Supplementary Material (ESI) for Dalton Transactions

Supporting Information for

Synthesis and Structural Studies of Amido, Hydrazido and Imido Zr(IV) Complexes Incorporating a Diamido/Diamine Cyclam-Based Ligand

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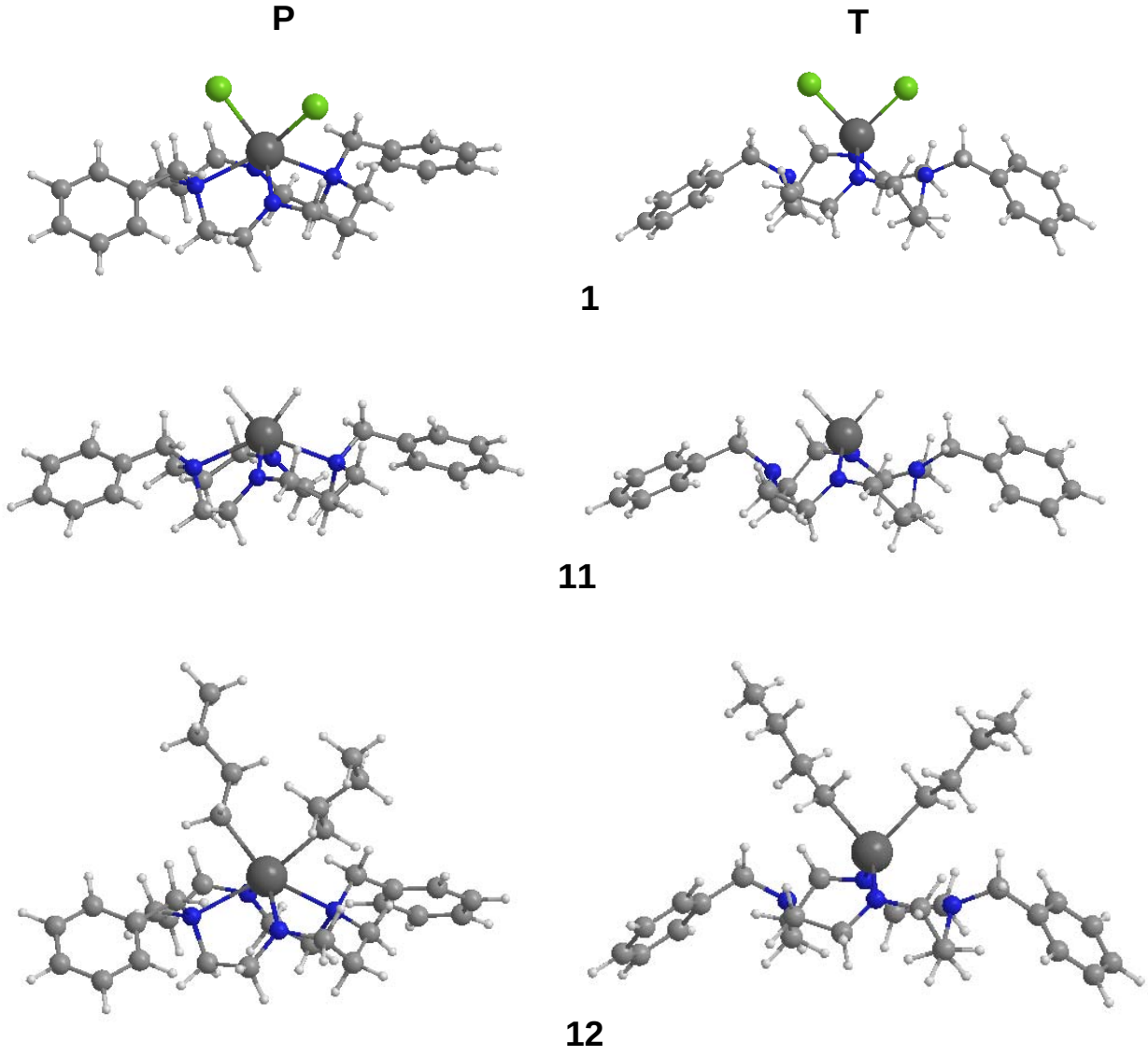

Figure S1. Optimized geometry for the **P** (left side) and the **T** (right side) isomers of the [(Bn_2Cyclam)ZrXY] complexes with equal ancillary ligands. X = Y = Cl (**1**, top), X = Y = H (**11**, middle), X = Y = *n*-Bu (**12**, bottom).

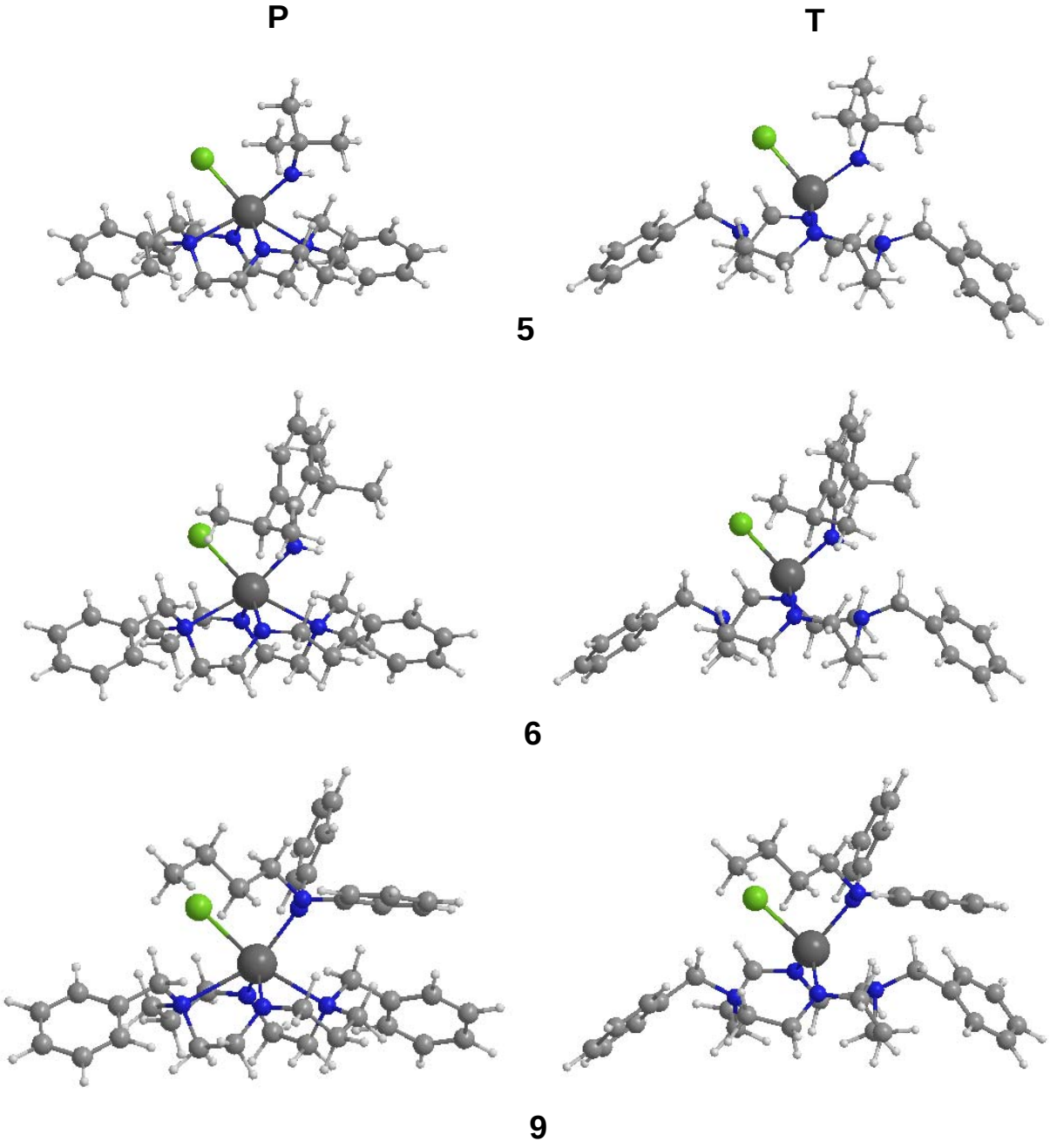

Figure S2. Optimized geometry for the **P** (left side) and the **T** (right side) isomers of the chloro amide complexes [(Bn_2Cyclam)ZrCl(NHR)]. R = *t*-Bu (**5**, top), R = 2,6-*i*-PrC_6H_4 (**6**, middle), R = N(Ph)N(Ph)(*n*-Bu) (**9**, bottom).

