

Supporting Information

for

**Comparing families of olefins polymerization
precatalysts using the percent of buried volume**

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Table S1. xyz coordinate data sets for **1-26** DFT optimized complexes.

1				2			
Zr	0.000000	0.000000	0.825137	Zr	0.000000	0.000000	0.669609
Si	0.000000	0.000000	-2.578424	Si	0.000000	0.000000	-2.707164
C	-0.746115	1.173953	-1.289703	C	-0.381035	1.341100	-1.424399
C	0.746115	-1.173953	-1.289703	C	0.381035	-1.341100	-1.424399
C	0.000000	2.142000	-0.528256	C	0.607896	2.071909	-0.674887
C	-0.749156	2.496591	0.639055	C	0.000000	2.661592	0.487332
C	-1.945205	1.733353	0.638820	C	-1.357547	2.231100	0.500950
C	-1.938230	0.904409	-0.528307	C	-1.593913	1.418540	-0.653167
H	0.982988	2.554344	-0.795617	H	1.663152	2.198017	-0.957548
H	-0.435529	3.207678	1.413298	H	-2.095961	2.478012	1.274834
H	-2.722585	1.747889	1.412654	H	-2.552930	0.944804	-0.905461
H	-2.726048	0.186664	-0.796806	C	-0.607896	-2.071909	-0.674887
C	0.000000	-2.142000	-0.528256	C	0.000000	-2.661592	0.487332
C	0.749156	-2.496591	0.639055	C	1.357547	-2.231100	0.500950
C	1.945205	-1.733353	0.638820	C	1.593913	-1.418540	-0.653167
C	1.938230	-0.904409	-0.528307	H	-1.663152	-2.198017	-0.957548
H	-0.982988	-2.554344	-0.795617	H	2.095961	-2.478012	1.274834
H	0.435529	-3.207678	1.413298	H	2.552930	-0.944804	-0.905461
H	2.722585	-1.747889	1.412654	C	0.652577	3.604173	1.456095
H	2.726048	-0.186664	-0.796806	H	0.755372	4.612742	0.999952
C	-1.324108	-0.839641	-3.626564	H	0.053935	3.709493	2.382183
H	-1.825109	-0.101825	-4.288018	H	1.664622	3.252091	1.741025
H	-0.874601	-1.625328	-4.269630	C	-0.652577	-3.604173	1.456095
H	-2.106911	-1.320001	-3.004050	H	-0.755372	-4.612742	0.999952
C	1.324108	0.839641	-3.626564	H	-0.053935	-3.709493	2.382183
H	1.825109	0.101825	-4.288018	H	-1.664622	-3.252091	1.741025
H	0.874601	1.625328	-4.269630	C	1.507751	0.428555	-3.757246
H	2.106911	1.320001	-3.004050	H	1.785700	-0.425526	-4.410023
Cl	-1.606678	-1.023048	2.355537	H	1.295340	1.302413	-4.408511
Cl	1.606678	1.023048	2.355537	H	2.390849	0.678549	-3.134057
				C	-1.507751	-0.428555	-3.757246
				H	-1.785700	0.425526	-4.410023
				H	-1.295340	-1.302413	-4.408511
				H	-2.390849	-0.678549	-3.134057
				Cl	-1.839170	-0.519959	2.198088
				Cl	1.839170	0.519959	2.198088

3				4			
Zr	0.000000	0.000000	0.155655	Zr	0.000000	0.000000	0.498694
Si	0.000000	0.000000	-3.195848	C	0.566501	1.297525	-1.587920
C	0.332646	1.359895	-1.934882	C	-0.566501	-1.297525	-1.587920
C	-0.332646	-1.359895	-1.934882	C	1.692340	1.421045	-0.707322
C	1.574010	1.464010	-1.205111	C	1.342318	2.218714	0.420795
C	1.387567	2.302318	-0.053821	C	0.000000	2.689571	0.222567
C	0.000000	2.630499	-0.023177	C	-0.499869	2.095657	-1.013505
C	-0.660945	2.073049	-1.168394	C	2.666732	0.937823	-0.865823
H	2.531283	1.026441	-1.519191	C	-0.824906	3.582048	0.969872
H	-0.498869	3.237315	0.743384	C	-1.821387	2.414246	-1.462363
C	-1.574010	-1.464010	-1.205111	C	-1.692340	-1.421045	-0.707322
C	-1.387567	-2.302318	-0.053821	C	-1.342318	-2.218714	0.420795
C	0.000000	-2.630499	-0.023177	C	0.000000	-2.689571	0.222567
C	0.660945	-2.073049	-1.168394	C	0.499869	-2.095657	-1.013505
H	-2.531283	-1.026441	-1.519191	H	-2.666732	-0.937823	-0.865823
H	0.498869	-3.237315	0.743384	C	0.824906	-3.582048	0.969872
C	2.473630	2.932983	0.823276	C	1.821387	-2.414246	-1.462363
C	-2.473630	-2.932983	0.823276	C	-2.094954	3.875527	0.496809
C	-2.656590	-4.389768	0.309137	C	-2.591140	3.294417	-0.713643
H	-3.457165	-4.900264	0.885994	H	-0.449095	4.027720	1.903506
H	-2.942390	-4.406456	-0.763429	H	-2.739452	4.569571	1.058620
H	-1.723287	-4.979278	0.423017	H	-3.602816	3.560284	-1.058630
C	2.656590	4.389768	0.309137	H	-2.208633	1.998054	-2.405242
H	3.457165	4.900264	0.885994	C	2.094954	-3.875527	0.496809
H	2.942390	4.406456	-0.763429	C	2.591140	-3.294417	-0.713643
H	1.723287	4.979278	0.423017	H	0.449095	-4.027720	1.903506
C	3.818632	2.187755	0.682294	H	2.739452	-4.569571	1.058620
H	3.726873	1.127881	0.991916	H	3.602816	-3.560284	-1.058630
H	4.197529	2.222203	-0.361020	H	2.208633	-1.998054	-2.405242
H	4.585314	2.669186	1.324378	C	-0.534866	-0.559434	-2.907162
C	-3.818632	-2.187755	0.682294	C	0.534866	0.559434	-2.907162
H	-3.726873	-1.127881	0.991916	H	-1.540038	-0.126096	-3.089131
H	-4.197529	-2.222203	-0.361020	H	-0.352130	-1.268528	-3.745328
H	-4.585314	-2.669186	1.324378	H	1.540038	0.126096	-3.089131
C	-2.051643	-2.976142	2.310582	H	0.352130	1.268528	-3.745328
H	-2.827367	-3.498879	2.908833	H	-1.997128	-2.462505	1.265662
H	-1.098756	-3.526945	2.452384	H	1.997128	2.462505	1.265662
H	-1.926668	-1.954622	2.720334	Cl	-1.786371	0.597900	2.038453
C	2.051643	2.976142	2.310582	Cl	1.786371	-0.597900	2.038453
H	2.827367	3.498879	2.908833				
H	1.098756	3.526945	2.452384				
H	1.926668	1.954622	2.720334				
C	-2.104685	2.314447	-1.528194				
H	-2.746372	2.327644	-0.624484				
H	-2.213430	3.298585	-2.034769				
H	-2.502138	1.548153	-2.223125				
C	2.104685	-2.314447	-1.528194				
H	2.746372	-2.327644	-0.624484				
H	2.213430	-3.298585	-2.034769				
H	2.502138	-1.548153	-2.223125				
H	-1.200677	0.265691	-4.055039				
H	1.200677	-0.265691	-4.055039				
Cl	-1.797180	0.600232	1.712847				
Cl	1.797180	-0.600232	1.712847				

