

**Rhodium-catalyzed cycloisomerization of ester-tethered 1,6-diynes with cyclopropanol moiety leading to tetralone/exocyclic diene hybrid molecules**

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**Supporting Information**

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Cartesian Coordinates of Optimized Structures

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Model A

C	5.110300	-2.228300	1.115300
C	4.040000	-2.779100	0.950600
C	1.007300	-1.555400	1.757700
C	0.805200	-0.299100	1.960200
O	2.040300	-3.762900	1.908800
P	0.122300	0.497500	-1.902600
P	-2.149900	-1.051500	0.071500
C	-3.214200	-0.481900	-1.329200
C	-3.129700	0.784300	-1.919500
C	-4.150900	-1.437200	-1.825800
C	-3.939600	1.068200	-3.081600
C	-2.294000	1.922300	-1.391000
C	-4.951100	-1.160900	-2.903900
H	-4.239000	-2.400400	-1.338700
C	-4.853100	0.080600	-3.576500
C	-0.904900	1.989800	-1.548300
C	-2.988000	3.039500	-0.801900
H	-5.663800	-1.901400	-3.257400
C	-0.205400	3.180600	-1.203100
C	-2.256500	4.217500	-0.431200
C	-0.862800	4.263700	-0.673700
H	0.865000	3.234400	-1.363300
H	-0.313100	5.169900	-0.431800
C	-2.205400	-2.890800	-0.000000
C	-2.621300	-3.668800	1.090900
C	-1.733700	-3.533200	-1.161700
C	-2.560700	-5.062600	1.021800
H	-2.994200	-3.197900	1.992900
C	-1.680400	-4.924000	-1.224400
H	-1.435100	-2.946900	-2.025300
C	-2.088600	-5.692400	-0.129900
H	-2.885600	-5.653300	1.873200
H	-1.324600	-5.408800	-2.129200
H	-2.043600	-6.776400	-0.178400
C	-2.990700	-0.545700	1.619100
C	-4.242000	0.089000	1.571800

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C	-2.412400	-0.833300	2.869000
C	-4.900200	0.435700	2.752200
H	-4.708500	0.305700	0.618600
C	-3.081700	-0.492900	4.043600
H	-1.456200	-1.340600	2.936800
C	-4.322100	0.147500	3.988600
H	-5.866500	0.928800	2.701500
H	-2.628100	-0.726900	5.001900
H	-4.836200	0.417600	4.906500
C	-0.321200	-0.211400	-3.533600
C	0.066300	-1.534300	-3.805000
C	-0.926000	0.546000	-4.545700
C	-0.162000	-2.093100	-5.062300
H	0.564200	-2.122300	-3.037500
C	-1.158400	-0.017800	-5.801900
H	-1.216100	1.574300	-4.358400
C	-0.779900	-1.336200	-6.061200
H	0.145500	-3.115300	-5.263500
H	-1.635300	0.576100	-6.576000
H	-0.960200	-1.771600	-7.039800
C	1.853000	1.075500	-2.157100
C	2.703200	1.226400	-1.047800
C	2.357700	1.340000	-3.442200
C	4.028800	1.629100	-1.215400
H	2.335500	1.040600	-0.043300
C	3.680600	1.751300	-3.605400
H	1.725400	1.221800	-4.315500
H	4.662600	1.712000	-0.338600
H	4.058000	1.954800	-4.603500
C	-2.939200	5.319500	0.151400
C	-4.394700	3.036700	-0.567700
C	-4.295600	5.273600	0.369800
H	-4.809200	6.120200	0.815600
C	-5.026300	4.117100	0.005500
H	-6.098800	4.084900	0.174900
H	-2.364800	6.202300	0.419800
H	-4.980200	2.170900	-0.852000
C	-3.865700	2.307300	-3.784400

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C	-5.647500	0.359900	-4.721000
C	-4.640600	2.545600	-4.897700
H	-4.559900	3.497800	-5.414000
C	-5.546100	1.566700	-5.372100
H	-6.157000	1.772200	-6.246200
H	-3.185800	3.077100	-3.440100
H	-6.336600	-0.403300	-5.072800
C	4.518200	1.891700	-2.496000
H	5.550700	2.201300	-2.631000
Rh	0.100700	-0.776500	0.084100
C	2.787100	-3.483800	0.701600
C	0.787500	0.816100	2.872200
C	0.976500	0.550300	4.246000
C	0.582200	2.137700	2.442500
C	0.977200	1.597400	5.162400
H	1.109700	-0.476300	4.574300
C	0.581500	3.178100	3.367600
H	0.424100	2.338800	1.388400
C	0.782300	2.911800	4.725000
H	1.126500	1.389900	6.218000
H	0.424400	4.198600	3.030900
H	0.783000	3.726800	5.443200
C	6.375600	-1.578000	1.273500
C	7.500000	-2.126800	0.630600
C	6.505500	-0.396100	2.049200
C	8.746700	-1.517000	0.742000
H	7.381800	-3.034300	0.046700
C	7.765100	0.200600	2.134200
C	8.878200	-0.349300	1.493700
H	9.608400	-1.951400	0.244000
H	7.877600	1.115900	2.706700
H	9.845000	0.138400	1.580500
C	1.214100	-2.842800	2.440400
O	0.607600	-3.091800	3.461700
H	2.982900	-4.472600	0.277200
H	2.150300	-2.930900	-0.000400
C	5.300800	0.181000	2.744800
C	4.904800	-0.336600	4.113400

C	5.421600	1.075600	3.942100
H	5.549000	-1.066900	4.594800
H	3.842300	-0.464200	4.298000
H	4.698900	1.883500	3.998500
H	6.404000	1.314700	4.336700
O	4.238600	0.537300	1.877700
H	3.898300	-0.294400	1.503500

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Model TS AB

C	2.631700	-1.564100	0.472400
C	1.947500	-2.293000	1.264000
C	0.610900	-1.323500	2.574900
C	0.483100	-0.049100	2.428600
O	1.051900	-3.581100	3.159500
Rh	0.518500	-0.850000	0.495900
C	1.753100	-3.620000	1.912400
C	0.484400	1.263100	3.011500
C	1.397200	1.544900	4.054700
C	-0.441300	2.247800	2.613600
C	1.365400	2.782800	4.687000
H	2.129100	0.799800	4.346600
C	-0.467800	3.478100	3.261800
H	-1.142300	2.032800	1.816100
C	0.432500	3.748800	4.296600
H	2.069300	2.994200	5.486200
H	-1.194300	4.225900	2.959200
H	0.409300	4.712300	4.797700
C	3.933300	-1.299600	-0.107200
C	4.097900	-1.301300	-1.502300
C	5.055800	-1.058300	0.733800
C	5.349600	-1.099200	-2.076600
H	3.236000	-1.472000	-2.137900
C	6.293800	-0.829400	0.128800
C	6.451900	-0.858000	-1.258300
H	5.457800	-1.119000	-3.156900
H	7.153300	-0.615100	0.755400
H	7.430800	-0.679900	-1.693900

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C	0.462600	-2.423000	3.532300
O	-0.142700	-2.332500	4.575200
H	2.737100	-4.057800	2.110200
H	1.192800	-4.285300	1.247900
C	4.900800	-1.018300	2.232700
C	5.034600	-2.289800	3.053500
C	6.067400	-1.190500	3.160700
H	5.323000	-3.205900	2.544400
H	4.343800	-2.418700	3.883100
H	6.050100	-0.570800	4.051400
H	7.056800	-1.380400	2.758100
O	3.952400	-0.075400	2.699200
H	3.073800	-0.457300	2.543100
P	0.640400	0.717200	-1.382200
P	-1.910300	-1.072700	0.357100
C	-2.678400	-0.695000	-1.285000
C	-2.598300	0.563000	-1.889200
C	-3.380000	-1.751100	-1.940000
C	-3.173800	0.752300	-3.200000
C	-2.019500	1.787700	-1.229200
C	-3.945300	-1.576400	-3.176800
H	-3.481100	-2.710100	-1.448200
C	-3.842500	-0.335600	-3.850500
C	-0.644800	2.039100	-1.146900
C	-2.950400	2.801200	-0.796700
H	-4.482000	-2.394200	-3.650800
C	-0.188400	3.314900	-0.709900
C	-2.461900	4.070100	-0.338500
C	-1.066200	4.301600	-0.335400
H	0.874100	3.517400	-0.674000
H	-0.690400	5.272400	-0.022400
C	-1.861000	-2.919200	0.424000
C	-2.388700	-3.638100	1.507000
C	-1.166600	-3.619000	-0.584000
C	-2.224600	-5.023900	1.581200
H	-2.929900	-3.124400	2.293900
C	-1.013100	-5.003500	-0.508900
H	-0.779100	-3.086100	-1.447700

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C	-1.538400	-5.709700	0.578100
H	-2.640700	-5.565400	2.425600
H	-0.492500	-5.531500	-1.303200
H	-1.419800	-6.787600	0.637000
C	-3.165900	-0.581000	1.612600
C	-4.486500	-0.303300	1.220600
C	-2.839600	-0.537500	2.980400
C	-5.453300	0.023800	2.171300
H	-4.766300	-0.352600	0.174700
C	-3.813300	-0.213500	3.926400
H	-1.843300	-0.779800	3.327400
C	-5.118900	0.073800	3.525400
H	-6.469500	0.235000	1.850800
H	-3.544600	-0.191800	4.978400
H	-5.873300	0.327600	4.264500
C	0.439400	0.042600	-3.081200
C	0.710700	-1.315800	-3.308400
C	0.079900	0.852000	-4.170200
C	0.637600	-1.852300	-4.595000
H	0.984700	-1.957600	-2.474900
C	0.004200	0.314900	-5.455900
H	-0.150700	1.901200	-4.015000
C	0.285200	-1.036000	-5.671300
H	0.853300	-2.904900	-4.755200
H	-0.281600	0.952000	-6.287600
H	0.225500	-1.451300	-6.673100
C	2.234800	1.645700	-1.435500
C	2.914400	1.888900	-0.230800
C	2.778500	2.139600	-2.631900
C	4.100200	2.623000	-0.219600
H	2.529700	1.494200	0.703200
C	3.967500	2.870300	-2.617900
H	2.286800	1.951200	-3.579500
H	4.613600	2.790200	0.722400
H	4.377100	3.243700	-3.552300
C	-3.379000	5.071500	0.082900
C	-4.362800	2.607600	-0.816300
C	-4.734000	4.841300	0.059100

H	-5.428000	5.611600	0.381900
C	-5.225900	3.594100	-0.395900
H	-6.297200	3.416200	-0.418100
H	-2.985100	6.027000	0.419900
H	-4.765300	1.667100	-1.171200
C	-3.105000	1.994400	-3.896600
C	-4.403800	-0.151500	-5.142500
C	-3.655600	2.142600	-5.150300
H	-3.588500	3.101500	-5.656400
C	-4.314100	1.061900	-5.783500
H	-4.749000	1.195300	-6.769700
H	-2.611000	2.839500	-3.432800
H	-4.908900	-0.990800	-5.613400
C	4.628700	3.116900	-1.413500
H	5.555400	3.683700	-1.406900

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Model B

C	2.401900	-1.719500	0.803500
C	2.134000	-2.063500	2.086100
C	1.258200	-1.236400	2.915600
C	0.649100	-0.116000	2.430200
O	2.000800	-2.962000	4.261400
P	0.845300	0.928300	-0.909400
P	-1.903700	-1.101900	0.268100
C	-2.546000	-0.585000	-1.384600
C	-2.374800	0.716800	-1.862700
C	-3.191000	-1.563000	-2.197400
C	-2.812000	1.037000	-3.201700
C	-1.885100	1.873300	-1.026300
C	-3.615300	-1.268400	-3.467500
H	-3.352400	-2.559000	-1.803400
C	-3.421000	0.024100	-4.012900
C	-0.537100	2.158200	-0.752300
C	-2.896600	2.817600	-0.614200
H	-4.109600	-2.027600	-4.068100
C	-0.190800	3.414500	-0.175600
C	-2.517000	4.065500	-0.016700