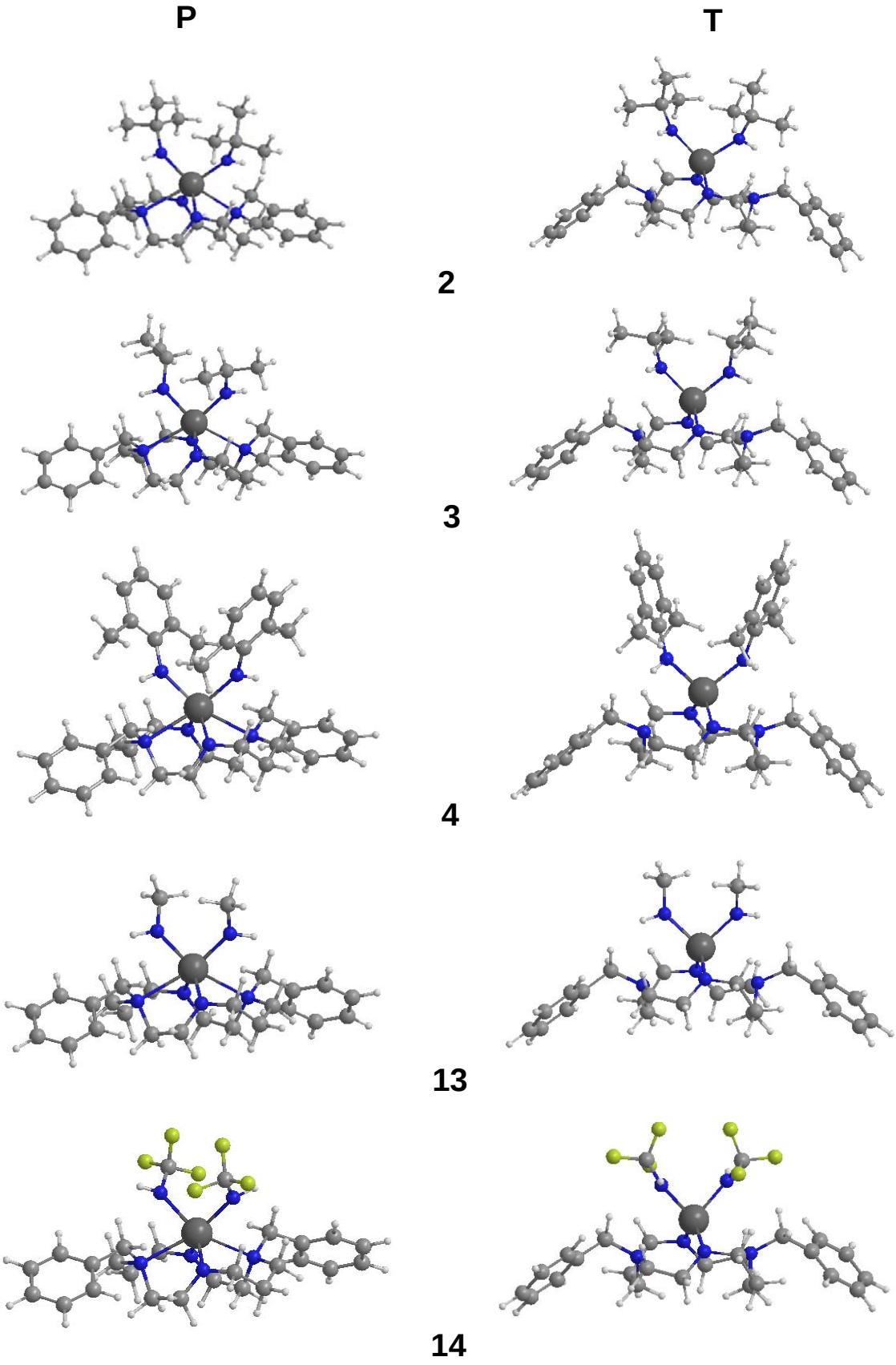

Figure S3. Optimized geometry for the **P** (left side) and the **T** (right side) isomers of the bis(amide) complexes [(Bn_2Cyclam)Zr($NHR)_2$]: R = *t*-Bu (**2**); R = *i*-Pr (**3**); R = 2,6-MeC_6H_4 (**4**); R = Me (**13**); R = CF_3 (**14**).

Atomic Coordinates for the optimized [(Bn_2Cyclam)ZrXY] complexes (B3LYP/VDZP)

(1) X = Y = Cl, isomer P

Zr	0.000002	0.564173	0.000020
Cl	1.472637	2.368787	0.898536
N	-0.105279	-0.602113	-1.731230
N	0.105264	-0.602202	1.731215
C	5.640312	-1.326045	-3.565805
Cl	-1.472600	2.368856	-0.898402
H	-5.690085	-1.956975	4.448851
C	-5.640207	-1.325933	3.565958
H	5.690233	-1.957166	-4.448638
N	-2.256958	-0.459745	0.421367
N	2.256938	-0.459786	-0.421389
C	-2.961966	0.410547	1.438819
H	3.083780	1.383690	-0.960550
C	2.961949	0.410485	-1.438859
H	-3.083866	1.383712	0.960445
C	-1.895774	-1.782772	0.991074
C	1.895711	-1.782784	-0.991122
H	2.265970	0.543364	-2.270863
H	-2.265966	0.543523	2.270788
C	-3.124014	-0.620736	-0.788390
C	3.124001	-0.620847	0.788353
H	1.465072	-2.371371	-0.179843
H	-1.465156	-2.371352	0.179780
H	2.787709	-2.311109	-1.354887
H	-2.787787	-2.311084	1.354823
C	-4.400107	-0.898079	3.088924
C	4.400183	-0.898215	-3.088822
H	3.419884	0.388430	1.086224
C	-4.304970	-0.079095	1.953716
C	4.304988	-0.079133	-1.953691
H	-3.419877	0.388561	-1.086212
C	-6.812495	-0.933303	2.918473
C	6.812572	-0.933291	-2.918345
H	-4.032440	-1.164759	-0.497806
H	4.032412	-1.164876	0.497738
C	5.494451	0.321066	-1.325223
C	-5.494460	0.320976	1.325219
H	-3.496379	-1.189461	3.617328
H	3.496476	-1.189698	-3.617206
H	7.778704	-1.261266	-3.290948
H	-7.778606	-1.261298	3.291117
C	-6.736369	-0.103413	1.798390
C	6.736388	-0.103299	-1.798341
H	5.445576	0.982912	-0.464637
H	-5.445629	0.982734	0.464564
C	2.494584	-1.319305	2.000689
C	-2.494609	-1.319143	-2.000762
C	0.853119	-1.631364	-2.094341
C	-0.853160	-1.631442	2.094286
H	-7.644049	0.221855	1.298080
H	7.644046	0.222069	-1.298055
C	-1.285452	-0.590337	-2.606189
C	1.285448	-0.590502	2.606162
H	-3.288817	-1.375079	-2.757803
H	3.288795	-1.375305	2.757722
H	-2.229389	-2.358295	-1.770672
H	2.229335	-2.358437	1.770540
H	-1.331101	-1.397358	3.062366
H	1.331079	-1.397242	-3.062402
H	-0.371762	-2.614555	2.236748
H	0.371694	-2.614456	-2.236858
H	1.032181	-1.063331	3.566342
H	-1.032188	-1.063125	-3.566390
H	1.570373	0.442380	2.831224
H	-1.570350	0.442563	-2.831200

(1) X = Y = Cl, isomer T

Zr	-1.764937	1.160210	-1.312699
N	-0.061471	2.595559	0.409254
N	0.053461	1.500778	-2.238608
N	-1.726841	-0.075718	0.347660
N	-1.054325	-1.441137	-2.081202
C	0.555982	1.556529	1.269871
H	1.421841	1.966349	1.812221
H	0.940822	0.780684	0.603997
C	1.252211	2.077985	-1.656323
H	1.842017	2.593332	-2.432478
H	1.925982	1.310001	-1.236344
Cl	-3.383205	0.666858	-3.083047
C	0.310576	0.768828	-3.479102
H	0.917407	1.388303	-4.158381
H	-0.642276	0.609273	-3.993648
Cl	-3.121830	3.109852	-0.718748
C	-1.794253	0.567795	1.660340
H	-2.345445	-0.077057	2.363151
H	-2.386468	1.483774	1.570523
C	0.897307	3.108531	-0.596511
H	1.815214	3.484496	-0.121306
H	0.407769	3.952343	-1.093060
C	-0.598428	3.745003	1.209740
H	-1.319099	3.343756	1.923590
H	-1.169786	4.360848	0.514319
C	0.429477	-1.422516	-2.123867
H	0.827566	-2.447564	-2.171121
H	0.769880	-0.996382	-1.177354
C	0.423732	4.605905	1.937974
C	-1.551778	-2.178099	-0.895859
H	-1.136372	-3.195593	-0.854210
H	-2.636511	-2.265284	-1.013238
C	-1.377620	-3.527881	-3.549882
C	-0.416243	0.906250	2.266285
H	-0.574014	1.544937	3.143163
H	0.070024	-0.001342	2.644172
C	-1.645045	-2.047061	-3.320401
H	-1.289659	-1.469209	-4.174939
H	-2.719798	-1.872649	-3.261520
C	1.014919	-0.588571	-3.273630
H	0.983512	-1.139783	-4.220425
H	2.078980	-0.440171	-3.053498
C	-1.274307	-1.454083	0.411711
H	-1.812392	-1.995536	1.207589
H	-0.204909	-1.531043	0.675699
C	0.870593	4.288360	3.229537
H	0.475151	3.411816	3.735068
C	0.920824	5.773250	1.338026
H	0.565015	6.057140	0.350880
C	2.296647	6.242072	3.270646
H	3.016894	6.872272	3.784355
C	-2.305080	-4.488772	-3.118270
H	-3.216188	-4.163829	-2.622428
C	1.849491	6.582850	1.992891
H	2.216283	7.483571	1.508810
C	1.800215	5.093944	3.889521
H	2.128883	4.829163	4.890610
C	-0.231609	-3.976013	-4.224238
H	0.486103	-3.254196	-4.603708
C	-0.006540	-5.336954	-4.438313
H	0.886707	-5.659446	-4.965941
C	-0.931548	-6.279440	-3.987004
H	-0.760130	-7.338560	-4.156375
C	-2.085997	-5.850372	-3.329818
H	-2.820883	-6.574458	-2.989509