5				6			
Zr	0.000000	0.000000	0.366861	Zr	0.000000	0.000000	0.692879
C	0.563588	1.296564	-1.694559	Si	0.000000	0.000000	-2.676320
C	-0.563588	-1.296564	-1.694559	C	0.901412	1.067308	-1.397874
C	1.694925	1.447066	-0.822542	C	-0.901412	-1.067308	-1.397874
C	1.362900	2.264093	0.301973	C	2.033805	0.578652	-0.644458
C	0.000000	2.696970	0.106148	C	2.235362	1.368968	0.521739
C	-0.505821	2.087265	-1.119058	C	1.261015	2.421625	0.510151
H	2.675709	0.977410	-0.987161	C	0.413305	2.224116	-0.664455
C	2.294727	2.724194	1.385785	H	2.639702	-0.299898	-0.910206
C	-0.826183	3.592689	0.848081	H	3.017098	1.218173	1.275945
C	-1.835762	2.386550	-1.556865	C	1.037184	3.528022	1.381943
C	-1.694925	-1.447066	-0.822542	C	-0.652083	3.148042	-0.914597
C	-1.362900	-2.264093	0.301973	C	-2.033805	-0.578652	-0.644458
C	0.000000	-2.696970	0.106148	C	-2.235362	-1.368968	0.521739
C	0.505821	-2.087265	-1.119058	C	-1.261015	-2.421625	0.510151
H	-2.675709	-0.977410	-0.987161	C	-0.413305	-2.224116	-0.664455
C	-2.294727	-2.724194	1.385785	H	-2.639702	0.299898	-0.910206
C	0.826183	-3.592689	0.848081	H	-3.017098	-1.218173	1.275945
C	1.835762	-2.386550	-1.556865	C	-1.037184	-3.528022	1.381943
C	-2.105407	3.867103	0.387130	C	0.652083	-3.148042	-0.914597
C	-2.608297	3.266403	-0.810518	C	0.000000	4.403337	1.097513
H	-0.447185	4.059268	1.770116	C	-0.839675	4.213706	-0.045962
H	-2.750329	4.561833	0.947686	H	1.680545	3.675235	2.263029
H	-3.626302	3.517007	-1.148314	H	-0.184468	5.264820	1.758297
H	-2.227928	1.955500	-2.490924	H	-1.647524	4.936709	-0.240566
C	2.105407	-3.867103	0.387130	H	-1.291991	3.032482	-1.801802
C	2.608297	-3.266403	-0.810518	C	0.000000	-4.403337	1.097513
H	0.447185	-4.059268	1.770116	C	0.839675	-4.213706	-0.045962
H	2.750329	-4.561833	0.947686	H	-1.680545	-3.675235	2.263029
H	3.626302	-3.517007	-1.148314	H	0.184468	-5.264820	1.758297
H	2.227928	-1.955500	-2.490924	H	1.647524	-4.936709	-0.240566
H	1.766349	2.863876	2.350339	H	1.291991	-3.032482	-1.801802
H	3.105620	1.989103	1.554206	C	1.227200	-0.941648	-3.761916
H	2.760487	3.697606	1.114400	H	0.718385	-1.752550	-4.324383
H	-1.766349	-2.863876	2.350339	H	1.679148	-0.246315	-4.500768
H	-3.105620	-1.989103	1.554206	H	2.057517	-1.394937	-3.183485
H	-2.760487	-3.697606	1.114400	C	-1.227200	0.941648	-3.761916
C	-0.535648	-0.557711	-3.014028	H	-0.718385	1.752550	-4.324383
C	0.535648	0.557711	-3.014028	H	-1.679148	0.246315	-4.500768
H	-1.540623	-0.122053	-3.192354	H	-2.057517	1.394937	-3.183485
H	-0.358744	-1.266706	-3.854199	Cl	-1.370373	1.279468	2.238123
H	1.540623	0.122053	-3.192354	Cl	1.370373	-1.279468	2.238123
H	0.358744	1.266706	-3.854199				
Cl	-1.785651	0.594905	1.913512				
Cl	1.785651	-0.594905	1.913512				

7				8			
Zr	0.000000	0.000000	0.660129	Zr	0.000000	0.000000	0.569916
C	0.000000	0.000000	-2.514261	Si	0.000000	0.000000	-2.766717
C	0.761181	0.910490	-1.519886	C	0.694664	1.215759	-1.495679
C	-0.761181	-0.910490	-1.519886	C	-0.694664	-1.215759	-1.495679
C	1.939714	0.478250	-0.811307	C	1.908824	0.963826	-0.750120
C	2.204087	1.343437	0.287759	C	1.986905	1.792213	0.409106
C	1.221720	2.383521	0.266778	C	0.806175	2.619853	0.403294
C	0.301824	2.116046	-0.844271	C	0.000000	2.258661	-0.759637
H	2.534203	-0.414010	-1.046941	H	2.677606	0.225611	-1.023936
H	3.033660	1.246536	0.997991	C	3.135851	1.894307	1.368274
C	1.050090	3.533540	1.094232	C	0.383465	3.669255	1.271609
C	-0.771139	3.043104	-1.071966	C	-1.226282	2.958357	-0.999467
C	-1.939714	-0.478250	-0.811307	C	-1.908824	-0.963826	-0.750120
C	-2.204087	-1.343437	0.287759	C	-1.986905	-1.792213	0.409106
C	-1.221720	-2.383521	0.266778	C	-0.806175	-2.619853	0.403294
C	-0.301824	-2.116046	-0.844271	C	0.000000	-2.258661	-0.759637
H	-2.534203	0.414010	-1.046941	H	-2.677606	-0.225611	-1.023936
H	-3.033660	-1.246536	0.997991	C	-3.135851	-1.894307	1.368274
C	-1.050090	-3.533540	1.094232	C	0.383465	-3.669255	1.271609
C	0.771139	-3.043104	-1.071966	C	1.226282	-2.958357	-0.999467
C	0.000000	4.397995	0.833995	C	-0.807726	4.326512	0.999836
C	-0.902284	4.151313	-0.248587	C	-1.608082	3.972242	-0.132133
H	1.750850	3.719668	1.922690	H	0.997173	3.949256	2.141739
H	-0.144393	5.291758	1.460684	H	-1.146465	5.139709	1.660812
H	-1.718985	4.866066	-0.436451	H	-2.542580	4.524257	-0.319747
H	-1.468204	2.904587	-1.908204	H	-1.841336	2.718287	-1.879203
C	0.000000	-4.397995	0.833995	C	0.807726	-4.326512	0.999836
C	0.902284	-4.151313	-0.248587	C	1.608082	-3.972242	-0.132133
H	-1.750850	-3.719668	1.922690	H	-0.997173	-3.949256	2.141739
H	0.144393	-5.291758	1.460684	H	1.146465	-5.139709	1.660812
H	1.718985	-4.866066	-0.436451	H	2.542580	-4.524257	-0.319747
H	1.468204	-2.904587	-1.908204	H	1.841336	-2.718287	-1.879203
C	0.981513	-0.755423	-3.436201	H	2.787894	2.057110	2.408199
H	0.452932	-1.552525	-3.998119	H	3.748101	0.971713	1.362654
H	1.419636	-0.046917	-4.169082	H	3.795173	2.748467	1.096579
H	1.824981	-1.219981	-2.894459	H	-2.787894	-2.057110	2.408199
C	-0.981513	0.755423	-3.436201	H	-3.748101	-0.971713	1.362654
H	-0.452932	1.552525	-3.998119	H	-3.795173	-2.748467	1.096579
H	-1.419636	0.046917	-4.169082	C	1.373213	-0.704857	-3.859787
H	-1.824981	1.219981	-2.894459	H	1.020581	-1.603876	-4.407770
Cl	-1.380724	1.292374	2.182871	H	1.672859	0.056292	-4.611170
Cl	1.380724	-1.292374	2.182871	H	2.281955	-0.983497	-3.289581
				C	-1.373213	0.704857	-3.859787
				H	-1.020581	1.603876	-4.407770
				H	-1.672859	-0.056292	-4.611170
				H	-2.281955	0.983497	-3.289581
				Cl	-1.579245	1.000025	2.123433
				Cl	1.579245	-1.000025	2.123433