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C	-1.142400	4.345600	0.155100
H	0.848600	3.651300	0.005700
H	-0.842900	5.301600	0.576200
C	-1.811400	-2.946000	0.159600
C	-2.412200	-3.783100	1.111900
C	-1.034100	-3.527000	-0.862000
C	-2.244000	-5.168400	1.040900
H	-3.018600	-3.360800	1.905700
C	-0.880900	-4.911700	-0.935700
H	-0.576500	-2.900400	-1.624300
C	-1.482100	-5.736300	0.019000
H	-2.720000	-5.802700	1.783000
H	-0.297200	-5.346100	-1.742700
H	-1.361800	-6.814200	-0.037900
C	-3.235800	-0.786300	1.492100
C	-4.566300	-0.583100	1.092800
C	-2.926100	-0.815300	2.862800
C	-5.567000	-0.406600	2.048800
H	-4.824100	-0.572700	0.038800
C	-3.932900	-0.647400	3.814500
H	-1.905000	-0.974000	3.196000
C	-5.252700	-0.438500	3.409100
H	-6.593400	-0.250200	1.729500
H	-3.680300	-0.675300	4.870300
H	-6.034400	-0.302900	4.151000
C	0.928300	0.366300	-2.652200
C	1.484600	-0.889200	-2.944500
C	0.523700	1.200300	-3.706700
C	1.624100	-1.305700	-4.269100
H	1.832000	-1.536700	-2.146700
C	0.666400	0.779600	-5.029000
H	0.096100	2.175000	-3.499400
C	1.213700	-0.473900	-5.312400
H	2.062900	-2.276500	-4.479900
H	0.343400	1.430800	-5.835700
H	1.323700	-0.798100	-6.343200
C	2.376500	1.924700	-0.663300
C	2.863500	2.149600	0.636200

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C	3.020000	2.543000	-1.750200
C	3.952000	2.997200	0.844500
H	2.388600	1.667300	1.482400
C	4.119100	3.376900	-1.535300
H	2.673600	2.371600	-2.763300
H	4.313600	3.167300	1.854400
H	4.615400	3.836800	-2.384500
C	-3.516200	4.996200	0.379400
C	-4.291000	2.568000	-0.784800
C	-4.849900	4.713500	0.204400
H	-5.607700	5.428600	0.510400
C	-5.235900	3.483400	-0.381200
H	-6.290500	3.261800	-0.516400
H	-3.202000	5.937700	0.822300
H	-4.613800	1.638400	-1.236300
C	-2.665400	2.336000	-3.771200
C	-3.839300	0.332400	-5.335300
C	-3.078700	2.605000	-5.057300
H	-2.954700	3.605000	-5.463200
C	-3.672000	1.595600	-5.852200
H	-3.998000	1.823400	-6.862800
H	-2.223100	3.130800	-3.182400
H	-4.299200	-0.452600	-5.930000
C	4.581600	3.612400	-0.239800
H	5.437000	4.261000	-0.076800
Rh	0.561000	-0.810000	0.548200
C	2.596900	-3.206500	2.972200
C	0.249400	1.087500	3.120200
C	1.006100	1.498400	4.247700
C	-0.875100	1.855400	2.751200
C	0.631300	2.614000	4.984900
H	1.878200	0.923800	4.539000
C	-1.244800	2.971200	3.495300
H	-1.466000	1.557300	1.895200
C	-0.496800	3.352800	4.612500
H	1.215700	2.907600	5.851800
H	-2.122200	3.540800	3.205000
H	-0.791100	4.222900	5.192600

C	3.301100	-2.431300	-0.123000
C	2.773600	-3.568600	-0.779500
C	4.651100	-2.076800	-0.371000
C	3.532800	-4.318300	-1.672700
H	1.751600	-3.865900	-0.562900
C	5.393100	-2.841400	-1.283200
C	4.852900	-3.946300	-1.936100
H	3.101300	-5.194400	-2.149600
H	6.423400	-2.553300	-1.471400
H	5.459400	-4.519100	-2.631900
C	1.189900	-1.861100	4.270600
O	0.559200	-1.522000	5.240100
H	3.684400	-3.240600	3.096500
H	2.255400	-4.184900	2.618500
C	5.343200	-0.879200	0.229100
C	5.371600	-0.601200	1.713100
C	6.624000	-1.058800	0.994600
H	4.892900	-1.296500	2.395100
H	5.316900	0.440500	2.013200
H	7.398400	-0.321100	0.807900
H	6.981800	-2.067000	1.182800
O	5.380000	0.234500	-0.635900
H	4.484600	0.606600	-0.679000

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Model TS BC

C	2.135200	-1.876200	1.546600
C	2.166000	-1.590100	2.878700
C	1.458500	-0.434900	3.366600
C	0.727100	0.308200	2.491000
O	2.436100	-1.444100	5.202800
P	0.826300	1.273100	-0.872300
P	-1.397900	-1.023400	-0.071800
C	-2.319900	-0.317100	-1.511700
C	-2.361200	1.041600	-1.837800
C	-2.965300	-1.272700	-2.354900
C	-2.961200	1.436900	-3.095200
C	-1.901500	2.164300	-0.943400

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C	-3.590800	-0.898000	-3.514400
H	-2.969200	-2.317500	-2.071300
C	-3.577400	0.453300	-3.936000
C	-0.560600	2.473400	-0.674800
C	-2.929000	3.054300	-0.458500
H	-4.087700	-1.642300	-4.131100
C	-0.227900	3.710800	-0.054000
C	-2.566600	4.296000	0.160500
C	-1.196300	4.609300	0.314600
H	0.810900	3.953300	0.128900
H	-0.915400	5.557700	0.763800
C	-1.045900	-2.749800	-0.607400
C	-1.605900	-3.866800	0.034800
C	-0.197800	-2.946800	-1.714800
C	-1.329500	-5.152800	-0.431200
H	-2.271200	-3.737000	0.881000
C	0.079400	-4.234900	-2.168400
H	0.223100	-2.096400	-2.242700
C	-0.487200	-5.340000	-1.529500
H	-1.781200	-6.008700	0.062000
H	0.733100	-4.373300	-3.024400
H	-0.277500	-6.343000	-1.889300
C	-2.566300	-1.153700	1.325400
C	-3.897800	-0.725200	1.207400
C	-2.116600	-1.689000	2.547600
C	-4.765400	-0.831800	2.295300
H	-4.257200	-0.311400	0.271700
C	-2.990500	-1.795700	3.627900
H	-1.086400	-2.013100	2.653500
C	-4.314200	-1.364400	3.504500
H	-5.794300	-0.498900	2.195700
H	-2.635400	-2.205600	4.568600
H	-4.990900	-1.441800	4.350400
C	1.011600	0.799200	-2.635500
C	1.920700	-0.227800	-2.953100
C	0.360100	1.487300	-3.668700
C	2.139900	-0.574800	-4.286800
H	2.497000	-0.718000	-2.171700

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C	0.586800	1.134300	-5.000200
H	-0.312900	2.305400	-3.443300
C	1.468200	0.097600	-5.311200
H	2.849600	-1.362300	-4.524200
H	0.073700	1.673900	-5.790800
H	1.643500	-0.174800	-6.348000
C	2.381500	2.217000	-0.563800
C	2.990900	2.222200	0.700700
C	2.976200	2.942700	-1.611200
C	4.167800	2.942000	0.915500
H	2.548300	1.665900	1.517400
C	4.147300	3.665900	-1.389000
H	2.531000	2.943300	-2.600200
H	4.628600	2.936900	1.899200
H	4.594700	4.224400	-2.206000
C	-3.580300	5.182800	0.614700
C	-4.319600	2.754700	-0.568900
C	-4.910100	4.856600	0.491900
H	-5.678100	5.537600	0.846500
C	-5.278300	3.623300	-0.098700
H	-6.329100	3.363100	-0.186900
H	-3.280200	6.122400	1.071000
H	-4.630200	1.824300	-1.029100
C	-2.950900	2.784400	-3.563800
C	-4.165200	0.840000	-5.170300
C	-3.512200	3.127300	-4.774000
H	-3.480900	4.161100	-5.105600
C	-4.135400	2.150300	-5.585800
H	-4.584300	2.437400	-6.532000
H	-2.487300	3.557200	-2.963000
H	-4.634000	0.074700	-5.783200
C	4.747100	3.665700	-0.127300
H	5.662600	4.225500	0.040100
Rh	0.821100	-0.625000	0.549600
C	2.815400	-2.250300	4.068500
C	0.070800	1.558300	2.884700
C	0.831700	2.531400	3.574100
C	-1.306300	1.799000	2.712500

C	0.236400	3.681100	4.081700
H	1.890800	2.362500	3.734800
C	-1.903900	2.935600	3.249300
H	-1.919200	1.072100	2.199000
C	-1.137500	3.882800	3.932500
H	0.841900	4.406400	4.617400
H	-2.973300	3.083100	3.131200
H	-1.607800	4.768400	4.350600
C	2.739300	-3.089200	0.952900
C	2.055400	-4.309000	1.127900
C	3.967200	-3.096200	0.236600
C	2.558600	-5.509200	0.631500
H	1.111300	-4.301800	1.665600
C	4.440500	-4.307600	-0.278700
C	3.755300	-5.508000	-0.083300
H	2.015700	-6.435500	0.797600
H	5.366500	-4.316000	-0.844400
H	4.155500	-6.432000	-0.491000
C	1.645000	-0.373200	4.846800
O	1.224400	0.398600	5.670600
H	3.909600	-2.268400	3.998000
H	2.470200	-3.276500	4.237500
C	4.756200	-1.826200	0.067200
C	5.809700	-1.434900	1.087300
C	6.208200	-1.817600	-0.320100
H	6.033100	-2.134700	1.888000
H	5.866600	-0.385000	1.362600
H	6.507300	-1.018400	-0.990600
H	6.737200	-2.753600	-0.464800
O	4.028000	-0.748100	-0.497000
H	3.508300	-0.348500	0.222500

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Model C

C	1.551200	-2.254700	1.496700
C	1.445300	-2.088700	2.824500
C	0.877600	-0.844200	3.281600
C	0.524700	0.103800	2.384000

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O	1.434900	-2.053400	5.167000
P	0.873600	1.425000	-1.127200
P	-1.255700	-1.233800	0.070100
C	-2.189900	-0.493100	-1.390500
C	-2.261400	0.848300	-1.794700
C	-2.881400	-1.479100	-2.165400
C	-2.885400	1.164500	-3.068600
C	-1.871000	2.070300	-0.998400
C	-3.530200	-1.177800	-3.332100
H	-2.908600	-2.502900	-1.820800
C	-3.510900	0.138600	-3.845900
C	-0.561900	2.548700	-0.890000
C	-2.956300	2.893600	-0.521100
H	-4.053500	-1.957500	-3.879300
C	-0.319100	3.863600	-0.405300
C	-2.684600	4.207900	-0.015000
C	-1.349000	4.675600	-0.002500
H	0.696800	4.236000	-0.358000
H	-1.144000	5.683800	0.347300
C	-1.045000	-2.976800	-0.517500
C	-1.697200	-4.066500	0.076100
C	-0.243100	-3.197000	-1.651200
C	-1.553600	-5.349900	-0.459900
H	-2.335700	-3.920800	0.940000
C	-0.110000	-4.476600	-2.187000
H	0.249100	-2.363100	-2.143900
C	-0.766900	-5.557500	-1.593800
H	-2.073000	-6.183400	0.004500
H	0.504200	-4.628100	-3.069900
H	-0.670000	-6.553700	-2.015700
C	-2.477400	-1.323400	1.436900
C	-3.751000	-0.748800	1.315700
C	-2.137900	-1.990100	2.627800
C	-4.662800	-0.826300	2.370500
H	-4.035100	-0.239800	0.403000
C	-3.055100	-2.072300	3.674000
H	-1.162100	-2.450100	2.730100
C	-4.316900	-1.484500	3.550400