(2) X = Y = NH(^{t}Bu), isomer P

Zr	-0.769571	0.935577	0.007973
N	0.755359	0.577245	2.319422
C	2.021138	1.861408	4.168542
C	3.391586	2.079531	3.963183
H	3.757967	2.267513	2.957745
C	1.960449	0.046532	1.655663
H	2.785482	-0.113090	2.368602
H	1.691839	-0.925622	1.240244
C	-0.422732	-2.224683	-0.467638
H	-1.219150	-2.890681	-0.851370
H	0.232370	-2.886462	0.126899
N	-0.985804	-1.153300	0.336990
C	-3.404009	1.825237	1.920857
C	-4.268266	1.115996	0.863815
C	1.035042	1.875571	3.008155
H	1.370159	2.577404	2.240903
H	0.078539	2.249771	3.385545
C	-3.454036	3.674201	-2.011364
H	-3.933451	3.486404	-1.049124
H	-3.905761	2.997801	-2.747113
H	-3.687330	4.701832	-2.316000
N	-0.229210	-0.547229	-2.279869
C	-1.429127	-1.658685	1.637103
H	-1.863669	-2.666849	1.519944
H	-2.227358	-1.019521	2.021205
C	-1.927548	3.441828	-1.931261

C	-1.307201	4.382150	-0.883268
C	0.674062	0.149618	-3.231941
H	0.079259	0.949423	-3.687500
H	0.964717	-0.538481	-4.040739
C	-1.334446	3.779582	-3.320192
H	-0.246304	3.667439	-3.326297
H	-1.569971	4.809662	-3.613231
H	-1.748402	3.116213	-4.090324
N	1.284356	1.388676	-0.300313
C	1.574186	1.662973	5.483821
H	0.512672	1.520905	5.670973
C	-1.176767	-1.527852	-5.439705
H	-1.143184	-0.460316	-5.642380
C	-1.482514	-0.976065	-2.976389
H	-1.950870	-0.070826	-3.374439
H	-2.153636	-1.371686	-2.210226
C	-1.313754	-4.263880	-4.949472
H	-1.379765	-5.330127	-4.751728
C	3.829320	1.863999	6.332902
H	4.525834	1.866267	7.166428
C	-1.349267	-1.973102	-4.120089
N	-1.977195	1.652661	1.587236
H	-1.443680	1.938215	2.404420
C	0.161578	-0.395257	3.273105
H	-0.699914	0.107378	3.727715
H	0.875974	-0.603249	4.084688
C	1.743992	1.879218	-1.600674
H	2.695810	2.425850	-1.481717
H	1.020241	2.597608	-1.991962
C	0.430770	-1.683633	-1.610819
H	1.365502	-1.307540	-1.193852
H	0.681663	-2.487240	-2.321383
N	-1.620235	2.042247	-1.580326
H	-1.891612	1.470425	-2.376530
C	4.288918	2.077731	5.032481
H	5.345630	2.251868	4.849752
C	-1.126296	-3.804173	-6.253848
H	-1.041040	-4.509611	-7.075431
C	-0.316732	-1.738622	2.701522
H	0.528885	-2.323045	2.319145
H	-0.696113	-2.306582	3.562875
C	2.466500	1.660325	6.556496
H	2.096386	1.507474	7.566428
C	-1.062485	-2.431077	-6.497084
H	-0.931860	-2.062245	-7.510586
C	-3.782193	3.322457	1.994883
H	-3.628336	3.816546	1.033993
H	-3.161605	3.837238	2.738173
H	-4.831558	3.457724	2.284642
C	-3.698801	1.203358	3.306745
H	-3.480443	0.131422	3.316780
H	-4.750397	1.336811	3.586726
H	-3.088846	1.681607	4.083905
C	2.407634	0.950673	0.510953
H	2.980944	1.816978	0.893142
H	3.139775	0.369978	-0.078601
C	1.953458	0.776629	-2.657622
H	2.626441	0.003608	-2.267101
H	2.480279	1.211656	-3.518862
C	-1.427478	-3.355725	-3.895509
H	-1.592763	-3.725280	-2.887302
H	-5.334792	1.258099	1.071252
H	-4.064386	0.039593	0.858185
H	-4.054651	1.503427	-0.134871
H	-0.215369	4.293771	-0.882471
H	-1.664631	4.135030	0.118976
H	-1.562103	5.426468	-1.095707

(2) X = Y = NH(^{t}Bu), isomer T

Zr	-0.711306	1.406154	-0.529956
N	1.209849	2.670179	1.261132
N	1.177045	1.627886	-1.463182
N	-0.608840	-0.004739	1.041511
N	0.171965	-1.534932	-1.396973
C	1.769188	1.530885	2.021558
H	2.676284	1.828842	2.572832
H	2.078796	0.784891	1.287849
C	-2.623294	1.318208	-3.301450
C	2.398902	2.155572	-0.881357
H	2.997333	2.677183	-1.650632
H	3.062565	1.357328	-0.500958
N	-1.845679	0.796616	-2.161350
C	1.466809	0.865994	-2.678286
H	2.075459	1.473811	-3.372559
H	0.521099	0.664680	-3.184091
N	-1.736261	3.143971	0.047383
C	-0.620463	0.604752	2.369765
H	-1.197563	-0.018115	3.076880
H	-1.152057	1.560404	2.309279
C	2.140986	3.164118	0.228684
H	3.104218	3.477338	0.662978
H	1.679640	4.055925	-0.212833
C	0.777909	3.788833	2.140861
H	0.056819	3.391539	2.856769
H	0.227770	4.489575	1.508079
C	1.633239	-1.353279	-1.336663
H	2.161577	-2.322276	-1.323952
H	1.850033	-0.865924	-0.384526
C	1.871523	4.543189	2.886434
C	-0.391385	-2.168899	-0.194357
H	-0.001367	-3.190374	-0.043537
H	-1.472063	-2.257763	-0.362377
C	0.142922	-3.690092	-2.788881
C	0.773773	0.868438	2.985479
H	0.638258	1.468148	3.894501
H	1.230160	-0.070669	3.320964
C	-0.279205	-2.235056	-2.623717
H	0.061866	-1.655148	-3.485229
H	-1.375043	-2.195018	-2.630259
C	2.210447	-0.473109	-2.456131
H	2.232754	-1.009688	-3.413347
H	3.262460	-0.292417	-2.201685
C	-0.171304	-1.387362	1.097412
H	-0.728845	-1.932255	1.881565
H	0.889772	-1.474956	1.395198
C	-3.051268	3.471590	0.631992
C	2.337759	4.109721	4.136780
H	1.902942	3.225658	4.594912
C	2.429215	5.710963	2.344870
H	2.067337	6.080763	1.388543
C	3.893716	5.958681	4.253182
H	4.671762	6.503838	4.779831
C	-0.676079	-4.728722	-2.321890
H	-1.627144	-4.487969	-1.852994
C	3.431051	6.412408	3.016799
H	3.845050	7.315870	2.577737
C	-3.840507	2.170424	0.864751
H	-3.946361	1.605436	-0.065025
H	-4.842517	2.389506	1.248914
H	-3.337389	1.527330	1.594267
C	3.340743	4.806048	4.813216
H	3.683951	4.452141	5.781423
C	-4.140898	1.202688	-3.035306
H	-4.415048	0.162367	-2.826334
H	-4.725976	1.540104	-3.899661
H	-4.432486	1.805757	-2.172201
C	-2.880921	4.201254	1.984306
H	-2.343727	3.575220	2.703061
H	-3.852997	4.460030	2.420743
H	-2.316038	5.132462	1.857460
C	1.349000	-4.032119	-3.417910
H	1.988611	-3.247683	-3.813226
C	1.733091	-5.366475	-3.560955
H	2.670249	-5.608134	-4.054736
C	-2.291786	0.502348	-4.570569
H	-1.223019	0.556992	-4.801521
H	-2.845653	0.879361	-5.437839
H	-2.560949	-0.553207	-4.441683
C	-2.243457	2.788666	-3.548866
H	-2.391599	3.382714	-2.644602
H	-2.849884	3.218639	-4.354155
H	-1.188834	2.867051	-3.834127
C	-3.851357	4.396850	-0.312077
H	-3.289779	5.316363	-0.517167
H	-4.811515	4.685781	0.132037
H	-4.051464	3.905877	-1.267239
C	0.911620	-6.387521	-3.080550
H	1.207166	-7.426563	-3.194527
C	-0.297858	-6.064537	-2.462823
H	-0.950532	-6.852199	-2.096702
H	-1.777292	-0.215391	-2.249917
H	-1.218178	4.012733	-0.091049

(3) X = Y = NH(^{i}Pr), isomer P

Zr	-0.531853	0.754062	0.021403
N	0.941363	0.510985	2.250210
C	2.024588	1.945782	4.104988
C	3.392599	2.220481	3.957057