9				10			
Zr	0.000000	0.000000	0.339044	Zr	0.000000	0.000000	0.167862
Si	0.000000	0.000000	-2.981118	Si	0.000000	0.000000	-3.211472
C	0.308699	1.362622	-1.711321	C	-0.437897	1.326428	-1.929800
C	1.542262	1.507078	-0.972105	C	0.437897	-1.326428	-1.929800
C	1.385700	2.373211	0.155033	C	0.575217	2.024567	-1.173634
C	0.000000	2.800831	0.142942	C	0.000000	2.610902	-0.008219
C	-0.663572	2.166331	-0.994752	C	-1.400141	2.321087	-0.015564
H	2.491205	1.027868	-1.249285	C	-1.672884	1.509222	-1.190849
C	2.528476	2.960809	0.995972	H	1.640496	2.086801	-1.437610
C	-0.744199	3.703865	0.962412	H	0.544320	3.195127	0.742867
C	-2.044904	2.438584	-1.254409	C	-2.470194	2.722681	0.876729
C	-2.080329	3.946619	0.675598	C	-3.023077	1.084014	-1.462531
C	-2.731118	3.317336	-0.429807	C	-0.575217	-2.024567	-1.173634
H	-0.269994	4.204166	1.818036	C	0.000000	-2.610902	-0.008219
H	-2.652636	4.642502	1.309035	C	1.400141	-2.321087	-0.015564
H	-3.790194	3.542715	-0.631237	C	1.672884	-1.509222	-1.190849
H	-2.546221	1.979118	-2.118629	H	-1.640496	-2.086801	-1.437610
C	2.243437	2.910161	2.517917	H	-0.544320	-3.195127	0.742867
C	3.852624	2.212591	0.720002	C	2.470194	-2.722681	0.876729
C	2.704123	4.442446	0.556243	C	3.023077	-1.084014	-1.462531
H	3.081228	3.385991	3.070155	C	-3.802664	2.287598	0.555060
H	1.317283	3.450786	2.794840	C	-4.037117	1.471823	-0.617108
H	2.144259	1.865139	2.869824	C	-2.260829	3.523424	2.026983
H	4.662664	2.638616	1.347876	C	-4.874243	2.681680	1.402742
H	3.763675	1.134648	0.962782	H	-5.074048	1.164720	-0.829565
H	4.170206	2.314712	-0.338944	H	-3.241966	0.480922	-2.355546
H	3.547389	4.906301	1.111223	C	3.802664	-2.287598	0.555060
H	2.926615	4.514556	-0.528956	C	4.037117	-1.471823	-0.617108
H	1.794392	5.044807	0.754777	C	2.260829	-3.523424	2.026983
C	-0.308699	-1.362622	-1.711321	C	4.874243	-2.681680	1.402742
C	-1.542262	-1.507078	-0.972105	H	5.074048	-1.164720	-0.829565
C	-1.385700	-2.373211	0.155033	H	3.241966	-0.480922	-2.355546
C	0.000000	-2.800831	0.142942	C	-3.331424	3.892561	2.844038
C	0.663572	-2.166331	-0.994752	H	-1.240517	3.850123	2.280446
H	-2.491205	-1.027868	-1.249285	H	-3.151724	4.511272	3.737334
C	-2.528476	-2.960809	0.995972	C	-4.645559	3.471316	2.529408
C	0.744199	-3.703865	0.962412	H	-5.895708	2.348065	1.157188
C	2.044904	-2.438584	-1.254409	H	-5.486682	3.765022	3.177104
C	2.080329	-3.946619	0.675598	C	3.331424	-3.892561	2.844038
C	2.731118	-3.317336	-0.429807	H	1.240517	-3.850123	2.280446
H	0.269994	-4.204166	1.818036	C	3.151724	-4.511272	3.737334
H	2.652636	-4.642502	1.309035	H	4.645559	-3.471316	2.529408
H	3.790194	-3.542715	-0.631237	H	5.895708	-2.348065	1.157188
H	2.546221	-1.979118	-2.118629	H	5.486682	-3.765022	3.177104
C	-2.243437	-2.910161	2.517917	C	-1.441400	-0.558322	-4.298426
C	-3.852624	-2.212591	0.720002	H	-1.877236	0.300713	-4.850526
C	-2.704123	-4.442446	0.556243	H	-1.077001	-1.293927	-5.046587
H	-3.081228	-3.385991	3.070155	H	-2.253585	-1.045831	-3.722672
H	-1.317283	-3.450786	2.794840	C	1.441400	0.558322	-4.298426
H	-2.144259	-1.865139	2.869824	H	1.877236	-0.300713	-4.850526
H	-4.662664	-2.638616	1.347876	H	1.077001	1.293927	-5.046587
H	-3.763675	-1.134648	0.962782	H	2.253585	1.045831	-3.722672
H	-4.170206	-2.314712	-0.338944	Cl	-1.813429	-0.499802	1.708099
H	-3.547389	-4.906301	1.111223	Cl	1.813429	0.499802	1.708099
H	-2.926615	-4.514556	-0.528956				
H	-1.794392	-5.044807	0.754777				
C	1.517105	-0.264185	-4.080370				
H	1.460328	-1.238899	-4.609070				
H	1.554413	0.537589	-4.848255				
H	2.473136	-0.230023	-3.520509				
C	-1.517105	0.264185	-4.080370				
H	-1.460328	1.238899	-4.609070				
H	-1.554413	-0.537589	-4.848255				
H	-2.473136	0.230023	-3.520509				
Cl	-1.773990	0.587810	1.893715				
Cl	1.773990	-0.587810	1.893715				

11				12			
Zr	0.000000	0.000000	0.276348	Zr	-0.955992	0.000000	-0.070311
Si	0.000000	0.000000	-3.092071	Si	1.298443	0.000000	2.405168
C	0.398509	1.351059	-1.809173	C	-0.597056	0.000000	2.429560
C	-0.398509	-1.351059	-1.809173	C	1.436477	0.000000	0.518260
C	1.616800	1.452118	-1.019045	C	-1.409662	1.148938	2.118717
C	1.348435	2.239504	0.143230	C	-2.701411	0.709675	1.682787
C	0.000000	2.704658	0.091141	C	-2.701411	-0.709675	1.682787
C	-0.595938	2.156918	-1.112386	C	-1.409662	-1.148938	2.118717
C	2.995696	0.938363	-1.354472	H	-1.101630	2.200563	2.201266
H	2.088826	2.472924	0.918190	H	-3.532282	1.357323	1.377455
C	-0.738106	3.600965	0.958170	H	-3.532282	-1.357323	1.377455
C	-1.941077	2.539644	-1.461777	H	-1.101630	-2.200563	2.201266
C	-1.616800	-1.452118	-1.019045	C	1.383021	-1.165977	-0.366325
C	-1.348435	-2.239504	0.143230	C	1.235274	-0.725872	-1.744427
C	0.000000	-2.704658	0.091141	C	1.235274	0.725872	-1.744427
C	0.595938	-2.156918	-1.112386	C	1.383021	1.165977	-0.366325
C	-2.995696	-0.938363	-1.354472	C	1.443021	-2.567993	-0.100690
H	-2.088826	-2.472924	0.918190	C	1.156713	-1.666036	-2.800943
C	0.738106	-3.600965	0.958170	C	1.156713	1.666036	-2.800943
C	1.941077	-2.539644	-1.461777	C	1.443021	2.567993	-0.100690
C	-2.078628	3.946682	0.570077	H	1.576110	-2.936379	0.925930
C	-2.638379	3.404209	-0.647572	H	1.048009	-1.323956	-3.841860
C	-0.196578	4.153384	2.145943	H	1.048009	1.323956	-3.841860
C	-2.821139	4.839829	1.390722	H	1.576110	2.936379	0.925930
H	-3.656699	3.717522	-0.929967	C	1.363674	-3.469872	-1.159327
H	-2.388672	2.191598	-2.403174	C	1.215406	-3.026123	-2.502831
C	2.078628	-3.946682	0.570077	C	1.215406	3.026123	-2.502831
C	2.638379	-3.404209	-0.647572	C	1.363674	3.469872	-1.159327
C	0.196578	-4.153384	2.145943	H	1.419702	-4.550439	-0.953105
C	2.821139	-4.839829	1.390722	H	1.153351	-3.768141	-3.313861
H	3.656699	-3.717522	-0.929967	H	1.419702	4.550439	-0.953105
H	2.388672	-2.191598	-2.403174	H	1.153351	3.768141	-3.313861
C	-0.949824	5.024029	2.935871	C	2.008023	1.540306	3.245627
H	0.825726	3.882456	2.451773	H	3.060101	1.716487	2.938290
H	-0.516980	5.439409	3.859601	H	1.995723	1.392687	4.346338
C	-2.268687	5.371073	2.555704	H	1.427958	2.459659	3.029903
H	-3.848633	5.105088	1.092478	H	2.008023	-1.540306	3.245627
H	-2.858464	6.058537	3.182459	H	1.995723	-1.392687	4.346338
C	0.949824	-5.024029	2.935871	H	3.060101	-1.716487	2.938290
H	-0.825726	-3.882456	2.451773	H	1.427958	-2.459659	3.029903
H	0.516980	-5.439409	3.859601	Cl	-1.982289	-1.861782	-1.248194
C	2.268687	-5.371073	2.555704	Cl	-1.982289	1.861782	-1.248194
H	3.848633	-5.105088	1.092478				
H	2.858464	-6.058537	3.182459				
H	3.666471	1.035003	-0.479170				
H	3.010923	-0.125397	-1.657960				
H	3.431485	1.530779	-2.188127				
H	-3.666471	-1.035003	-0.479170				
H	-3.010923	0.125397	-1.657960				
H	-3.431485	-1.530779	-2.188127				
C	1.448154	-0.395742	-4.248389				
H	1.234599	-1.325115	-4.817887				
H	1.545156	0.432239	-4.982991				
H	2.428563	-0.511778	-3.750918				
C	-1.448154	0.395742	-4.248389				
H	-1.234599	1.325115	-4.817887				
H	-1.545156	-0.432239	-4.982991				
H	-2.428563	0.511778	-3.750918				
Cl	-1.805100	0.528198	1.823234				
Cl	1.805100	-0.528198	1.823234				

