H | -3.66351000 | -7.01571400 | -3.71615100 |
| H | -2.65622400 | -7.65048500 | -2.39920500 |

P₃-P

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|---|-------------|------------|-------------|
| C | 0.62274400 | 3.13164600 | 1.12008700 |
| H | 0.49310100 | 3.23911800 | 2.18790400 |
| C | 1.86055000 | 3.11791400 | 0.42862000 |
| H | 2.84036800 | 3.21793900 | 0.87835400 |
| C | 1.58543600 | 3.00115600 | -0.96166300 |
| C | -0.41034900 | 2.98226800 | 0.16493600 |
| H | -1.47294400 | 2.97512800 | 0.37297300 |
| C | 0.18561000 | 2.90298800 | -1.12642800 |
| H | -0.34061100 | 2.81192300 | -2.06864400 |

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|----|-------------|-------------|-------------|
| C | 3.10656500 | 0.19771800 | -0.84713400 |
| C | 2.14770500 | -0.09316600 | -1.85915400 |
| H | 2.05988400 | 0.40293300 | -2.81687800 |
| C | 1.35684600 | -1.17598700 | -1.40514100 |
| C | 2.90374400 | -0.70741700 | 0.22697400 |
| H | 3.48073700 | -0.75123300 | 1.14065600 |
| C | 1.81486300 | -1.54510800 | -0.11354000 |
| H | 1.42180200 | -2.34775200 | 0.49652300 |
| H | 0.55216900 | -1.64874500 | -1.95552100 |
| Zr | 0.89372400 | 0.82288500 | 0.10056100 |
| C | -2.48429600 | -1.33240400 | -0.91270500 |
| H | -1.77923200 | -2.15452000 | -1.08619800 |
| H | -2.70749200 | -0.89610300 | -1.89188900 |
| H | 2.32013200 | 2.98959400 | -1.75570700 |
| H | 3.88418200 | 0.94809500 | -0.90470800 |
| C | -1.33991800 | -0.77376900 | 1.32077700 |
| C | -1.79336800 | -0.25962100 | -0.05820000 |
| H | -0.69193900 | -1.65171000 | 1.20211800 |
| H | -2.25395000 | -1.15513500 | 1.78528500 |
| H | -2.46226300 | 0.59900300 | 0.07582800 |
| H | -0.98846400 | 0.12297600 | -0.74271800 |
| C | -0.70201100 | 0.23844400 | 2.31581000 |
| C | 0.84426100 | 0.37924400 | 2.27642700 |
| H | -0.96152400 | -0.10279000 | 3.32349300 |
| H | -1.20017500 | 1.21188300 | 2.21166500 |
| H | 1.30090800 | -0.57786600 | 2.54005600 |
| H | 1.17829900 | 1.12264100 | 3.00021900 |
| C | -3.77441500 | -1.87670200 | -0.26536300 |
| H | -4.53416500 | -2.00518000 | -1.04449400 |
| H | -4.17944300 | -1.11151600 | 0.40949300 |
| C | -3.61241800 | -3.21319800 | 0.48362300 |
| H | -4.29428200 | -3.23434900 | 1.34057800 |
| H | -2.59670800 | -3.29271600 | 0.89587300 |
| C | -3.89279700 | -4.44147900 | -0.38854200 |
| H | -4.93845200 | -4.40663400 | -0.71791400 |
| H | -3.79520900 | -5.34052200 | 0.22925000 |
| C | -2.98282900 | -4.56746000 | -1.60981000 |
| H | -3.20067200 | -5.48256900 | -2.16555500 |
| H | -3.11402400 | -3.72848800 | -2.30228000 |
| H | -1.92731300 | -4.60407400 | -1.31443400 |

P₄-R

| | | | |
|---|-------------|-------------|-------------|
| C | 0.40415800 | 3.18978100 | 1.60077500 |
| H | 0.35755600 | 3.18043200 | 2.68241600 |
| C | 1.57104400 | 3.39689000 | 0.82162800 |
| H | 2.56989100 | 3.57791200 | 1.19838700 |
| C | 1.18311400 | 3.39196500 | -0.54511800 |
| C | -0.69458300 | 3.01832300 | 0.72675700 |
| H | -1.72447800 | 2.86329800 | 1.01932400 |
| C | -0.21028100 | 3.15707300 | -0.60502300 |
| H | -0.80806300 | 3.12099200 | -1.50657800 |
| C | 2.98272700 | 0.79967400 | -1.02078500 |
| C | 1.98396100 | 0.08573200 | -1.72851600 |
| H | 1.61262600 | 0.31850300 | -2.71870700 |
| C | 1.62790800 | -1.05409900 | -0.94596200 |
| C | 3.20390100 | 0.14506600 | 0.21310900 |

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|----|-------------|-------------|-------------|
| H | 3.93091100 | 0.43606000 | 0.96001900 |
| C | 2.37056000 | -1.01355900 | 0.24618600 |
| H | 2.31953200 | -1.74527900 | 1.04281500 |
| H | 0.91949800 | -1.82173700 | -1.22621900 |
| Zr | 0.82794800 | 1.03114400 | 0.29892700 |
| C | -1.75751600 | -1.05134600 | -1.67710800 |
| H | -1.19682500 | -1.92856700 | -1.33622500 |
| H | -1.42831000 | -0.84012100 | -2.70143100 |
| H | 1.83098000 | 3.56318600 | -1.39398600 |
| H | 3.48890900 | 1.69287300 | -1.36087000 |
| C | -1.07656400 | -0.15687100 | 0.67175200 |
| C | -1.42847200 | 0.14378200 | -0.76277200 |
| H | -0.90026800 | -1.21856400 | 0.85019000 |
| H | -1.78552100 | 0.24072700 | 1.39539200 |
| H | -2.21390900 | 0.90566600 | -0.82485500 |
| H | -0.56917600 | 0.67704700 | -1.30605000 |
| C | 0.46986900 | 0.22320100 | 3.01778300 |
| C | 1.76501000 | 0.58666000 | 2.96593600 |
| H | 0.17629500 | -0.82040600 | 2.97488700 |
| H | -0.31967100 | 0.94195400 | 3.21476300 |
| H | 2.54959400 | -0.15828300 | 2.89260300 |
| H | 2.08273200 | 1.61278000 | 3.12811100 |
| C | -3.25564500 | -1.37646300 | -1.70373600 |
| H | -3.42516400 | -2.15069900 | -2.46022700 |
| H | -3.79924100 | -0.49099400 | -2.05693100 |
| C | -3.85426500 | -1.82887000 | -0.36924500 |
| H | -4.92629600 | -1.99887300 | -0.52580600 |
| H | -3.78420100 | -1.01128500 | 0.36090300 |
| C | -3.25068600 | -3.09706400 | 0.24964700 |
| H | -3.80806400 | -3.29856700 | 1.17090600 |
| H | -2.21959100 | -2.90860000 | 0.57284700 |
| C | -3.29416900 | -4.35339400 | -0.63711700 |
| H | -4.21594300 | -4.33836100 | -1.23341000 |
| H | -3.37135400 | -5.23476300 | 0.01096000 |
| C | -2.09188200 | -4.57693100 | -1.56724700 |
| H | -2.28157000 | -5.48254500 | -2.15373600 |
| H | -2.00369700 | -3.76523000 | -2.29821800 |
| C | -0.76435700 | -4.74895600 | -0.82730900 |
| H | -0.82390400 | -5.56918500 | -0.10449200 |
| H | 0.04882200 | -4.97545500 | -1.52287500 |
| H | -0.48218500 | -3.84750500 | -0.26853300 |

P4-TS

| | | | |
|---|-------------|-------------|-------------|
| C | -0.50134900 | -0.48503600 | -0.05852100 |
| H | -0.59895600 | -0.47852100 | 1.01891700 |
| C | 0.69338000 | -0.26293800 | -0.78784900 |
| H | 1.66876800 | -0.05423700 | -0.36696700 |
| C | 0.36900600 | -0.30270700 | -2.17150200 |
| C | -1.54805200 | -0.71217300 | -0.97937000 |
| H | -2.58522800 | -0.89464000 | -0.72853000 |
| C | -1.00893200 | -0.58770600 | -2.29270000 |
| H | -1.56226300 | -0.66485000 | -3.22002600 |
| C | 2.29335500 | -2.81718100 | -2.44893600 |
| C | 1.32466100 | -3.31211600 | -3.36502900 |
| H | 1.06028800 | -2.86882800 | -4.31661400 |
| C | 0.83027100 | -4.53907500 | -2.84602400 |

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|----|-------------|-------------|-------------|
| C | 2.36421800 | -3.71023500 | -1.35581800 |
| H | 3.02028500 | -3.61574300 | -0.50137400 |
| C | 1.45023400 | -4.77378100 | -1.60059800 |
| H | 1.27798400 | -5.62682000 | -0.95617000 |
| H | 0.10010700 | -5.18100000 | -3.32299900 |
| Zr | 0.05969800 | -2.65766900 | -1.29673000 |
| C | -2.64546800 | -4.78649700 | -3.18531800 |
| H | -2.08342100 | -5.69083100 | -2.92627000 |
| H | -2.35222100 | -4.51424000 | -4.20608200 |
| H | 1.05416000 | -0.13530100 | -2.99181700 |
| H | 2.88493900 | -1.91951500 | -2.57024200 |
| C | -1.85781300 | -4.12954800 | -0.81842300 |
| C | -2.23778700 | -3.64438900 | -2.22160800 |
| H | -1.45981300 | -5.14391100 | -0.86904200 |
| H | -2.74591000 | -4.12378400 | -0.19559400 |
| H | -3.03595600 | -2.89881600 | -2.15520900 |
| H | -1.43363300 | -3.10786200 | -2.79175600 |
| C | -0.90648000 | -3.57868700 | 0.96636200 |
| C | 0.45411900 | -3.16833100 | 0.95941500 |
| H | -1.13107800 | -4.60539900 | 1.23125300 |
| H | -1.65525700 | -2.86443200 | 1.29733600 |
| H | 1.19343400 | -3.95212300 | 1.07897000 |
| H | 0.70801800 | -2.23606700 | 1.45018300 |
| C | -4.14909400 | -5.08244900 | -3.18504900 |
| H | -4.34470400 | -5.82728400 | -3.96432100 |
| H | -4.68277900 | -4.17655100 | -3.49898600 |
| C | -4.73804500 | -5.56962400 | -1.85872000 |
| H | -5.80892000 | -5.74531100 | -2.01593200 |
| H | -4.68323000 | -4.76315300 | -1.11414900 |
| C | -4.12312700 | -6.84402600 | -1.26456700 |
| H | -4.66183500 | -7.05370900 | -0.33399300 |
| H | -3.08386100 | -6.66378800 | -0.96256700 |
| C | -4.19193600 | -8.09187600 | -2.16172600 |
| H | -5.13417200 | -8.07439400 | -2.72488400 |
| H | -4.24433400 | -8.97815600 | -1.51808900 |
| C | -3.02274600 | -8.30582900 | -3.13499100 |
| H | -3.23109000 | -9.21026900 | -3.71677600 |
| H | -2.96553500 | -7.49261800 | -3.86755000 |
| C | -1.66790200 | -8.47656400 | -2.44579300 |
| H | -1.70246500 | -9.28980700 | -1.71359000 |
| H | -0.88418900 | -8.71325000 | -3.17082800 |
| H | -1.35700300 | -7.57125100 | -1.90860900 |

P₄-P

| | | | |
|---|-------------|------------|-------------|
| C | 0.58858600 | 3.36964200 | 1.42656300 |
| H | 0.41473700 | 3.39657700 | 2.49304400 |
| C | 1.85199900 | 3.44393300 | 0.78640100 |
| H | 2.80994200 | 3.54308800 | 1.28123200 |
| C | 1.63368400 | 3.42154800 | -0.61873200 |
| C | -0.40147000 | 3.25728200 | 0.42266300 |
| H | -1.47045200 | 3.19853700 | 0.58549600 |
| C | 0.24586900 | 3.29132200 | -0.84618000 |
| H | -0.24072900 | 3.25284100 | -1.81297300 |
| C | 3.24160800 | 0.69483600 | -0.68079500 |
| C | 2.31078600 | 0.38809400 | -1.71253500 |
| H | 2.20129100 | 0.91628600 | -2.65084000 |

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|----|-------------|-------------|-------------|
| C | 1.58278300 | -0.75935200 | -1.30913200 |
| C | 3.08283300 | -0.26090600 | 0.35674000 |
| H | 3.65151700 | -0.30521200 | 1.27583100 |
| C | 2.05568300 | -1.15335100 | -0.03167000 |
| H | 1.70864900 | -2.00276200 | 0.54200100 |
| H | 0.81197200 | -1.25896200 | -1.88427200 |
| Zr | 0.98097000 | 1.14951800 | 0.25952000 |
| C | -2.05260600 | -1.07166800 | -1.22747000 |
| H | -1.40243000 | -1.94837200 | -1.11882800 |
| H | -1.85286400 | -0.66013400 | -2.22356800 |
| H | 2.39713500 | 3.49112100 | -1.38202200 |
| H | 3.97242800 | 1.49251400 | -0.69901900 |
| C | -1.19909000 | -0.63304800 | 1.17401100 |
| C | -1.64616800 | -0.02741300 | -0.17212700 |
| H | -0.45663400 | -1.42202100 | 0.99809700 |
| H | -2.07703700 | -1.15842500 | 1.55388900 |
| H | -2.46065600 | 0.68735100 | 0.00246500 |
| H | -0.88420100 | 0.60420700 | -0.70299300 |
| C | -0.70307200 | 0.33276800 | 2.29257100 |
| C | 0.83286000 | 0.54785100 | 2.39083300 |
| H | -1.02388200 | -0.09443700 | 3.24807800 |
| H | -1.24220200 | 1.28700800 | 2.21824200 |
| H | 1.31966900 | -0.40348900 | 2.61821400 |
| H | 1.07227200 | 1.25053600 | 3.18840900 |
| C | -3.52669600 | -1.49816900 | -1.19524400 |
| H | -3.70799200 | -2.11794200 | -2.08029000 |
| H | -4.15135900 | -0.60546600 | -1.32546100 |
| C | -3.99793100 | -2.25798200 | 0.04881200 |
| H | -5.04493800 | -2.54029400 | -0.11401100 |
| H | -4.01660900 | -1.58119300 | 0.91372600 |
| C | -3.20960800 | -3.52429800 | 0.41080600 |
| H | -3.65822000 | -3.92970100 | 1.32417500 |
| H | -2.17652100 | -3.27158600 | 0.68313400 |
| C | -3.20510500 | -4.62713900 | -0.66215600 |
| H | -4.18094300 | -4.63810200 | -1.16488400 |
| H | -3.11612700 | -5.59776300 | -0.15966300 |
| C | -2.09160400 | -4.55881500 | -1.71833300 |
| H | -2.24664100 | -5.38184500 | -2.42439600 |
| H | -2.17030000 | -3.64220600 | -2.31422000 |
| C | -0.68169000 | -4.68021900 | -1.13739100 |
| H | -0.57854500 | -5.60154100 | -0.55511300 |
| H | 0.07149200 | -4.70087400 | -1.93031000 |
| H | -0.43482800 | -3.84668900 | -0.46746500 |