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H	-5.643400	-0.371500	2.264900
H	-2.780200	-2.586900	4.589900
H	-5.025800	-1.541700	4.371200
C	0.979000	0.937100	-2.896100
C	1.709000	-0.220900	-3.216500
C	0.428200	1.704000	-3.932100
C	1.871700	-0.608800	-4.547100
H	2.174900	-0.806800	-2.427400
C	0.585700	1.309100	-5.262100
H	-0.125000	2.608500	-3.704200
C	1.304400	0.152900	-5.571700
H	2.442800	-1.502500	-4.782700
H	0.145300	1.907000	-6.054600
H	1.426600	-0.151100	-6.607300
C	2.391600	2.469100	-0.915200
C	2.825700	2.789400	0.387100
C	3.168300	2.893800	-2.005200
C	4.002200	3.516300	0.588100
H	2.223900	2.503500	1.244500
C	4.344800	3.618400	-1.799000
H	2.860400	2.660100	-3.018100
H	4.313300	3.765300	1.598900
H	4.930900	3.939900	-2.655200
C	-3.753400	5.021200	0.451500
C	-4.316700	2.465800	-0.543000
C	-5.050100	4.564300	0.431400
H	-5.859700	5.191700	0.792100
C	-5.329400	3.271100	-0.072200
H	-6.355100	2.914400	-0.096100
H	-3.522700	6.015100	0.826300
H	-4.562300	1.491400	-0.947900
C	-2.904900	2.486600	-3.606300
C	-4.117100	0.450300	-5.092100
C	-3.488800	2.760600	-4.823500
H	-3.479100	3.777800	-5.204600
C	-4.107500	1.736300	-5.577600
H	-4.572500	1.968700	-6.531100
H	-2.447600	3.297800	-3.054100



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H	-4.588400	-0.351900	-5.653900
C	4.768000	3.928200	-0.505500
H	5.684000	4.490600	-0.350000
Rh	0.949000	-0.559600	0.450500
C	1.904100	-2.844300	4.051900
C	0.125500	1.462200	2.761500
C	1.037200	2.260800	3.487400
C	-1.180900	1.946400	2.567000
C	0.654400	3.497000	3.999600
H	2.035800	1.879100	3.680200
C	-1.567700	3.171600	3.105200
H	-1.905500	1.339200	2.038100
C	-0.652900	3.953100	3.815100
H	1.365400	4.089500	4.568400
H	-2.589100	3.514900	2.973700
H	-0.960700	4.906800	4.234500
C	2.430700	-3.195600	0.793400
C	2.076600	-4.530600	0.544900
C	3.700400	-2.730100	0.351200
C	2.949400	-5.392500	-0.118700
H	1.107300	-4.887300	0.877500
C	4.548100	-3.596800	-0.343200
C	4.181800	-4.924600	-0.574700
H	2.661700	-6.426600	-0.286500
H	5.509700	-3.238900	-0.698200
H	4.858600	-5.586900	-1.106400
C	0.860600	-0.864700	4.772500
O	0.441800	-0.065700	5.570500
H	2.994600	-2.935400	4.127000
H	1.470400	-3.845400	4.142800
C	4.122700	-1.333400	0.692200
C	4.793600	-1.001600	2.001000
C	5.550300	-0.867400	0.692200
H	5.052200	-1.823700	2.661800
H	4.487700	-0.091700	2.511800
H	5.749600	0.136300	0.322400
H	6.341000	-1.577400	0.472600
O	3.149900	-0.376900	0.207000

H	3.479100	0.538100	0.293400
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Model TS CD

C	2.132200	-2.573400	1.544400
C	1.777400	-2.849700	2.820800
C	1.229300	-1.739400	3.544900
C	1.119200	-0.547500	2.892400
O	1.426900	-3.470300	5.052400
Rh	1.515500	-0.749100	0.895900
C	1.933700	-3.988200	3.801800
C	1.015200	0.778000	3.498900
C	1.776200	1.067700	4.655600
C	0.193500	1.794900	2.972200
C	1.705400	2.317400	5.262300
H	2.411900	0.299300	5.080400
C	0.121100	3.044100	3.588100
H	-0.415600	1.591500	2.099600
C	0.877000	3.311100	4.731800
H	2.291800	2.514200	6.155200
H	-0.534300	3.804500	3.175100
H	0.816300	4.283800	5.211700
C	3.015300	-3.332700	0.664700
C	3.023300	-4.741800	0.626300
C	3.897500	-2.649900	-0.204800
C	3.848000	-5.438600	-0.253000
H	2.340200	-5.286600	1.268700
C	4.704200	-3.355300	-1.110900
C	4.679600	-4.748500	-1.138700
H	3.828800	-6.524800	-0.260000
H	5.369200	-2.811800	-1.775800
H	5.308600	-5.287200	-1.840500
C	1.001600	-2.165600	4.949900
O	0.523700	-1.573100	5.885800
H	2.972200	-4.307300	3.952100
H	1.334600	-4.868800	3.544300
C	4.157600	-1.183700	-0.138300
C	3.624800	-0.197400	1.564000

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C	4.970600	-0.579000	0.907500
H	3.559100	-0.619200	2.560800
H	3.475800	0.876200	1.513600
H	5.578800	0.272200	0.588600
H	5.560300	-1.290200	1.483700
O	3.952900	-0.542500	-1.287900
H	4.303400	0.372700	-1.261700
P	1.222900	1.312100	-0.849600
P	-0.865700	-1.410000	0.480000
C	-1.503000	-0.926800	-1.221600
C	-1.717800	0.398300	-1.630000
C	-1.791200	-1.984200	-2.133900
C	-2.178100	0.658100	-2.978500
C	-1.574200	1.633700	-0.771700
C	-2.246600	-1.748900	-3.406000
H	-1.678600	-3.010200	-1.815700
C	-2.442000	-0.429900	-3.872000
C	-0.339700	2.260000	-0.561200
C	-2.781200	2.306600	-0.361200
H	-2.470900	-2.584200	-4.064700
C	-0.292600	3.571400	-0.013900
C	-2.705200	3.610500	0.232400
C	-1.438200	4.228000	0.363800
H	0.660400	4.074100	0.092700
H	-1.381400	5.239000	0.760200
C	-0.931000	-3.266500	0.493800
C	-1.755900	-3.963400	1.389600
C	-0.115400	-4.007700	-0.379400
C	-1.780700	-5.361300	1.394500
H	-2.387000	-3.425700	2.086600
C	-0.164200	-5.400700	-0.394200
H	0.555000	-3.497700	-1.065100
C	-0.998000	-6.084000	0.495400
H	-2.426100	-5.879800	2.097700
H	0.458400	-5.950800	-1.093900
H	-1.033700	-7.169700	0.487400
C	-2.315600	-0.998900	1.562500
C	-3.606700	-1.181500	1.031600

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C	-2.190500	-0.667600	2.918700
C	-4.735300	-1.018800	1.832800
H	-3.733400	-1.470300	-0.006300
C	-3.324500	-0.497300	3.717500
H	-1.217200	-0.562000	3.373600
C	-4.598300	-0.669500	3.178100
H	-5.722300	-1.168600	1.404200
H	-3.200200	-0.239600	4.765000
H	-5.478600	-0.542000	3.801700
C	1.242900	0.977100	-2.663400
C	1.472600	-0.320200	-3.142500
C	1.041200	2.017800	-3.586700
C	1.509600	-0.572700	-4.514900
H	1.622500	-1.137400	-2.444900
C	1.084900	1.765200	-4.957300
H	0.849900	3.027600	-3.234500
C	1.319800	0.469300	-5.423600
H	1.685200	-1.583500	-4.872000
H	0.927400	2.578100	-5.660200
H	1.350200	0.273100	-6.491500
C	2.638100	2.492700	-0.629100
C	2.869900	3.083900	0.628700
C	3.603000	2.683700	-1.637400
C	4.005800	3.862400	0.857300
H	2.163600	2.935700	1.440500
C	4.751000	3.448200	-1.397200
H	3.447300	2.265000	-2.626300
H	4.151400	4.319500	1.832000
H	5.474900	3.589200	-2.195300
C	-3.895000	4.275900	0.633700
C	-4.075700	1.744100	-0.551700
C	-5.125300	3.691100	0.448000
H	-6.030400	4.207300	0.754200
C	-5.211200	2.413700	-0.155200
H	-6.185200	1.958500	-0.310100
H	-3.812500	5.261900	1.083700
H	-4.166000	0.771800	-1.018700
C	-2.388300	1.977100	-3.480300

C	-2.907300	-0.176800	-5.190500
C	-2.839100	2.193700	-4.763500
H	-2.991500	3.211200	-5.112400
C	-3.107500	1.109500	-5.631500
H	-3.468900	1.296400	-6.638500
H	-2.189500	2.830600	-2.845200
H	-3.105300	-1.024400	-5.841600
C	4.954700	4.043800	-0.152300
H	5.840800	4.644600	0.030000

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Model D

C	2.001900	-1.724900	0.972000
C	1.687800	-2.527200	2.051800
C	0.987400	-1.950100	3.148300
C	0.650200	-0.608100	2.999300
O	1.575200	-4.096600	3.776800
Rh	1.001600	0.019300	1.100100
C	2.067600	-3.936400	2.438800
C	0.210700	0.351200	4.005500
C	-0.080800	0.012300	5.349500
C	0.093600	1.715800	3.636400
C	-0.460800	0.992400	6.262400
H	-0.013500	-1.022400	5.663700
C	-0.277700	2.692500	4.553400
H	0.294800	2.015600	2.608600
C	-0.557700	2.331800	5.875400
H	-0.681500	0.706700	7.286900
H	-0.356400	3.729700	4.240100
H	-0.853200	3.089500	6.595800
C	2.944700	-2.105900	-0.052900
C	2.855100	-3.390700	-0.649200
C	3.982200	-1.235900	-0.557700
C	3.620500	-3.742000	-1.747600
H	2.103100	-4.079500	-0.284400
C	4.703700	-1.595700	-1.739700
C	4.529000	-2.826700	-2.324900
H	3.494600	-4.726000	-2.191400