H	3.802131	2.376953	2.962897
C	2.210586	0.056661	1.636149
H	3.012034	-0.021319	2.387147
H	2.030353	-0.944297	1.240075
C	-0.132497	-2.381399	-0.490412
H	-0.916962	-3.069908	-0.858897
H	0.564366	-3.026719	0.074855
N	-0.707333	-1.336867	0.338259
C	-3.217150	1.871453	1.534023
H	-3.477439	2.059203	0.486298
C	1.099662	1.855248	2.899924
H	1.431911	2.542234	2.118574
H	0.099700	2.182858	3.192893
C	-2.046767	3.706126	-3.024827
H	-2.717897	3.063399	-3.607930
H	-1.048967	3.651843	-3.475865
H	-2.410552	4.735874	-3.120409
N	-0.037575	-0.649770	-2.267917
C	-1.112676	-1.850027	1.646915
H	-1.497749	-2.879306	1.546688
H	-1.939669	-1.246031	2.032957
C	-2.001115	3.264916	-1.552753
H	-3.025147	3.386190	-1.152949
C	0.816272	0.074841	-3.246422
H	0.188479	0.872078	-3.661583
H	1.081365	-0.598325	-4.075845
C	-1.093804	4.196990	-0.739617
H	-1.038173	3.872997	0.303509
H	-1.478598	5.222831	-0.758715
H	-0.077760	4.207527	-1.149541
N	1.493305	1.307636	-0.346183
C	1.520352	1.792932	5.405499
H	0.458250	1.608815	5.547587
C	-1.102323	-1.581641	-5.404982
H	-1.075662	-0.510749	-5.589878
C	-1.315355	-1.073522	-2.922355
H	-1.795034	-0.159764	-3.285200
H	-1.953865	-1.486815	-2.137431
C	-1.223468	-4.325803	-4.957792
H	-1.283170	-5.395313	-4.776319
C	3.716524	2.146482	6.353577
H	4.367933	2.225018	7.219267
C	-1.224234	-2.049877	-4.087632
N	-1.821814	1.425224	1.551334
H	-1.539904	1.319381	2.523691
C	0.434485	-0.483868	3.235006
H	-0.439249	-0.031603	3.719646
H	1.184785	-0.632189	4.026207
C	1.899877	1.815266	-1.655344
H	2.835248	2.394401	-1.565512
H	1.141452	2.510386	-2.030918
C	0.665346	-1.794447	-1.653599
H	1.609588	-1.411874	-1.263852
H	0.900574	-2.574116	-2.395202
N	-1.571187	1.867776	-1.430339
H	-2.020526	1.333050	-2.169821
C	4.232402	2.316524	5.067954
H	5.287907	2.533099	4.928671
C	-1.085897	-3.843406	-6.260181
H	-1.033357	-4.534383	-7.096669
C	0.020292	-1.860213	2.692467
H	0.888939	-2.400474	2.297247
H	-0.308790	-2.436190	3.569094
C	2.354738	1.888247	6.519778
H	1.939935	1.769068	7.516811
C	-1.029844	-2.466274	-6.481606
H	-0.938034	-2.079798	-7.492795
C	-3.410480	3.180132	2.320402
H	-2.760798	3.969449	1.932018
H	-3.163447	3.032067	3.380522
H	-4.447982	3.532134	2.270424
C	-4.177320	0.787303	2.059348
H	-4.080843	-0.130483	1.471318
H	-5.222464	1.117849	2.014327
H	-3.951741	0.543590	3.106109
C	2.631911	0.963425	0.481057
H	3.147384	1.868191	0.859170
H	3.407881	0.413886	-0.083169
C	2.105981	0.718472	-2.717023
H	2.804029	-0.040706	-2.343753
H	2.596388	1.161343	-3.595770
C	-1.295306	-3.436159	-3.884561
H	-1.422136	-3.823042	-2.877285

(3) X = Y = NH(^{i}Pr), isomer T

Zr	-0.403864	1.327301	-0.656461
N	1.388254	2.620650	1.234803
N	1.508496	1.634202	-1.504980
N	-0.378474	-0.050904	0.954220
N	0.422604	-1.437727	-1.512009
C	1.933762	1.496588	2.028162
H	2.809825	1.816817	2.616328
H	2.291350	0.753837	1.312210
C	-2.563215	1.578684	-3.106586
C	2.698707	2.142098	-0.847160
H	3.340375	2.676097	-1.571599
H	3.338700	1.335831	-0.442399
N	-1.592967	0.842233	-2.294445
C	1.833449	0.915268	-2.733677
H	2.486186	1.530987	-3.378389
H	0.906502	0.764151	-3.293821
N	-1.453115	3.067592	-0.177038
C	-0.452442	0.532331	2.288388
H	-1.036273	-0.117567	2.965458
H	-1.008889	1.474029	2.224295
C	2.372037	3.135055	0.261915
H	3.306996	3.450128	0.753423
H	1.929501	4.027304	-0.196613
C	0.866348	3.725753	2.083229
H	0.108152	3.305086	2.746614
H	0.339685	4.411681	1.415288
C	1.894283	-1.330639	-1.434442
H	2.367807	-2.326618	-1.446661
H	2.123305	-0.885769	-0.464237
C	1.885087	4.510904	2.899239
C	-0.161452	-2.143183	-0.352609
H	0.221501	-3.173444	-0.269349
H	-1.240035	-2.205107	-0.538785
C	0.334894	-3.526160	-3.012566
C	0.914466	0.815671	2.953607
H	0.740487	1.407555	3.861285
H	1.373804	-0.119465	3.297284
C	-0.041272	-2.067865	-2.777367
H	0.324620	-1.459094	-3.608565
H	-1.134654	-1.995192	-2.780865
C	2.528387	-0.451203	-2.523580
H	2.560056	-0.971728	-3.488981
H	3.577771	-0.307061	-2.237526
C	0.046214	-1.434852	0.981309
H	-0.533793	-2.007923	1.728790
H	1.101135	-1.547628	1.296318
C	-2.851562	3.411508	0.094621
C	2.276764	4.094784	4.180618
H	1.836478	3.200398	4.612520
C	2.445249	5.692759	2.391733
H	2.138980	6.049403	1.411353
C	3.767156	5.988613	4.394796
H	4.490799	6.557781	4.971265
C	-0.526167	-4.557909	-2.609913
H	-1.472321	-4.308610	-2.135922
C	3.377880	6.425053	3.127362
H	3.794580	7.339139	2.713536
C	-3.636818	2.171491	0.538323
H	-3.542063	1.362993	-0.192594
H	-4.700842	2.406652	0.649774
H	-3.267948	1.802860	1.502277
C	3.210322	4.821924	4.920933
H	3.495911	4.480991	5.912244
H	-2.798245	2.503180	-2.567588
C	-2.965555	4.528404	1.144398
H	-2.542647	4.202721	2.101462
H	-4.011739	4.811916	1.308821
H	-2.425503	5.427558	0.823940
C	1.533105	-3.877972	-3.651120
H	2.204789	-3.098255	-3.999082
C	1.869914	-5.215807	-3.863702
H	2.802261	-5.464309	-4.363063
C	-3.867993	0.785398	-3.293128
H	-3.676269	-0.147270	-3.840333
H	-4.608082	1.357262	-3.865303
H	-4.308175	0.522384	-2.326696
C	-1.972895	1.977168	-4.471957
H	-1.066870	2.575629	-4.336900
H	-2.688507	2.559081	-5.065747
H	-1.705813	1.085036	-5.053256
H	-3.334832	3.788582	-0.825738
C	1.007838	-6.230470	-3.445192
H	1.266775	-7.271962	-3.612919

C	-0.194990	-5.897031	-2.820189
H	-0.879383	-6.678634	-2.502368
H	-1.442598	-0.071460	-2.713555
H	-0.915290	3.926919	-0.289261