P5-R

| | | | |
|---|-------------|-------------|-------------|
| C | 1.23182500 | 3.36759700 | 1.59417800 |
| H | 1.26571300 | 3.36571000 | 2.67632500 |
| C | 2.35264600 | 3.30010000 | 0.72750800 |
| H | 3.39194900 | 3.24389200 | 1.02596100 |
| C | 1.87174300 | 3.38885500 | -0.60631600 |
| C | 0.06050300 | 3.45837300 | 0.80696700 |
| H | -0.95204200 | 3.54572200 | 1.17766700 |
| C | 0.46137100 | 3.48405600 | -0.55921100 |
| H | -0.19501200 | 3.59052400 | -1.41318200 |
| C | 2.94608600 | 0.44148500 | -1.20831800 |
| C | 1.74860000 | -0.04077000 | -1.79287900 |

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|----|-------------|-------------|-------------|
| H | 1.34169100 | 0.25420900 | -2.75202600 |
| C | 1.22717800 | -1.05912800 | -0.93874500 |
| C | 3.13806700 | -0.22792400 | 0.02314400 |
| H | 3.98170300 | -0.09652300 | 0.68823500 |
| C | 2.07636300 | -1.16932500 | 0.17532600 |
| H | 1.94276500 | -1.86028000 | 0.99866900 |
| H | 0.34292100 | -1.65551900 | -1.12233100 |
| Zr | 1.04271500 | 1.17245900 | 0.29825200 |
| C | -2.09263300 | -0.25131000 | -1.43182900 |
| H | -1.70498200 | -1.22997600 | -1.12974600 |
| H | -1.81425200 | -0.10894700 | -2.48295400 |
| H | 2.47562400 | 3.40758600 | -1.50324300 |
| H | 3.60215400 | 1.19184000 | -1.62793600 |
| C | -1.04823200 | 0.46221800 | 0.84334600 |
| C | -1.43584400 | 0.83768700 | -0.56383700 |
| H | -1.10705900 | -0.61149000 | 1.02560900 |
| H | -1.58405900 | 1.01301800 | 1.61399300 |
| H | -2.03158400 | 1.75755000 | -0.57802500 |
| H | -0.52405100 | 1.16463400 | -1.18060500 |
| C | 0.73951100 | 0.46007300 | 3.05116500 |
| C | 2.07449700 | 0.52852300 | 2.89216100 |
| H | 0.21961000 | -0.49226300 | 3.04274900 |
| H | 0.14717600 | 1.33450300 | 3.30286700 |
| H | 2.66743100 | -0.37023400 | 2.76342500 |
| H | 2.62268900 | 1.45796400 | 3.01695200 |
| C | -3.62243300 | -0.24906700 | -1.32924700 |
| H | -4.01562000 | -0.95922000 | -2.06496800 |
| H | -3.99209500 | 0.73612500 | -1.64105900 |
| C | -4.19509900 | -0.57841500 | 0.05205200 |
| H | -5.28813500 | -0.52924200 | -0.02270900 |
| H | -3.90838400 | 0.20672600 | 0.76476500 |
| C | -3.81303800 | -1.94164900 | 0.64616600 |
| H | -4.34698700 | -2.03315500 | 1.59843000 |
| H | -2.74945100 | -1.95469000 | 0.91161300 |
| C | -4.14509300 | -3.17004700 | -0.21793000 |
| H | -5.10265200 | -2.99981300 | -0.72729900 |
| H | -4.30870900 | -4.02631300 | 0.44756200 |
| C | -3.09096800 | -3.59004900 | -1.25385800 |
| H | -3.48152800 | -4.45387000 | -1.80571900 |
| H | -2.94201000 | -2.80636400 | -2.00648100 |
| C | -1.73622000 | -3.98077000 | -0.66057800 |
| H | -1.87120900 | -4.82097900 | 0.03437600 |
| H | -1.32554900 | -3.15804000 | -0.05262700 |
| C | -0.70845600 | -4.35996900 | -1.72615600 |
| H | -1.11492800 | -5.16527600 | -2.34950300 |
| H | -0.55774600 | -3.50627300 | -2.40413200 |
| C | 0.62810000 | -4.79851700 | -1.13189800 |
| H | 1.06079600 | -4.01016000 | -0.50414400 |
| H | 0.50097400 | -5.68480100 | -0.50286500 |
| H | 1.35649000 | -5.04105500 | -1.90985000 |

P₅-TS

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|---|------------|-------------|-------------|
| C | 0.17773300 | 0.09870800 | -0.46668800 |
| H | 0.10373400 | 0.34629400 | 0.58401000 |
| C | 1.36488900 | -0.25352800 | -1.15604000 |
| H | 2.35655700 | -0.31812400 | -0.72662500 |

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|----|-------------|-------------|-------------|
| C | 1.02992000 | -0.44885000 | -2.52291800 |
| C | -0.89340000 | 0.07460500 | -1.38664200 |
| H | -1.92536300 | 0.31531000 | -1.16510500 |
| C | -0.36279500 | -0.25787300 | -2.66693600 |
| H | -0.92050900 | -0.31960900 | -3.59282700 |
| C | 1.97913400 | -3.48725800 | -2.12299100 |
| C | 0.96638200 | -3.66910000 | -3.10676100 |
| H | 0.97381400 | -3.27268000 | -4.11376600 |
| C | -0.01665300 | -4.52953600 | -2.55851100 |
| C | 1.60461000 | -4.20954700 | -0.96793700 |
| H | 2.18528700 | -4.29192100 | -0.06026900 |
| C | 0.35418700 | -4.83846700 | -1.22871100 |
| H | -0.19020700 | -5.48456000 | -0.55064300 |
| H | -0.89673500 | -4.89294300 | -3.07487300 |
| Zr | -0.07797300 | -2.33072500 | -1.24554900 |
| C | -3.40523600 | -3.73474000 | -2.71458000 |
| H | -2.92592100 | -4.69294900 | -2.48595700 |
| H | -3.31549000 | -3.59002700 | -3.79832300 |
| H | 1.72113900 | -0.69564700 | -3.31773800 |
| H | 2.88925800 | -2.91440000 | -2.24396100 |
| C | -2.38264900 | -2.86065200 | -0.52700500 |
| C | -2.61479200 | -2.60823300 | -2.02031300 |
| H | -2.42476800 | -3.93081200 | -0.32282900 |
| H | -3.16235000 | -2.35463400 | 0.03215200 |
| H | -3.10835700 | -1.64315800 | -2.16628000 |
| H | -1.69606200 | -2.52112000 | -2.66325500 |
| C | -1.20825800 | -2.35789600 | 1.12914100 |
| C | 0.20447900 | -2.50121200 | 1.07824000 |
| H | -1.78617300 | -3.14630600 | 1.59681100 |
| H | -1.61759000 | -1.36335100 | 1.28158700 |
| H | 0.59509000 | -3.46579200 | 1.38071100 |
| H | 0.81557500 | -1.65638500 | 1.37505000 |
| C | -4.89466400 | -3.80185200 | -2.35300400 |
| H | -5.39549700 | -4.38372200 | -3.13432200 |
| H | -5.32486800 | -2.79401800 | -2.41702200 |
| C | -5.24814700 | -4.41381400 | -0.99062000 |
| H | -6.34180700 | -4.47159700 | -0.93414000 |
| H | -4.95044400 | -3.73529100 | -0.18216700 |
| C | -4.68030300 | -5.80947100 | -0.69511500 |
| H | -5.04223600 | -6.09374100 | 0.29902100 |
| H | -3.58650800 | -5.76985000 | -0.60116900 |
| C | -5.07371700 | -6.91621100 | -1.68830200 |
| H | -6.11653400 | -6.76061900 | -1.99393000 |
| H | -5.05705900 | -7.87666300 | -1.15930100 |
| C | -4.19787800 | -7.06784900 | -2.94106400 |
| H | -4.64021000 | -7.84851400 | -3.57180900 |
| H | -4.21691000 | -6.15605400 | -3.55066000 |
| C | -2.74590900 | -7.45732100 | -2.65778700 |
| H | -2.72520000 | -8.41973400 | -2.12848200 |
| H | -2.27194000 | -6.73459100 | -1.97363100 |
| C | -1.89983000 | -7.55629800 | -3.92669400 |
| H | -2.38325600 | -8.24639100 | -4.62852100 |
| H | -1.89026600 | -6.57832300 | -4.43195500 |
| C | -0.47100200 | -8.02069500 | -3.65298500 |
| H | 0.03819200 | -7.34954100 | -2.95165100 |
| H | -0.46828300 | -9.02139800 | -3.21032300 |

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|---|------------|-------------|-------------|
| H | 0.12272500 | -8.05977000 | -4.56989300 |
|---|------------|-------------|-------------|

P₅-P

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|----|-------------|-------------|-------------|
| C | 1.47400800 | 3.59501900 | 1.24432500 |
| H | 1.38318000 | 3.75598400 | 2.30922000 |
| C | 2.67259200 | 3.30023500 | 0.54521800 |
| H | 3.65708300 | 3.20266800 | 0.98515000 |
| C | 2.36218600 | 3.21328200 | -0.84012000 |
| C | 0.42177100 | 3.64480100 | 0.30059800 |
| H | -0.61644500 | 3.86561900 | 0.51490300 |
| C | 0.97233400 | 3.41065700 | -0.99254500 |
| H | 0.42755900 | 3.41089800 | -1.92858600 |
| C | 3.27117700 | 0.18531800 | -0.68319400 |
| C | 2.22868200 | 0.00204500 | -1.63399300 |
| H | 2.18304800 | 0.43947900 | -2.62291500 |
| C | 1.28436900 | -0.89336500 | -1.07092400 |
| C | 2.96493600 | -0.59144900 | 0.46493600 |
| H | 3.56635600 | -0.67165200 | 1.36054800 |
| C | 1.73710500 | -1.25196000 | 0.22378400 |
| H | 1.24033800 | -1.92959500 | 0.90635600 |
| H | 0.38424100 | -1.25832600 | -1.55340900 |
| Zr | 1.24223300 | 1.25535400 | 0.28781600 |
| C | -2.32456300 | -0.23464100 | -0.91268200 |
| H | -1.86447200 | -1.22480000 | -0.80691800 |
| H | -2.13577800 | 0.08409600 | -1.94443500 |
| H | 3.06694000 | 3.02678500 | -1.63940800 |
| H | 4.16302200 | 0.78177400 | -0.82300900 |
| C | -1.25019400 | 0.14512700 | 1.41158100 |
| C | -1.60849400 | 0.74186800 | 0.03578900 |
| H | -0.72506500 | -0.80944900 | 1.27783700 |
| H | -2.20616100 | -0.12649600 | 1.86181900 |
| H | -2.20404900 | 1.65291100 | 0.17702800 |
| H | -0.74272900 | 1.11212700 | -0.57653900 |
| C | -0.48754200 | 1.04643100 | 2.43105700 |
| C | 1.05870100 | 0.89829700 | 2.47093100 |
| H | -0.85554400 | 0.78116500 | 3.42730800 |
| H | -0.78989900 | 2.09305800 | 2.29068200 |
| H | 1.32013600 | -0.11707000 | 2.77772800 |
| H | 1.49212800 | 1.59201200 | 3.19060800 |
| C | -3.84661600 | -0.33601900 | -0.73554500 |
| H | -4.23487000 | -0.90333300 | -1.58818200 |
| H | -4.27820000 | 0.66859700 | -0.82889900 |
| C | -4.35796000 | -0.97940900 | 0.55930200 |
| H | -5.44705200 | -1.07355800 | 0.47167800 |
| H | -4.19975700 | -0.29569500 | 1.40350500 |
| C | -3.78303600 | -2.35819300 | 0.91232000 |
| H | -4.21888800 | -2.64778000 | 1.87479900 |
| H | -2.70215400 | -2.29059200 | 1.09232500 |
| C | -4.07151400 | -3.47720500 | -0.10290600 |
| H | -5.09310300 | -3.35130800 | -0.48422000 |
| H | -4.06706700 | -4.43575900 | 0.42988700 |
| C | -3.10488400 | -3.60820800 | -1.28884700 |
| H | -3.48505900 | -4.39698200 | -1.94953400 |
| H | -3.09985700 | -2.69601500 | -1.89834500 |
| C | -1.66835600 | -3.96868600 | -0.90603500 |
| H | -1.66666500 | -4.91982500 | -0.35639100 |

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|---|-------------|-------------|-------------|
| H | -1.24827700 | -3.22355300 | -0.21019900 |
| C | -0.74750700 | -4.08075800 | -2.12081400 |
| H | -1.17548300 | -4.79893100 | -2.83040800 |
| H | -0.72984100 | -3.11594100 | -2.65016700 |
| C | 0.67273000 | -4.50689700 | -1.75675600 |
| H | 1.13059800 | -3.80488400 | -1.05044700 |
| H | 0.67176500 | -5.49385000 | -1.28432000 |
| H | 1.31664800 | -4.55935500 | -2.63856900 |

P6-R

| | | | |
|----|-------------|-------------|-------------|
| C | 0.97663100 | 2.95196900 | 2.24908300 |
| H | 0.93062200 | 2.53496300 | 3.24732000 |
| C | 2.16046900 | 3.23097900 | 1.50528900 |
| H | 3.17942900 | 3.09972600 | 1.84571800 |
| C | 1.76915200 | 3.79422200 | 0.26774500 |
| C | -0.13241800 | 3.31782100 | 1.46461300 |
| H | -1.17068600 | 3.23321400 | 1.75694500 |
| C | 0.35305800 | 3.82391400 | 0.22237200 |
| H | -0.25132300 | 4.22097300 | -0.58334900 |
| C | 2.25787500 | 1.56377600 | -1.95556500 |
| C | 1.05038500 | 0.88910600 | -2.25102900 |
| H | 0.26442800 | 1.25294600 | -2.90061800 |
| C | 1.07972600 | -0.37763400 | -1.59710400 |
| C | 3.03244000 | 0.73104500 | -1.10589500 |
| H | 4.02193400 | 0.95561700 | -0.72806200 |
| C | 2.30867700 | -0.47494500 | -0.90926100 |
| H | 2.64008600 | -1.33241100 | -0.33635200 |
| H | 0.31994900 | -1.14595300 | -1.65368300 |
| Zr | 0.97758500 | 1.38576200 | 0.22898100 |
| C | -2.23566700 | 0.09353500 | -1.30775100 |
| H | -1.90244100 | -0.93705100 | -1.14215000 |
| H | -1.88994700 | 0.37685000 | -2.30867500 |
| H | 2.43754200 | 4.14714600 | -0.50526000 |
| H | 2.54630800 | 2.53539400 | -2.33229400 |
| C | -0.89520800 | 0.28357600 | 0.90003700 |
| C | -1.59690600 | 0.99576200 | -0.23042900 |
| H | -0.89324900 | -0.80013900 | 0.78069000 |
| H | -1.25340000 | 0.56035600 | 1.89137200 |
| H | -2.31193000 | 1.73565400 | 0.14499200 |
| H | -0.88839900 | 1.69098300 | -0.80676200 |
| C | 1.44326800 | -0.56649100 | 2.27369700 |
| C | 2.58437200 | 0.14778200 | 2.24948500 |
| H | 1.29719800 | -1.43110700 | 1.63145500 |
| H | 0.67240900 | -0.37316000 | 3.01258600 |
| H | 3.41042700 | -0.11729400 | 1.59616200 |
| H | 2.77170800 | 0.92942300 | 2.97781100 |
| C | -3.76825100 | 0.15045500 | -1.29748600 |
| H | -4.14066800 | -0.51949200 | -2.08107800 |
| H | -4.08363900 | 1.15996100 | -1.59037800 |
| C | -4.42824200 | -0.20182300 | 0.03810300 |
| H | -5.51333800 | -0.11072100 | -0.09150500 |
| H | -4.15632500 | 0.54945200 | 0.79266300 |
| C | -4.11871300 | -1.59183700 | 0.60662400 |
| H | -4.68002200 | -1.68450100 | 1.54265000 |
| H | -3.06254200 | -1.64872800 | 0.89729400 |
| C | -4.48442900 | -2.77671900 | -0.30526400 |