H	5.435800	-0.900300	-2.133000
H	5.098600	-3.103100	-3.206200
C	0.921500	-2.974300	4.224600
O	0.408900	-2.965100	5.320400
H	3.148700	-4.119000	2.433300
H	1.581800	-4.694500	1.815800
C	4.448000	-0.140500	0.202400
C	2.754200	0.881200	1.838800
C	4.091800	0.135800	1.619600
H	2.651900	1.015300	2.918400
H	2.831700	1.871000	1.388900
H	4.918300	0.712300	2.067400
H	4.041900	-0.822100	2.149600
O	5.356600	0.634500	-0.375600
H	5.623900	1.359100	0.217400
P	1.124600	1.302200	-1.235600
P	-1.378200	-0.941000	0.397900
C	-1.990100	-0.664000	-1.339900
C	-2.024500	0.621600	-1.881000
C	-2.500500	-1.756400	-2.099600
C	-2.532700	0.819000	-3.218000
C	-1.679600	1.876400	-1.119600
C	-2.983300	-1.584500	-3.371800
H	-2.523800	-2.747100	-1.665500
C	-2.999000	-0.303900	-3.974500
C	-0.378200	2.387600	-1.003000
C	-2.796700	2.662700	-0.655000
H	-3.370800	-2.435400	-3.926800
C	-0.201400	3.715400	-0.516300
C	-2.579200	3.974900	-0.121500
C	-1.259600	4.484000	-0.098400
H	0.783100	4.159300	-0.517800
H	-1.089800	5.502200	0.243300
C	-1.308000	-2.781600	0.585500
C	-1.814400	-3.396300	1.742400
C	-0.657800	-3.586600	-0.366100
C	-1.703600	-4.777200	1.926800
H	-2.306400	-2.802200	2.504500

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C	-0.571500	-4.969500	-0.194200
H	-0.237100	-3.138700	-1.261200
C	-1.095100	-5.570900	0.954100
H	-2.102500	-5.228700	2.830300
H	-0.100400	-5.578400	-0.961900
H	-1.029000	-6.646800	1.087800
C	-2.904300	-0.509500	1.355600
C	-4.113400	-1.180300	1.091300
C	-2.894300	0.509700	2.313300
C	-5.273000	-0.848700	1.788300
H	-4.150000	-1.968000	0.344900
C	-4.058900	0.843200	3.010600
H	-1.981300	1.050000	2.524300
C	-5.247500	0.163300	2.753500
H	-6.196800	-1.381100	1.579600
H	-4.028100	1.633900	3.754600
H	-6.152000	0.417900	3.298700
C	0.962500	0.547100	-2.907800
C	1.215100	-0.820600	-3.077300
C	0.666500	1.330500	-4.036400
C	1.170200	-1.397200	-4.348800
H	1.448600	-1.437300	-2.216000
C	0.622700	0.754000	-5.304600
H	0.472500	2.392900	-3.924200
C	0.874700	-0.611600	-5.463200
H	1.368300	-2.458900	-4.466000
H	0.385000	1.369100	-6.167500
H	0.839800	-1.059300	-6.452300
C	2.592700	2.432800	-1.483800
C	3.004700	3.356100	-0.500300
C	3.418200	2.285600	-2.613800
C	4.167900	4.114200	-0.652800
H	2.417200	3.507100	0.397000
C	4.584700	3.038400	-2.763800
H	3.155900	1.579100	-3.391000
H	4.440700	4.832800	0.115600
H	5.192600	2.904500	-3.654200
C	-3.681300	4.747300	0.333800

C	-4.138600	2.185300	-0.708000
C	-4.961400	4.249200	0.271200
H	-5.799800	4.845200	0.619700
C	-5.186200	2.953300	-0.252200
H	-6.197500	2.559600	-0.294400
H	-3.491600	5.742200	0.728600
H	-4.335700	1.193800	-1.096300
C	-2.592100	2.101100	-3.837200
C	-3.486600	-0.115500	-5.295300
C	-3.071600	2.254500	-5.119600
H	-3.107400	3.244900	-5.564800
C	-3.523700	1.137700	-5.861200
H	-3.903300	1.274200	-6.869700
H	-2.254200	2.973900	-3.291400
H	-3.836500	-0.983500	-5.848400
C	4.965400	3.959400	-1.788100
H	5.866900	4.552800	-1.912000

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Model TS DE

C	2.269600	-1.622800	1.035400
C	1.879500	-2.488400	2.070000
C	1.068600	-1.981100	3.107400
C	0.572900	-0.682900	2.920100
O	1.816100	-4.059300	3.796900
P	1.016500	1.233900	-1.181900
P	-1.387600	-0.886900	0.460000
C	-1.955400	-0.695700	-1.307200
C	-2.050800	0.568000	-1.894700
C	-2.368400	-1.841800	-2.045500
C	-2.527100	0.690000	-3.251200
C	-1.762000	1.855300	-1.168300
C	-2.822000	-1.740600	-3.336700
H	-2.343900	-2.817700	-1.579600
C	-2.903000	-0.483600	-3.981300
C	-0.464700	2.349500	-0.984900
C	-2.891000	2.656800	-0.771400
H	-3.136300	-2.632000	-3.874100



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C	-0.286200	3.666400	-0.474000
C	-2.680900	3.968000	-0.231200
C	-1.355700	4.451200	-0.117500
H	0.709800	4.080500	-0.389600
H	-1.190500	5.461100	0.250000
C	-1.342800	-2.712600	0.755700
C	-1.955000	-3.274200	1.887000
C	-0.594000	-3.553800	-0.085100
C	-1.844800	-4.641100	2.154600
H	-2.522100	-2.649400	2.567800
C	-0.508900	-4.924300	0.167100
H	-0.090800	-3.143500	-0.955300
C	-1.132500	-5.473300	1.290700
H	-2.322300	-5.052000	3.039100
H	0.040500	-5.565100	-0.518400
H	-1.063100	-6.538700	1.490300
C	-2.932300	-0.375100	1.344000
C	-4.144300	-1.029600	1.052100
C	-2.937300	0.672800	2.269700
C	-5.322300	-0.655600	1.694500
H	-4.168400	-1.837900	0.327300
C	-4.121000	1.050100	2.910200
H	-2.021500	1.199600	2.499800
C	-5.312600	0.385000	2.628900
H	-6.248100	-1.176500	1.466300
H	-4.103300	1.863300	3.629900
H	-6.231600	0.673800	3.131100
C	0.955800	0.610300	-2.913800
C	1.218900	-0.743900	-3.160900
C	0.690300	1.461900	-3.999900
C	1.224600	-1.237700	-4.467200
H	1.412500	-1.414700	-2.330100
C	0.699900	0.968300	-5.303800
H	0.471100	2.511400	-3.825900
C	0.968000	-0.382800	-5.539600
H	1.427200	-2.290100	-4.644500
H	0.487100	1.635500	-6.133800
H	0.971000	-0.766600	-6.555800

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C	2.478500	2.394900	-1.225100
C	2.865800	3.070700	-0.050600
C	3.273700	2.568800	-2.370000
C	3.995300	3.891100	-0.022300
H	2.276600	2.966200	0.854900
C	4.408100	3.385000	-2.343900
H	3.018200	2.061300	-3.292000
H	4.257500	4.413800	0.893800
H	5.001200	3.502500	-3.246500
C	-3.795500	4.760400	0.154800
C	-4.234300	2.197200	-0.893700
C	-5.077600	4.281800	0.021800
H	-5.924800	4.893400	0.318100
C	-5.293500	2.984800	-0.503300
H	-6.307200	2.606800	-0.598900
H	-3.613300	5.754100	0.556100
H	-4.422800	1.205000	-1.285000
C	-2.643500	1.945400	-3.915700
C	-3.367200	-0.367400	-5.319000
C	-3.099200	2.028000	-5.213000
H	-3.181800	2.999400	-5.692500
C	-3.465900	0.862400	-5.926600
H	-3.828000	0.943400	-6.947500
H	-2.370900	2.853500	-3.391700
H	-3.649400	-1.272400	-5.851100
C	4.777200	4.048400	-1.172000
H	5.651800	4.692900	-1.156500
Rh	0.851300	-0.090800	0.991300
C	2.336300	-3.871900	2.474500
C	0.175700	0.280900	3.941500
C	-0.036200	-0.049400	5.303600
C	0.072200	1.649900	3.581900
C	-0.324200	0.939800	6.239800
H	0.020500	-1.085300	5.614800
C	-0.187900	2.637100	4.526400
H	0.188800	1.935800	2.538300
C	-0.392200	2.284200	5.864000
H	-0.490500	0.657300	7.275500

H	-0.251900	3.677300	4.219000
H	-0.612700	3.049400	6.603100
C	3.068400	-2.053700	-0.084600
C	2.893800	-3.372500	-0.590700
C	4.007000	-1.225100	-0.817900
C	3.493000	-3.804200	-1.757400
H	2.201200	-4.032000	-0.086700
C	4.557800	-1.676300	-2.063600
C	4.315000	-2.942700	-2.525100
H	3.301300	-4.814800	-2.108200
H	5.211700	-1.006200	-2.609200
H	4.753300	-3.287600	-3.455900
C	1.053500	-2.992300	4.201300
O	0.490600	-3.016500	5.271500
H	3.426700	-3.983300	2.502500
H	1.921600	-4.673200	1.854000
C	4.533600	-0.066600	-0.241400
C	2.946700	0.161800	1.817500
C	4.332100	0.311900	1.190400
H	3.037400	-0.239300	2.822900
H	2.496100	1.161800	1.929800
H	4.708100	1.332400	1.336100
H	5.032300	-0.345000	1.734000
O	5.435600	0.614100	-0.935200
H	5.646300	1.462100	-0.501500

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Model E

C	3.060200	-2.243500	1.360800
C	2.056800	-2.461400	2.335900
C	1.200200	-1.510000	2.922900
C	0.716600	-0.256600	2.455100
O	1.073600	-3.397000	4.270900
P	0.504500	1.659300	-1.395800
P	-1.505400	-0.775500	0.230500
C	-2.247700	-0.445000	-1.454300
C	-2.470900	0.834500	-1.984100
C	-2.562900	-1.589700	-2.244800

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C	-2.975000	0.963200	-3.332300
C	-2.259100	2.130900	-1.240700
C	-3.060900	-1.477400	-3.518000
H	-2.417900	-2.578700	-1.830800
C	-3.270200	-0.207600	-4.103800
C	-0.990700	2.705300	-1.109900
C	-3.412400	2.862000	-0.788500
H	-3.300400	-2.371000	-4.089000
C	-0.849500	4.009700	-0.563700
C	-3.244000	4.162700	-0.204800
C	-1.942800	4.715800	-0.123800
H	0.135200	4.457400	-0.494500
H	-1.819100	5.716400	0.283300
C	-1.214800	-2.606700	0.232200
C	-2.071600	-3.505400	0.885300
C	-0.096600	-3.114400	-0.451200
C	-1.818600	-4.879800	0.848700
H	-2.940200	-3.140500	1.421700
C	0.141700	-4.487200	-0.506900
H	0.584500	-2.425700	-0.943400
C	-0.718400	-5.374900	0.147800
H	-2.490300	-5.561200	1.363100
H	1.000900	-4.862800	-1.055300
H	-0.533900	-6.445000	0.107800
C	-2.921600	-0.598400	1.403200
C	-4.245100	-0.549200	0.936100
C	-2.695700	-0.620900	2.789800
C	-5.313200	-0.500500	1.833400
H	-4.446600	-0.564000	-0.128600
C	-3.765900	-0.580800	3.683800
H	-1.692600	-0.690800	3.191800
C	-5.077000	-0.512000	3.208700
H	-6.330200	-0.458700	1.453700
H	-3.565700	-0.607100	4.750900
H	-5.909400	-0.475400	3.905700
C	0.599600	1.297000	-3.192000
C	1.018700	0.022100	-3.598500
C	0.306200	2.265500	-4.165800