(4) X = Y = NH(2,6-MeC_6H_4), isomer P

Zr	0.768153	0.441998	-0.782736
N	1.369220	0.672805	1.841541
C	1.903258	2.424396	3.669918
C	3.255001	2.723128	3.897083
H	3.948698	2.736186	3.061019
C	2.742009	0.120629	1.791876
H	3.240446	0.198069	2.769830
H	2.648841	-0.938165	1.550171
C	1.278948	-2.698621	-0.491446
H	0.660310	-3.484070	-0.965361
H	1.727374	-3.187316	0.392295
N	0.472869	-1.547801	-0.130840
C	1.385876	2.112101	2.272860
H	1.967639	2.656620	1.526095
H	0.358453	2.477685	2.205247
C	-3.014592	2.671951	0.425427
C	0.213341	3.770220	-2.749698
C	-0.436536	2.444926	-4.696109
C	-3.091770	0.853943	-1.203968
C	-0.197028	4.917772	-3.433846
C	-4.344685	2.973917	0.124968
N	1.989864	-1.319016	-2.428915
H	-4.824790	3.795753	0.651719
H	-0.088509	5.880562	-2.939239
C	-0.403610	-1.831057	1.008920
H	-0.748459	-2.877865	0.965023
H	-1.299214	-1.204405	0.946806
C	3.145707	-0.754851	-3.183334
C	0.798824	3.919355	-1.368169
C	-2.302912	3.485938	1.481046
H	1.710781	3.325714	-1.242374
H	-1.391022	3.963115	1.100849
H	2.723309	-0.092828	-3.947702
H	3.665615	-1.565750	-3.713995
H	-2.012082	2.878547	2.351587
H	0.093534	3.588420	-0.599642
H	-2.952586	4.280738	1.857110
H	1.047482	4.965557	-1.164130
C	-0.724013	4.860549	-4.721384
C	-5.057197	2.250361	-0.827268
H	-1.036190	5.765630	-5.233722
H	-6.090184	2.497206	-1.053310
N	2.793296	0.981294	-0.505302
C	1.025595	2.462096	4.764397
H	-0.032227	2.266112	4.608275
C	2.058687	-2.869442	-5.507547
C	-2.353375	1.606154	-0.251138
C	0.086654	2.498794	-3.371629
H	2.127288	-1.849833	-5.878379
C	1.013905	-1.951528	-3.380275
H	0.664353	-1.162294	-4.050121
C	-4.419990	1.194774	-1.474151
H	0.154183	-2.268137	-2.785891
C	-0.831412	3.618814	-5.341517
C	1.840652	-5.492988	-4.603643
H	-1.231632	3.550240	-6.350673
H	-4.965873	0.604168	-2.206662
C	-0.565693	1.130293	-5.429955
C	-2.484593	-0.325255	-1.921301
H	1.740663	-6.515045	-4.249328
C	2.836576	3.040308	6.258591
H	-1.941000	-0.985582	-1.236819
H	-1.185486	0.405361	-4.887528
H	3.196217	3.278491	7.255418
H	0.409964	0.653107	-5.608338
H	-1.772830	-0.003351	-2.687708
H	-1.024354	1.280729	-6.410853
H	-3.260329	-0.918389	-2.415620
C	1.510623	-3.107068	-4.237629
N	-1.018440	1.294407	0.054612
H	-0.787557	1.749882	0.930921
C	0.493004	-0.122849	2.747517
H	-0.479220	0.382930	2.761777
H	0.892340	-0.081081	3.771270
C	3.643760	1.288533	-1.658024
H	4.500974	1.904201	-1.337268
H	3.079737	1.889528	-2.378596
C	2.433639	-2.288028	-1.401157
H	3.187921	-1.784130	-0.795907
H	2.905583	-3.170277	-1.859282
N	0.498563	1.321312	-2.726019
H	0.584998	0.596779	-3.430686
C	3.719924	3.024312	5.178301
H	4.770551	3.255283	5.329906
C	2.398652	-5.237808	-5.857106
H	2.739490	-6.058813	-6.481216
C	0.258943	-1.594578	2.378457
H	1.189258	-2.170205	2.452755
H	-0.397417	-1.995727	3.163236
C	1.484891	2.762910	6.047027
H	0.786041	2.788979	6.878258
C	2.502045	-3.921359	-6.309765
H	2.919680	-3.713018	-7.290682
C	3.573311	0.796187	0.704281
H	3.985203	1.759199	1.060920
H	4.458231	0.156186	0.536281
C	4.184628	0.042236	-2.381401
H	4.713190	-0.606527	-1.672610
H	4.942974	0.357778	-3.111436
C	1.398155	-4.436918	-3.805299
H	0.945316	-4.650095	-2.841036

(4) X = Y = NH(2,6-MeC_6H_4), isomer T

Zr	-0.000531	0.823001	0.000630
N	-0.340829	1.997141	-1.704467
N	2.501214	2.467719	-0.241950
C	0.775077	2.132377	-2.640326
H	0.405094	2.132330	-3.680533
H	1.414398	1.249338	-2.543951
C	5.872440	2.715309	0.341439
H	5.668926	1.990027	1.125334
N	1.581651	-0.531506	-0.361444
C	4.995618	2.814920	-0.749473
C	1.639313	3.396187	-2.432106
H	1.111922	4.287603	-2.793079
H	2.531856	3.309162	-3.063355
C	2.013353	3.661039	-0.966401
H	2.746590	4.482301	-0.914444
H	1.119252	4.005554	-0.444150
C	1.151055	-2.518334	-1.734700
C	2.880366	-2.582448	-0.005281
C	6.440170	4.542906	-1.678977
H	6.661228	5.245986	-2.477137
C	1.447774	-3.848696	-2.040700
H	0.894677	-4.332715	-2.842290
C	3.759249	1.928419	-0.830602
H	3.555435	1.668596	-1.871580
H	3.977612	0.988278	-0.316253
C	7.294177	4.440660	-0.579885
H	8.180051	5.065832	-0.515412
C	0.110421	-1.780610	-2.537139
H	0.516662	-0.858953	-2.969791
H	-0.748433	-1.494979	-1.922516
H	-0.260245	-2.402415	-3.357321
C	2.433882	-4.556074	-1.355843
H	2.648078	-5.590225	-1.608609
C	-1.364925	3.001463	-1.938462
H	-1.614428	3.046961	-3.013514
H	-1.016933	4.018590	-1.683156
C	5.304991	3.734903	-1.762110
H	4.660663	3.811489	-2.633478
C	1.860747	-1.869665	-0.692607
C	7.008865	3.520008	0.429876
H	7.674705	3.421919	1.282667
C	3.146092	-3.910960	-0.348503
H	3.925565	-4.444364	0.191016
C	3.689146	-1.922468	1.087518
H	3.056995	-1.492657	1.874481
H	4.323115	-1.109000	0.704661
H	4.359239	-2.645110	1.560984
C	-2.670979	2.715612	-1.204894
H	-3.373628	3.541975	-1.400484
H	-3.113834	1.807841	-1.632387
N	0.339676	1.998890	1.704224
N	-2.503057	2.468407	0.240737
C	-0.776182	2.135339	2.640040
H	-0.406003	2.137014	3.680162
H	-1.415201	1.251976	2.544986
C	-5.873784	2.721521	-0.342813
H	-5.671172	1.996006	-1.126720
C	-4.997028	2.819806	0.748273
C	-1.640487	3.398818	2.429998

H	-1.113281	4.290723	2.790050
H	-2.533187	3.312489	3.061115
C	-2.014147	3.662125	0.963915
H	-2.746603	4.484007	0.910903
H	-1.119668	4.005162	0.441362
C	-6.439272	4.549772	1.677649
H	-6.659469	5.253097	2.475830
C	-3.762021	1.931408	0.829629
H	-3.558616	1.671398	1.870647
H	-3.982239	0.991662	0.315257
C	-7.293222	4.448828	0.578395
H	-8.178196	5.075261	0.513814
C	1.363806	3.003573	1.936744
H	1.613395	3.050415	3.011702
H	1.015783	4.020363	1.680165
C	-5.305263	3.740144	1.760926
H	-4.660983	3.815761	2.632409
C	-7.009039	3.527855	-0.431390
H	-7.674859	3.430788	-1.284313
C	2.669684	2.716614	1.203273
H	3.372612	3.543024	1.397695
H	3.112492	1.809313	1.631838
N	-1.582745	-0.529441	0.370025
C	-1.147702	-2.520255	1.736338
C	-2.875892	-2.582578	0.005700
C	-1.440468	-3.852841	2.036602
H	-0.886599	-4.338433	2.836700
C	-0.110840	-1.782258	2.543514
H	-0.520784	-0.863059	2.977885
H	0.748535	-1.492081	1.931824
H	0.259511	-2.405699	3.362607
C	-2.423905	-4.560413	1.348132
H	-2.634977	-5.596288	1.596440
C	-1.858518	-1.869740	0.696199
C	-3.137771	-3.913322	0.343232
H	-3.915457	-4.446828	-0.198757
C	-3.686516	-1.920144	-1.084216
H	-3.055484	-1.483863	-1.868499
H	-4.323605	-1.110999	-0.697410
H	-4.353750	-2.642807	-1.561674
H	-2.393235	-0.134698	-0.100679
H	2.388832	-0.138681	0.116638

(5) X = Cl, Y = NH(^{t}Bu), isomer P

Zr	-0.622991	1.496405	0.050508
N	0.811872	1.286933	2.291805
C	1.961998	2.715341	4.116037
C	3.323840	3.000534	3.937232
H	3.708721	3.169436	2.935473
C	2.075860	0.786928	1.706215
H	2.867866	0.702064	2.465220
H	1.874443	-0.214325	1.321941
C	-0.297533	-1.610111	-0.433299
H	-1.105037	-2.276870	-0.788428
H	0.403149	-2.271103	0.107232
N	-0.834589	-0.563777	0.421444
C	-3.392017	2.418569	1.609768
C	-4.122861	1.526823	0.590307
C	1.008160	2.631836	2.932651
H	1.323324	3.316510	2.141962
H	0.023785	2.964093	3.272654
N	-0.220263	0.191193	-2.140137
C	-1.264029	-1.079299	1.720563
H	-1.630613	-2.113565	1.613731
H	-2.105218	-0.482934	2.087729
C	0.621567	0.901516	-3.148389
H	-0.000199	1.710004	-3.543570
H	0.841375	0.214846	-3.977789
N	1.378576	2.065012	-0.259755
C	1.489203	2.547795	5.426756
H	0.431985	2.356554	5.592902
C	-1.514200	-0.483065	-5.265106
H	-1.494384	0.598382	-5.371259
C	-1.554817	-0.156022	-2.748597
H	-2.026313	0.798375	-2.988613
H	-2.149179	-0.619268	-1.957075
C	-1.624119	-3.253458	-5.012491
H	-1.680015	-4.333285	-4.906264
C	3.705804	2.905210	6.324299
H	4.377539	2.979317	7.174608
C	-1.546059	-1.047002	-3.980127
N	-1.933056	2.204080	1.506150
H	-1.501415	2.696399	2.285237
C	0.243927	0.333937	3.287921
H	-0.652518	0.816335	3.692504
H	0.953467	0.212951	4.119244
C	1.782383	2.593857	-1.568928
H	2.736810	3.134557	-1.466616
H	1.046301	3.327100	-1.912468
C	0.468586	-1.009029	-1.610439
H	1.450740	-0.685713	-1.260274
H	0.628091	-1.759440	-2.398904
Cl	-1.676034	3.035167	-1.682670
C	4.189540	3.091059	5.028474
H	5.239852	3.315884	4.865819
C	-1.574498	-2.676508	-6.282289
H	-1.586660	-3.304044	-7.168879
C	-0.152638	-1.060715	2.784029
H	0.722808	-1.613618	2.422285
H	-0.500262	-1.608160	3.671426
C	2.349996	2.637426	6.521139
H	1.960159	2.506568	7.526626
C	-1.524226	-1.286760	-6.405488
H	-1.502008	-0.827147	-7.389631
C	-3.726223	3.900737	1.336833
H	-3.376218	4.188566	0.342827
H	-3.234641	4.546964	2.074304
H	-4.805994	4.083092	1.399801
C	-3.860605	2.045446	3.033123
H	-3.656638	0.991600	3.250329
H	-4.936303	2.216894	3.155011
H	-3.342296	2.654195	3.784843
C	2.520471	1.673010	0.544962
H	3.069783	2.560296	0.910504
H	3.262156	1.098295	-0.037612
C	1.939985	1.510019	-2.650329
H	2.633729	0.732744	-2.306701
H	2.413348	1.957864	-3.535032
C	-1.613699	-2.444444	-3.874824
H	-1.676375	-2.904741	-2.892323
H	-5.207409	1.641628	0.691480
H	-3.878599	0.470848	0.749657
H	-3.852145	1.800612	-0.432959