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|---|-------------|-------------|-------------|
| H | -5.37880200 | -2.51824700 | -0.88715300 |
| H | -4.77417300 | -3.62512800 | 0.32609100 |
| C | -3.38511300 | -3.27492500 | -1.25552700 |
| H | -3.79062600 | -4.11141400 | -1.83821200 |
| H | -3.11663400 | -2.50581200 | -1.99129700 |
| C | -2.12528100 | -3.75427300 | -0.53318300 |
| H | -2.41070800 | -4.47974200 | 0.24154100 |
| H | -1.65877500 | -2.91478900 | 0.00158100 |
| C | -1.09407400 | -4.39952900 | -1.45990800 |
| H | -1.55470800 | -5.26426100 | -1.95112300 |
| H | -0.82748000 | -3.69844400 | -2.26600400 |
| C | 0.17566500 | -4.84296400 | -0.72510400 |
| H | -0.10838300 | -5.38270100 | 0.18852300 |
| H | 0.73633500 | -5.55552300 | -1.34111100 |
| C | 1.10816800 | -3.68533900 | -0.36129600 |
| H | 1.51259200 | -3.25975700 | -1.28972300 |
| H | 0.52472400 | -2.88465100 | 0.12147500 |
| C | 2.25243000 | -4.11541000 | 0.55552300 |
| H | 1.86826800 | -4.49704100 | 1.50667900 |
| H | 2.84021000 | -4.91336400 | 0.09235000 |
| H | 2.94303600 | -3.29417900 | 0.78236200 |

P₆-TS

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|----|-------------|-------------|-------------|
| C | 0.05207300 | -0.22975900 | 0.10342500 |
| H | 0.14499500 | -0.35348000 | 1.17412200 |
| C | 1.11941500 | -0.03529300 | -0.80844000 |
| H | 2.17133600 | 0.01850500 | -0.55807100 |
| C | 0.55629300 | 0.13782400 | -2.10249400 |
| C | -1.15891300 | -0.22931600 | -0.62378900 |
| H | -2.15072700 | -0.33801900 | -0.20372800 |
| C | -0.84590500 | 0.01051900 | -1.99308000 |
| H | -1.55746600 | 0.10911200 | -2.80300300 |
| C | 2.05582600 | -2.49694400 | -3.04132900 |
| C | 0.87999100 | -2.81230400 | -3.77562300 |
| H | 0.48185600 | -2.25427700 | -4.61364500 |
| C | 0.37214800 | -4.03951800 | -3.26678500 |
| C | 2.24551700 | -3.49673000 | -2.06017000 |
| H | 3.06006600 | -3.54309700 | -1.35006300 |
| C | 1.19851400 | -4.45055000 | -2.20070500 |
| H | 1.06493800 | -5.34570400 | -1.60600700 |
| H | -0.50466400 | -4.56494000 | -3.62741000 |
| Zr | 0.11683500 | -2.26910400 | -1.44841400 |
| C | -3.16900900 | -3.81871500 | -3.01586600 |
| H | -2.81850300 | -4.84788100 | -2.86943700 |
| H | -2.93455100 | -3.55121400 | -4.05259400 |
| H | 1.10263500 | 0.34186700 | -3.01357700 |
| H | 2.70236700 | -1.64584300 | -3.20856700 |
| C | -1.86501100 | -3.58216400 | -0.80398100 |
| C | -2.40465400 | -2.87311600 | -2.05137100 |
| H | -1.62573900 | -4.62127300 | -1.03918900 |
| H | -2.62987300 | -3.55471000 | -0.03436800 |
| H | -3.04798200 | -2.03942600 | -1.75546200 |
| H | -1.64024200 | -2.38968700 | -2.71337600 |
| C | -0.55994200 | -3.38830600 | 0.82936900 |
| C | 0.81885200 | -3.11138300 | 0.62632000 |
| H | -0.85787100 | -4.41622700 | 1.00115900 |

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|---|-------------|-------------|-------------|
| H | -1.15264500 | -2.65976500 | 1.37544100 |
| H | 1.47321400 | -3.96864100 | 0.51709300 |
| H | 1.25643200 | -2.28118300 | 1.16807500 |
| C | -4.68920100 | -3.73800800 | -2.83095400 |
| H | -5.16126600 | -4.38780000 | -3.57535600 |
| H | -5.01314500 | -2.71869700 | -3.07646200 |
| C | -5.20565300 | -4.09484900 | -1.43475100 |
| H | -6.29573900 | -3.97680900 | -1.44110300 |
| H | -4.83846500 | -3.35442500 | -0.70900800 |
| C | -4.87385400 | -5.50206800 | -0.92200700 |
| H | -5.30706500 | -5.58700800 | 0.08077500 |
| H | -3.79114600 | -5.61123500 | -0.78168000 |
| C | -5.40517200 | -6.65960300 | -1.78467300 |
| H | -6.38380500 | -6.37716300 | -2.19427100 |
| H | -5.59124200 | -7.52124800 | -1.13249600 |
| C | -4.49548500 | -7.13772800 | -2.92563600 |
| H | -5.02125800 | -7.93093800 | -3.47124500 |
| H | -4.32638700 | -6.33949500 | -3.65941400 |
| C | -3.14497200 | -7.68515300 | -2.46294600 |
| H | -3.30886300 | -8.49504700 | -1.73814400 |
| H | -2.58941600 | -6.90563900 | -1.92297400 |
| C | -2.29331100 | -8.20673600 | -3.62072800 |
| H | -2.86067400 | -8.97849500 | -4.15440700 |
| H | -2.12784300 | -7.39464500 | -4.34558900 |
| C | -0.94203700 | -8.78087400 | -3.18862200 |
| H | -1.10098500 | -9.55271500 | -2.42344800 |
| H | -0.47316700 | -9.28584500 | -4.04180700 |
| C | 0.03487500 | -7.73288500 | -2.65381800 |
| H | 0.18472600 | -6.96612100 | -3.42719200 |
| H | -0.40756500 | -7.22526100 | -1.78375300 |
| C | 1.38334500 | -8.33470300 | -2.26177700 |
| H | 1.26167000 | -9.08004200 | -1.46997400 |
| H | 1.84732400 | -8.83295100 | -3.11816100 |
| H | 2.08617100 | -7.57581600 | -1.90294800 |

P₆-P

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|----|-------------|-------------|-------------|
| C | 1.22350600 | 3.77461600 | 1.72075400 |
| H | 1.27085300 | 3.71856400 | 2.79890300 |
| C | 2.33333600 | 3.84676700 | 0.83950700 |
| H | 3.37604700 | 3.85968700 | 1.13072200 |
| C | 1.83361500 | 3.96257100 | -0.48758700 |
| C | 0.04611800 | 3.79803600 | 0.93728000 |
| H | -0.96897200 | 3.77634400 | 1.31317300 |
| C | 0.42385900 | 3.91892800 | -0.43112700 |
| H | -0.25053000 | 3.98946500 | -1.27570000 |
| C | 3.30070200 | 1.18567000 | -0.98598900 |
| C | 2.20474100 | 0.97184100 | -1.86702700 |
| H | 1.97059700 | 1.55640300 | -2.74731600 |
| C | 1.50296500 | -0.17385800 | -1.41119900 |
| C | 3.26723100 | 0.17894000 | 0.01455600 |
| H | 3.97014500 | 0.06436600 | 0.82895900 |
| C | 2.15559000 | -0.65625500 | -0.24965700 |
| H | 1.86244100 | -1.52253700 | 0.32928500 |
| H | 0.62656700 | -0.61310200 | -1.87468500 |
| Zr | 1.23659900 | 1.65267500 | 0.32998700 |
| C | -2.26159700 | -0.16424800 | -0.86404200 |

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|---|-------------|-------------|-------------|
| H | -1.90523400 | -1.19905800 | -0.77128200 |
| H | -2.03762100 | 0.14643800 | -1.89047800 |
| H | 2.42945000 | 4.06318600 | -1.38499600 |
| H | 4.05137800 | 1.95921200 | -1.08041000 |
| C | -0.93402300 | -0.06082000 | 1.33928700 |
| C | -1.47508300 | 0.72294100 | 0.12510300 |
| H | -0.31166000 | -0.89779900 | 0.99406600 |
| H | -1.81909000 | -0.53227200 | 1.77231100 |
| H | -2.10083100 | 1.55409400 | 0.47374700 |
| H | -0.70905400 | 1.22030100 | -0.52579700 |
| C | -0.22009200 | 0.71870600 | 2.48691900 |
| C | 1.32487400 | 0.85632600 | 2.39956300 |
| H | -0.43557000 | 0.17414000 | 3.41191600 |
| H | -0.70366200 | 1.69596600 | 2.61589900 |
| H | 1.78578000 | -0.13134400 | 2.47266000 |
| H | 1.69976900 | 1.46580900 | 3.22098600 |
| C | -3.78327000 | -0.09435100 | -0.67445100 |
| H | -4.25619000 | -0.65211600 | -1.48920500 |
| H | -4.09795100 | 0.94884800 | -0.80641300 |
| C | -4.31929800 | -0.60498500 | 0.66611600 |
| H | -5.40722500 | -0.46827900 | 0.66082500 |
| H | -3.95225600 | 0.03685400 | 1.48048700 |
| C | -4.02148300 | -2.07168700 | 1.00794600 |
| H | -4.48540200 | -2.27290800 | 1.97969400 |
| H | -2.94595100 | -2.22240400 | 1.16351400 |
| C | -4.53840400 | -3.10612100 | -0.00659800 |
| H | -5.50405900 | -2.76583100 | -0.40307100 |
| H | -4.74679200 | -4.04019100 | 0.52847400 |
| C | -3.60053800 | -3.44607000 | -1.17454000 |
| H | -4.11094600 | -4.16896600 | -1.82291000 |
| H | -3.41767800 | -2.56605900 | -1.80401200 |
| C | -2.25690200 | -4.04107700 | -0.75163500 |
| H | -2.42952000 | -4.94114000 | -0.14532600 |
| H | -1.72211800 | -3.33729000 | -0.09948700 |
| C | -1.37166000 | -4.39706000 | -1.94659700 |
| H | -1.89454700 | -5.13651700 | -2.56460800 |
| H | -1.24312900 | -3.50636000 | -2.58120000 |
| C | 0.00605200 | -4.93970400 | -1.55893000 |
| H | -0.11348600 | -5.77308700 | -0.85353200 |
| H | 0.49555600 | -5.35696000 | -2.44726500 |
| C | 0.93558300 | -3.88956200 | -0.94779500 |
| H | 1.04623600 | -3.06224400 | -1.66350400 |
| H | 0.47365100 | -3.46769600 | -0.04309200 |
| C | 2.31212800 | -4.45501000 | -0.60200100 |
| H | 2.22809500 | -5.25939800 | 0.13493000 |
| H | 2.79418400 | -4.86962200 | -1.49239600 |
| H | 2.98065400 | -3.69195700 | -0.19055100 |

P7-R

| | | | |
|---|-------------|------------|-------------|
| C | 1.40639800 | 3.25972100 | 2.01186800 |
| H | 1.83432200 | 2.93244900 | 2.95098200 |
| C | 2.13604000 | 3.69580500 | 0.87886700 |
| H | 3.21394100 | 3.75663300 | 0.79659200 |
| C | 1.19821700 | 4.09180100 | -0.11308900 |
| C | 0.02286900 | 3.35219700 | 1.71852000 |
| H | -0.79093100 | 3.11462300 | 2.39053300 |

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|----|-------------|-------------|-------------|
| C | -0.10134000 | 3.88604500 | 0.40686300 |
| H | -1.02873700 | 4.11550900 | -0.10158100 |
| C | 2.45833500 | 1.75732600 | -1.89033600 |
| C | 1.18691600 | 1.33999200 | -2.35642300 |
| H | 0.53709600 | 1.89625300 | -3.02062200 |
| C | 0.95909500 | 0.01515300 | -1.87361400 |
| C | 2.99023900 | 0.72917700 | -1.07818000 |
| H | 3.96041700 | 0.73867000 | -0.59837300 |
| C | 2.06206300 | -0.35553800 | -1.08690000 |
| H | 2.17904800 | -1.30288800 | -0.57818200 |
| H | 0.09092100 | -0.59865700 | -2.07742500 |
| Zr | 0.94040900 | 1.58740800 | 0.13744300 |
| C | -2.40365700 | 0.23040400 | -1.25057900 |
| H | -2.04268600 | -0.80275200 | -1.17199900 |
| H | -2.20791100 | 0.55854100 | -2.27825100 |
| H | 1.43131500 | 4.50656200 | -1.08454200 |
| H | 2.93724400 | 2.70239700 | -2.10891000 |
| C | -0.85935500 | 0.38597300 | 0.83626500 |
| C | -1.63074100 | 1.10744800 | -0.24015500 |
| H | -0.76432300 | -0.68530800 | 0.64256300 |
| H | -1.23419000 | 0.56107600 | 1.84328700 |
| H | -2.28627800 | 1.86885800 | 0.19583800 |
| H | -0.95074800 | 1.76347200 | -0.88909800 |
| C | 1.39760300 | 0.04485300 | 2.50944300 |
| C | 2.62433500 | 0.23621800 | 1.98886400 |
| H | 0.88216400 | -0.90293500 | 2.39492700 |
| H | 0.92157500 | 0.78183400 | 3.14948600 |
| H | 3.12718500 | -0.56292000 | 1.45278700 |
| H | 3.20756300 | 1.13006000 | 2.19609200 |
| C | -3.91812200 | 0.27944500 | -1.00751800 |
| H | -4.40910200 | -0.36770800 | -1.74293100 |
| H | -4.26992400 | 1.29696700 | -1.22049600 |
| C | -4.36605300 | -0.10786200 | 0.40459500 |
| H | -5.45533600 | 0.00890500 | 0.45417000 |
| H | -3.95803500 | 0.61105600 | 1.12886000 |
| C | -4.00675400 | -1.52395400 | 0.86851300 |
| H | -4.39235400 | -1.63316900 | 1.88804900 |
| H | -2.91796000 | -1.62451200 | 0.95741600 |
| C | -4.57522500 | -2.66023700 | 0.00075800 |
| H | -5.54667000 | -2.34878200 | -0.40516700 |
| H | -4.78334500 | -3.52281400 | 0.64501600 |
| C | -3.67854500 | -3.15382100 | -1.14315500 |
| H | -4.21609100 | -3.94308000 | -1.68366200 |
| H | -3.49997900 | -2.35951900 | -1.87964900 |
| C | -2.33707200 | -3.71641900 | -0.67298200 |
| H | -2.51111700 | -4.43981500 | 0.13601300 |
| H | -1.72545400 | -2.91585300 | -0.23074400 |
| C | -1.54295000 | -4.40187200 | -1.78571100 |
| H | -2.09757700 | -5.28501100 | -2.12217400 |
| H | -1.47220900 | -3.73398000 | -2.65749000 |
| C | -0.13433200 | -4.80312800 | -1.33717100 |
| H | -0.19267300 | -5.23528700 | -0.32876500 |
| H | 0.26337100 | -5.59181800 | -1.98544500 |
| C | 0.84998000 | -3.62864000 | -1.34518700 |
| H | 1.10627900 | -3.39282000 | -2.38569700 |
| H | 0.34797200 | -2.73392900 | -0.94052900 |