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C	1.151000	-0.279700	-4.955000
H	1.231500	-0.736300	-2.849600
C	0.438800	1.962100	-5.520700
H	-0.029400	3.254100	-3.865100
C	0.862400	0.690500	-5.916400
H	1.472200	-1.271600	-5.260200
H	0.206800	2.716000	-6.267500
H	0.961600	0.456000	-6.972500
C	1.981700	2.722800	-1.065800
C	2.252900	3.084000	0.269900
C	2.915200	3.066600	-2.056000
C	3.418200	3.777400	0.600600
H	1.535700	2.845100	1.053200
C	4.081700	3.759200	-1.721500
H	2.733700	2.797800	-3.090900
H	3.601100	4.060200	1.633700
H	4.787200	4.027300	-2.503300
C	-4.381600	4.882800	0.251000
C	-4.740000	2.358400	-0.909700
C	-5.645500	4.355300	0.130600
H	-6.509000	4.914400	0.479000
C	-5.822000	3.081200	-0.460800
H	-6.823100	2.673000	-0.566300
H	-4.231700	5.865400	0.691300
H	-4.899000	1.392700	-1.373800
C	-3.195800	2.229300	-3.951000
C	-3.771600	-0.079400	-5.427100
C	-3.680000	2.323100	-5.236700
H	-3.839800	3.302200	-5.679600
C	-3.976000	1.159800	-5.986200
H	-4.363300	1.249800	-6.996900
H	-2.979600	3.136800	-3.401200
H	-3.991900	-0.984100	-5.987900
C	4.337700	4.115700	-0.395900
H	5.241900	4.661900	-0.141800
Rh	0.495200	0.281900	0.570200
C	1.871400	-3.740100	3.138900
C	0.555600	0.861800	3.383400

C	1.424100	1.010000	4.495000
C	-0.371000	1.903800	3.123100
C	1.377000	2.144600	5.293900
H	2.144400	0.227900	4.710600
C	-0.421900	3.034200	3.933600
H	-1.066700	1.792400	2.298800
C	0.452300	3.159300	5.017300
H	2.052500	2.240000	6.139100
H	-1.150100	3.812800	3.726600
H	0.409900	4.041000	5.650900
C	3.852600	-3.248300	0.741900
C	3.551800	-4.648200	0.788300
C	5.028000	-2.894100	-0.065200
C	4.292900	-5.585200	0.111500
H	2.671400	-4.986400	1.311300
C	5.764500	-3.906500	-0.775900
C	5.416700	-5.221400	-0.685800
H	3.999000	-6.629900	0.167800
H	6.614500	-3.595700	-1.372800
H	5.978100	-5.983900	-1.215600
C	0.656500	-2.099400	4.184500
O	-0.074100	-1.609000	5.013100
H	2.811600	-4.177800	3.489300
H	1.312500	-4.498300	2.577200
C	5.507000	-1.594800	-0.048500
C	3.350700	-0.816300	0.921000
C	4.845100	-0.531100	0.762900
H	2.953800	-0.104600	1.647900
H	2.852900	-0.614500	-0.043700
H	4.989800	0.456700	0.306200
H	5.344700	-0.502500	1.747400
O	6.653200	-1.312200	-0.676600
H	6.867100	-0.368000	-0.588200

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Model F

C	3.006800	-2.336800	1.282100
C	2.112300	-2.435100	2.301400

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C	1.340000	-1.356000	2.960700
C	0.739100	-0.194200	2.439100
O	1.443700	-3.096000	4.467400
P	0.452700	1.693800	-1.393700
P	-1.488100	-0.785000	0.137400
C	-2.276700	-0.400000	-1.518100
C	-2.512800	0.892800	-2.009900
C	-2.602900	-1.522800	-2.335600
C	-3.025900	1.056500	-3.351300
C	-2.303900	2.171000	-1.235700
C	-3.118300	-1.377500	-3.598300
H	-2.450100	-2.523000	-1.953600
C	-3.330700	-0.093300	-4.149900
C	-1.035900	2.741100	-1.090300
C	-3.457800	2.893100	-0.770900
H	-3.364300	-2.256200	-4.189200
C	-0.894600	4.036900	-0.524400
C	-3.288800	4.181300	-0.159900
C	-1.987900	4.734200	-0.070800
H	0.090000	4.483900	-0.450400
H	-1.864800	5.728100	0.352400
C	-1.177700	-2.611700	0.041500
C	-2.060400	-3.559700	0.582400
C	-0.035600	-3.063700	-0.639600
C	-1.806600	-4.926800	0.439700
H	-2.953400	-3.239100	1.107200
C	0.204400	-4.427800	-0.802000
H	0.662800	-2.337700	-1.046000
C	-0.680200	-5.364400	-0.258200
H	-2.499400	-5.647400	0.865200
H	1.084700	-4.759000	-1.345400
H	-0.494100	-6.427700	-0.382200
C	-2.888600	-0.704700	1.344800
C	-4.216100	-0.537200	0.925000
C	-2.638400	-0.906000	2.712900
C	-5.262400	-0.547400	1.850600
H	-4.439100	-0.410800	-0.127200
C	-3.683600	-0.926900	3.635300

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H	-1.621900	-1.062200	3.057300
C	-5.000300	-0.739700	3.206700
H	-6.283200	-0.409700	1.505800
H	-3.470000	-1.089800	4.688000
H	-5.814900	-0.750100	3.925100
C	0.571000	1.386400	-3.196300
C	0.993800	0.125700	-3.641200
C	0.298900	2.392400	-4.137600
C	1.148900	-0.126000	-5.005300
H	1.196700	-0.659500	-2.917800
C	0.453700	2.138300	-5.500100
H	-0.034600	3.371800	-3.806100
C	0.879500	0.880100	-5.934800
H	1.475900	-1.105900	-5.341200
H	0.239900	2.920800	-6.222400
H	0.998400	0.684900	-6.996800
C	1.938600	2.710700	-0.991200
C	2.148100	3.078600	0.354700
C	2.946900	2.985000	-1.928800
C	3.329300	3.712000	0.744700
H	1.371700	2.895000	1.094800
C	4.127000	3.618100	-1.533400
H	2.813900	2.705200	-2.968200
H	3.468300	3.998500	1.783400
H	4.894800	3.828600	-2.272400
C	-4.426500	4.891800	0.311200
C	-4.786600	2.395500	-0.907100
C	-5.691000	4.368500	0.178800
H	-6.554200	4.921300	0.537600
C	-5.868500	3.108800	-0.442800
H	-6.870400	2.706300	-0.562600
H	-4.276200	5.865400	0.770900
H	-4.947300	1.444600	-1.400800
C	-3.243500	2.338400	-3.938100
C	-3.841200	0.069000	-5.465900
C	-3.734200	2.465600	-5.218400
H	-3.888800	3.455800	-5.637400
C	-4.042600	1.322400	-5.993300



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H	-4.435300	1.439000	-6.999200
H	-3.016800	3.231600	-3.369500
H	-4.068700	-0.820800	-6.047300
C	4.322900	3.981400	-0.199200
H	5.242700	4.474400	0.102000
Rh	0.481500	0.308100	0.533600
C	1.945500	-3.642200	3.201300
C	0.518700	0.967600	3.330000
C	1.531400	1.366200	4.244100
C	-0.622600	1.797300	3.212400
C	1.397400	2.524900	5.009000
H	2.443700	0.779300	4.312500
C	-0.755400	2.945200	3.990100
H	-1.405600	1.518500	2.518100
C	0.250500	3.314400	4.888900
H	2.192400	2.815100	5.690000
H	-1.647300	3.556700	3.890800
H	0.144700	4.214800	5.486900
C	3.848900	-3.470500	0.835900
C	3.391500	-4.801400	0.842100
C	5.160400	-3.225900	0.347400
C	4.208400	-5.850300	0.420600
H	2.366800	-5.016800	1.122800
C	5.970700	-4.288000	-0.072200
C	5.506800	-5.599000	-0.030600
H	3.823300	-6.866300	0.433500
H	6.969400	-4.052100	-0.425400
H	6.143300	-6.416800	-0.354700
C	1.118000	-1.839700	4.275500
O	0.536200	-1.288500	5.314400
H	2.868600	-4.178200	3.426100
H	1.179500	-4.353000	2.874000
C	5.727600	-1.844900	0.274700
C	3.337800	-1.034200	0.585700
C	4.832600	-0.710200	0.750700
H	2.742900	-0.201300	0.986400
H	3.103100	-1.110600	-0.483300
H	5.112800	0.199200	0.210900

H	5.056800	-0.538000	1.813900
O	6.856400	-1.632400	-0.135600
H	0.420000	-0.329200	5.145300

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Model G

C	3.979000	-3.299700	2.420900
C	2.624200	-3.216800	2.432100
C	1.697900	-2.149000	1.960700
C	1.647000	-1.187800	0.981100
O	0.541800	-3.353800	3.558400
P	-0.169700	2.357100	-0.782900
P	-1.625900	-0.637400	-0.041900
C	-2.228100	-0.248800	-1.765100
C	-2.685000	1.022100	-2.140800
C	-2.103200	-1.267200	-2.752800
C	-2.973200	1.287500	-3.529200
C	-2.956000	2.135400	-1.162500
C	-2.401400	-1.032600	-4.071300
H	-1.787900	-2.260200	-2.462600
C	-2.829800	0.244900	-4.502100
C	-1.930800	2.881400	-0.577000
C	-4.326400	2.485300	-0.894400
H	-2.313300	-1.835000	-4.799600
C	-2.242700	3.987700	0.260200
C	-4.618300	3.596400	-0.036300
C	-3.545800	4.335200	0.519800
H	-1.440800	4.571500	0.696400
H	-3.766600	5.189700	1.154700
C	-1.610800	-2.494500	0.059500
C	-2.542200	-3.235600	0.802500
C	-0.573900	-3.188300	-0.592000
C	-2.451300	-4.628600	0.873400
H	-3.336100	-2.734700	1.343000
C	-0.495400	-4.579600	-0.537300
H	0.176100	-2.631700	-1.146500
C	-1.436100	-5.306000	0.198500
H	-3.181500	-5.181100	1.457900

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H	0.300700	-5.095700	-1.067400
H	-1.376700	-6.389900	0.244600
C	-3.000900	-0.130500	1.073700
C	-4.323200	-0.531500	0.814500
C	-2.740200	0.643200	2.212600
C	-5.350600	-0.188700	1.692600
H	-4.552500	-1.107700	-0.077300
C	-3.769700	0.991800	3.087800
H	-1.728800	0.990300	2.406100
C	-5.075100	0.570300	2.832600
H	-6.367600	-0.504800	1.480200
H	-3.551300	1.593800	3.965200
H	-5.877300	0.838500	3.514000
C	0.235700	2.695500	-2.541100
C	1.031800	1.780100	-3.244100
C	-0.212200	3.857900	-3.190800
C	1.383400	2.027500	-4.572500
H	1.370300	0.873400	-2.751500
C	0.145400	4.104400	-4.516000
H	-0.842200	4.568200	-2.662500
C	0.943900	3.189800	-5.208100
H	1.996800	1.310400	-5.110700
H	-0.204200	5.006300	-5.010500
H	1.216800	3.381500	-6.242000
C	0.819700	3.580100	0.187400
C	0.848600	3.442300	1.588500
C	1.602100	4.581400	-0.406600
C	1.625600	4.294000	2.373700
H	0.256700	2.664100	2.064300
C	2.385500	5.428800	0.382100
H	1.605300	4.703800	-1.484200
H	1.629000	4.179300	3.454100
H	2.983900	6.200900	-0.093600
C	-5.970400	3.944200	0.230100
C	-5.426000	1.767200	-1.447400
C	-7.005500	3.229400	-0.325700
H	-8.035600	3.506200	-0.120800
C	-6.725600	2.129500	-1.171700