13				14			
Zr	0.905805	0.000000	0.191134	Zr	0.888445	-0.481514	0.000000
C	-1.744803	0.000000	1.925392	C	-1.809821	-2.129854	0.000000
C	-0.270120	0.000000	2.370219	C	-0.351331	-2.624726	0.000000
C	-1.544840	0.000000	0.380833	C	-1.560964	-0.599639	0.000000
C	0.592869	1.150921	2.378338	C	0.510696	-2.657633	1.151142
C	1.955717	0.708477	2.429743	C	1.871809	-2.745598	0.708711
C	1.955717	-0.708477	2.429743	C	1.871809	-2.745598	-0.708711
C	0.592869	-1.150921	2.378338	C	0.510696	-2.657633	-1.151142
H	0.278803	2.201306	2.334814	H	0.195985	-2.607278	2.200984
H	2.838711	1.358650	2.443064	H	2.754292	-2.783783	1.358649
H	2.838711	-1.358650	2.443064	H	2.754292	-2.783783	-1.358649
H	0.278803	-2.201306	2.334814	H	0.195985	-2.607278	-2.200984
C	-1.322095	-1.172645	-0.471355	C	-1.316976	0.248488	-1.186662
C	-0.893627	-0.723408	-1.790574	C	-0.862210	1.530590	-0.701914
C	-0.893627	0.723408	-1.790574	C	-0.862210	1.530590	0.701914
C	-1.322095	1.172645	-0.471355	C	-1.316976	0.248488	1.186662
C	-1.426200	-2.587566	-0.263488	C	-1.376556	0.146428	-2.609847
C	-0.588920	-1.643677	-2.824787	C	-0.498269	2.667113	-1.470984
C	-0.588920	1.643677	-2.824787	C	-0.498269	2.667113	1.470984
C	-1.426200	2.587566	-0.263488	C	-1.376556	0.146428	2.609847
H	-1.768792	-2.997339	0.693266	H	-1.716964	-0.765127	-3.117909
H	-0.266529	-1.274782	-3.810686	H	-1.716964	-0.765127	3.117909
H	-0.266529	1.274782	-3.810686	C	-1.011610	1.258824	-3.397000
H	-1.768792	2.997339	0.693266	C	-0.576390	2.498768	-2.871907
C	-1.125549	-3.467233	-1.299688	C	-0.576390	2.498768	2.871907
C	-0.700619	-3.007597	-2.576459	C	-1.011610	1.258824	3.397000
C	-0.700619	3.007597	-2.576459	H	-1.070986	1.150631	-4.491925
C	-1.125549	3.467233	-1.299688	H	-0.309034	3.320219	-3.554872
H	-1.221958	-4.550262	-1.123159	H	-1.070986	1.150631	4.491925
H	-0.466448	-3.735286	-3.368418	H	-0.309034	3.320219	3.554872
H	-1.221958	4.550262	-1.123159	C	-2.584658	-2.617402	1.241336
H	-0.466448	3.735286	-3.368418	H	-3.570188	-2.112556	1.305508
C	-2.505356	1.235500	2.456884	H	-2.757352	-3.710973	1.169275
H	-3.484162	1.342259	1.946409	H	-2.048002	-2.436105	2.189676
H	-2.692636	1.113395	3.543257	C	-2.584658	-2.617402	-1.241336
H	-1.950155	2.181920	2.337092	H	-2.757352	-3.710973	-1.169275
C	-2.505356	-1.235500	2.456884	H	-3.570188	-2.112556	-1.305508
H	-2.692636	-1.113395	3.543257	H	-2.048002	-2.436105	-2.189676
H	-3.484162	-1.342259	1.946409	C	-0.110060	3.828130	-0.695410
H	-1.950155	-2.181920	2.337092	C	-0.110060	3.828130	0.695410
Cl	2.198767	-1.877471	-0.651726	H	0.196666	4.741442	-1.230676
Cl	2.198767	1.877471	-0.651726	H	0.196666	4.741442	1.230676
XX	2.198767	0.000000	-0.651726	Cl	2.202846	0.350013	-1.867225
				Cl	2.202846	0.350013	1.867225

15				16			
Zr	0.000000	0.000000	1.080931	Zr	0.000000	0.000000	0.997678
N	1.320295	0.697349	-0.953414	N	1.316273	0.699012	-1.039251
C	1.828030	2.103816	-0.757232	C	1.821268	2.106465	-0.843138
C	0.771380	3.185913	-0.754989	C	0.765466	3.189899	-0.837324
C	-0.402575	3.036067	0.040312	C	-0.394874	3.047654	-0.026083
C	-1.360834	4.076978	0.082061	C	-1.358982	4.092793	0.062111
C	-1.154317	5.256357	-0.649474	C	-1.135125	5.265269	-0.685185
C	0.000000	5.412386	-1.438817	C	0.000000	5.413999	-1.502287
C	0.947645	4.375425	-1.488961	C	0.942745	4.376412	-1.576383
O	-0.592479	1.905558	0.730833	O	-0.580237	1.911336	0.661487
C	0.439262	0.622392	-2.150975	C	0.436424	0.624044	-2.237241
C	2.494924	-0.198421	-1.095923	C	2.491116	-0.195149	-1.184354
H	1.050297	0.644148	-3.085278	H	1.047798	0.650042	-3.171187
H	-0.185159	1.538382	-2.163498	H	-0.190634	1.538426	-2.247094
H	3.120802	0.110146	-1.966388	H	3.117185	0.115944	-2.053848
H	2.172704	-1.246845	-1.232960	H	2.167599	-1.242641	-1.326615
H	3.105870	-0.147859	-0.174280	H	3.102270	-0.146866	-0.262797
H	2.376033	2.094496	0.209818	H	2.371907	2.097472	0.122440
H	2.572603	2.326357	-1.557884	H	2.563628	2.329727	-1.645568
H	1.853639	4.491176	-2.107941	H	1.838793	4.487320	-2.210037
H	-2.253979	3.936953	0.709976	C	-2.556227	3.921555	0.963176
H	-1.903884	6.062633	-0.602418	H	-1.872988	6.082374	-0.620946
H	0.161607	6.336333	-2.014986	H	0.149467	6.339742	-2.079128
N	-1.320295	-0.697349	-0.953414	N	-1.316273	-0.699012	-1.039251
C	-1.828030	-2.103816	-0.757232	C	-1.821268	-2.106465	-0.843138
C	-0.771380	-3.185913	-0.754989	C	-0.765466	-3.189899	-0.837324
C	0.402575	-3.036067	0.040312	C	0.394874	-3.047654	-0.026083
C	1.360834	-4.076978	0.082061	C	1.358982	-4.092793	0.062111
C	1.154317	-5.256357	-0.649474	C	1.135125	-5.265269	-0.685185
C	0.000000	-5.412386	-1.438817	C	0.000000	-5.413999	-1.502287
C	-0.947645	-4.375425	-1.488961	C	-0.942745	-4.376412	-1.576383
O	0.592479	-1.905558	0.730833	O	0.580237	-1.911336	0.661487
C	-0.439262	-0.622392	-2.150975	C	-0.436424	-0.624044	-2.237241
C	-2.494924	0.198421	-1.095923	C	-2.491116	0.195149	-1.184354
H	-1.050297	-0.644148	-3.085278	H	-1.047798	-0.650042	-3.171187
H	0.185159	-1.538382	-2.163498	H	0.190634	-1.538426	-2.247094
H	-3.120802	-0.110146	-1.966388	H	-3.117185	-0.115944	-2.053848
H	-2.172704	1.246845	-1.232960	H	-2.167599	1.242641	-1.326615
H	-3.105870	0.147859	-0.174280	H	-3.102270	0.146866	-0.262797
H	-2.376033	-2.094496	0.209818	H	-2.371907	-2.097472	0.122440
H	-2.572603	-2.326357	-1.557884	H	-2.563628	-2.329727	-1.645568
H	-1.853639	-4.491176	-2.107941	H	-1.838793	-4.487320	-2.210037
H	2.253979	-3.936953	0.709976	C	2.556227	-3.921555	0.963176
H	1.903884	-6.062633	-0.602418	H	1.872988	-6.082374	-0.620946
H	-0.161607	-6.336333	-2.014986	H	-0.149467	-6.339742	-2.079128
Cl	1.898615	0.556440	2.498732	H	-3.214341	4.812054	0.932626
Cl	-1.898615	-0.556440	2.498732	H	-3.158308	3.031389	0.682246
				H	-2.242032	3.752288	2.015149
				H	3.214341	-4.812054	0.932626
				H	3.158308	-3.031389	0.682246
				H	2.242032	-3.752288	2.015149
				Cl	1.903756	0.546534	2.417312
				Cl	-1.903756	-0.546534	2.417312