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|---|------------|-------------|-------------|
| C | 2.11946200 | -3.89168000 | -0.52623000 |
| H | 2.43710600 | -4.93308200 | -0.66687700 |
| H | 2.95298200 | -3.27937200 | -0.89682300 |
| C | 1.92263400 | -3.61815600 | 0.96610700 |
| H | 1.57379500 | -2.57867600 | 1.08701000 |
| H | 1.11031400 | -4.24504400 | 1.35355400 |
| C | 3.18803200 | -3.83647800 | 1.79144700 |
| H | 3.52037600 | -4.87642400 | 1.72471300 |
| H | 4.00969800 | -3.20933300 | 1.42607700 |
| H | 3.02841800 | -3.60514600 | 2.84832500 |

P₇-TS

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|----|-------------|-------------|-------------|
| C | 0.09150500 | -0.17035600 | 0.00813300 |
| H | 0.29378900 | -0.33136000 | 1.05861300 |
| C | 1.05484800 | 0.11504500 | -0.99137000 |
| H | 2.12235500 | 0.21285700 | -0.83986200 |
| C | 0.36140200 | 0.30912100 | -2.21732600 |
| C | -1.18302000 | -0.20356900 | -0.60015200 |
| H | -2.12319200 | -0.38025100 | -0.09334400 |
| C | -1.01604400 | 0.10580600 | -1.98098600 |
| H | -1.80655900 | 0.19883200 | -2.71479000 |
| C | 1.90140600 | -2.20803500 | -3.39623500 |
| C | 0.67838600 | -2.53892000 | -4.04162000 |
| H | 0.18654100 | -1.95993500 | -4.81296700 |
| C | 0.26547400 | -3.80907200 | -3.55381700 |
| C | 2.21555800 | -3.24381300 | -2.48719200 |
| H | 3.09119800 | -3.28876800 | -1.85393900 |
| C | 1.19685300 | -4.23338400 | -2.58349900 |
| H | 1.14980100 | -5.15988000 | -2.02443300 |
| H | -0.61918800 | -4.35318200 | -3.86375100 |
| Zr | 0.10354300 | -2.14050000 | -1.63160100 |
| C | -3.23283200 | -3.80358600 | -2.95255500 |
| H | -2.81016400 | -4.81406900 | -2.88991100 |
| H | -3.11965900 | -3.47912200 | -3.99336800 |
| H | 0.80678900 | 0.57598800 | -3.16636600 |
| H | 2.49704900 | -1.32281400 | -3.57528600 |
| C | -1.74158900 | -3.57728700 | -0.86220200 |
| C | -2.43107700 | -2.85298100 | -2.02423700 |
| H | -1.47441600 | -4.59286000 | -1.16116300 |
| H | -2.43075700 | -3.61846800 | -0.02474700 |
| H | -3.08534200 | -2.06677800 | -1.63639400 |
| H | -1.75722900 | -2.30481100 | -2.73275100 |
| C | -0.29906700 | -3.37816700 | 0.64956500 |
| C | 1.04016000 | -3.02862300 | 0.32880200 |
| H | -0.53369400 | -4.42462300 | 0.80688500 |
| H | -0.86857100 | -2.69883000 | 1.27759900 |
| H | 1.71703100 | -3.84949100 | 0.12100500 |
| H | 1.49188900 | -2.19994100 | 0.86135200 |
| C | -4.72906100 | -3.82589700 | -2.61726600 |
| H | -5.23356200 | -4.47545700 | -3.34036000 |
| H | -5.13526100 | -2.82045600 | -2.78565600 |
| C | -5.08291000 | -4.26594700 | -1.19442800 |
| H | -6.17329500 | -4.21596300 | -1.09038900 |
| H | -4.68974100 | -3.53098900 | -0.47687600 |
| C | -4.62093100 | -5.66777500 | -0.77624500 |
| H | -4.94531600 | -5.81497100 | 0.25990700 |

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|---|-------------|--------------|-------------|
| H | -3.52522100 | -5.71643000 | -0.74849600 |
| C | -5.16924600 | -6.82360700 | -1.63026200 |
| H | -6.19782300 | -6.58611100 | -1.93178100 |
| H | -5.24135500 | -7.71733200 | -0.99904800 |
| C | -4.35107600 | -7.20639900 | -2.87189600 |
| H | -4.88130800 | -8.01301000 | -3.39300700 |
| H | -4.30372200 | -6.37609800 | -3.58792900 |
| C | -2.93093200 | -7.68359400 | -2.56608200 |
| H | -2.97124900 | -8.51227500 | -1.84475100 |
| H | -2.36218700 | -6.88239700 | -2.07308400 |
| C | -2.18208100 | -8.13870700 | -3.81890600 |
| H | -2.76852700 | -8.92121300 | -4.31518900 |
| H | -2.12434500 | -7.30154500 | -4.53158600 |
| C | -0.77185600 | -8.66412700 | -3.54149400 |
| H | -0.83371400 | -9.49538000 | -2.82835800 |
| H | -0.35294700 | -9.07987600 | -4.46680600 |
| C | 0.18762100 | -7.59436100 | -3.01407100 |
| H | 0.11003400 | -6.71227300 | -3.66706400 |
| H | -0.12833300 | -7.27578100 | -2.00824100 |
| C | 1.64901000 | -8.04762000 | -2.95751900 |
| H | 1.98213700 | -8.31449000 | -3.96956800 |
| H | 2.28417300 | -7.20653900 | -2.64360600 |
| C | 1.89924000 | -9.22741200 | -2.01718800 |
| H | 1.48483000 | -8.99458800 | -1.02644300 |
| H | 1.35775200 | -10.10885000 | -2.37853700 |
| C | 3.38378100 | -9.56311900 | -1.89186200 |
| H | 3.80978300 | -9.81417400 | -2.86843500 |
| H | 3.94685000 | -8.71279900 | -1.49274100 |
| H | 3.54739800 | -10.41502600 | -1.22726300 |

P₇-P

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|----|-------------|-------------|-------------|
| C | 0.93010600 | 4.14524200 | 1.72839000 |
| H | 1.04374200 | 4.06821100 | 2.80034300 |
| C | 1.98161100 | 4.28522400 | 0.78622400 |
| H | 3.03818000 | 4.33787600 | 1.01673500 |
| C | 1.39984000 | 4.40513500 | -0.50647900 |
| C | -0.29162700 | 4.13198100 | 1.01566000 |
| H | -1.28076100 | 4.05687800 | 1.44944800 |
| C | -0.00113400 | 4.29721700 | -0.36926700 |
| H | -0.72656400 | 4.35442200 | -1.17146900 |
| C | 2.93878800 | 1.69886400 | -1.16896100 |
| C | 1.79579400 | 1.47075100 | -1.98481000 |
| H | 1.48574200 | 2.07068300 | -2.83057100 |
| C | 1.16406600 | 0.28913800 | -1.51992700 |
| C | 3.00436900 | 0.66389300 | -0.19949400 |
| H | 3.76235300 | 0.55141700 | 0.56415200 |
| C | 1.90558800 | -0.20145400 | -0.41607300 |
| H | 1.67945100 | -1.09318400 | 0.15446100 |
| H | 0.27465200 | -0.16694000 | -1.94029800 |
| Zr | 0.95101300 | 2.05505700 | 0.29009100 |
| C | -2.54556200 | 0.09188600 | -0.66548500 |
| H | -2.12459300 | -0.92216100 | -0.63657600 |
| H | -2.42920100 | 0.44315300 | -1.69669000 |
| H | 1.93685600 | 4.55026400 | -1.43439400 |
| H | 3.65562100 | 2.50061900 | -1.28811100 |
| C | -1.05903800 | 0.22040200 | 1.43361600 |

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|---|-------------|-------------|-------------|
| C | -1.72722300 | 0.99705000 | 0.28008800 |
| H | -0.42943300 | -0.58230800 | 1.02606200 |
| H | -1.88505000 | -0.29697800 | 1.92621100 |
| H | -2.36166100 | 1.79222600 | 0.69133500 |
| H | -1.03516300 | 1.54058800 | -0.41555100 |
| C | -0.29230800 | 1.01603600 | 2.53453800 |
| C | 1.23351300 | 1.22434500 | 2.32869300 |
| H | -0.40944500 | 0.45049600 | 3.46467700 |
| H | -0.80728800 | 1.96853100 | 2.71738400 |
| H | 1.73995900 | 0.25653100 | 2.34387300 |
| H | 1.64594700 | 1.83433400 | 3.13170200 |
| C | -4.04707400 | 0.06689900 | -0.34673200 |
| H | -4.55435200 | -0.49888600 | -1.13493600 |
| H | -4.43101100 | 1.09233100 | -0.42271500 |
| C | -4.43897600 | -0.50560900 | 1.01862300 |
| H | -5.52991900 | -0.43670100 | 1.10488700 |
| H | -4.04607900 | 0.14016300 | 1.81751500 |
| C | -4.02686300 | -1.95814700 | 1.29546200 |
| H | -4.39049000 | -2.20665100 | 2.29850800 |
| H | -2.93481200 | -2.04762700 | 1.35218200 |
| C | -4.57118400 | -3.00070700 | 0.30396300 |
| H | -5.58566300 | -2.71010200 | 0.00088400 |
| H | -4.67835300 | -3.95578300 | 0.83179000 |
| C | -3.72170200 | -3.26247100 | -0.94846000 |
| H | -4.24398800 | -4.00434600 | -1.56517300 |
| H | -3.64793700 | -2.36247800 | -1.57216900 |
| C | -2.31261300 | -3.78112900 | -0.65886900 |
| H | -2.37460000 | -4.69188400 | -0.04660000 |
| H | -1.75825800 | -3.04956700 | -0.05523700 |
| C | -1.52666400 | -4.07917100 | -1.93568000 |
| H | -2.07347800 | -4.82701600 | -2.52240900 |
| H | -1.48957500 | -3.17067700 | -2.55678500 |
| C | -0.10013600 | -4.57312100 | -1.68558200 |
| H | -0.13514200 | -5.47587400 | -1.06338500 |
| H | 0.35002500 | -4.87251900 | -2.64087600 |
| C | 0.80454000 | -3.52435500 | -1.03170000 |
| H | 0.66951700 | -2.57359200 | -1.57001100 |
| H | 0.48352200 | -3.35014400 | 0.00663100 |
| C | 2.28890700 | -3.89933900 | -1.03909500 |
| H | 2.62622700 | -4.01480500 | -2.07819600 |
| H | 2.88071300 | -3.07329200 | -0.61889300 |
| C | 2.60994500 | -5.17607700 | -0.26075600 |
| H | 2.19360800 | -5.09568300 | 0.75273400 |
| H | 2.11180300 | -6.03063800 | -0.73241500 |
| C | 4.11122200 | -5.44528200 | -0.18424600 |
| H | 4.54084600 | -5.54393300 | -1.18627300 |
| H | 4.63196800 | -4.62534500 | 0.32161500 |
| H | 4.32575300 | -6.36640900 | 0.36317600 |

Ps-R

| | | | |
|---|-------------|------------|-------------|
| C | 1.30756500 | 3.86723600 | 1.59743000 |
| H | 1.89449500 | 3.65698100 | 2.48255900 |
| C | 1.82519400 | 4.22297000 | 0.32734500 |
| H | 2.87134600 | 4.33138500 | 0.06999700 |
| C | 0.72263100 | 4.46971900 | -0.53486700 |
| C | -0.10675000 | 3.85747200 | 1.51963500 |

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|----|-------------|-------------|-------------|
| H | -0.79023000 | 3.64604800 | 2.33116200 |
| C | -0.46561200 | 4.24839300 | 0.19986200 |
| H | -1.47308200 | 4.37664100 | -0.17416600 |
| C | 1.80754900 | 2.02101500 | -2.28701100 |
| C | 0.49843700 | 1.51321200 | -2.47938800 |
| H | -0.28663600 | 1.97654400 | -3.06393400 |
| C | 0.43064700 | 0.23414300 | -1.84800000 |
| C | 2.52690000 | 1.09759700 | -1.49422000 |
| H | 3.56377900 | 1.19111100 | -1.19852600 |
| C | 1.67134000 | -0.01693100 | -1.23829300 |
| H | 1.92794900 | -0.90685300 | -0.67607100 |
| H | -0.42608200 | -0.42749200 | -1.83817200 |
| Zr | 0.67088400 | 1.99185800 | -0.01793600 |
| C | -2.80521800 | 0.33812000 | -0.58447400 |
| H | -2.30681400 | -0.63838400 | -0.63141500 |
| H | -2.97037900 | 0.66293800 | -1.61847000 |
| H | 0.77694100 | 4.79534400 | -1.56498700 |
| H | 2.19027400 | 2.95708700 | -2.67124700 |
| C | -0.87478800 | 0.76092700 | 1.10774700 |
| C | -1.89110600 | 1.33802100 | 0.15481100 |
| H | -0.73740300 | -0.31503100 | 0.97697600 |
| H | -1.06432100 | 0.99679000 | 2.15327600 |
| H | -2.49018100 | 2.11233600 | 0.64718600 |
| H | -1.39465100 | 1.94419400 | -0.68089700 |
| C | 1.64546700 | 0.71428100 | 2.33359700 |
| C | 2.75239800 | 0.94933200 | 1.60355200 |
| H | 1.19640900 | -0.27254900 | 2.36675800 |
| H | 1.22459900 | 1.46345800 | 2.99763200 |
| H | 3.22393800 | 0.14791000 | 1.04388900 |
| H | 3.28848600 | 1.89379200 | 1.65226100 |
| C | -4.16771000 | 0.20140000 | 0.10752800 |
| H | -4.79114000 | -0.48184200 | -0.47913400 |
| H | -4.67315600 | 1.17482100 | 0.06837400 |
| C | -4.11586800 | -0.26692200 | 1.56445800 |
| H | -5.14245200 | -0.27543500 | 1.95027800 |
| H | -3.57747000 | 0.47714300 | 2.16769000 |
| C | -3.49487300 | -1.64698300 | 1.81561100 |
| H | -3.53556400 | -1.82283400 | 2.89632700 |
| H | -2.42717900 | -1.63534500 | 1.56338400 |
| C | -4.19008800 | -2.81808500 | 1.10079600 |
| H | -5.26949400 | -2.62085100 | 1.06156100 |
| H | -4.07322900 | -3.72045100 | 1.71302600 |
| C | -3.68474000 | -3.15597700 | -0.30887500 |
| H | -4.29735300 | -3.97680300 | -0.70246800 |
| H | -3.83820900 | -2.31626200 | -0.99844600 |
| C | -2.21762400 | -3.58319700 | -0.36262000 |
| H | -2.04598400 | -4.38685800 | 0.36805700 |
| H | -1.56968700 | -2.75059500 | -0.05064000 |
| C | -1.79601200 | -4.07087400 | -1.75006600 |
| H | -2.41554500 | -4.93449000 | -2.01863500 |
| H | -2.01738100 | -3.29212300 | -2.49567200 |
| C | -0.31572500 | -4.45328500 | -1.83698000 |
| H | -0.07265200 | -5.10730700 | -0.98946600 |
| H | -0.13512800 | -5.04414700 | -2.74315100 |
| C | 0.61397800 | -3.23870200 | -1.85509800 |
| H | 0.39683400 | -2.65472500 | -2.76045600 |