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H	-7.545300	1.567300	-1.610100
H	-6.169900	4.791900	0.880700
H	-5.234900	0.922600	-2.098700
C	-3.403500	2.565500	-3.991800
C	-3.128900	0.502500	-5.866800
C	-3.681700	2.787100	-5.321900
H	-4.007800	3.771600	-5.645400
C	-3.549500	1.747100	-6.272600
H	-3.778900	1.935800	-7.317300
H	-3.511700	3.378400	-3.284500
H	-3.018700	-0.306700	-6.584200
C	2.398500	5.289900	1.770500
H	3.007000	5.952000	2.379800
Rh	0.477100	0.245000	0.185100
C	1.711600	-4.178100	3.177800
C	2.662800	-0.762300	0.026000
C	3.143900	-1.560400	-1.043700
C	3.046600	0.605900	0.084000
C	3.987300	-1.011400	-1.996400
H	2.857700	-2.606600	-1.095700
C	3.891100	1.145900	-0.903600
H	2.792600	1.202100	0.958700
C	4.361100	0.344800	-1.934400
H	4.369000	-1.637600	-2.798200
H	4.187300	2.188300	-0.835600
H	5.026400	0.756900	-2.686900
C	4.706900	-4.490500	2.914400
C	4.208700	-5.795600	2.748300
C	5.977400	-4.339200	3.527600
C	4.916600	-6.904200	3.210000
H	3.283900	-5.953100	2.202400
C	6.678600	-5.459300	3.989500
C	6.151900	-6.739000	3.842700
H	4.510100	-7.900500	3.059800
H	7.641300	-5.293800	4.462400
H	6.702300	-7.602700	4.203500
C	0.548600	-2.297500	2.800500
O	-0.434300	-1.470500	2.919500

H	2.127300	-4.578900	4.101700
H	1.292000	-4.988500	2.573800
C	6.604000	-2.993500	3.702700
C	4.876800	-2.152900	2.015800
C	5.816900	-1.800700	3.185200
H	4.300200	-1.271100	1.743200
H	5.475500	-2.432000	1.137900
H	6.528100	-1.017100	2.907500
H	5.222400	-1.411200	4.025000
O	7.688800	-2.855600	4.242900
H	-0.278600	-0.745200	2.229900

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Model H

C	3.898600	-3.117300	2.523200
C	2.549300	-3.219900	2.392000
C	1.558400	-2.237500	1.907900
C	1.585600	-1.349200	0.895100
O	0.437300	-3.715100	3.307900
P	-0.130100	2.333100	-0.834900
P	-1.669900	-0.732100	-0.040800
C	-2.253100	-0.283900	-1.752000
C	-2.676700	1.006100	-2.115900
C	-2.150400	-1.293700	-2.753900
C	-2.961000	1.289300	-3.500800
C	-2.921100	2.121100	-1.132500
C	-2.440100	-1.036700	-4.069900
H	-1.867200	-2.298900	-2.474600
C	-2.840500	0.254100	-4.485700
C	-1.878800	2.856800	-0.564200
C	-4.283300	2.496100	-0.856200
H	-2.371100	-1.833300	-4.806200
C	-2.163300	3.968400	0.275400
C	-4.547700	3.608600	0.009100
C	-3.458200	4.330400	0.554600
H	-1.347700	4.542700	0.698200
H	-3.659400	5.185400	1.195000
C	-1.681900	-2.576900	0.018400

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C	-2.649100	-3.283700	0.747300
C	-0.684100	-3.299400	-0.659500
C	-2.631700	-4.679700	0.775300
H	-3.404700	-2.753900	1.313600
C	-0.675200	-4.693300	-0.637800
H	0.089600	-2.773600	-1.210800
C	-1.651800	-5.388200	0.080900
H	-3.384300	-5.210200	1.351000
H	0.094000	-5.235900	-1.180700
H	-1.644400	-6.474200	0.102100
C	-2.955600	-0.179500	1.136700
C	-4.304000	-0.424900	0.822700
C	-2.634900	0.409000	2.366800
C	-5.309600	-0.088000	1.727600
H	-4.571500	-0.875800	-0.128100
C	-3.645300	0.754600	3.263600
H	-1.598600	0.564900	2.640100
C	-4.981900	0.505700	2.947900
H	-6.347300	-0.280000	1.472500
H	-3.384200	1.207500	4.215500
H	-5.766000	0.770500	3.651400
C	0.247400	2.747100	-2.583600
C	1.045900	1.872900	-3.335300
C	-0.214300	3.934400	-3.175800
C	1.381900	2.180900	-4.655000
H	1.411100	0.951800	-2.889000
C	0.126400	4.241800	-4.492700
H	-0.838100	4.618700	-2.607400
C	0.923900	3.365500	-5.233800
H	1.998400	1.495400	-5.229400
H	-0.233100	5.163200	-4.941700
H	1.184600	3.605500	-6.260600
C	0.907200	3.494700	0.158800
C	0.880400	3.399200	1.563800
C	1.788100	4.410600	-0.436700
C	1.701600	4.208400	2.348400
H	0.207100	2.697700	2.048000
C	2.616000	5.213500	0.352900

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H	1.831000	4.504200	-1.516100
H	1.660200	4.127600	3.431000
H	3.289900	5.919000	-0.124900
C	-5.890900	3.978200	0.290500
C	-5.400400	1.805300	-1.408700
C	-6.943500	3.287000	-0.262000
H	-7.966500	3.580600	-0.046000
C	-6.690800	2.190500	-1.121000
H	-7.524200	1.649300	-1.560000
H	-6.069200	4.824400	0.948900
H	-5.231900	0.964000	-2.070600
C	-3.367400	2.580900	-3.949600
C	-3.136500	0.531600	-5.847100
C	-3.644200	2.821100	-5.276200
H	-3.952400	3.814600	-5.589000
C	-3.533900	1.788300	-6.238100
H	-3.762100	1.992500	-7.280100
H	-3.458900	3.388400	-3.234200
H	-3.044300	-0.272000	-6.573000
C	2.575300	5.116400	1.744000
H	3.218400	5.743400	2.354600
Rh	0.450700	0.117600	0.021300
C	1.690900	-4.343200	2.955200
C	2.629500	-0.999100	-0.061500
C	3.050800	-1.869700	-1.099800
C	3.072600	0.353900	-0.099100
C	3.910300	-1.417600	-2.090900
H	2.716800	-2.902800	-1.087700
C	3.925900	0.800100	-1.123300
H	2.846500	1.014800	0.736200
C	4.348200	-0.080600	-2.110500
H	4.252700	-2.106200	-2.858500
H	4.267000	1.830900	-1.119900
H	5.023300	0.256000	-2.891500
C	4.748900	-4.242500	2.970900
C	4.446800	-5.578600	2.647800
C	5.945500	-3.991800	3.691600
C	5.270100	-6.626000	3.056000

H	3.583600	-5.799000	2.029000
C	6.765500	-5.052000	4.096700
C	6.430800	-6.367200	3.791400
H	5.012500	-7.646400	2.786000
H	7.664900	-4.811100	4.654300
H	7.071000	-7.184200	4.110400
C	0.312000	-2.515400	2.691400
O	-0.676500	-1.829900	2.824700
H	2.103800	-4.799400	3.856700
H	1.460400	-5.132100	2.228500
C	6.367000	-2.603000	4.044200
C	4.640100	-1.812000	2.337500
C	5.438400	-1.481000	3.612900
H	3.947400	-0.996900	2.131900
H	5.328800	-1.879200	1.483400
H	6.034300	-0.571400	3.492400
H	4.736800	-1.299700	4.440800
O	7.397400	-2.378400	4.658000
H	0.075700	0.456600	1.459400

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Model TS HI

C	3.924400	-3.189600	2.506500
C	2.571100	-3.248600	2.378900
C	1.599400	-2.210900	1.993700
C	1.619100	-1.216200	1.082700
O	0.452400	-3.777300	3.272100
P	-0.175100	2.317700	-0.865200
P	-1.682700	-0.639800	-0.047900
C	-2.303000	-0.258800	-1.762500
C	-2.741600	1.014300	-2.154600
C	-2.208500	-1.294800	-2.736500
C	-3.042600	1.263600	-3.542200
C	-2.973200	2.146400	-1.190400
C	-2.517000	-1.074000	-4.055200
H	-1.909700	-2.289200	-2.434800
C	-2.927600	0.203900	-4.500700
C	-1.920200	2.874200	-0.632800



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C	-4.329500	2.535300	-0.908500
H	-2.451600	-1.889000	-4.771600
C	-2.189900	4.003900	0.188300
C	-4.579200	3.666200	-0.063000
C	-3.479700	4.387300	0.462200
H	-1.368300	4.576200	0.600900
H	-3.668400	5.257000	1.086500
C	-1.643100	-2.484500	0.046700
C	-2.595900	-3.212800	0.773100
C	-0.615500	-3.182600	-0.612300
C	-2.533000	-4.607300	0.821200
H	-3.377200	-2.699900	1.320400
C	-0.562600	-4.575500	-0.573500
H	0.144400	-2.634000	-1.161200
C	-1.523800	-5.292400	0.145200
H	-3.274400	-5.155000	1.395300
H	0.227000	-5.100200	-1.104800
H	-1.483000	-6.377400	0.179400
C	-2.972600	-0.110000	1.135100
C	-4.325700	-0.370600	0.858500
C	-2.623000	0.492700	2.351000
C	-5.309300	-0.036000	1.788100
H	-4.613000	-0.830200	-0.082600
C	-3.611600	0.832400	3.274600
H	-1.579700	0.672400	2.582200
C	-4.953400	0.567700	2.996200
H	-6.352200	-0.238600	1.563800
H	-3.330500	1.295900	4.215700
H	-5.721000	0.829600	3.718900
C	0.234100	2.617500	-2.627400
C	1.060800	1.704600	-3.298900
C	-0.227600	3.756500	-3.307500
C	1.424900	1.929100	-4.627600
H	1.420500	0.818100	-2.783100
C	0.141200	3.979400	-4.633800
H	-0.875100	4.467100	-2.801500
C	0.966900	3.066300	-5.295000
H	2.062200	1.214700	-5.140900

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H	-0.219900	4.862700	-5.152700
H	1.248800	3.240200	-6.329600
C	0.853000	3.521400	0.085000
C	0.851700	3.441000	1.491100
C	1.685700	4.462500	-0.538200
C	1.654300	4.290800	2.251900
H	0.216300	2.714100	1.990000
C	2.494300	5.307100	0.227800
H	1.707600	4.541500	-1.619600
H	1.635300	4.222400	3.335900
H	3.131600	6.033100	-0.269100
C	-5.917400	4.051100	0.221000
C	-5.455400	1.838200	-1.435100
C	-6.978800	3.353700	-0.306300
H	-7.998100	3.657700	-0.087200
C	-6.740600	2.236000	-1.142000
H	-7.581400	1.688800	-1.559000
H	-6.085000	4.912200	0.862800
H	-5.297000	0.981400	-2.079300
C	-3.457500	2.542000	-4.018900
C	-3.237400	0.446200	-5.866000
C	-3.746300	2.748100	-5.348900
H	-4.060900	3.732400	-5.683900
C	-3.641500	1.691600	-6.285300
H	-3.879500	1.868700	-7.330000
H	-3.546500	3.366600	-3.322500
H	-3.149300	-0.375200	-6.572300
C	2.480900	5.224900	1.620700
H	3.109100	5.884300	2.212500
Rh	0.432300	0.204900	0.125000
C	1.691100	-4.398300	2.854300
C	2.669900	-0.748200	0.180800
C	3.201100	-1.558600	-0.854900
C	3.048500	0.620100	0.230900
C	4.094300	-1.025700	-1.772500
H	2.916300	-2.605100	-0.903500
C	3.938600	1.147500	-0.721100
H	2.735000	1.235900	1.070500