(5) X = Cl, Y = NH(^{t}Bu), isomer T

Zr	-0.588586	1.102502	-1.314838
N	1.363649	2.703205	0.512028
N	1.212010	1.641374	-2.214728
N	-0.317874	-0.067407	0.397916
N	0.266818	-1.409406	-2.106521
C	2.006891	1.599027	1.251200
H	2.925440	1.939460	1.758506
H	2.316484	0.861129	0.508384
C	2.443391	2.211035	-1.699750
H	2.975576	2.750720	-2.502305
H	3.151037	1.435131	-1.356867
Cl	-2.337325	0.507029	-2.977740
C	1.402898	0.945471	-3.488326
H	1.905174	1.607679	-4.212618
H	0.418669	0.731881	-3.924414
N	-1.625101	2.720538	-0.591175
C	-0.309701	0.538283	1.726894
H	-0.794857	-0.134818	2.455430
H	-0.916796	1.445573	1.685416
C	2.205263	3.218814	-0.580050
H	3.181785	3.578850	-0.214878
H	1.680842	4.082091	-1.006556
C	0.910090	3.807096	1.395724
H	0.211338	3.387782	2.123119
H	0.333954	4.499845	0.772519
C	1.740005	-1.274998	-2.224092
H	2.215489	-2.264168	-2.311442
H	2.094489	-0.835705	-1.289104
C	1.989970	4.601733	2.120597
C	-0.119407	-2.163426	-0.889893
H	0.350014	-3.158402	-0.870511
H	-1.203571	-2.309030	-0.946193
C	0.038935	-3.510014	-3.572271
C	1.094461	0.893873	2.266010
H	0.967941	1.496874	3.173713
H	1.622826	-0.011854	2.588793
C	-0.339347	-2.058761	-3.313058
H	-0.083298	-1.448789	-4.181244
H	-1.420332	-1.975594	-3.193796
C	2.195327	-0.376665	-3.383565
H	2.124588	-0.898387	-4.345242
H	3.262718	-0.173827	-3.234490
C	0.197930	-1.426304	0.404802

H	-0.262027	-2.008055	1.223030
H	1.284908	-1.463781	0.601675
C	-3.009566	3.203763	-0.400129
C	2.462067	4.209429	3.381783
H	2.039074	3.332791	3.864474
C	2.531520	5.760457	1.544301
H	2.162870	6.099048	0.579107
C	3.993019	6.081524	3.443996
H	4.763539	6.652048	3.954501
C	-0.766997	-4.550334	-3.084779
H	-1.665903	-4.308318	-2.523524
C	3.524413	6.493648	2.195298
H	3.925895	7.389937	1.730801
C	-3.931861	2.013597	-0.082437
H	-3.942100	1.295375	-0.905381
H	-4.958532	2.359675	0.079839
H	-3.597436	1.499820	0.825288
C	3.455612	4.938344	4.037465
H	3.803471	4.617316	5.015366
C	-3.040599	4.190324	0.785054
H	-2.698195	3.705602	1.705564
H	-4.054948	4.567441	0.955394
H	-2.395060	5.056805	0.593643
C	1.170584	-3.853699	-4.327366
H	1.793798	-3.069955	-4.748944
C	1.499797	-5.188856	-4.567493
H	2.379622	-5.429677	-5.157699
C	-3.498230	3.921252	-1.676699
H	-2.852258	4.776305	-1.907828
H	-4.522245	4.294750	-1.555026
H	-3.474664	3.235636	-2.527255
C	0.695341	-6.210662	-4.061218
H	0.947533	-7.250132	-4.250474
C	-0.443712	-5.886806	-3.322021
H	-1.085841	-6.673963	-2.936844
H	-0.984296	3.495712	-0.425347

(6) X = Cl, Y = NH(2,6-^{i}PrC$_6$H$_4$), isomer P

Zr	1.287947	0.326962	0.453579
Cl	3.236197	-0.464548	1.821964
N	-1.099668	1.596669	0.333418
N	-0.239411	-0.823252	1.307209
N	1.844718	-1.911264	-0.697265
N	1.049581	0.553111	-1.615786
N	1.801515	2.295966	1.044236
H	0.986275	2.793629	1.384609
C	-1.931933	0.409596	0.033285
H	-1.652795	0.068308	-0.964451
H	-3.002205	0.663535	0.013021
C	-1.659604	-0.717956	1.027349
H	-2.232631	-0.572252	1.960529
H	-2.065152	-1.644562	0.584123
C	0.108927	-2.094352	1.954692
H	-0.703678	-2.393779	2.635538
H	0.998924	-1.955194	2.576601
C	0.372080	-3.238060	0.959008
H	0.446202	-4.182610	1.515182
H	-0.487359	-3.359099	0.288087
C	1.682563	-3.117287	0.168961
H	2.511875	-3.087745	0.881922
H	1.806731	-4.019605	-0.445888
C	0.847901	-1.888160	-1.794201
H	-0.135604	-2.008090	-1.335737
H	0.996101	-2.729356	-2.486911
C	0.883793	-0.555361	-2.542611
H	1.686040	-0.551862	-3.302585
H	-0.056807	-0.478499	-3.116308
C	0.750650	1.846918	-2.230254
H	1.050940	1.837100	-3.290500
H	1.347632	2.626416	-1.745119
C	-0.733222	2.239778	-2.138929
H	-0.908354	3.122293	-2.769548
H	-1.361008	1.446362	-2.562093
C	-1.209579	2.630903	-0.734170
H	-0.609962	3.484903	-0.397438
H	-2.251480	2.975409	-0.802664
C	-1.478856	2.196119	1.658979
H	-0.793366	3.027958	1.836918
H	-1.271658	1.439668	2.419217
C	-2.898249	2.724956	1.813719
C	-3.203237	4.056928	1.492606
H	-2.415458	4.713406	1.132354
C	-4.496493	4.557763	1.645301
H	-4.707402	5.592962	1.392577
C	-5.512618	3.733948	2.132682
H	-6.519354	4.122368	2.256386
C	-5.222510	2.412347	2.474388
H	-6.002243	1.768020	2.870584
C	-3.927027	1.916396	2.319437
H	-3.710381	0.892440	2.610262
C	3.254645	-1.861081	-1.229065
H	3.897103	-1.760376	-0.353129
H	3.343667	-0.933557	-1.799100
C	3.718607	-3.035751	-2.075258
C	4.373205	-4.125967	-1.481117
H	4.544169	-4.123658	-0.407851
C	4.822389	-5.201872	-2.247521
H	5.329547	-6.032987	-1.765632
C	4.631211	-5.204660	-3.630489
H	4.983938	-6.039282	-4.229567
C	3.997705	-4.120770	-4.239924
H	3.859511	-4.105470	-5.317434
C	3.550490	-3.046906	-3.468266
H	3.080607	-2.198136	-3.957852
C	2.961815	2.966863	1.506952
C	2.950615	3.623830	2.773332
C	4.086461	4.317615	3.197675
H	4.072544	4.822889	4.158865
C	5.242886	4.363172	2.424158
H	6.118674	4.903270	2.772495
C	5.260569	3.699308	1.203361
H	6.161588	3.730725	0.596558
C	4.146055	3.000492	0.724930
C	1.711990	3.595818	3.665336
H	1.129654	2.709788	3.388475
C	2.031721	3.440106	5.162742
H	1.106716	3.297946	5.732826
H	2.530524	4.324315	5.573784
H	2.677845	2.575110	5.338334
C	0.831117	4.842365	3.431590
H	-0.101371	4.787867	4.006185
H	0.573286	4.967850	2.373215
H	1.363934	5.749403	3.737990
C	4.239156	2.357281	-0.654472
H	3.328124	1.775915	-0.824050
C	4.293684	3.429191	-1.762515
H	4.300547	2.965661	-2.756247
H	5.198402	4.041134	-1.673435
H	3.433326	4.104087	-1.705881
C	5.428154	1.386046	-0.776331
H	5.420605	0.891636	-1.755254
H	5.385838	0.619775	0.002301
H	6.386961	1.907772	-0.685482