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|---|------------|-------------|-------------|
| H | 0.37434200 | -2.58739400 | -1.00541600 |
| C | 2.10702600 | -3.58748000 | -1.85316300 |
| H | 2.30249500 | -4.22691300 | -2.72322900 |
| H | 2.69740300 | -2.67509400 | -2.01961600 |
| C | 2.64300300 | -4.29870000 | -0.60497600 |
| H | 2.04109200 | -5.19076300 | -0.39150700 |
| H | 3.64641200 | -4.66948200 | -0.84223000 |
| C | 2.75251100 | -3.46182300 | 0.67618100 |
| H | 3.34762400 | -4.04024700 | 1.39420400 |
| H | 3.34524700 | -2.55493300 | 0.47429600 |
| C | 1.43683300 | -3.07898500 | 1.37408000 |
| H | 1.00372400 | -2.17300000 | 0.92351000 |
| H | 0.69058200 | -3.86871200 | 1.21663700 |
| C | 1.63360300 | -2.85596600 | 2.87396200 |
| H | 1.92500700 | -3.78870000 | 3.36519300 |
| H | 2.43284800 | -2.12958800 | 3.06534600 |
| H | 0.71916400 | -2.49884500 | 3.35927100 |

P8-TS

| | | | |
|----|-------------|-------------|-------------|
| C | 0.92010800 | -0.35586300 | -0.59213500 |
| H | 1.39313400 | -0.53592500 | 0.36400300 |
| C | 1.58250100 | -0.01590200 | -1.79773400 |
| H | 2.64995000 | 0.11178400 | -1.92566900 |
| C | 0.58921800 | 0.18502700 | -2.79525000 |
| C | -0.46808700 | -0.41483200 | -0.84971700 |
| H | -1.23963700 | -0.63497200 | -0.12285800 |
| C | -0.67364200 | -0.06664200 | -2.21564800 |
| H | -1.62973200 | 0.01786500 | -2.71639500 |
| C | 1.83479100 | -2.24496500 | -4.40893000 |
| C | 0.50594600 | -2.64169700 | -4.72064300 |
| H | -0.19805400 | -2.08995000 | -5.33070700 |
| C | 0.30110700 | -3.93490700 | -4.16290400 |
| C | 2.42700400 | -3.26128900 | -3.62501800 |
| H | 3.43588400 | -3.25835800 | -3.23453900 |
| C | 1.47290300 | -4.30686700 | -3.47392000 |
| H | 1.62250100 | -5.23014600 | -2.92852000 |
| H | -0.60200000 | -4.52895400 | -4.24226200 |
| Zr | 0.55364200 | -2.28579000 | -2.23665600 |
| C | -2.97258200 | -4.02170600 | -2.72869200 |
| H | -2.51565400 | -5.01651700 | -2.80553100 |
| H | -3.14743100 | -3.67588600 | -3.75390200 |
| H | 0.76506400 | 0.48854300 | -3.81853000 |
| H | 2.31535400 | -1.32744500 | -4.72133500 |
| C | -1.01544200 | -3.77702400 | -1.07516800 |
| C | -1.98642800 | -3.05743600 | -2.01843800 |
| H | -0.80792700 | -4.78162900 | -1.45068600 |
| H | -1.47692000 | -3.84949200 | -0.09563800 |
| H | -2.54157600 | -2.29163300 | -1.46858200 |
| H | -1.52049800 | -2.48681800 | -2.86320600 |
| C | 0.74501600 | -3.57046700 | 0.04349600 |
| C | 1.95984100 | -3.20482600 | -0.59487200 |
| H | 0.56483000 | -4.62166000 | 0.23688100 |
| H | 0.34248500 | -2.90415300 | 0.80162900 |
| H | 2.56379300 | -4.01920900 | -0.98239500 |
| H | 2.52934900 | -2.38161200 | -0.17893600 |
| C | -4.32638200 | -4.10485900 | -2.01252900 |

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|---|-------------|-------------|-------------|
| H | -4.98205400 | -4.76383500 | -2.59130700 |
| H | -4.79511800 | -3.11321300 | -2.04702700 |
| C | -4.28072900 | -4.57296300 | -0.55533800 |
| H | -5.30708000 | -4.56289500 | -0.16941300 |
| H | -3.73840500 | -3.83113500 | 0.04862100 |
| C | -3.68332100 | -5.96244300 | -0.29709500 |
| H | -3.71253100 | -6.12563400 | 0.78610400 |
| H | -2.61938200 | -5.98058000 | -0.56640800 |
| C | -4.41230900 | -7.12749400 | -0.98757100 |
| H | -5.48994500 | -6.91794200 | -0.99531300 |
| H | -4.28678400 | -8.02825700 | -0.37492700 |
| C | -3.95136400 | -7.47392500 | -2.41010100 |
| H | -4.58320900 | -8.28919200 | -2.78403400 |
| H | -4.11775600 | -6.63459700 | -3.09703800 |
| C | -2.49089900 | -7.91498000 | -2.50704000 |
| H | -2.31043600 | -8.73690300 | -1.79950500 |
| H | -1.82514700 | -7.09785500 | -2.19182900 |
| C | -2.10610800 | -8.37209400 | -3.91517800 |
| H | -2.71969100 | -9.24100900 | -4.17998000 |
| H | -2.36288100 | -7.58420300 | -4.63947300 |
| C | -0.62258300 | -8.72491000 | -4.05251100 |
| H | -0.33616500 | -9.36992100 | -3.21177500 |
| H | -0.46101800 | -9.31572700 | -4.96216500 |
| C | 0.28283200 | -7.49265500 | -4.10855000 |
| H | 0.02796500 | -6.92135400 | -5.01227800 |
| H | 0.05562700 | -6.83592400 | -3.25836500 |
| C | 1.78088300 | -7.81916100 | -4.15228000 |
| H | 1.95442700 | -8.46032700 | -5.02577200 |
| H | 2.35275200 | -6.90076900 | -4.34397100 |
| C | 2.37193400 | -8.52020000 | -2.92264600 |
| H | 1.79812400 | -9.42649100 | -2.69222700 |
| H | 3.37431600 | -8.86806300 | -3.19603300 |
| C | 2.50900100 | -7.68625700 | -1.64157100 |
| H | 3.15013900 | -8.25024100 | -0.95230700 |
| H | 3.06371900 | -6.75958100 | -1.85891500 |
| C | 1.21158800 | -7.35272600 | -0.88845000 |
| H | 0.71260800 | -6.48223800 | -1.33963900 |
| H | 0.50177800 | -8.18418600 | -0.99030500 |
| C | 1.46577900 | -7.07522800 | 0.59329100 |
| H | 1.87733100 | -7.96099000 | 1.08556100 |
| H | 2.19295800 | -6.26458000 | 0.72572400 |
| H | 0.54585300 | -6.80450100 | 1.12258900 |

P8-P

| | | | |
|---|-------------|------------|-------------|
| C | 1.23154800 | 4.25621200 | 1.34172200 |
| H | 1.65085300 | 4.17438200 | 2.33437200 |
| C | 1.96264600 | 4.44433000 | 0.14031200 |
| H | 3.03837700 | 4.53579200 | 0.05886300 |
| C | 1.03027600 | 4.55160900 | -0.92863600 |
| C | -0.14205200 | 4.20100800 | 1.00933300 |
| H | -0.96151900 | 4.08321600 | 1.70710900 |
| C | -0.26762400 | 4.38812100 | -0.39752100 |
| H | -1.19437400 | 4.42353700 | -0.95688900 |
| C | 2.40123400 | 1.90438600 | -2.05809400 |
| C | 1.07956900 | 1.63877300 | -2.51306400 |
| H | 0.51944900 | 2.23089600 | -3.22516100 |

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|----|-------------|-------------|-------------|
| C | 0.64798400 | 0.43309800 | -1.90309300 |
| C | 2.77791500 | 0.86801000 | -1.16363900 |
| H | 3.72636500 | 0.77923600 | -0.65061900 |
| C | 1.69174800 | -0.03377900 | -1.06600800 |
| H | 1.66731600 | -0.93070600 | -0.45964200 |
| H | -0.30723700 | -0.05683900 | -2.05668300 |
| Zr | 0.91123600 | 2.17953000 | -0.07986600 |
| C | -2.62575200 | 0.09933700 | -0.06339700 |
| H | -2.16202400 | -0.88386600 | -0.22490900 |
| H | -2.84152000 | 0.50437100 | -1.05827300 |
| H | 1.27272100 | 4.72465200 | -1.96871600 |
| H | 3.02597300 | 2.73205900 | -2.36718700 |
| C | -0.60360800 | 0.25111800 | 1.53173900 |
| C | -1.61345200 | 1.01779600 | 0.65264300 |
| H | -0.07853700 | -0.50133500 | 0.92907300 |
| H | -1.22117800 | -0.33232000 | 2.21871500 |
| H | -2.14001300 | 1.76228400 | 1.26309200 |
| H | -1.17929500 | 1.62540100 | -0.18437300 |
| C | 0.41079000 | 1.06386800 | 2.39583900 |
| C | 1.80525300 | 1.34657100 | 1.77224800 |
| H | 0.58457300 | 0.47488500 | 3.30278800 |
| H | -0.06756900 | 1.98877200 | 2.74509000 |
| H | 2.33522400 | 0.40409800 | 1.61399700 |
| H | 2.40410000 | 1.96571000 | 2.43926300 |
| C | -3.95865900 | -0.04418500 | 0.68395500 |
| H | -4.65788800 | -0.58470600 | 0.03788100 |
| H | -4.38886900 | 0.95688600 | 0.81573100 |
| C | -3.89061000 | -0.73945300 | 2.04649100 |
| H | -4.90471700 | -0.75579600 | 2.46328900 |
| H | -3.30163800 | -0.12963800 | 2.74633300 |
| C | -3.35115600 | -2.17642000 | 2.04098000 |
| H | -3.35811700 | -2.52630300 | 3.07914700 |
| H | -2.29580700 | -2.19526300 | 1.73497700 |
| C | -4.15682400 | -3.16845400 | 1.18235600 |
| H | -5.22091300 | -2.90422000 | 1.24016900 |
| H | -4.07125700 | -4.16487000 | 1.63185000 |
| C | -3.74264300 | -3.29731700 | -0.29139900 |
| H | -4.42391500 | -4.00778500 | -0.77604300 |
| H | -3.87493600 | -2.34897900 | -0.82753700 |
| C | -2.30878700 | -3.78545600 | -0.48880600 |
| H | -2.16091100 | -4.71774800 | 0.07472800 |
| H | -1.60407400 | -3.06270500 | -0.05561900 |
| C | -1.94212100 | -4.02729900 | -1.95396400 |
| H | -2.57235600 | -4.83262600 | -2.34836300 |
| H | -2.18059200 | -3.13179300 | -2.54797100 |
| C | -0.46192500 | -4.38167800 | -2.13346000 |
| H | -0.18164000 | -5.09983300 | -1.35233300 |
| H | -0.30465600 | -4.89308600 | -3.09024700 |
| C | 0.45662000 | -3.15714800 | -2.08064600 |
| H | 0.29926000 | -2.56880300 | -2.99541300 |
| H | 0.14748700 | -2.50617500 | -1.25230700 |
| C | 1.95014000 | -3.49532300 | -1.97660700 |
| H | 2.20922600 | -4.10968400 | -2.84833200 |
| H | 2.53952900 | -2.57340800 | -2.07973500 |
| C | 2.42297000 | -4.24001500 | -0.71816600 |
| H | 1.82812600 | -5.14918800 | -0.56691400 |

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|---|------------|-------------|-------------|
| H | 3.44294100 | -4.58710200 | -0.91675300 |
| C | 2.45270600 | -3.44139900 | 0.59283100 |
| H | 3.09537900 | -3.97619800 | 1.30381900 |
| H | 2.95309300 | -2.47408000 | 0.42335100 |
| C | 1.10197100 | -3.21524300 | 1.27898300 |
| H | 0.44912300 | -2.59499000 | 0.65404100 |
| H | 0.58287600 | -4.17750700 | 1.37749000 |
| C | 1.24582900 | -2.56203600 | 2.65214400 |
| H | 1.82838200 | -3.19335100 | 3.32960200 |
| H | 1.76921000 | -1.60051100 | 2.57532600 |
| H | 0.27080700 | -2.38334600 | 3.11824400 |

P9-R

| | | | |
|----|-------------|-------------|-------------|
| C | 0.73832500 | 3.60926100 | 2.17592300 |
| H | 1.11706500 | 3.29157300 | 3.13917600 |
| C | 1.52584800 | 3.96131600 | 1.04991400 |
| H | 2.60750800 | 3.96361400 | 1.00002100 |
| C | 0.64178200 | 4.37023500 | 0.01586000 |
| C | -0.62573800 | 3.76168100 | 1.83450100 |
| H | -1.47035200 | 3.58895900 | 2.48811600 |
| C | -0.68256700 | 4.24554600 | 0.49652500 |
| H | -1.58107400 | 4.50133000 | -0.05009000 |
| C | 1.73377500 | 1.89308000 | -1.71213400 |
| C | 0.41251100 | 1.61433000 | -2.14553500 |
| H | -0.18841700 | 2.23218800 | -2.80113900 |
| C | 0.05503900 | 0.32565800 | -1.64661100 |
| C | 2.16954200 | 0.81824900 | -0.90522800 |
| H | 3.14987400 | 0.71894300 | -0.45570400 |
| C | 1.12386900 | -0.15479800 | -0.87092600 |
| H | 1.15205600 | -1.10356300 | -0.34774600 |
| H | -0.88207100 | -0.18691800 | -1.82334800 |
| Zr | 0.24001100 | 1.89417800 | 0.34593300 |
| C | -3.29575400 | 0.62233200 | -0.73745100 |
| H | -2.91805700 | -0.40839600 | -0.75274100 |
| H | -3.27919600 | 0.98341500 | -1.77240000 |
| H | 0.92730700 | 4.73184400 | -0.96284300 |
| H | 2.30929000 | 2.77740900 | -1.95162400 |
| C | -1.54584200 | 0.76478900 | 1.18469400 |
| C | -2.37600100 | 1.48821800 | 0.15175500 |
| H | -1.49675000 | -0.31088100 | 1.00182700 |
| H | -1.84988400 | 0.96229800 | 2.21123300 |
| H | -2.94854400 | 2.30055600 | 0.61332800 |
| H | -1.72389500 | 2.07079400 | -0.58584400 |
| C | 0.80194300 | 0.36264300 | 2.69397700 |
| C | 2.01619000 | 0.61763900 | 2.17146400 |
| H | 0.32048300 | -0.59881600 | 2.54780100 |
| H | 0.30736700 | 1.05674500 | 3.36668000 |
| H | 2.54347100 | -0.14054800 | 1.60223700 |
| H | 2.56737700 | 1.52482800 | 2.40481300 |
| C | -4.74710500 | 0.64858400 | -0.23794100 |
| H | -5.35966500 | 0.03724800 | -0.90922600 |
| H | -5.12531100 | 1.67402200 | -0.33840200 |
| C | -4.94962300 | 0.19315700 | 1.21002800 |
| H | -6.01172500 | 0.31521200 | 1.45476200 |
| H | -4.41032500 | 0.87362300 | 1.88371300 |
| C | -4.54092800 | -1.24791000 | 1.53851100 |