17				18			
Zr	0.000000	0.000000	0.662262	Zr	0.000000	0.000000	0.079476
N	1.446006	0.301700	-1.363091	N	1.474458	-0.039697	-1.942127
C	2.324242	1.508837	-1.161055	C	2.602927	0.935130	-1.729605
C	1.632829	2.854524	-1.133790	C	2.240586	2.403810	-1.698860
C	0.531415	3.079985	-0.254110	C	1.209663	2.882039	-0.833707
C	0.000000	4.398423	-0.067928	C	1.000804	4.290768	-0.654478
C	0.559723	5.425352	-0.859875	C	1.804776	5.153934	-1.432987
C	1.602315	5.201846	-1.774686	C	2.781819	4.690863	-2.329044
C	2.146987	3.917618	-1.899041	C	3.005955	3.314531	-2.450741
O	0.029334	2.013380	0.392770	O	0.462847	1.961702	-0.194336
C	0.587941	0.482321	-2.564254	C	0.684520	0.332503	-3.145809
C	2.326533	-0.882309	-1.518511	C	2.065899	-1.391536	-2.096944
H	1.188753	0.346797	-3.495342	H	1.238741	0.057563	-4.074960
H	0.234990	1.533890	-2.566795	H	0.586124	1.437235	-3.152372
H	2.995754	-0.759582	-2.402566	H	2.758238	-1.416848	-2.971198
H	1.727383	-1.802958	-1.640708	H	1.276422	-2.152612	-2.234715
H	2.947243	-0.997742	-0.610197	H	2.631382	-1.648034	-1.181401
H	2.859867	1.335318	-0.202641	H	3.081238	0.639009	-0.770999
H	3.091480	1.519469	-1.970743	H	3.356921	0.774344	-2.535982
H	2.991397	3.732124	-2.584041	H	3.793693	2.933081	-3.122018
C	-1.085189	4.703924	0.993021	C	0.000000	4.856913	0.372751
H	0.171578	6.448134	-0.757601	H	1.669138	6.239335	-1.335802
H	1.998564	6.036438	-2.373561	H	3.376047	5.407896	-2.916393
N	-1.446006	-0.301700	-1.363091	N	-1.474458	0.039697	-1.942127
C	-2.324242	-1.508837	-1.161055	C	-2.602927	-0.935130	-1.729605
C	-1.632829	-2.854524	-1.133790	C	-2.240586	-2.403810	-1.698860
C	-0.531415	-3.079985	-0.254110	C	-1.209663	-2.882039	-0.833707
C	0.000000	-4.398423	-0.067928	C	-1.000804	-4.290768	-0.654478
C	-0.559723	-5.425352	-0.859875	C	-1.804776	-5.153934	-1.432987
C	-1.602315	-5.201846	-1.774686	C	-2.781819	-4.690863	-2.329044
C	-2.146987	-3.917618	-1.899041	C	-3.005955	-3.314531	-2.450741
O	-0.029334	-2.013380	0.392770	O	-0.462847	-1.961702	-0.194336
C	-0.587941	-0.482321	-2.564254	C	-0.684520	-0.332503	-3.145809
C	-2.326533	0.882309	-1.518511	C	-2.065899	1.391536	-2.096944
H	-1.188753	-0.346797	-3.495342	H	-1.238741	-0.057563	-4.074960
H	-0.234990	-1.533890	-2.566795	H	-0.586124	-1.437235	-3.152372
H	-2.995754	0.759582	-2.402566	H	-2.758238	1.416848	-2.971198
H	-1.727383	1.802958	-1.640708	H	-1.276422	2.152612	-2.234715
H	-2.947243	0.997742	-0.610197	H	-2.631382	1.648034	-1.181401
H	-2.859867	-1.335318	-0.202641	H	-3.081238	0.639009	-0.770999
H	-3.091480	-1.519469	-1.970743	H	-3.356921	-0.774344	-2.535982
H	-2.991397	-3.732124	-2.584041	H	-3.793693	-2.933081	-3.122018
C	1.085189	-4.703924	0.993021	C	0.000000	-4.856913	0.372751
H	-0.171578	-6.448134	-0.757601	H	-1.669138	-6.239335	-1.335802
H	-1.998564	-6.036438	-2.373561	H	-3.376047	-5.407896	-2.916393
C	-1.441113	6.207479	1.031311	C	0.011518	6.413553	0.403747
C	-2.389329	3.922122	0.692795	C	-1.461282	4.411789	0.054759
C	-0.550093	4.306044	2.395415	C	0.366112	4.360364	1.809292
H	-2.202865	6.382673	1.818908	C	-0.979766	6.969489	1.450922
H	-0.563731	6.842306	1.274282	H	1.035340	6.780173	0.639046
H	-1.871172	6.562303	0.070920	H	-0.252485	6.815710	-0.600135
H	-3.174301	4.197700	1.428876	C	-2.452508	4.963136	1.105719
H	-2.775775	4.165842	-0.319957	H	-1.739278	4.771015	-0.962356
H	-2.231167	2.830836	0.767057	H	-1.511420	3.306424	0.047088
H	-1.314218	4.525783	3.171231	C	-0.632531	4.910856	2.853743
H	-0.310210	3.226938	2.448903	H	0.365002	3.252075	1.832645
H	0.366246	4.880209	2.646730	H	1.399988	4.691252	2.054128
C	1.441113	-6.207479	1.031311	C	-0.011518	-6.413553	0.403747
C	2.389329	-3.922122	0.692795	C	1.461282	-4.411789	0.054759
C	0.550093	-4.306044	2.395415	C	-0.366112	-4.360364	1.809292
H	2.202865	-6.382673	1.818908	C	0.979766	-6.969489	1.450922
H	0.563731	-6.842306	1.274282	H	-1.035340	-6.780173	0.639046
H	1.871172	-6.562303	0.070920	H	0.252485	-6.815710	-0.600135
H	3.174301	-4.197700	1.428876	C	2.452508	-4.963136	1.105719
H	2.775775	-4.165842	-0.319957	H	1.739278	-4.771015	-0.962356
H	2.231167	-2.830836	0.767057	H	1.511420	-3.306424	0.047088
H	1.314218	-4.525783	3.171231	C	0.632531	-4.910856	2.853743
H	0.310210	-3.226938	2.448903	H	-0.365002	-3.252075	1.832645
H	-0.366246	-4.880209	2.646730	H	-1.399988	-4.691252	2.054128
Cl	1.993993	-0.058658	2.069160	H	-0.931089	8.081017	1.432609
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				C	-0.590708	6.453970	2.853634
				H	-3.477752	4.613692	0.849886
				C	-2.060780	4.434057	2.504466
				H	-0.347154	4.526461	3.857876
				H	0.931089	-8.081017	1.432609
				C	2.411371	-6.505475	1.104744
				C	0.590708	-6.453970	2.853634
				H	3.477752	-4.613692	0.849886
				C	2.060780	-4.434057	2.504466
				H	0.347154	-4.526461	3.857876
				H	-2.711814	6.899632	0.107757
				H	-3.136883	6.913079	1.843689
				H	0.427856	6.812142	3.123896
				H	-1.288807	6.860805	3.618973
				H	-2.107678	3.323992	2.518116
				H	-2.783657	4.801147	3.266968
				H	2.711814	-6.899632	0.107757
				H	3.136883	-6.913079	1.843689
				H	-0.427856	-6.812142	3.123896
				H	1.288807	-6.860805	3.618973
				H	2.107678	-3.323992	2.518116
				H	2.783657	-4.801147	3.266968
				Cl	1.932261	-0.483410	1.492712
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19				20			
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N	-0.771284	1.627800	-0.212030	N	-1.55925290	0.83973314	-0.25161510
C	-2.022067	1.802386	-0.587618	C	-2.66934372	0.23909059	-0.63271510
C	-3.155307	0.964780	-0.294643	C	-3.10515821	-1.09640582	-0.32190010
C	-3.050782	-0.243278	0.478255	C	-2.32844519	-1.99848161	0.47972590
C	-4.214569	-1.025179	0.693942	C	-2.80300784	-3.32027448	0.73994890
C	-5.445455	-0.617978	0.171337	C	-4.03818191	-3.69904719	0.19246090
C	-5.561514	0.572105	-0.586408	C	-4.81623597	-2.82253604	-0.60078310
C	-4.426011	1.346101	-0.814485	C	-4.35196714	-1.53593146	-0.85486110
O	-1.892243	-0.620897	0.984167	O	-1.16967943	-1.61630069	0.98698590
C	0.133725	2.661130	-0.583393	C	-1.42178449	2.19470627	-0.66537510
H	-2.250779	2.688887	-1.215858	H	-3.36303979	0.81051712	-1.28467510
H	-4.496875	2.274626	-1.404929	H	-4.94273788	-0.83758837	-1.47019710
H	-4.116182	-1.942926	1.292462	C	-1.97419965	-4.23683257	1.60204390
H	-6.339673	-1.234652	0.356784	H	-4.41150841	-4.71707869	0.39345590
H	-6.537214	0.880565	-0.990421	H	-5.77994469	-3.15989643	-1.01081310
N	0.771284	-1.627800	-0.212030	N	1.55925290	-0.83973314	-0.25161510
C	2.022067	-1.802386	-0.587618	C	2.66934372	-0.23909059	-0.63271510
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C	4.214569	1.025179	0.693942	C	2.80300784	3.32027448	0.73994890
C	5.445455	0.617978	0.171337	C	4.03818191	3.69904719	0.19246090
C	5.561514	-0.572105	-0.586408	C	4.81623597	2.82253604	-0.60078310
C	4.426011	-1.346101	-0.814485	C	4.35196714	1.53593146	-0.85486110
O	1.892243	0.620897	0.984167	O	1.16967943	1.61630069	0.98698590
C	-0.133725	-2.661130	-0.583393	C	1.42178449	-2.19470627	-0.66537510
H	2.250779	-2.688887	-1.215858	H	3.36303979	-0.81051712	-1.28467510
H	4.496875	-2.274626	-1.404929	H	4.94273788	0.83758837	-1.47019710
H	4.116182	1.942926	1.292462	C	1.97419965	4.23683257	1.60204390
H	6.339673	1.234652	0.356784	H	4.41150841	4.71707869	0.39345590
H	6.537214	-0.880565	-0.990421	H	5.77994469	3.15989643	-1.01081310
C	1.231401	2.387617	-1.426845	C	-0.38459415	2.57821649	-1.54216810
C	2.182332	3.372252	-1.740672	C	-0.19237488	3.91901378	-1.91448110
C	2.040713	4.670714	-1.215016	C	-1.05506787	4.91262248	-1.41331710
C	0.948416	4.972288	-0.381465	C	-2.10286599	4.55477281	-0.54514810
C	0.000000	3.976820	-0.082166	C	-2.28813392	3.20568975	-0.18902710
F	1.374261	1.162064	-1.955160	F	0.43747897	1.64586956	-2.04784510
F	3.210022	3.087243	-2.548938	F	0.79417136	4.25314205	-2.75456810
F	2.939575	5.614477	-1.510829	F	-0.88287036	6.18986397	-1.76702410
F	0.810143	6.205894	0.116390	F	-2.92716724	5.49549327	-0.07132610
F	-1.034798	4.293295	0.706617	F	-3.30127598	2.89174702	0.62780690
C	-1.231401	-2.387617	-1.426845	C	0.38459415	-2.57821649	-1.54216810
C	-2.182332	-3.372252	-1.740672	C	0.19237488	-3.91901378	-1.91448110
C	-2.040713	-4.670714	-1.215016	C	1.05506787	-4.91262248	-1.41331710
C	-0.948416	-4.972288	-0.381465	C	2.10286599	-4.55477281	-0.54514810
C	0.000000	-3.976820	-0.082166	C	2.28813392	-3.20568975	-0.18902710
F	-1.374261	-1.162064	-1.955160	F	-0.43747897	-1.64586956	-2.04784510
F	-3.210022	-3.087243	-2.548938	F	-0.79417136	-4.25314205	-2.75456810
F	-2.939575	-5.614477	-1.510829	F	0.88287036	-6.18986397	-1.76702410
F	-0.810143	-6.205894	0.116390	F	2.92716724	-5.49549327	-0.07132610
F	1.034798	-4.293295	0.706617	F	3.30127598	-2.89174702	0.62780690
Cl	-0.534576	1.741091	3.038311	H	-2.40939571	-5.25389986	1.64656090
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				H	-1.89322938	-3.84281140	2.63780490
				H	2.40939571	5.25389986	1.64656090
				H	0.93315763	4.30900507	1.22355390
				H	1.89322938	3.84281140	2.63780490
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				Cl	1.45646425	-1.10944508	3.01614690