(6) X = Cl, Y = NH(2,6-^{i}PrC$_6$H$_4$), isomer T

Zr	-0.093016	1.171985	0.543711
N	-0.356376	2.280098	-1.204812
N	2.524006	2.717182	0.175301
C	0.721969	2.393593	-2.182002
H	0.309461	2.405440	-3.205268
H	1.338831	1.493563	-2.109768
C	5.930082	2.821850	0.630289
H	5.731050	2.113034	1.430241
N	1.363857	-0.230198	0.064178
C	5.012666	2.947099	-0.423729
C	1.619301	3.638077	-2.007518
H	1.099706	4.538758	-2.357623
H	2.489133	3.527073	-2.666349
C	2.046964	3.909290	-0.557697
H	2.803231	4.711174	-0.540998
H	1.178898	4.286129	-0.012912
C	0.831455	-2.259698	-1.226738
C	2.236515	-2.417947	0.780957
C	6.485253	4.603812	-1.434384
H	6.700539	5.288903	-2.249576
C	0.988136	-3.639337	-1.403933
H	0.507451	-4.119800	-2.251782
C	3.737503	2.112984	-0.440666
H	3.488783	1.838108	-1.468148
H	3.937077	1.178326	0.094801
C	7.380791	4.476998	-0.371479
H	8.293699	5.065199	-0.352417
C	0.034754	-1.474348	-2.264261
H	-0.093328	-0.454269	-1.894121
C	-1.374691	-2.049572	-2.494503
C	0.812093	-1.377426	-3.592876
C	1.754449	-4.407677	-0.533963
H	1.866627	-5.476067	-0.695917

C	-1.422825	3.243109	-1.419282
H	-1.714006	3.265766	-2.483831
H	-1.111060	4.276486	-1.181851
C	5.315352	3.842936	-1.459771
H	4.638572	3.937496	-2.304339
C	1.472185	-1.633582	-0.126702
C	7.101615	3.579198	0.660271
H	7.799243	3.461705	1.484690
C	2.371569	-3.790225	0.549860
H	2.963131	-4.389275	1.237075
C	2.916892	-1.799730	2.000845
C	2.590927	-2.552334	3.304763
H	2.521064	-0.786688	2.127579
C	4.442376	-1.689350	1.800839
C	-2.672853	2.880321	-0.626392
H	-3.430780	3.667767	-0.750620
H	-3.084832	1.953669	-1.039494
N	0.450401	2.326496	2.187210
N	-2.402361	2.617674	0.809492
C	-0.630384	2.420624	3.168361
H	-0.217147	2.443435	4.190047
H	-1.229967	1.502409	3.119979
C	-5.815764	2.550913	0.329344
H	-5.579318	1.820040	-0.439780
C	-4.907954	2.762306	1.378580
C	-1.563541	3.636325	2.976451
H	-1.066570	4.556177	3.307846
H	-2.431173	3.513847	3.635184
C	-1.995242	3.857692	1.518677
H	-2.801767	4.605495	1.480259
H	-1.150637	4.275388	0.966252
C	-6.466356	4.382000	2.321883
H	-6.719009	5.085645	3.110169
C	-3.605143	1.978387	1.437716
H	-3.355410	1.756015	2.476768
H	-3.731307	1.014376	0.942819
C	-7.349776	4.171044	1.262320
H	-8.290466	4.712359	1.218524
C	1.481271	3.328981	2.376309
H	1.762400	3.389878	3.441804
H	1.133242	4.343428	2.110860
C	-5.260610	3.680980	2.378820
H	-4.594642	3.838719	3.222695
C	-7.022598	3.248384	0.267056
H	-7.710657	3.064042	-0.553184
C	2.755548	3.002084	1.604218
H	3.478733	3.821786	1.746121
H	3.197274	2.099191	2.041541
Cl	-1.668693	-0.637700	1.105074
H	2.269295	0.149840	0.325812
H	-1.934613	-1.412820	-3.189667
H	-1.930569	-2.106402	-1.554862
H	-1.339716	-3.053996	-2.930993
H	0.262127	-0.773277	-4.324117
H	0.971080	-2.369538	-4.030559
H	1.796570	-0.921196	-3.444368
H	3.019635	-2.026607	4.165737
H	3.001076	-3.567737	3.305209
H	1.509608	-2.627153	3.453021
H	4.918393	-1.194697	2.656133
H	4.692587	-1.123735	0.895901
H	4.895011	-2.681609	1.694861

(9) X = Cl, Y = NH{N(Ph)N(Ph)(*n*Bu)}, isomer P

Zr	-0.560675	-0.400699	0.263143
Cl	-0.718291	1.948569	1.237331
N	-2.602912	-0.471062	2.025725
N	-0.353382	-2.105941	-1.703012
N	2.264864	-0.185381	0.632870
N	1.382181	0.277235	-0.388911
N	-2.202928	-0.193410	-1.008446
C	3.115192	1.882505	-1.165670
H	3.868639	1.439991	-0.525817
N	-0.581064	-2.203637	1.317263
C	0.141342	-1.389386	-2.931476
H	-0.491527	-0.510988	-3.059905
H	1.135871	-1.021623	-2.683800
C	3.578253	-1.379659	-1.090957
H	3.001132	-0.899823	-1.868521
C	4.606260	-2.259034	-1.430634
H	4.790978	-2.471646	-2.480674
C	1.803571	1.367052	-1.171489
C	-3.742542	0.436548	1.714964
H	-4.580216	0.215652	2.392592
H	-3.392571	1.446918	1.944142
C	0.502770	-3.303821	-1.448370
H	0.380836	-4.014419	-2.277870
H	1.538127	-2.953063	-1.474867
C	3.464393	2.952992	-1.990162
H	4.485332	3.325440	-1.963540
C	-3.063436	-0.316266	4.561322
C	0.286998	-4.050052	-0.126675
H	-0.697846	-4.531713	-0.098346
H	1.018158	-4.869531	-0.121126
C	-4.269541	0.427872	0.273477
H	-4.720741	-0.540532	0.023674
H	-5.097396	1.149686	0.252131
C	3.319122	-1.057302	0.254260
C	1.222542	3.043318	-2.846460
H	0.471386	3.495072	-3.489347
C	4.144994	-1.637950	1.238665
H	3.980585	-1.415860	2.285642
C	0.861197	1.980623	-2.025952
H	-0.165621	1.626337	-2.024765
C	5.409026	-2.841191	-0.448941
H	6.208455	-3.524269	-0.718543
C	-2.663223	-1.237234	-1.916777
H	-3.694047	-1.556795	-1.688293
H	-2.704454	-0.849222	-2.949943
C	-0.898180	-2.211734	-5.108242
H	-1.797500	-1.652519	-4.864455
C	-2.085866	-0.173340	3.404617
H	-1.224801	-0.825587	3.566355
H	-1.710722	0.850638	3.363935
C	2.530693	0.753633	1.758617
H	3.612466	0.922586	1.835033
H	2.064113	1.703877	1.491314
C	-1.778386	-2.480391	-1.839822
H	-1.940181	-3.125867	-2.715716
H	-2.045416	-3.056752	-0.952338
C	-3.223887	-1.534428	5.239206
H	-2.634957	-2.396605	4.937676
C	-3.241250	0.824320	-0.799903
H	-2.773338	1.770366	-0.515260
H	-3.769984	1.004602	-1.749779
C	1.985869	0.300537	3.118630
H	0.908482	0.123698	3.032954
H	2.431252	-0.657383	3.415328
C	0.193238	-2.184477	-4.226962
C	5.170344	-2.514372	0.886463
H	5.784436	-2.947308	1.671626
C	-1.733561	-2.787668	1.989705
H	-2.002882	-3.770814	1.566443
H	-1.491144	-2.988079	3.048707
C	2.529071	3.541478	-2.839937
H	2.807058	4.374268	-3.478651
C	-2.967328	-1.892527	1.875704
H	-3.731644	-2.198372	2.606709
H	-3.403054	-2.011623	0.881719
C	0.489167	-3.183332	1.126731
H	1.452661	-2.669556	1.050804
H	0.562548	-3.834257	2.012961
C	1.356105	-2.878429	-4.595908
H	2.224425	-2.848592	-3.943042
C	-0.840393	-2.926903	-6.305700
H	-1.697053	-2.930651	-6.973825
C	1.419745	-3.594385	-5.791640
H	2.331834	-4.121367	-6.057276
C	-3.804502	0.788957	5.007983
H	-3.673548	1.750167	4.517783
C	0.318284	-3.624776	-6.648912
H	0.366833	-4.178498	-7.582123
C	-4.852181	-0.547019	6.730662
H	-5.539931	-0.635520	7.566806
C	-4.692387	0.677026	6.078391
H	-5.252541	1.547561	6.408112
C	-4.111250	-1.652498	6.310449
H	-4.216290	-2.605312	6.821905
C	2.240239	1.347279	4.211338
H	1.760269	2.290113	3.919739
H	3.317289	1.556365	4.273634
C	1.725976	0.913722	5.587913
H	1.921429	1.678981	6.346223
H	0.644909	0.735208	5.568865
H	2.208631	-0.013246	5.919034