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|---|-------------|-------------|-------------|
| H | -4.71908800 | -1.39300700 | 2.60983500 |
| H | -3.45990200 | -1.37498500 | 1.40316400 |
| C | -5.29961400 | -2.33815200 | 0.76279200 |
| H | -6.33221300 | -2.00397200 | 0.59659800 |
| H | -5.37226700 | -3.23083000 | 1.39565300 |
| C | -4.68607600 | -2.77642200 | -0.57373700 |
| H | -5.34649000 | -3.52962400 | -1.02188600 |
| H | -4.65731800 | -1.94441300 | -1.28924400 |
| C | -3.28292900 | -3.37265700 | -0.45468400 |
| H | -3.27150400 | -4.13344800 | 0.33832700 |
| H | -2.57312700 | -2.59583400 | -0.13673400 |
| C | -2.80070600 | -4.00342400 | -1.76305000 |
| H | -3.40648900 | -4.89405200 | -1.96549400 |
| H | -2.99143500 | -3.30924800 | -2.59493600 |
| C | -1.31422500 | -4.37384600 | -1.75328100 |
| H | -1.08152500 | -4.90675300 | -0.82189500 |
| H | -1.09869700 | -5.07010100 | -2.57278600 |
| C | -0.40591500 | -3.15227400 | -1.90505600 |
| H | -0.65695400 | -2.65003100 | -2.84951200 |
| H | -0.63103800 | -2.43395300 | -1.10029900 |
| C | 1.09229100 | -3.46257400 | -1.88039200 |
| H | 1.32203400 | -4.21508500 | -2.64598300 |
| H | 1.64412500 | -2.56042800 | -2.17289900 |
| C | 1.59292100 | -3.96205200 | -0.52074700 |
| H | 1.14563000 | -3.35188500 | 0.28309600 |
| H | 1.23059100 | -4.98173400 | -0.35215800 |
| C | 3.11792500 | -3.93268700 | -0.37434800 |
| H | 3.41105000 | -4.51354600 | 0.50830100 |
| H | 3.57786500 | -4.42995600 | -1.23864400 |
| C | 3.68868600 | -2.52006400 | -0.23966700 |
| H | 3.44339900 | -1.92420200 | -1.12975500 |
| H | 3.19455800 | -2.02749200 | 0.61516400 |
| C | 5.19863700 | -2.47690400 | -0.02075000 |
| H | 5.45570100 | -3.04943800 | 0.88032500 |
| H | 5.70204700 | -2.97707700 | -0.85843000 |
| C | 5.73623900 | -1.05246800 | 0.11174800 |
| H | 5.49220900 | -0.49154500 | -0.80125100 |
| H | 5.21612700 | -0.54855600 | 0.94101200 |
| C | 7.24329200 | -1.00533500 | 0.35395900 |
| H | 7.50638900 | -1.53636300 | 1.27386600 |
| H | 7.78235000 | -1.48169100 | -0.47046400 |
| H | 7.60690400 | 0.02168000 | 0.44262700 |

P₉-TS

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|---|-------------|-------------|-------------|
| C | 0.88492500 | -0.72843500 | -0.02823100 |
| H | 1.23773200 | -1.00320600 | 0.95686300 |
| C | 1.69668900 | -0.38512400 | -1.13819800 |
| H | 2.77865000 | -0.34956800 | -1.15107100 |
| C | 0.83430900 | -0.04090500 | -2.21465800 |
| C | -0.46801000 | -0.64700000 | -0.42571100 |
| H | -1.32675700 | -0.83415300 | 0.20638400 |
| C | -0.49942800 | -0.20964600 | -1.78152300 |
| H | -1.38738900 | -0.01192100 | -2.36844600 |
| C | 2.04739500 | -2.50070900 | -3.83665700 |
| C | 0.72278500 | -2.67883300 | -4.32421600 |
| H | 0.17594100 | -1.98778900 | -4.95308500 |

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|----|-------------|-------------|-------------|
| C | 0.28266700 | -3.96591100 | -3.91117100 |
| C | 2.40388100 | -3.64974600 | -3.09493500 |
| H | 3.35440700 | -3.82859900 | -2.60832200 |
| C | 1.30311500 | -4.55126700 | -3.13311000 |
| H | 1.26513100 | -5.52435800 | -2.65919700 |
| H | -0.67567500 | -4.41698900 | -4.14133500 |
| Zr | 0.53014900 | -2.52334900 | -1.82559300 |
| C | -3.08084400 | -3.91023600 | -2.71062700 |
| H | -2.73299900 | -4.94772200 | -2.79473600 |
| H | -3.11221800 | -3.50610800 | -3.72883200 |
| H | 1.14255200 | 0.29857800 | -3.19450700 |
| H | 2.67974200 | -1.64056800 | -4.01287800 |
| C | -1.24468700 | -3.96208200 | -0.90251000 |
| C | -2.07116600 | -3.09423800 | -1.85909800 |
| H | -1.08852900 | -4.95185900 | -1.33686400 |
| H | -1.79206000 | -4.06176000 | 0.02950400 |
| H | -2.59867600 | -2.31920900 | -1.29571800 |
| H | -1.49140100 | -2.51485800 | -2.62325000 |
| C | 0.43075300 | -3.97708600 | 0.36002700 |
| C | 1.71839200 | -3.64179300 | -0.13830500 |
| H | 0.17176100 | -5.02616700 | 0.44779500 |
| H | 0.00418700 | -3.34977300 | 1.13772900 |
| H | 2.31167100 | -4.45907700 | -0.53363600 |
| H | 2.29000800 | -2.88946500 | 0.39263000 |
| C | -4.50029700 | -3.86256100 | -2.13129100 |
| H | -5.16507500 | -4.41995400 | -2.79955200 |
| H | -4.84958100 | -2.82268900 | -2.16182100 |
| C | -4.64784600 | -4.38692800 | -0.70050000 |
| H | -5.69628500 | -4.26277600 | -0.40433000 |
| H | -4.07584400 | -3.74353000 | -0.01596600 |
| C | -4.24892700 | -5.84885900 | -0.46243700 |
| H | -4.38707800 | -6.04765900 | 0.60619600 |
| H | -3.17673200 | -5.98886700 | -0.64944100 |
| C | -5.05483900 | -6.88647200 | -1.26277900 |
| H | -6.09081500 | -6.53584000 | -1.35825500 |
| H | -5.10511700 | -7.81334200 | -0.67909100 |
| C | -4.50994400 | -7.24974000 | -2.65094100 |
| H | -5.19983600 | -7.96829800 | -3.11103100 |
| H | -4.50602100 | -6.37736000 | -3.31695200 |
| C | -3.11134400 | -7.86633400 | -2.63389600 |
| H | -3.08576500 | -8.69916500 | -1.91754100 |
| H | -2.37974400 | -7.13253200 | -2.26552700 |
| C | -2.67086200 | -8.37399700 | -4.00849400 |
| H | -3.29458400 | -9.23258600 | -4.28179500 |
| H | -2.86705300 | -7.60024600 | -4.76576700 |
| C | -1.18963200 | -8.76187700 | -4.05800900 |
| H | -0.94236400 | -9.33956700 | -3.15784600 |
| H | -1.00101100 | -9.42283300 | -4.91210300 |
| C | -0.26736300 | -7.54619000 | -4.17683700 |
| H | -0.46640700 | -7.05329800 | -5.13796000 |
| H | -0.53006300 | -6.81470000 | -3.39394100 |
| C | 1.22467800 | -7.87105300 | -4.06767700 |
| H | 1.47947600 | -8.65915100 | -4.78827900 |
| H | 1.80368000 | -6.99047800 | -4.37147800 |
| C | 1.65136200 | -8.31843400 | -2.66479200 |
| H | 1.18574300 | -7.65978400 | -1.91058700 |

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|---|------------|-------------|-------------|
| H | 1.25385600 | -9.31925600 | -2.46543900 |
| C | 3.16807900 | -8.32426200 | -2.44751000 |
| H | 3.39945700 | -8.86255600 | -1.52053100 |
| H | 3.65073800 | -8.88536000 | -3.25873400 |
| C | 3.78093800 | -6.92533800 | -2.36474200 |
| H | 3.60814000 | -6.37892600 | -3.30224800 |
| H | 3.26126400 | -6.36036600 | -1.57215000 |
| C | 5.27746100 | -6.92297400 | -2.06376500 |
| H | 5.46251800 | -7.45383300 | -1.12036700 |
| H | 5.80670400 | -7.48614600 | -2.84371800 |
| C | 5.86130900 | -5.51342100 | -1.97513400 |
| H | 5.68679000 | -4.99261200 | -2.92699200 |
| H | 5.31864900 | -4.94906900 | -1.20165400 |
| C | 7.35468100 | -5.50824700 | -1.65596200 |
| H | 7.54948300 | -5.99962200 | -0.69775800 |
| H | 7.91696000 | -6.04581000 | -2.42552900 |
| H | 7.75232700 | -4.49161500 | -1.59949100 |

P₉-P

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|----|-------------|-------------|-------------|
| C | 0.88865000 | 3.95227900 | 1.85463100 |
| H | 1.26173200 | 3.70901700 | 2.83923800 |
| C | 1.67787100 | 4.23827500 | 0.71053300 |
| H | 2.75979600 | 4.25419300 | 0.67286300 |
| C | 0.79836600 | 4.55849700 | -0.36098500 |
| C | -0.47135200 | 4.05085800 | 1.47834600 |
| H | -1.32393300 | 3.90894900 | 2.13034600 |
| C | -0.52759800 | 4.43068400 | 0.10646600 |
| H | -1.42671600 | 4.61198100 | -0.46954600 |
| C | 2.04760200 | 1.98042000 | -1.76656900 |
| C | 0.73842700 | 1.86813800 | -2.31267300 |
| H | 0.25930700 | 2.58048800 | -2.97182200 |
| C | 0.19677200 | 0.62967400 | -1.88036000 |
| C | 2.30661200 | 0.81867900 | -0.99263000 |
| H | 3.21775400 | 0.59420500 | -0.45168300 |
| C | 1.15942500 | -0.00754100 | -1.05978900 |
| H | 1.04700300 | -0.96674900 | -0.57106000 |
| H | -0.77802300 | 0.23075500 | -2.13891200 |
| Zr | 0.47263700 | 2.11186000 | 0.15800400 |
| C | -3.24649800 | 0.35000200 | -0.22446400 |
| H | -2.90911200 | -0.67948000 | -0.40466600 |
| H | -3.33429800 | 0.82039500 | -1.20987400 |
| H | 1.09335700 | 4.84600200 | -1.36141700 |
| H | 2.74033400 | 2.79356300 | -1.93941100 |
| C | -1.29856400 | 0.12924200 | 1.44287600 |
| C | -2.17321200 | 1.08682000 | 0.60664500 |
| H | -0.81868400 | -0.60856700 | 0.78491400 |
| H | -2.01692800 | -0.44690100 | 2.03053300 |
| H | -2.64438000 | 1.82565300 | 1.26687900 |
| H | -1.63635900 | 1.70779100 | -0.15729900 |
| C | -0.26377800 | 0.72974800 | 2.44376000 |
| C | 1.18060800 | 0.96507900 | 1.92263000 |
| H | -0.18724400 | 0.01834300 | 3.27252800 |
| H | -0.68196700 | 1.64107500 | 2.89160900 |
| H | 1.64018700 | 0.00671500 | 1.66808500 |
| H | 1.78975600 | 1.43815200 | 2.69223500 |
| C | -4.63577600 | 0.36079800 | 0.42815100 |

| | | | |
|---|-------------|-------------|-------------|
| H | -5.34920400 | -0.08270900 | -0.27419400 |
| H | -4.94881700 | 1.40567400 | 0.55070100 |
| C | -4.74816900 | -0.34872200 | 1.78045500 |
| H | -5.77767300 | -0.22167100 | 2.13588100 |
| H | -4.12103800 | 0.16656400 | 2.52291500 |
| C | -4.41815000 | -1.84768900 | 1.79505600 |
| H | -4.56900700 | -2.19705100 | 2.82226000 |
| H | -3.35407900 | -2.01364300 | 1.58539900 |
| C | -5.26316300 | -2.71816700 | 0.84904500 |
| H | -6.28450800 | -2.31720700 | 0.80866300 |
| H | -5.35151900 | -3.71923200 | 1.28738100 |
| C | -4.72522600 | -2.89065700 | -0.57906800 |
| H | -5.42750700 | -3.52584400 | -1.13344200 |
| H | -4.70830200 | -1.93350200 | -1.11580600 |
| C | -3.33662400 | -3.52552100 | -0.65439800 |
| H | -3.32765200 | -4.45867300 | -0.07436500 |
| H | -2.59227500 | -2.87188100 | -0.17675500 |
| C | -2.89319000 | -3.82366600 | -2.08814100 |
| H | -3.51670600 | -4.62961100 | -2.49110400 |
| H | -3.08206400 | -2.94457000 | -2.72268600 |
| C | -1.41144500 | -4.20264000 | -2.17916500 |
| H | -1.16702000 | -4.87730000 | -1.34844700 |
| H | -1.21753100 | -4.76462300 | -3.09991400 |
| C | -0.48631900 | -2.98173300 | -2.15861600 |
| H | -0.61900700 | -2.43278200 | -3.10042700 |
| H | -0.80470000 | -2.29570000 | -1.35430900 |
| C | 0.99391100 | -3.32216900 | -1.96145500 |
| H | 1.28055800 | -4.11828800 | -2.66118700 |
| H | 1.60317900 | -2.45217900 | -2.23438500 |
| C | 1.32802100 | -3.76587400 | -0.53262200 |
| H | 0.85793300 | -3.07265200 | 0.18692300 |
| H | 0.87177200 | -4.74255200 | -0.33857600 |
| C | 2.82926200 | -3.84079700 | -0.23624800 |
| H | 2.98457600 | -4.36528000 | 0.71421200 |
| H | 3.32404200 | -4.44627700 | -1.00724500 |
| C | 3.50635800 | -2.47188500 | -0.15434100 |
| H | 3.40912900 | -1.94386000 | -1.11314400 |
| H | 2.97810100 | -1.86021800 | 0.59659700 |
| C | 4.98466300 | -2.53697800 | 0.22114300 |
| H | 5.09568900 | -3.05306100 | 1.18417900 |
| H | 5.52188300 | -3.14516700 | -0.51859100 |
| C | 5.63522000 | -1.15691700 | 0.30832600 |
| H | 5.53165500 | -0.64984100 | -0.66128700 |
| H | 5.08740600 | -0.54893800 | 1.04370500 |
| C | 7.11080400 | -1.22005000 | 0.69662800 |
| H | 7.23608200 | -1.70000100 | 1.67210000 |
| H | 7.67957900 | -1.80152200 | -0.03535000 |
| H | 7.55696300 | -0.22371000 | 0.75255000 |