21				22			
Zr	0.000000	0.000000	1.124889	Zr	0.000000	0.000000	0.991169
N	1.593284	0.638031	-0.585598	N	-0.332627	1.708217	-0.712949
C	1.829804	1.870060	-0.995956	C	-1.501909	2.164825	-1.122166
C	1.148675	3.086911	-0.645699	C	-2.817341	1.706571	-0.770055
C	0.057224	3.129386	0.292250	C	-3.054883	0.628841	0.153054
C	-0.518078	4.389697	0.675816	C	-4.386609	0.286354	0.541707
C	0.000000	5.537473	0.048167	C	-5.439377	0.999798	-0.063852
C	1.045266	5.506097	-0.903987	C	-5.229515	2.031060	-1.010576
C	1.624038	4.290143	-1.239974	C	-3.928177	2.386904	-1.347142
O	-0.378740	1.986997	0.795413	O	-2.021796	-0.031703	0.652544
C	2.552256	-0.328531	-1.002785	C	0.787624	2.483185	-1.125551
H	2.674849	2.011004	-1.702206	H	-1.491130	3.024771	-1.824436
H	2.457931	4.239339	-1.959082	H	-3.736692	3.207084	-2.058917
C	-1.624829	4.483884	1.751730	H	-6.477753	0.754919	0.214472
H	-0.421414	6.517901	0.311165	H	-6.087131	2.555611	-1.458288
H	1.401015	6.443053	-1.358235	N	0.332627	-1.708217	-0.712949
N	-1.593284	-0.638031	-0.585598	C	1.501909	-2.164825	-1.122166
C	-1.829804	-1.870060	-0.995956	C	2.817341	-1.706571	-0.770055
C	-1.148675	-3.086911	-0.645699	C	3.054883	-0.628841	0.153054
C	-0.057224	-3.129386	0.292250	C	4.386609	-0.286354	0.541707
C	0.518078	-4.389697	0.675816	C	5.439377	-0.999798	-0.063852
C	0.000000	-5.537473	0.048167	C	5.229515	-2.031060	-1.010576
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C	-1.624038	-4.290143	-1.239974	O	2.021796	0.031703	0.652544
O	0.378740	-1.986997	0.795413	C	-0.787624	-2.483185	-1.125551
C	-2.552256	0.328531	-1.002785	H	1.491130	-3.024771	-1.824436
H	-2.674849	-2.011004	-1.702206	H	3.736692	-3.207084	-2.058917
H	-2.457931	-4.239339	-1.959082	H	6.477753	-0.754919	0.214472
C	1.624829	-4.483884	1.751730	H	6.087131	-2.555611	-1.458288
H	0.421414	-6.517901	0.311165	C	1.798021	1.932713	-1.941789
H	-1.401015	-6.443053	-1.358235	C	2.934904	2.672280	-2.306458
C	2.197127	-1.390099	-1.861297	C	3.072418	4.001710	-1.867019
C	3.119699	-2.385648	-2.222036	C	2.069910	4.583170	-1.070691
C	4.439355	-2.322115	-1.738144	C	0.938354	3.828654	-0.712781
C	4.825322	-1.263849	-0.896127	F	1.671977	0.678339	-2.402478
C	3.890213	-0.272901	-0.545849	F	3.883207	2.120976	-3.072739
F	0.952239	-1.456465	-2.358657	F	4.163115	4.703040	-2.190691
F	2.750148	-3.391025	-3.024043	F	2.201282	5.844445	-0.646858
F	5.316716	-3.276458	-2.062484	F	0.000000	4.404052	0.051010
F	6.077827	-1.202813	-0.431672	C	-1.798021	-1.932713	-1.941789
F	4.284523	0.727811	0.251423	C	-2.934904	-2.672280	-2.306458
C	-2.197127	1.390099	-1.861297	C	-3.072418	-4.001710	-1.867019
C	-3.119699	2.385648	-2.222036	C	-2.069910	-4.583170	-1.070691
C	-4.439355	2.322115	-1.738144	C	-0.938354	-3.828654	-0.712781
C	-4.825322	1.263849	-0.896127	F	-1.671977	-0.678339	-2.402478
C	-3.890213	0.272901	-0.545849	F	-3.883207	-2.120976	-3.072739
F	-0.952239	1.456465	-2.358657	F	4.163115	-4.703040	-2.190691
F	-2.750148	3.391025	-3.024043	F	-2.201282	-5.844445	-0.646858
F	-5.316716	3.276458	-2.062484	F	0.000000	-4.404052	0.051010
F	-6.077827	1.202813	-0.431672	C	-6.605069	-1.105066	2.170199
F	-4.284523	-0.727811	0.251423	C	-4.086050	-2.718081	1.408064
C	-2.061528	5.946002	1.996185	C	-3.906241	-0.442648	3.528232
C	-2.878341	3.689716	1.302071	H	-6.830528	-1.849233	2.963798
C	-1.087488	3.921820	3.095420	H	-7.036084	-0.135594	2.498419
H	-2.855905	5.963577	2.770331	H	-7.141141	-1.430013	1.253282
H	-1.227834	6.578060	2.367436	H	-4.279318	-3.455784	2.215835
H	-2.480968	6.420231	1.083965	H	-4.590515	-3.082554	0.488856
H	-3.660185	3.738868	2.088998	H	-2.991812	-2.690848	1.231126
H	-3.306362	4.122833	0.373274	H	-4.153485	-1.147601	4.350584
H	-2.645046	2.623031	1.124804	H	-2.802179	-0.408163	3.432682
H	-1.867110	4.014172	3.880657	H	-4.260473	0.566644	3.825139
H	-0.811212	2.853894	3.021239	C	6.605069	1.105066	2.170199
H	-0.195325	4.490190	3.431693	C	4.086050	2.718081	1.408064
C	2.061528	-5.946002	1.996185	C	3.906241	0.442648	3.528232
C	2.878341	-3.689716	1.302071	H	6.830528	1.849233	2.963798
C	1.087488	-3.921820	3.095420	H	7.036084	0.135594	2.498419
H	2.855905	-5.963577	2.770331	H	7.141141	1.430013	1.253282
H	1.227834	-6.578060	2.367436	H	4.279318	3.455784	2.215835
H	2.480968	-6.420231	1.083965	H	4.590515	3.082554	0.488856
H	3.660185	-3.738868	2.088998	H	2.991812	2.690848	1.231126
H	3.306362	-4.122833	0.373274	H	4.153485	1.147601	4.350584
H	2.645046	-2.623031	1.124804	H	2.802179	0.408163	3.432682
H	1.867110	-4.014172	3.880657	H	4.260473	-0.566644	3.825139
H	0.811212	-2.853894	3.021239	Si	4.723613	1.008743	1.917210
H	0.195325	-4.490190	3.431693	Si	-4.723613	-1.008743	1.917210
Cl	1.833852	0.272300	2.692602	Cl	0.022025	1.850944	2.561775
Cl	-1.833852	-0.272300	2.692602	Cl	-0.022025	-1.850944	2.561775