C	4.463200	0.330700	-1.713600
H	4.514300	-1.664600	-2.544600
H	4.226200	2.192400	-0.656300
H	5.164800	0.732600	-2.438400
C	4.747200	-4.368700	2.854400
C	4.413100	-5.664800	2.419300
C	5.948700	-4.207400	3.592100
C	5.211900	-6.761900	2.735300
H	3.545000	-5.811300	1.785500
C	6.742800	-5.317100	3.905200
C	6.377300	-6.593300	3.489000
H	4.931000	-7.749400	2.379700
H	7.646800	-5.146000	4.480800
H	6.997900	-7.449200	3.736800
C	0.353100	-2.530200	2.764400
O	-0.602100	-1.815500	2.971000
H	2.100800	-4.935700	3.711200
H	1.436800	-5.117100	2.066400
C	6.402400	-2.863000	4.060700
C	4.699300	-1.893600	2.423700
C	5.504300	-1.686000	3.721000
H	4.032100	-1.044800	2.280000
H	5.387300	-1.915600	1.566900
H	6.124200	-0.786000	3.670900
H	4.807600	-1.550900	4.561700
O	7.435100	-2.717000	4.693400
H	0.377100	-0.200600	1.656800

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Model I

C	3.311200	-3.155900	3.280100
C	2.161700	-2.552200	3.701600
C	1.824700	-1.131600	3.731100
C	2.038300	-0.036100	2.955500
O	0.542300	-2.157000	5.379300
C	1.088400	-3.212600	4.560100
C	2.552700	0.105200	1.600600
C	2.551800	-0.948700	0.637200

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C	2.937600	1.381800	1.136300
C	3.082000	-0.775400	-0.658100
H	2.181600	-1.925700	0.925600
C	3.378500	1.579700	-0.191100
H	2.891800	2.232400	1.807300
C	3.513600	0.493300	-1.082900
H	3.126700	-1.625800	-1.328100
H	3.654500	2.578800	-0.510400
H	3.923400	0.641700	-2.075700
C	3.524700	-4.616600	3.352000
C	2.470000	-5.532800	3.178100
C	4.831500	-5.138600	3.537300
C	2.691600	-6.907400	3.229200
H	1.474200	-5.167800	2.950400
C	5.041800	-6.521400	3.587600
C	3.979000	-7.408100	3.444900
H	1.858300	-7.590300	3.088800
H	6.056600	-6.873500	3.743200
H	4.149700	-8.479600	3.489700
C	0.905800	-0.940000	4.906000
O	0.487500	0.096900	5.363800
H	1.480400	-3.987900	5.221400
H	0.255600	-3.629200	3.980900
C	6.017300	-4.241000	3.688100
C	4.516200	-2.369900	2.815700
C	5.746300	-2.746800	3.664300
H	4.342800	-1.296400	2.896400
H	4.726900	-2.586800	1.758300
H	6.648900	-2.239500	3.311600
H	5.580900	-2.424500	4.702700
O	7.144100	-4.684600	3.832600
H	1.676700	0.889500	3.403500
P	0.053000	2.592700	-1.284400
P	-0.808900	-0.534400	-0.794500
C	-1.837400	-0.149300	-2.290300
C	-2.536600	1.056100	-2.403600
C	-1.818000	-1.055900	-3.387900
C	-3.168600	1.395000	-3.653900

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C	-2.731000	2.003300	-1.252000
C	-2.440900	-0.757400	-4.574000
H	-1.322500	-2.012200	-3.287500
C	-3.112300	0.475400	-4.751600
C	-1.714100	2.832400	-0.768400
C	-4.053400	2.098100	-0.687100
H	-2.424400	-1.473600	-5.391700
C	-2.015900	3.808000	0.223400
C	-4.322700	3.068100	0.332800
C	-3.277900	3.926100	0.750200
H	-1.247000	4.489700	0.560100
H	-3.485200	4.687700	1.497600
C	-0.307500	-2.309100	-0.989900
C	-0.786700	-3.319000	-0.142100
C	0.625300	-2.655800	-1.985900
C	-0.350100	-4.639100	-0.292300
H	-1.505100	-3.084100	0.634800
C	1.050000	-3.974600	-2.141600
H	1.013900	-1.888000	-2.649100
C	0.564700	-4.971900	-1.290500
H	-0.738600	-5.408300	0.369500
H	1.758000	-4.224700	-2.927000
H	0.897100	-5.999100	-1.408800
C	-1.957500	-0.552800	0.639100
C	-3.235600	-1.128100	0.542400
C	-1.521400	-0.057400	1.875800
C	-4.053700	-1.208900	1.669300
H	-3.591500	-1.511900	-0.409400
C	-2.339300	-0.142300	3.004400
H	-0.538800	0.397600	1.949900
C	-3.606300	-0.719800	2.900000
H	-5.042500	-1.650400	1.585100
H	-1.979700	0.234800	3.957500
H	-4.246100	-0.787000	3.775300
C	0.088200	2.842300	-3.104200
C	0.883300	2.013100	-3.906800
C	-0.626700	3.894700	-3.700000
C	0.967600	2.233000	-5.282800

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H	1.423700	1.191100	-3.445500
C	-0.537300	4.114700	-5.074000
H	-1.252000	4.542200	-3.091800
C	0.259800	3.284800	-5.866800
H	1.583000	1.582400	-5.897900
H	-1.094400	4.930000	-5.526300
H	0.325200	3.456700	-6.937400
C	0.974400	4.052100	-0.610000
C	1.133800	4.184300	0.783000
C	1.587800	4.996900	-1.446500
C	1.862100	5.243900	1.322100
H	0.680100	3.456900	1.450100
C	2.331100	6.049900	-0.903800
H	1.490900	4.919900	-2.523200
H	1.958000	5.338700	2.400200
H	2.798900	6.770600	-1.568300
C	-5.625700	3.164500	0.891200
C	-5.126200	1.253500	-1.096300
C	-6.636000	2.333100	0.468600
H	-7.629800	2.414100	0.899100
C	-6.377700	1.367200	-0.533500
H	-7.177100	0.709900	-0.863900
H	-5.807200	3.910600	1.660500
H	-4.954300	0.507200	-1.862400
C	-3.854600	2.627600	-3.858400
C	-3.738300	0.805400	-5.983800
C	-4.447400	2.922000	-5.065800
H	-4.963800	3.869200	-5.194000
C	-4.394900	2.003200	-6.141300
H	-4.873000	2.247200	-7.085500
H	-3.909700	3.346800	-3.050300
H	-3.687800	0.089600	-6.800200
C	2.466900	6.180000	0.477700
H	3.039100	7.002700	0.896300
Rh	1.096100	0.707000	-0.509100

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C	3.393200	-1.861700	0.221900
C	2.732500	-2.640800	1.120400
C	1.906200	-2.222300	2.273500
C	1.105800	-1.067300	2.410200
O	2.569200	-4.390100	2.680100
P	0.406200	1.530700	-1.086500
P	-1.648900	-0.563200	0.632500
C	-2.026300	-0.724100	-1.180800
C	-2.315000	0.343400	-2.033300
C	-1.849800	-2.032100	-1.725400
C	-2.509600	0.093500	-3.442700
C	-2.367700	1.771700	-1.567200
C	-2.033200	-2.282800	-3.060000
H	-1.575200	-2.850200	-1.069300
C	-2.387700	-1.240200	-3.952200
C	-1.190200	2.458400	-1.256100
C	-3.624900	2.463000	-1.529400
H	-1.907800	-3.290500	-3.448400
C	-1.239100	3.844300	-0.946500
C	-3.653800	3.859000	-1.203300
C	-2.433600	4.524600	-0.929900
H	-0.320500	4.376000	-0.726000
H	-2.452100	5.588100	-0.704800
C	-2.345100	-2.153400	1.309800
C	-3.529600	-2.719700	0.801900
C	-1.715300	-2.799900	2.381200
C	-4.066800	-3.879900	1.360900
H	-4.027100	-2.271500	-0.051800
C	-2.244600	-3.969000	2.935400
H	-0.792000	-2.396900	2.772300
C	-3.427200	-4.509900	2.430300
H	-4.981600	-4.297700	0.950200
H	-1.713800	-4.475500	3.738600
H	-3.839000	-5.420900	2.854600
C	-2.803400	0.688100	1.377100
C	-2.271300	1.873300	1.907800
C	-4.187700	0.471600	1.478600
C	-3.095700	2.819400	2.518000

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H	-1.202200	2.047600	1.837200
C	-5.012100	1.417500	2.087800
H	-4.634400	-0.436700	1.092100
C	-4.469700	2.593100	2.610200
H	-2.663100	3.732500	2.917400
H	-6.080500	1.233200	2.154000
H	-5.114200	3.326400	3.086500
C	0.833400	0.986900	-2.790000
C	1.373600	-0.294200	-2.975600
C	0.661100	1.824500	-3.904700
C	1.758100	-0.722400	-4.247900
H	1.476300	-0.961200	-2.124200
C	1.045400	1.394500	-5.174400
H	0.221600	2.810600	-3.781200
C	1.599000	0.122700	-5.346800
H	2.178800	-1.715500	-4.377800
H	0.909200	2.049900	-6.029900
H	1.898000	-0.209100	-6.337000
C	1.680200	2.803000	-0.662800
C	1.762700	3.222300	0.679500
C	2.619300	3.299200	-1.580200
C	2.744100	4.126300	1.086700
H	1.055500	2.834000	1.408900
C	3.607100	4.197400	-1.167800
H	2.589800	2.982900	-2.617000
H	2.787900	4.443900	2.124900
H	4.328200	4.568600	-1.890400
C	-4.898600	4.544200	-1.169200
C	-4.862900	1.812400	-1.799000
C	-6.074600	3.883900	-1.439700
H	-7.020500	4.417100	-1.414100
C	-6.052900	2.503300	-1.754400
H	-6.985000	1.986600	-1.965500
H	-4.902700	5.603600	-0.925700
H	-4.861900	0.756200	-2.044700
C	-2.813800	1.129300	-4.372000
C	-2.601200	-1.492600	-5.332700
C	-3.014800	0.854400	-5.707200



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H	-3.252800	1.663800	-6.391600
C	-2.915200	-0.468600	-6.196400
H	-3.081000	-0.670800	-7.250600
H	-2.893800	2.151500	-4.023800
H	-2.510100	-2.513700	-5.694400
C	3.671300	4.614800	0.162500
H	4.440900	5.313200	0.478500
Rh	0.576700	-0.041300	0.775800
C	2.977600	-4.121800	1.310400
C	0.945800	-0.473800	3.750700
C	2.039600	-0.464400	4.651300
C	-0.230500	0.200700	4.147900
C	1.952600	0.166800	5.890900
H	2.972100	-0.935500	4.356300
C	-0.323500	0.817000	5.394800
H	-1.079400	0.224000	3.477400
C	0.769100	0.804300	6.273000
H	2.810000	0.164500	6.557600
H	-1.243700	1.322300	5.675600
H	0.700600	1.297700	7.238100
C	4.326200	-2.412400	-0.787000
C	4.078100	-3.619200	-1.465400
C	5.500400	-1.689600	-1.125600
C	4.973500	-4.111500	-2.414400
H	3.152900	-4.157000	-1.285200
C	6.394300	-2.196900	-2.076600
C	6.141600	-3.405900	-2.717400
H	4.751900	-5.044000	-2.926200
H	7.286500	-1.617900	-2.292500
H	6.840600	-3.793200	-3.452500
C	1.948300	-3.330800	3.171400
O	1.413300	-3.582100	4.324900
H	4.022000	-4.422200	1.207200
H	2.355100	-4.776300	0.690900
C	5.827900	-0.382500	-0.479000
C	3.393600	-0.349700	0.246300
C	4.818200	0.167500	0.523100
H	2.730500	0.065900	1.030900