T(P₅)-R

| | | | |
|---|------------|------------|-------------|
| C | 1.55064446 | 1.54237543 | -0.63953922 |
| H | 1.46660942 | 1.58708866 | 0.43728784 |
| C | 2.75595511 | 1.39245940 | -1.37546968 |
| H | 3.74884208 | 1.28757344 | -0.95466883 |
| C | 2.43784686 | 1.43881222 | -2.75821119 |
| C | 0.48669203 | 1.67378644 | -1.56999358 |

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|----|-------------|-------------|-------------|
| H | -0.55685646 | 1.83055564 | -1.32499454 |
| C | 1.03355021 | 1.60401921 | -2.88078567 |
| H | 0.48145217 | 1.69793670 | -3.80749255 |
| C | 2.88944609 | -1.87392946 | -3.41575068 |
| C | 1.70931604 | -1.57602702 | -4.15463801 |
| H | 1.64309653 | -0.90833862 | -5.00389446 |
| C | 0.64219198 | -2.31829189 | -3.59224897 |
| C | 2.54834196 | -2.82471963 | -2.41376273 |
| H | 3.22805530 | -3.26504531 | -1.69497214 |
| C | 1.16419916 | -3.08756954 | -2.51325829 |
| H | 0.60191043 | -3.76967438 | -1.88865126 |
| H | -0.38288294 | -2.32781118 | -3.94224171 |
| Zr | 1.38253061 | -0.65539136 | -1.85192495 |
| C | -2.42757883 | -0.17453967 | 3.00473414 |
| H | -1.92289694 | 0.79367402 | 3.12517764 |
| H | -3.39078376 | 0.03347207 | 2.51797830 |
| H | 3.14435311 | 1.37261611 | -3.57543542 |
| H | 3.88185286 | -1.49293027 | -3.62058112 |
| C | -1.32969129 | -0.43806060 | 0.72921367 |
| C | -1.58159440 | -1.06888514 | 2.09920074 |
| H | -0.82502070 | 0.52890304 | 0.85785462 |
| H | -2.29015121 | -0.23588615 | 0.24018639 |
| H | -2.08663393 | -2.03470954 | 1.96360701 |
| H | -0.62270206 | -1.28463114 | 2.58842093 |
| C | -0.47279380 | -1.34142193 | -0.16253880 |
| C | 0.99250730 | -1.43336631 | 0.20333109 |
| H | -0.63369856 | -0.91307304 | -1.23220283 |
| H | -0.93244792 | -2.32780060 | -0.27931258 |
| H | 1.33925304 | -2.45023894 | 0.38084240 |
| H | 1.25968617 | -0.78276149 | 1.03535679 |
| C | -2.67444354 | -0.80240877 | 4.37638014 |
| H | -3.10623957 | -1.80187871 | 4.23629495 |
| H | -1.70755035 | -0.94996749 | 4.87730244 |
| C | -3.58989454 | 0.01334558 | 5.29510567 |
| H | -3.70907947 | -0.54610614 | 6.22860747 |
| H | -4.59141043 | 0.07515300 | 4.84774640 |
| C | -3.08048433 | 1.43292124 | 5.60026605 |
| H | -3.30366308 | 1.68866699 | 6.64251075 |
| H | -1.98343373 | 1.45478859 | 5.51710436 |
| C | -3.68266754 | 2.52176331 | 4.70878870 |
| H | -3.54655633 | 2.26751090 | 3.64863804 |
| H | -4.76853488 | 2.55303287 | 4.87306581 |
| C | -3.09288943 | 3.90576645 | 4.97260742 |
| H | -2.00935218 | 3.87566519 | 4.79582495 |
| H | -3.22236438 | 4.15579969 | 6.03304948 |
| C | -3.72736014 | 4.99208995 | 4.10684725 |
| H | -3.29017861 | 5.97376401 | 4.30737849 |
| H | -3.58989648 | 4.77417800 | 3.04203702 |
| H | -4.80365635 | 5.06072565 | 4.29391058 |

T(P₅)-TS

| | | | |
|---|------------|-------------|-------------|
| C | 0.15862500 | 0.00851300 | -0.11144800 |
| H | 0.15817900 | 0.03510000 | 0.97023600 |
| C | 1.31165300 | -0.08770500 | -0.93997400 |
| H | 2.33671700 | -0.17190400 | -0.59953000 |
| C | 0.88773500 | -0.01591400 | -2.28803000 |

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|----|-------------|-------------|-------------|
| C | -0.97780700 | 0.14648300 | -0.95073100 |
| H | -2.00026200 | 0.28348900 | -0.62645800 |
| C | -0.52718800 | 0.11295800 | -2.29793200 |
| H | -1.15230800 | 0.21059300 | -3.17582900 |
| C | 1.02592200 | -3.17820500 | -3.36572500 |
| C | -0.33474800 | -2.92910400 | -3.70433500 |
| H | -0.68351600 | -2.23572400 | -4.45819500 |
| C | -1.15014600 | -3.78685500 | -2.92125700 |
| C | 1.04737000 | -4.18728100 | -2.37226500 |
| H | 1.93482300 | -4.60990700 | -1.91585000 |
| C | -0.29219700 | -4.55404600 | -2.08669200 |
| H | -0.60524000 | -5.32005800 | -1.38850700 |
| H | -2.22657200 | -3.86883000 | -2.97621200 |
| Zr | -0.05911500 | -2.15261000 | -1.35645500 |
| C | -3.91114400 | -1.70768000 | 3.50901300 |
| H | -3.37549300 | -0.76899800 | 3.70352000 |
| H | -4.77099900 | -1.45375200 | 2.87369900 |
| H | 1.52960100 | -0.04450700 | -3.15863000 |
| H | 1.89177300 | -2.71159700 | -3.81647600 |
| C | -2.47582800 | -2.04898900 | 1.43933400 |
| C | -2.98636700 | -2.66389000 | 2.75582100 |
| H | -1.90517600 | -1.13918500 | 1.66016900 |
| H | -3.33009700 | -1.76934100 | 0.81487200 |
| H | -3.52125500 | -3.59778600 | 2.54024500 |
| H | -2.13027500 | -2.92900000 | 3.38874000 |
| C | -1.60902200 | -3.04530700 | 0.72536800 |
| C | -0.24584200 | -3.13002200 | 0.90935300 |
| H | -1.84027100 | -2.25648800 | -0.99061500 |
| H | -2.12606700 | -3.90389600 | 0.29596500 |
| H | 0.27462100 | -4.06558400 | 0.71330600 |
| H | 0.24794900 | -2.41219500 | 1.56148400 |
| C | -4.40624700 | -2.30435900 | 4.82641400 |
| H | -4.86935700 | -3.27853900 | 4.62305000 |
| H | -3.54048700 | -2.50103400 | 5.47367300 |
| C | -5.40460600 | -1.42463200 | 5.58622200 |
| H | -5.70316800 | -1.96581900 | 6.48977900 |
| H | -6.31716600 | -1.30865700 | 4.98567100 |
| C | -4.86454100 | -0.03468000 | 5.96581200 |
| H | -5.23369300 | 0.24517400 | 6.95912900 |
| H | -3.76890100 | -0.07890500 | 6.05781900 |
| C | -5.25151500 | 1.07843700 | 4.98892400 |
| H | -4.96642000 | 0.80517500 | 3.96349000 |
| H | -6.34571700 | 1.17681000 | 4.98001600 |
| C | -4.62677500 | 2.42720300 | 5.34036400 |
| H | -3.53287100 | 2.32989500 | 5.33663600 |
| H | -4.90583400 | 2.69619500 | 6.36677600 |
| C | -5.04960600 | 3.54016900 | 4.38401000 |
| H | -4.59003300 | 4.49570700 | 4.64977300 |
| H | -4.75983700 | 3.30292900 | 3.35441900 |
| H | -6.13567900 | 3.67562400 | 4.39900300 |

T(P₅)-P

| | | | |
|---|------------|------------|-------------|
| C | 1.42356900 | 1.70409900 | -0.98531800 |
| H | 1.06263500 | 1.88914500 | 0.01821300 |
| C | 2.75977900 | 1.39079700 | -1.34876200 |
| H | 3.59759500 | 1.28282300 | -0.67023100 |

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|----|-------------|-------------|-------------|
| C | 2.81153800 | 1.25423000 | -2.75574700 |
| C | 0.64689500 | 1.78542400 | -2.17168800 |
| H | -0.39906300 | 2.04915700 | -2.23188300 |
| C | 1.50286700 | 1.49040600 | -3.26528800 |
| H | 1.22039300 | 1.49158500 | -4.30973600 |
| C | 2.35268500 | -1.82277400 | -3.92062600 |
| C | 0.96083100 | -1.68459300 | -4.17621300 |
| H | 0.51480600 | -1.11040200 | -4.97759000 |
| C | 0.25520700 | -2.47905700 | -3.23412300 |
| C | 2.50942200 | -2.67734500 | -2.80555000 |
| H | 3.45225600 | -2.99219800 | -2.37455600 |
| C | 1.21255700 | -3.07622600 | -2.37393400 |
| H | 0.99902900 | -3.76785600 | -1.56817400 |
| H | -0.81547300 | -2.61901600 | -3.19801000 |
| Zr | 1.34934700 | -0.61218600 | -1.95713400 |
| C | -2.37908900 | -0.20448700 | 3.12176100 |
| H | -1.82702200 | 0.68137100 | 3.46231600 |
| H | -3.12289700 | 0.14813400 | 2.39366300 |
| H | 3.69617200 | 1.04327400 | -3.34159400 |
| H | 3.15213500 | -1.36636400 | -4.48897100 |
| C | -0.68042300 | -0.49158300 | 1.25271100 |
| C | -1.40906300 | -1.16362200 | 2.43257600 |
| H | -0.12512200 | 0.38295000 | 1.60994200 |
| H | -1.42588000 | -0.14893600 | 0.52410500 |
| H | -1.95623000 | -2.04308100 | 2.06999000 |
| H | -0.66903000 | -1.52598700 | 3.15681100 |
| C | 0.24646300 | -1.45712200 | 0.59223600 |
| C | 1.59431100 | -1.34531200 | 0.56392000 |
| H | -0.44715700 | -0.48510000 | -1.85821600 |
| H | -0.21888200 | -2.34726500 | 0.16207100 |
| H | 2.21879500 | -2.17130000 | 0.21609000 |
| H | 2.09076600 | -0.51612600 | 1.06293800 |
| C | -3.08992800 | -0.85820000 | 4.30656900 |
| H | -3.56915200 | -1.78532300 | 3.96639000 |
| H | -2.33810600 | -1.15229800 | 5.05177000 |
| C | -4.14042500 | 0.02814200 | 4.98404100 |
| H | -4.59141700 | -0.55304300 | 5.79473800 |
| H | -4.95120800 | 0.23868200 | 4.27324400 |
| C | -3.59065200 | 1.35461800 | 5.53694900 |
| H | -4.08385900 | 1.59005000 | 6.48699300 |
| H | -2.52321700 | 1.23833900 | 5.77726300 |
| C | -3.77726800 | 2.55121500 | 4.60071800 |
| H | -3.35913500 | 2.33124400 | 3.60860300 |
| H | -4.85258200 | 2.71334900 | 4.44402300 |
| C | -3.14662900 | 3.83494300 | 5.13676900 |
| H | -2.06978000 | 3.67510100 | 5.28097700 |
| H | -3.55914400 | 4.05040800 | 6.13030700 |
| C | -3.37230100 | 5.03186300 | 4.21559800 |
| H | -2.91091600 | 5.93922400 | 4.61395600 |
| H | -2.94759800 | 4.84732100 | 3.22266200 |
| H | -4.44129500 | 5.22887600 | 4.08676800 |

T(P₉)-R

| | | | |
|---|------------|-------------|-------------|
| C | 1.35515400 | 0.09167500 | 0.16427200 |
| H | 1.13755200 | -0.10613800 | 1.20477700 |
| C | 2.64227600 | 0.07074800 | -0.43795900 |

| | | | |
|----|-------------|-------------|-------------|
| H | 3.57458600 | -0.16385800 | 0.06168000 |
| C | 2.49969500 | 0.45269900 | -1.79781700 |
| C | 0.41806900 | 0.47676800 | -0.82892200 |
| H | -0.64615100 | 0.61789400 | -0.67810000 |
| C | 1.12300900 | 0.69265000 | -2.04410900 |
| H | 0.69146600 | 1.02076000 | -2.98195500 |
| C | 3.00448700 | -2.70565700 | -3.08702600 |
| C | 1.98770300 | -2.14308500 | -3.90936700 |
| H | 2.10257800 | -1.29277100 | -4.56915600 |
| C | 0.80384300 | -2.89666300 | -3.71886400 |
| C | 2.44790600 | -3.82783300 | -2.41154800 |
| H | 2.96896900 | -4.47989500 | -1.72180300 |
| C | 1.09147900 | -3.93704100 | -2.78933700 |
| H | 0.39559200 | -4.69084600 | -2.44395900 |
| H | -0.14364000 | -2.73423100 | -4.21802800 |
| Zr | 1.30806400 | -1.75327300 | -1.53165100 |
| C | -3.08069900 | -1.87351600 | 2.76130400 |
| H | -2.47233000 | -1.03559300 | 3.12939100 |
| H | -3.93481700 | -1.42768400 | 2.23174000 |
| H | 3.30022600 | 0.55376000 | -2.51942900 |
| H | 4.03397700 | -2.37491400 | -3.03284400 |
| C | -1.73145000 | -1.84051800 | 0.61989700 |
| C | -2.24385400 | -2.69326900 | 1.78063700 |
| H | -1.17724900 | -0.98150100 | 1.02205800 |
| H | -2.58422300 | -1.43509700 | 0.06158700 |
| H | -2.84223500 | -3.52508400 | 1.38592300 |
| H | -1.39435100 | -3.14303400 | 2.31126800 |
| C | -0.82056200 | -2.63583100 | -0.32045700 |
| C | 0.56482400 | -2.93989400 | 0.20713200 |
| H | -0.79113900 | -1.99931100 | -1.29325600 |
| H | -1.32583200 | -3.53099400 | -0.69665300 |
| H | 0.82368900 | -3.99737200 | 0.18156200 |
| H | 0.73753000 | -2.52322500 | 1.19892900 |
| C | -3.58321600 | -2.70008400 | 3.94438800 |
| H | -4.14631700 | -3.56254700 | 3.56536400 |
| H | -2.71562100 | -3.10768100 | 4.48185700 |
| C | -4.45641500 | -1.92212300 | 4.93534500 |
| H | -4.74530400 | -2.60766000 | 5.73843900 |
| H | -5.38992000 | -1.62063200 | 4.44078000 |
| C | -3.77019500 | -0.67832500 | 5.52588600 |
| H | -4.05204000 | -0.55921600 | 6.57839300 |
| H | -2.68003400 | -0.82894700 | 5.52555600 |
| C | -4.10780100 | 0.62168900 | 4.79033900 |
| H | -3.99526400 | 0.48387700 | 3.70912100 |
| H | -5.16958700 | 0.85185500 | 4.95249600 |
| C | -3.26351700 | 1.80689100 | 5.26149400 |
| H | -2.19715700 | 1.57672300 | 5.11433700 |
| H | -3.39989400 | 1.90945900 | 6.34506000 |
| C | -3.59713900 | 3.14119800 | 4.57343000 |
| H | -3.45646300 | 3.96099000 | 5.28582900 |
| H | -4.66185600 | 3.15301500 | 4.30258000 |
| C | -2.75494700 | 3.45511000 | 3.33217000 |
| H | -3.03709300 | 4.44929100 | 2.95923900 |
| H | -1.70218200 | 3.52792500 | 3.63494700 |
| C | -2.89078000 | 2.45156600 | 2.18320300 |
| H | -2.40933200 | 1.50070000 | 2.45888700 |