23				24			
Zr	0.000000	0.000000	1.475930	Zr	0.000000	0.000000	1.366327
N	-1.177922	1.032889	-0.388202	N	1.504514	0.297136	-0.513654
C	-2.238823	0.545435	-0.993161	C	1.748997	1.432866	-1.131550
C	-2.969057	-0.662962	-0.690286	C	1.267294	2.755119	-0.812674
C	-2.581810	-1.560234	0.362616	C	0.381303	3.010194	0.285678
C	-3.372212	-2.711583	0.612710	C	0.000000	4.349709	0.605141
C	-4.510542	-2.967666	-0.156881	C	0.493243	5.388017	-0.199461
C	-4.899561	-2.093188	-1.199359	C	1.349515	5.150989	-1.300615
C	-4.133138	-0.957138	-1.455630	C	1.734940	3.846961	-1.598808
O	-1.511482	-1.313671	1.091555	O	-0.074010	2.010059	1.017495
C	-0.657255	2.253827	-0.930800	C	2.145244	-0.860867	-1.065097
H	-2.660353	1.140378	-1.832460	H	2.449021	1.395442	-1.994383
H	-4.424949	-0.259757	-2.258814	H	2.415595	3.641991	-2.441726
H	-3.062148	-3.382572	1.427122	H	0.200852	6.423660	0.042338
H	-5.113673	-3.865502	0.054578	H	1.713671	5.993891	-1.907313
H	-5.798742	-2.305424	-1.797099	N	-1.504514	-0.297136	-0.513654
N	1.177922	-1.032889	-0.388202	C	-1.748997	-1.432866	-1.131550
C	2.238823	-0.545435	-0.993161	C	-1.267294	-2.755119	-0.812674
C	2.969057	0.662962	-0.690286	C	0.381303	-3.010194	0.285678
C	2.581810	1.560234	0.362616	C	0.000000	-4.349709	0.605141
C	3.372212	2.711583	0.612710	C	0.493243	-5.388017	-0.199461
C	4.510542	2.967666	-0.156881	C	-1.349515	-5.150989	-1.300615
C	4.899561	2.093188	-1.199359	C	-1.734940	-3.846961	-1.598808
C	4.133138	0.957138	-1.455630	O	0.074010	-2.010059	1.017495
O	1.511482	1.313671	1.091555	C	-2.145244	0.860867	-1.065097
C	0.657255	-2.253827	-0.930800	H	-2.449021	-1.395442	-1.994383
H	2.660353	-1.140378	-1.832460	H	-2.415595	-3.641991	-2.441726
H	4.424949	0.259757	-2.258814	H	0.200852	-6.423660	0.042338
H	3.062148	3.382572	1.427122	H	-1.713671	-5.993891	-1.907313
H	5.113673	3.865502	0.054578	C	1.965982	-1.207874	-2.423300
H	5.798742	2.305424	-1.797099	C	2.610573	-2.337528	-2.955060
C	-0.304349	2.340098	-2.296618	C	3.440469	-3.126163	-2.140796
C	0.198837	3.542242	-2.821861	C	3.618492	-2.780519	-0.788353
C	0.349731	4.666644	-1.993289	C	2.971195	-1.660377	-0.244320
C	0.000000	4.579609	-0.632918	H	1.303326	-0.595720	-3.055389
C	-0.493690	3.381117	-0.095493	H	2.456851	-2.603750	-4.012888
H	-0.408053	1.451409	-2.939237	H	3.946331	-4.010882	-2.558011
H	0.479744	3.595443	-3.885742	H	4.274681	-3.388777	-0.145716
H	0.744034	5.608837	-2.405097	H	3.108394	-1.378864	0.810661
H	0.110034	5.458247	0.022276	C	-1.965982	1.207874	-2.423300
H	-0.771858	3.305721	0.966409	C	-2.610573	2.337528	-2.955060
C	0.304349	-2.340098	-2.296618	C	-3.440469	3.126163	-2.140796
C	-0.198837	-3.542242	-2.821861	C	-3.618492	2.780519	-0.788353
C	-0.349731	-4.666644	-1.993289	C	-2.971195	1.660377	-0.244320
C	0.000000	-4.579609	-0.632918	H	-1.303326	0.595720	-3.055389
C	0.493690	-3.381117	-0.095493	H	-2.456851	2.603750	-4.012888
H	0.408053	-1.451409	-2.939237	H	-3.946331	4.010882	-2.558011
H	-0.479744	-3.595443	-3.885742	H	-4.274681	3.388777	-0.145716
H	-0.744034	-5.608837	-2.405097	H	-3.108394	1.378864	0.810661
H	-0.110034	-5.458247	0.022276	C	-0.899334	4.591771	1.789197
H	0.771858	-3.305721	0.966409	H	-0.443309	4.197994	2.722223
Cl	-1.222969	1.457917	2.991780	H	-1.105921	5.671268	1.924962
Cl	1.222969	-1.457917	2.991780	H	-1.865271	4.057270	1.672286
				C	0.899334	-4.591771	1.789197
				H	0.443309	-4.197994	2.722223
				H	1.105921	-5.671268	1.924962
				H	1.865271	-4.057270	1.672286
				Cl	1.910235	0.032145	2.879538
				Cl	-1.910235	-0.032145	2.879538

