

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

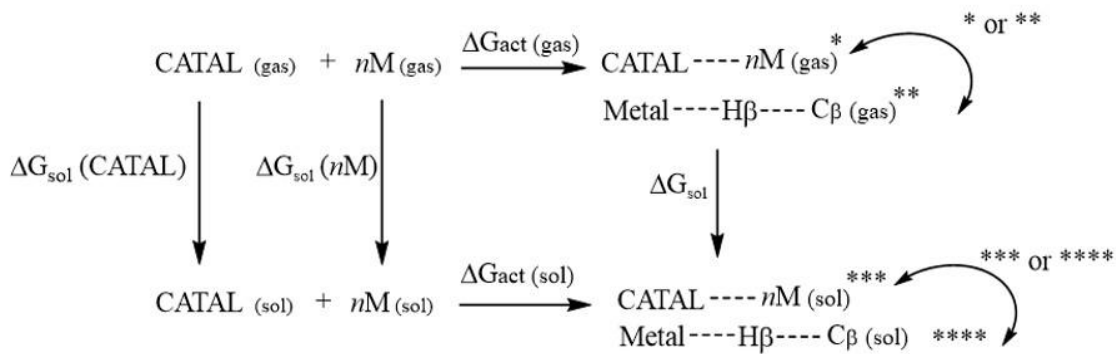


Figure S1. Thermodynamic cycle used for calculating activation free energies in gas and solution phases for an ethylene polymerization process. n denotes the number of M monomers of ethylene, CATAL corresponds to the catalyst and H β /C β the hydrogen and carbon atom in β -position.

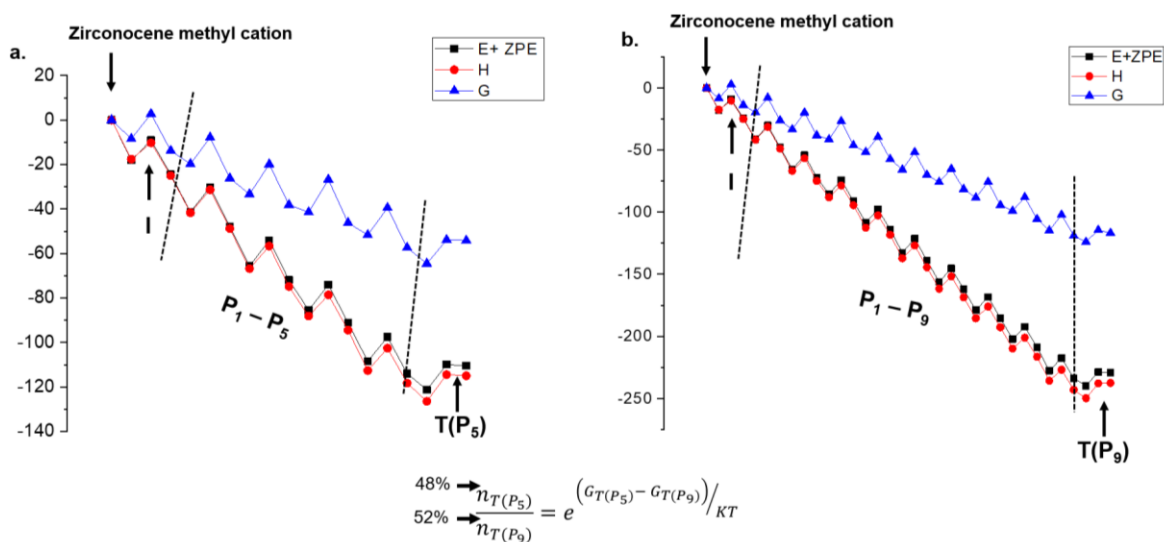


Figure S2. Relative energy data for an earlier chain termination (a) and later chain termination (b) on zirconocene ethylene polymerization reaction. Boltzmann distribution is obtained from the Gibbs free energies of the reactants and products involved in the propagation paths P_5 - P/P_9 - P and $T(P_5)$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

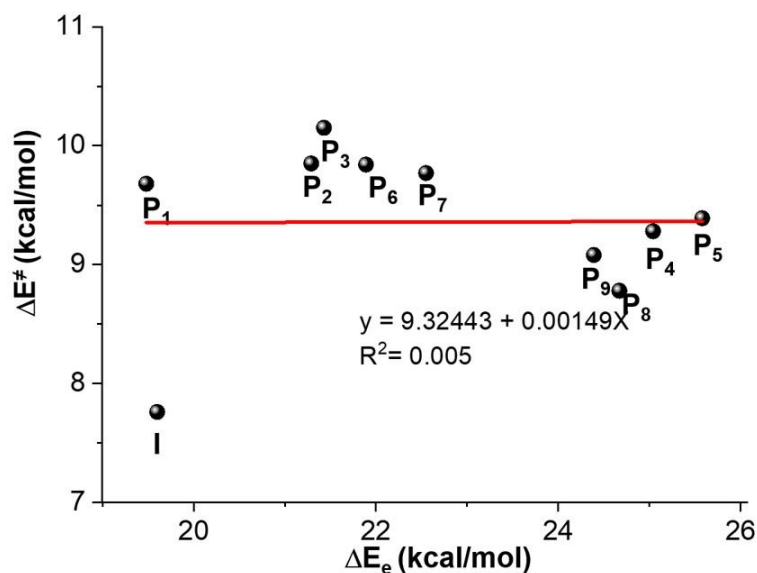


Figure S3. Correlation of the activation energy from the chain initiation to chain propagation of the ethylene polymerization reaction with the electrostatic energy difference (ΔE_e).

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

P1-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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

H 0.12272500 -8.05977000 -4.56989300

P5-P

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

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

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

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

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

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

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

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

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

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

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

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

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

P8-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

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

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

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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

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

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

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

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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

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

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

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

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

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

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

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

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

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

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

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

H 3.32149000 3.28313100 -4.67033100

T(P₉)-P

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

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