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|---|-------------|------------|-------------|
| H | -3.95412500 | 2.22581100 | 2.02835100 |
| C | -2.29535500 | 2.95626200 | 0.86532600 |
| H | -2.49505800 | 2.21943100 | 0.07230100 |
| H | -2.81927100 | 3.87282100 | 0.56187900 |
| C | -0.79271200 | 3.23285300 | 0.91668700 |
| H | -0.57477000 | 3.99061900 | 1.67884700 |
| H | -0.26735400 | 2.32017600 | 1.24135000 |
| C | -0.22502400 | 3.70047700 | -0.42345500 |
| H | -0.65733300 | 4.67664400 | -0.67951500 |
| H | -0.55087000 | 3.01480700 | -1.22059000 |
| C | 1.29960800 | 3.79495000 | -0.43790100 |
| H | 1.62840100 | 4.53978500 | 0.29909000 |
| H | 1.72557000 | 2.83540300 | -0.10817500 |
| C | 1.87031200 | 4.14508500 | -1.81042800 |
| H | 1.48875000 | 5.12401300 | -2.13020700 |
| H | 1.49408400 | 3.41911800 | -2.54512600 |
| C | 3.39873700 | 4.16870900 | -1.83576800 |
| H | 3.74867700 | 4.95401000 | -1.15500500 |
| H | 3.78346800 | 3.21942800 | -1.43037200 |
| C | 3.98833100 | 4.39583900 | -3.23121900 |
| H | 3.48932200 | 5.25410600 | -3.69767700 |
| H | 5.04571400 | 4.66625400 | -3.14174900 |
| C | 3.86935000 | 3.17333800 | -4.14237500 |
| H | 4.45425700 | 2.33875900 | -3.73717000 |
| H | 2.82869300 | 2.84496100 | -4.24655200 |
| H | 4.24878000 | 3.38244900 | -5.14589800 |

T(P₉)-TS

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|----|-------------|-------------|-------------|
| C | 0.36145300 | -0.07368400 | 0.60114300 |
| H | 0.23575000 | -0.28052200 | 1.65599900 |
| C | 1.60314400 | -0.02528500 | -0.09472700 |
| H | 2.58128700 | -0.21537900 | 0.33046600 |
| C | 1.33926000 | 0.36161500 | -1.43001600 |
| C | -0.66741300 | 0.28719200 | -0.30672900 |
| H | -1.71897900 | 0.39450800 | -0.07431300 |
| C | -0.06335000 | 0.53629700 | -1.56804500 |
| H | -0.58138100 | 0.84910900 | -2.46582200 |
| C | 1.62478500 | -2.52677000 | -3.10406400 |
| C | 0.34056500 | -2.13321400 | -3.57707300 |
| H | 0.13093400 | -1.27317200 | -4.19935700 |
| C | -0.60766400 | -3.09122500 | -3.13291500 |
| C | 1.46629600 | -3.72601200 | -2.36727900 |
| H | 2.26071800 | -4.28670900 | -1.88875900 |
| C | 0.09034000 | -4.06818900 | -2.37173300 |
| H | -0.34743200 | -4.94586200 | -1.91319700 |
| H | -1.66386500 | -3.09745500 | -3.36263300 |
| Zr | 0.26351400 | -1.89602900 | -1.10243800 |
| C | -4.11649000 | -2.08315600 | 3.26119500 |
| H | -3.52281200 | -1.25309000 | 3.66833900 |
| H | -4.88032200 | -1.63245000 | 2.61208000 |
| H | 2.07585500 | 0.50839600 | -2.20939500 |
| H | 2.56080400 | -2.02250500 | -3.30485200 |
| C | -2.49128000 | -2.18585200 | 1.31802400 |
| C | -3.20265000 | -2.98123300 | 2.42769700 |
| H | -1.90363100 | -1.38130700 | 1.77590400 |
| H | -3.23896100 | -1.72546700 | 0.66423500 |

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|---|-------------|-------------|-------------|
| H | -3.78798400 | -3.79551400 | 1.98201000 |
| H | -2.45193600 | -3.44911800 | 3.07680800 |
| C | -1.59584800 | -3.09865300 | 0.53077600 |
| C | -0.27648700 | -3.32369300 | 0.85447300 |
| H | -1.55338100 | -1.97820800 | -1.02657500 |
| H | -2.09613900 | -3.81217200 | -0.12435100 |
| H | 0.21830500 | -4.23694100 | 0.53041500 |
| H | 0.16436700 | -2.78762100 | 1.69308600 |
| C | -4.79070100 | -2.84356600 | 4.40301400 |
| H | -5.34150000 | -3.69739600 | 3.98819800 |
| H | -4.01116900 | -3.26286600 | 5.05407500 |
| C | -5.74024100 | -1.99447300 | 5.25543000 |
| H | -6.15579800 | -2.63948400 | 6.03611900 |
| H | -6.59186500 | -1.67108700 | 4.64146000 |
| C | -5.07268800 | -0.76183400 | 5.88923000 |
| H | -5.46038700 | -0.60532300 | 6.90228500 |
| H | -3.99542500 | -0.95141800 | 6.01019300 |
| C | -5.27978000 | 0.53027300 | 5.09358800 |
| H | -5.06186900 | 0.35821000 | 4.03356700 |
| H | -6.34284500 | 0.80328800 | 5.13935000 |
| C | -4.44164700 | 1.69286200 | 5.62879500 |
| H | -3.37327300 | 1.43921400 | 5.55151200 |
| H | -4.64897800 | 1.78826300 | 6.70192100 |
| C | -4.69708400 | 3.04461800 | 4.94275600 |
| H | -4.53988700 | 3.84943900 | 5.66884200 |
| H | -5.75314900 | 3.10538000 | 4.64580800 |
| C | -3.81197200 | 3.33864000 | 3.72703400 |
| H | -4.04423300 | 4.34936600 | 3.36420700 |
| H | -2.76404200 | 3.36405200 | 4.05366900 |
| C | -3.96264800 | 2.36055000 | 2.55806300 |
| H | -3.50314300 | 1.39443600 | 2.81811700 |
| H | -5.02954700 | 2.16089300 | 2.39227700 |
| C | -3.34658100 | 2.87699600 | 1.25475200 |
| H | -3.54813400 | 2.15660900 | 0.44794200 |
| H | -3.85381900 | 3.80595100 | 0.96092000 |
| C | -1.84086200 | 3.13094300 | 1.32681000 |
| H | -1.62309100 | 3.89502900 | 2.08298000 |
| H | -1.33373200 | 2.21473600 | 1.67007200 |
| C | -1.24742600 | 3.57054400 | -0.01150700 |
| H | -1.66417100 | 4.54743800 | -0.29004500 |
| H | -1.56910800 | 2.87369200 | -0.80014100 |
| C | 0.27808100 | 3.64647600 | -0.00319600 |
| H | 0.60422500 | 4.39267400 | 0.73378500 |
| H | 0.68616300 | 2.68378000 | 0.33943700 |
| C | 0.87566800 | 3.98128300 | -1.36823000 |
| H | 0.50365900 | 4.95873400 | -1.70384800 |
| H | 0.51186200 | 3.24905500 | -2.10291100 |
| C | 2.40440800 | 4.00116100 | -1.36174200 |
| H | 2.74112800 | 4.77428800 | -0.66043800 |
| H | 2.77812700 | 3.04427000 | -0.96405300 |
| C | 3.02633100 | 4.25235000 | -2.73875600 |
| H | 2.55257100 | 5.13151500 | -3.19255300 |
| H | 4.08615600 | 4.50131500 | -2.61966900 |
| C | 2.90531800 | 3.05733100 | -3.68514300 |
| H | 3.45660200 | 2.19758200 | -3.28500100 |
| H | 1.86087000 | 2.75891700 | -3.83067000 |

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| H | 3.32149000 | 3.28313100 | -4.67033100 |
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T(P₉)-P

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|----|-------------|-------------|-------------|
| C | 1.39300800 | 0.07094000 | 0.13041900 |
| H | 1.29181500 | -0.14925200 | 1.18540500 |
| C | 2.61859000 | 0.11704500 | -0.59595300 |
| H | 3.60689100 | -0.07695600 | -0.19769000 |
| C | 2.32050500 | 0.52867400 | -1.91760000 |
| C | 0.34412700 | 0.44423400 | -0.74531700 |
| H | -0.70307000 | 0.54064100 | -0.48991700 |
| C | 0.91747100 | 0.70847700 | -2.01813900 |
| H | 0.37546500 | 1.02354500 | -2.90094700 |
| C | 2.84133200 | -2.38386000 | -3.41635200 |
| C | 1.61598100 | -1.99834700 | -4.03192400 |
| H | 1.47443600 | -1.14423600 | -4.68139600 |
| C | 0.62649900 | -2.95641800 | -3.68942300 |
| C | 2.60436500 | -3.57260000 | -2.68706200 |
| H | 3.34316200 | -4.12465600 | -2.11805700 |
| C | 1.23585900 | -3.91816500 | -2.83994200 |
| H | 0.74857400 | -4.78924500 | -2.41978300 |
| H | -0.39765200 | -2.96727300 | -4.03300800 |
| Zr | 1.26167500 | -1.73452800 | -1.59039100 |
| C | -3.05549800 | -1.99038900 | 2.87949700 |
| H | -2.44945400 | -1.18735200 | 3.32101300 |
| H | -3.75395900 | -1.50826700 | 2.18120600 |
| H | 3.03709900 | 0.68368100 | -2.71396700 |
| H | 3.79218800 | -1.87691200 | -3.51450500 |
| C | -1.30068000 | -2.18507900 | 1.05599100 |
| C | -2.13684700 | -2.93887100 | 2.10949800 |
| H | -0.70551500 | -1.41166000 | 1.55516900 |
| H | -1.97708700 | -1.69227100 | 0.34817200 |
| H | -2.73337900 | -3.71803200 | 1.61884900 |
| H | -1.46132300 | -3.44788800 | 2.80811100 |
| C | -0.41249900 | -3.13688400 | 0.32363700 |
| C | 0.92338400 | -3.26094200 | 0.51749300 |
| H | -0.52996900 | -1.73412100 | -1.80243400 |
| H | -0.91059100 | -3.83943500 | -0.34684100 |
| H | 1.47023800 | -4.10480500 | 0.10040900 |
| H | 1.42853000 | -2.65306500 | 1.26725200 |
| C | -3.83548700 | -2.71122600 | 3.97881800 |
| H | -4.39935100 | -3.54045100 | 3.53282900 |
| H | -3.11889700 | -3.16304900 | 4.67854900 |
| C | -4.79478100 | -1.81342800 | 4.76801900 |
| H | -5.28764300 | -2.43409100 | 5.52301000 |
| H | -5.59079100 | -1.45431400 | 4.10156200 |
| C | -4.11086100 | -0.60957300 | 5.43888000 |
| H | -4.54800000 | -0.43436000 | 6.42844600 |
| H | -3.05130000 | -0.84480100 | 5.62064200 |
| C | -4.21735800 | 0.68886800 | 4.63350600 |
| H | -3.94562400 | 0.50514600 | 3.58805400 |
| H | -5.26930000 | 1.00515800 | 4.61783400 |
| C | -3.36413400 | 1.81566800 | 5.21998200 |
| H | -2.30140400 | 1.53272700 | 5.17294700 |
| H | -3.60535200 | 1.89413300 | 6.28754600 |
| C | -3.55737400 | 3.19123500 | 4.56258900 |
| H | -3.36406300 | 3.97042100 | 5.30784900 |

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|---|-------------|------------|-------------|
| H | -4.61006700 | 3.30579700 | 4.26949400 |
| C | -2.66221900 | 3.47752200 | 3.35245900 |
| H | -2.85053800 | 4.50767600 | 3.01995000 |
| H | -1.61299600 | 3.44779100 | 3.67486900 |
| C | -2.85967600 | 2.54201200 | 2.15563400 |
| H | -2.42206000 | 1.55613900 | 2.37601800 |
| H | -3.93414400 | 2.37593300 | 2.00237700 |
| C | -2.25164800 | 3.08385000 | 0.85906700 |
| H | -2.47887800 | 2.39170300 | 0.03487600 |
| H | -2.74364600 | 4.03104900 | 0.59973500 |
| C | -0.74023400 | 3.30530200 | 0.91725200 |
| H | -0.49770600 | 4.05284500 | 1.68253000 |
| H | -0.24842900 | 2.37357100 | 1.24006500 |
| C | -0.15405000 | 3.75149000 | -0.42198500 |
| H | -0.55514800 | 4.73966100 | -0.68322900 |
| H | -0.49851200 | 3.07071200 | -1.21491100 |
| C | 1.37258500 | 3.79767500 | -0.43171800 |
| H | 1.72261800 | 4.53045400 | 0.30776800 |
| H | 1.76561500 | 2.82396900 | -0.10283700 |
| C | 1.95962800 | 4.13315600 | -1.80122100 |
| H | 1.60335200 | 5.12108700 | -2.12291900 |
| H | 1.57142100 | 3.41546100 | -2.53774300 |
| C | 3.48840700 | 4.12223400 | -1.81404400 |
| H | 3.84937900 | 4.87817100 | -1.10605300 |
| H | 3.84769600 | 3.15239800 | -1.43465500 |
| C | 4.09876300 | 4.38131700 | -3.19474500 |
| H | 3.64038600 | 5.27880200 | -3.62797500 |
| H | 5.16559400 | 4.60328200 | -3.08508000 |
| C | 3.93762800 | 3.20576300 | -4.15932800 |
| H | 4.47034400 | 2.32545400 | -3.77898700 |
| H | 2.88449700 | 2.93707600 | -4.29968800 |
| H | 4.35030800 | 3.43718100 | -5.14467300 |