25				26			
Zr	0.000000	0.000000	0.955232	Zr	0.000000	0.000000	0.790099
N	1.372551	0.557063	-0.941940	N	-0.851704	1.211410	-1.114682
C	1.414568	1.732196	-1.534991	C	-2.012051	0.999713	-1.700028
C	0.806527	2.979587	-1.140561	C	-3.084216	0.123885	-1.296971
C	0.000000	3.109492	0.043184	C	-3.016312	-0.710639	-0.128131
C	-0.434879	4.406389	0.484872	C	-4.163613	-1.440416	0.312438
C	-0.112526	5.496370	-0.344340	C	-5.321038	-1.368066	-0.486956
C	0.624864	5.374304	-1.544590	C	-5.389950	-0.601446	-1.674343
C	1.097509	4.126270	-1.930531	C	-4.284326	0.149704	-2.062163
O	-0.302695	2.010646	0.710649	O	-1.881279	-0.775670	0.547331
C	2.138048	-0.480678	-1.569833	C	0.000000	2.173935	-1.750026
H	2.050478	1.807598	-2.443398	H	-2.234602	1.607793	-2.603506
H	1.710672	4.009124	-2.839353	H	-4.326742	0.786295	-2.961937
H	-0.442770	6.501707	-0.046946	H	-6.219693	-1.925104	-0.174439
H	0.838397	6.268393	-2.149798	H	-6.316148	-0.582062	-2.268783
N	-1.372551	-0.557063	-0.941940	N	0.851704	-1.211410	-1.114682
C	-1.414568	-1.732196	-1.534991	C	2.012051	-0.999713	-1.700028
C	-0.806527	-2.979587	-1.140561	C	3.084216	-0.123885	-1.296971
C	0.000000	-3.109492	0.043184	C	3.016312	0.710639	-0.128131
C	0.434879	-4.406389	0.484872	C	4.163613	1.440416	0.312438
C	0.112526	-5.496370	-0.344340	C	5.321038	1.368066	-0.486956
C	-0.624864	-5.374304	-1.544590	C	5.389950	0.601446	-1.674343
C	-1.097509	-4.126270	-1.930531	C	4.284326	-0.149704	-2.062163
O	0.302695	-2.010646	0.710649	O	1.881279	0.775670	0.547331
C	-2.138048	0.480678	-1.569833	C	0.000000	-2.173935	-1.750026
H	-2.050478	-1.807598	-2.443398	H	2.234602	-1.607793	-2.603506
H	-1.710672	-4.009124	-2.839353	H	4.326742	-0.786295	-2.961937
H	0.442770	-6.501707	-0.046946	H	6.219693	1.925104	-0.174439
H	-0.838397	-6.268393	-2.149798	H	6.316148	0.582062	-2.268783
C	1.942997	-0.801764	-2.932747	C	0.330361	2.057829	-3.119955
C	2.716883	-1.803011	-3.541975	C	1.154237	3.016301	-3.732960
C	3.693957	-2.489144	-2.801007	C	1.651275	4.099673	-2.989140
C	3.887600	-2.170283	-1.444528	C	1.322928	4.214987	-1.626082
C	3.112186	-1.178792	-0.823485	C	0.509302	3.257175	-1.001508
H	1.173036	-0.266248	-3.509980	H	-0.053281	1.202526	-3.697997
H	2.550544	-2.049032	-4.602792	H	1.411578	2.910619	-4.798880
H	4.302173	-3.273164	-3.278438	H	2.296362	4.851777	-3.469519
H	4.657792	-2.696056	-0.858726	H	1.700237	5.065701	-1.037473
H	3.265513	-0.917428	0.234255	H	0.242782	3.345813	0.061896
C	-1.942997	0.801764	-2.932747	C	-0.330361	-2.057829	-3.119955
C	-2.716883	1.803011	-3.541975	C	-1.154237	-3.016301	-3.732960
C	-3.693957	2.489144	-2.801007	C	-1.651275	-4.099673	-2.989140
C	-3.887600	2.170283	-1.444528	C	-1.322928	-4.214987	-1.626082
C	-3.112186	1.178792	-0.823485	C	-0.509302	-3.257175	-1.001508
H	-1.173036	0.266248	-3.509980	H	0.053281	1.202526	-3.697997
H	-2.550544	2.049032	-4.602792	H	-1.411578	-2.910619	-4.798880
H	-4.302173	3.273164	-3.278438	H	-2.296362	-4.851777	-3.469519
H	-4.657792	2.696056	-0.858726	H	-1.700237	-5.065701	-1.037473
H	-3.265513	0.917428	0.234255	H	0.242782	3.345813	0.061896
C	-1.176982	4.598849	1.828126	C	-2.874725	-3.757920	2.040592
C	1.176982	-4.598849	1.828126	H	-3.012168	-4.473311	1.203150
C	-2.502808	3.796187	1.842926	H	-1.846311	-3.345569	1.994320
H	-3.166543	4.114201	1.011739	H	-2.969408	-4.325200	2.991439
H	-2.323825	2.708540	1.756928	C	2.874725	3.757920	2.040592
H	-3.040930	3.977282	2.797682	C	3.012168	4.473311	1.203150
C	2.502808	-3.796187	1.842926	H	1.846311	3.345569	1.994320
H	3.166543	-4.114201	1.011739	H	2.969408	4.325200	2.991439
H	2.323825	-2.708540	1.756928	C	3.879762	1.139887	3.393143
H	3.040930	-3.977282	2.797682	H	2.892137	0.644248	3.300321
C	0.258609	-4.123042	2.986856	H	4.659511	0.349508	3.399151
H	-0.016749	-3.056133	2.885090	H	3.911729	1.658528	4.375207
H	-0.676242	-4.720939	3.021449	C	5.893521	3.156252	2.195271
H	0.779974	-4.249220	3.959456	H	5.939316	3.696781	3.164916
C	1.524025	-6.083575	2.079956	H	6.703323	2.396191	2.205159
H	2.046799	-6.174757	3.054326	H	6.122518	3.893711	1.396608
H	0.619940	-6.725966	2.130846	C	-5.893521	-3.156252	2.195271
H	2.201666	-6.495671	1.302477	H	-5.939316	-3.696781	3.164916
C	-1.524025	6.083575	2.079956	H	-6.703323	-2.396191	2.205159
H	-2.046799	6.174757	3.054326	H	-6.122518	-3.893711	1.396608
H	-0.619940	6.725966	2.130846	C	-3.879762	-1.139887	3.393143
H	-2.201666	6.495671	1.302477	H	-2.892137	-0.644248	3.300321
C	-0.258609	4.123042	2.986856	H	-4.659511	-0.349508	3.399151
H	0.016749	3.056133	2.885090	H	-3.911729	-1.658528	4.375207
H	0.676242	4.720939	3.021449	Si	-4.169682	-2.376291	1.986954
H	-0.779974	4.249220	3.959456	Si	4.169682	2.376291	1.986954
Cl	1.925550	0.234340	2.437349	Cl	-0.693779	1.816888	2.263886
Cl	-1.925550	-0.234340	2.437349	Cl	0.693779	-1.816888	2.263886