H	3.069500	0.043500	-0.721500
H	4.864400	1.259900	0.489900
H	5.140400	-0.144400	1.527000
O	6.856200	0.222500	-0.730700
H	0.776400	-2.921700	4.738700
O	-0.504500	-2.520000	5.710700
H	-0.533200	-1.568600	5.913800
H	-1.365000	-2.718800	5.306300

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Model TS JK

C	3.262400	-2.250200	0.836900
C	2.652400	-2.477500	2.049900
C	1.837100	-1.576100	2.829600
C	0.964400	-0.512300	2.500000
O	2.549500	-3.235200	4.294000
P	0.203100	1.660600	-1.170700
P	-1.741300	-0.746900	0.203600
C	-2.321500	-0.493500	-1.568100
C	-2.616100	0.740700	-2.161100
C	-2.294200	-1.658800	-2.393500
C	-2.936100	0.803300	-3.569400
C	-2.573300	2.060200	-1.444300
C	-2.606300	-1.613800	-3.727800
H	-2.017300	-2.612800	-1.970100
C	-2.949700	-0.394500	-4.354000
C	-1.352200	2.664100	-1.129200
C	-3.801000	2.758600	-1.184200
H	-2.583800	-2.525800	-4.319100
C	-1.330200	3.986800	-0.607200
C	-3.757900	4.086800	-0.644000
C	-2.497000	4.679400	-0.383400
H	-0.380300	4.461900	-0.391700
H	-2.461100	5.696400	-0.000500
C	-1.847300	-2.585600	0.378900
C	-3.055000	-3.287200	0.190800
C	-0.683500	-3.313900	0.654300

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C	-3.096000	-4.674900	0.311100
H	-3.962100	-2.752400	-0.075300
C	-0.725700	-4.706600	0.768400
H	0.259600	-2.789100	0.765300
C	-1.930300	-5.388700	0.606400
H	-4.035500	-5.200200	0.164500
H	0.186500	-5.257600	0.979800
H	-1.963400	-6.470500	0.697300
C	-3.030300	-0.118200	1.407500
C	-3.129500	1.264800	1.645300
C	-3.820300	-0.975800	2.198500
C	-4.020500	1.774200	2.591000
H	-2.489900	1.951200	1.107500
C	-4.693800	-0.464000	3.164600
H	-3.756200	-2.049900	2.082300
C	-4.808600	0.913100	3.356000
H	-4.088100	2.849100	2.732000
H	-5.290300	-1.151100	3.758400
H	-5.495000	1.308800	4.098700
C	0.512300	1.228800	-2.925000
C	0.982600	-0.053700	-3.240500
C	0.339000	2.170500	-3.953000
C	1.288900	-0.387600	-4.561100
H	1.094200	-0.792500	-2.451700
C	0.646700	1.834400	-5.270800
H	-0.036100	3.164200	-3.724400
C	1.124400	0.556600	-5.575600
H	1.652300	-1.384000	-4.796200
H	0.510700	2.568100	-6.060100
H	1.363700	0.298000	-6.603100
C	1.589900	2.783800	-0.706400
C	1.677700	3.218500	0.631700
C	2.625900	3.117800	-1.594900
C	2.764200	3.982100	1.061200
H	0.891000	2.969400	1.339200
C	3.712200	3.878900	-1.158700
H	2.587700	2.787700	-2.627100
H	2.811000	4.311100	2.095100

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H	4.502800	4.133100	-1.858900
C	-4.972900	4.777200	-0.384100
C	-5.077500	2.174000	-1.425500
C	-6.187700	4.181600	-0.632600
H	-7.111100	4.716700	-0.431300
C	-6.236400	2.865000	-1.152800
H	-7.199000	2.398100	-1.340600
H	-4.922900	5.786800	0.015900
H	-5.131200	1.167200	-1.824100
C	-3.227900	2.027900	-4.239800
C	-3.277200	-0.339500	-5.734800
C	-3.537100	2.052600	-5.581800
H	-3.759000	3.001100	-6.062700
C	-3.571200	0.859200	-6.340700
H	-3.823300	0.894700	-7.396500
H	-3.209100	2.959200	-3.688600
H	-3.287100	-1.266000	-6.303100
C	3.784200	4.313100	0.166800
H	4.631600	4.905200	0.500300
Rh	0.301500	0.164900	0.646500
C	3.027100	-3.619900	2.988400
C	0.975200	0.648200	3.418700
C	2.188300	1.074000	4.014400
C	-0.175200	1.441400	3.643700
C	2.239000	2.210300	4.814500
H	3.094000	0.505800	3.826200
C	-0.122300	2.579000	4.444100
H	-1.117700	1.155500	3.190000
C	1.083800	2.967600	5.036000
H	3.181100	2.511000	5.264400
H	-1.024000	3.161600	4.612000
H	1.124400	3.855100	5.661100
C	4.199400	-3.210100	0.218900
C	4.004400	-4.603400	0.290900
C	5.310600	-2.739700	-0.533600
C	4.885600	-5.492100	-0.320800
H	3.125400	-4.997900	0.788000
C	6.192200	-3.642900	-1.138700

C	5.991900	-5.015500	-1.030800
H	4.700900	-6.560500	-0.252600
H	7.034100	-3.235400	-1.689100
H	6.682000	-5.709400	-1.501200
C	1.806400	-2.116100	4.206200
O	1.064100	-1.780600	5.131900
H	4.104700	-3.794100	3.045100
H	2.533200	-4.570600	2.764600
C	5.584200	-1.279800	-0.693700
C	3.196300	-0.930600	0.102200
C	4.606600	-0.327200	-0.022900
H	2.545900	-0.214800	0.626200
H	2.777800	-1.071100	-0.900800
H	4.594900	0.611000	-0.585600
H	4.999000	-0.099500	0.979100
O	6.544500	-0.867800	-1.322900
H	-0.437000	-1.653300	4.383300
O	-1.054300	-1.673000	3.572400
H	-1.846500	-1.120800	3.728200
H	-0.337100	-1.144400	2.748200

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Model K

C	5.067000	-2.660300	0.456400
C	4.863300	-2.310100	1.758200
C	3.663400	-1.741000	2.378800
C	2.368900	-2.062800	2.094400
O	5.459200	-1.199900	3.742400
C	5.937500	-2.210500	2.826200
C	1.118700	-1.540500	2.640400
C	0.967500	-0.203500	3.119700
C	-0.018400	-2.372500	2.671500
C	-0.190800	0.227300	3.786200
H	1.797700	0.475900	3.031300
C	-1.228500	-1.899700	3.222600
H	0.032400	-3.384400	2.281300
C	-1.311000	-0.624600	3.829800

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H	-0.191800	1.207800	4.248300
H	-2.095800	-2.549400	3.229000
H	-2.227800	-0.318000	4.321500
C	6.342100	-3.235200	-0.026200
C	7.119300	-4.096200	0.770600
C	6.785600	-2.978100	-1.350300
C	8.306700	-4.647800	0.293200
H	6.767800	-4.381700	1.755900
C	7.982300	-3.534400	-1.817400
C	8.749200	-4.360000	-1.001300
H	8.880300	-5.315600	0.929700
H	8.287300	-3.299900	-2.832100
H	9.676600	-4.787300	-1.370700
C	4.154300	-0.923500	3.540200
O	3.563300	-0.143700	4.258300
H	6.909800	-1.889300	2.447000
H	6.070600	-3.127400	3.411800
C	6.001900	-2.112700	-2.281400
C	4.060600	-2.386600	-0.641100
C	4.709200	-1.526300	-1.741600
H	3.180900	-1.865200	-0.262900
H	3.714400	-3.334100	-1.078400
H	4.024100	-1.368700	-2.579900
H	4.943500	-0.534100	-1.327900
O	6.381600	-1.877300	-3.417200
H	2.232000	-2.879800	1.389300
P	-0.198700	1.185300	-0.204700
P	-3.007500	-0.329000	0.515700
C	-3.182700	-0.189400	-1.327100
C	-2.889500	1.002100	-1.996700
C	-3.555900	-1.343300	-2.072900
C	-2.907500	1.027600	-3.437600
C	-2.604300	2.293900	-1.281400
C	-3.604700	-1.323100	-3.444300
H	-3.826600	-2.254000	-1.555400
C	-3.265400	-0.153800	-4.165500
C	-1.404900	2.538800	-0.605500
C	-3.596600	3.336700	-1.363900

H	-3.906000	-2.213200	-3.990900
C	-1.155000	3.828900	-0.058200
C	-3.325100	4.623200	-0.793400
C	-2.079000	4.838800	-0.157700
H	-0.211600	4.029500	0.432900
H	-1.857800	5.820400	0.253800
C	-3.697000	-1.995700	0.937300
C	-4.872700	-2.160700	1.683200
C	-2.965000	-3.141700	0.571100
C	-5.310100	-3.439200	2.045400
H	-5.453000	-1.297500	1.988500
C	-3.410700	-4.415100	0.920100
H	-2.039600	-3.033000	0.012000
C	-4.586000	-4.567400	1.663000
H	-6.222000	-3.547000	2.625800
H	-2.840400	-5.288900	0.616700
H	-4.930600	-5.559000	1.941900
C	-4.232800	0.866800	1.189400
C	-3.886600	1.701800	2.260200
C	-5.533300	0.933000	0.660400
C	-4.826200	2.580700	2.802700
H	-2.873700	1.670500	2.650200
C	-6.471700	1.806200	1.209300
H	-5.813600	0.303000	-0.179200
C	-6.120000	2.630100	2.281900
H	-4.545500	3.228800	3.628200
H	-7.475000	1.848500	0.795300
H	-6.851500	3.312900	2.704400
C	0.235900	0.361000	-1.792300
C	0.436800	-1.026200	-1.811500
C	0.446700	1.097400	-2.969200
C	0.845700	-1.666800	-2.983200
H	0.258300	-1.598400	-0.904600
C	0.859300	0.457300	-4.138000
H	0.285600	2.171400	-2.975100
C	1.061100	-0.925300	-4.147100
H	0.989000	-2.744000	-2.989700
H	1.014700	1.037000	-5.042900

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H	1.378200	-1.422200	-5.059400
C	1.372000	2.044200	0.276200
C	1.477800	2.620700	1.555100
C	2.482800	2.112500	-0.581100
C	2.651700	3.253500	1.964900
H	0.642400	2.569700	2.245600
C	3.656300	2.750900	-0.172000
H	2.443200	1.671100	-1.569400
H	2.708900	3.650600	2.972900
H	4.501800	2.799300	-0.853000
C	-4.296700	5.656000	-0.883800
C	-4.861600	3.145900	-1.992100
C	-5.503000	5.436200	-1.506100
H	-6.239300	6.231800	-1.573200
C	-5.785600	4.164700	-2.059700
H	-6.742100	3.991000	-2.544600
H	-4.065500	6.625500	-0.449900
H	-5.102100	2.181200	-2.422100
C	-2.565100	2.189100	-4.189800
C	-3.281500	-0.131600	-5.586100
C	-2.582300	2.178500	-5.566800
H	-2.316200	3.078200	-6.114400
C	-2.947800	1.009700	-6.276800
H	-2.963400	1.018700	-7.362800
H	-2.284300	3.096800	-3.669400
H	-3.562600	-1.037800	-6.116600
C	3.745000	3.321200	1.098200
H	4.662400	3.809400	1.414700
Rh	-0.935100	-0.206600	1.469600
H	2.671000	1.522200	4.903600
O	2.033800	2.251000	5.010600
H	2.147500	2.543400	5.927100