(9) X = Cl, Y = NH{N(Ph)N(Ph)(*n*Bu)}, isomer T

Zr	0.302601	0.623561	0.737729

N	-0.169317	1.610199	-1.027456
N	2.485404	2.235998	0.536398
C	0.950281	1.687790	-1.960442
H	0.593599	1.614367	-3.000616
N	1.362747	-1.597205	-0.773497
N	1.694667	-0.993191	0.477741
H	1.593081	0.813145	-1.816676
C	5.865741	2.368999	1.294211
H	5.608807	1.692548	2.105392
C	2.980504	-3.012823	1.154680
H	2.888321	-3.450566	0.168441
C	5.026337	2.448791	0.172415
C	1.803451	2.966442	-1.809484
H	1.297647	3.821336	-2.274652
H	2.734306	2.830081	-2.371949
C	2.082746	3.360152	-0.351541
C	3.705085	-1.310276	-1.537051
H	4.012664	-1.062225	-0.532597
H	2.846170	4.151903	-0.324881
C	4.653151	-1.346556	-2.560075
H	1.172574	3.785996	0.076588
H	5.684406	-1.092895	-2.328886
C	2.400805	-1.756714	1.423636
C	6.573468	4.061690	-0.799032
H	6.849710	4.710414	-1.625542
C	3.766495	1.597701	0.092567
H	3.625064	1.243216	-0.927764
C	3.688279	-3.696322	2.144037
H	3.889506	0.713141	0.719757
H	4.125653	-4.662080	1.903981
C	7.387592	3.983336	0.331890
H	8.297081	4.574042	0.392822
C	2.360889	-1.640619	-1.785438
C	-1.228749	2.556185	-1.326865
H	-1.438388	2.555630	-2.410144
C	3.258603	-1.921021	3.703211
H	-0.945062	3.596541	-1.087292
H	3.346270	-1.491059	4.697811
C	2.013674	-2.029880	-3.095353
C	5.408132	3.297570	-0.877764
H	0.989170	-2.287566	-3.330381
H	4.798944	3.350015	-1.775511
C	2.546208	-1.231214	2.727458
H	2.066195	-0.288048	2.977831
C	7.032899	3.129095	1.377349
H	7.668521	3.047348	2.254511
C	4.298106	-1.722842	-3.855272
H	5.039471	-1.752155	-4.647827
C	-2.526580	2.188423	-0.619795
H	-3.291530	2.949438	-0.844241
H	-2.879088	1.238247	-1.034659
N	0.393653	1.866924	2.424666
C	0.393339	-2.727922	-0.736439
N	-2.360829	1.988666	0.830863
H	0.866205	-3.614734	-1.178488
C	-0.748954	1.961105	3.338005
H	0.206959	-2.945411	0.316967
H	-0.385462	2.095556	4.370649
H	-1.283376	1.010603	3.322186
C	-5.710383	1.619093	0.106890
H	-5.367891	0.869237	-0.601828
C	-4.898959	1.949869	1.202760
C	-1.732384	3.108449	3.017821
H	-1.324047	4.071924	3.347952
H	-2.639325	2.955380	3.614864
C	-0.951535	-2.468734	-1.430641
C	-2.066823	3.258439	1.526730
H	-1.372188	-1.528317	-1.061413
H	-2.894608	3.977257	1.407466
H	-0.815172	-2.343992	-2.511838
H	-1.199754	3.697802	1.027065
C	-6.630682	3.499458	1.939674
H	-6.988285	4.223650	2.666458
C	2.970304	-2.071205	-4.107705
C	-3.545584	1.277706	1.392076
H	2.666039	-2.372108	-5.106725
H	-3.360806	1.110368	2.454373
H	-3.558487	0.288148	0.930496
C	-7.417714	3.168983	0.835443
H	-8.387894	3.637038	0.695249
C	3.841329	-3.160274	3.422429
H	4.392665	-3.698983	4.186886
C	1.302198	2.988962	2.595482
H	1.495661	3.165514	3.667430
H	0.881127	3.938144	2.217556
C	-5.386795	2.892204	2.120775
H	-4.796663	3.142143	2.998210
C	-6.955045	2.221681	-0.079471
H	-7.566490	1.944953	-0.933905
C	2.638794	2.706991	1.934864
H	3.286707	3.594149	1.984846
H	3.133413	1.903263	2.488111
Cl	-1.272757	-1.037042	1.724758
C	-1.946837	-3.607549	-1.173687
H	-2.099744	-3.707243	-0.091848
H	-1.513614	-4.558166	-1.515075
C	-3.297671	-3.387302	-1.861913
H	-3.988329	-4.212842	-1.660797
H	-3.771904	-2.464628	-1.508226
H	-3.183912	-3.305789	-2.949371

(11) X = Y = H, isomer P

Zr	0.000006	0.497365	0.000036
H	1.178311	1.976501	0.127143
N	-0.096216	-0.565453	-1.796582
N	0.096222	-0.565504	1.796625
C	5.680325	-1.321920	-3.572425
H	-1.178202	1.976580	-0.127038
H	-5.728665	-1.939071	4.465228
C	-5.680436	-1.321926	3.572354
H	5.728500	-1.939057	-4.465307
N	-2.292563	-0.478162	0.441462
N	2.292585	-0.478117	-0.441422
C	-3.005614	0.405275	1.431273
H	3.117964	1.371116	-0.935268
C	3.005642	0.405334	-1.431217
H	-3.117893	1.371076	0.935350
C	-1.896552	-1.778841	1.041879
C	1.896571	-1.778783	-1.041868
H	2.313879	0.562830	-2.261835
H	-2.313867	0.562726	2.261914
C	-3.139244	-0.667532	-0.771849
C	3.139261	-0.667524	0.771887
H	1.452709	-2.374150	-0.240657
H	-1.452685	-2.374188	0.240657
H	2.773675	-2.327834	-1.414833
H	-2.773653	-2.327903	1.414831
C	-4.442489	-0.886395	3.096408
C	4.442412	-0.886356	-3.096423
H	3.472729	0.333677	1.066406
C	-4.348541	-0.085518	1.948174
C	4.348535	-0.085490	-1.948176
H	-3.472715	0.333679	-1.066332
C	-6.853279	-0.955409	2.910602
C	6.853207	-0.955444	-2.910717
H	-4.037430	-1.240959	-0.501092
H	4.037449	-1.240940	0.501115
C	5.539222	0.287562	-1.305513
C	-5.539191	0.287576	1.305466
H	-3.538267	-1.157936	3.634702
H	3.538159	-1.157866	-3.634681
H	7.817755	-1.289568	-3.282141
H	-7.817852	-1.289508	3.281983
C	-6.779391	-0.143969	1.776932
C	6.779390	-0.144015	-1.777034
H	5.492937	0.934672	-0.433444
H	-5.492850	0.934694	0.433406
C	2.483537	-1.328483	1.994511
C	-2.483524	-1.328444	-1.994499
C	0.853973	-1.601686	-2.155015
C	-0.853955	-1.601759	2.155029
H	-7.687636	0.160669	1.264513
H	7.687665	0.160591	-1.264650
C	-1.313111	-0.535846	-2.606153
C	1.313119	-0.535913	2.606194
H	-3.282444	-1.421881	-2.743345
H	3.282456	-1.421945	2.743356
H	-2.161905	-2.353149	-1.771815
H	2.161923	-2.353181	1.771788
H	-1.347954	-1.369221	3.116273
H	1.347971	-1.369117	-3.116253
H	-0.373270	-2.585040	2.306289
H	0.373299	-2.584969	-2.306302
H	1.102873	-0.924510	3.614479
H	-1.102860	-0.924409	-3.614449
H	1.637968	0.504448	2.750510
H	-1.637968	0.504518	-2.750437

(11) X = Y = H, isomer T

Zr	-1.298806	0.993362	-1.182202
N	0.181937	2.516227	0.432037
N	0.485961	1.391583	-2.177602
N	-1.328364	-0.243845	0.491256
N	-0.786053	-1.480837	-2.024063
C	0.835710	1.579128	1.384686
H	1.641886	2.091537	1.931862
H	1.312904	0.806635	0.776314
C	1.642055	2.001834	-1.556224
H	2.258190	2.530133	-2.304188
H	2.323123	1.271420	-1.079581
H	-2.740062	0.593076	-2.328220
C	0.716113	0.684430	-3.427074
H	1.362079	1.276713	-4.095429
H	-0.244126	0.602963	-3.955165
H	-2.311893	2.568103	-0.976759
C	-1.440357	0.406794	1.786428
H	-1.941400	-0.254427	2.511986
H	-2.109713	1.271369	1.676418
C	1.179480	3.044891	-0.538957
H	2.044110	3.477858	-0.014937
H	0.682078	3.846629	-1.092393
C	-0.514364	3.655443	1.115907
H	-1.239812	3.226397	1.809778
H	-1.092940	4.158840	0.338843
C	0.693570	-1.569165	-2.147280
H	1.005619	-2.619127	-2.257998
H	1.101502	-1.219038	-1.195649
C	0.366054	4.657546	1.848302
C	-1.252294	-2.267683	-0.848793
H	-0.870114	-3.298070	-0.892088
H	-2.343382	-2.308895	-0.913254
C	-1.415692	-3.414398	-3.602262
C	-0.104409	0.893186	2.390341
H	-0.327736	1.554020	3.236964
H	0.452017	0.047379	2.813217
C	-1.507458	-1.934975	-3.258822
H	-1.133624	-1.338963	-4.093623
H	-2.550383	-1.645259	-3.116219
C	1.316393	-0.731713	-3.276600
H	1.234369	-1.246439	-4.241779
H	2.390890	-0.668372	-3.063756
C	-0.891915	-1.623514	0.489986
H	-1.408462	-2.200955	1.276096
H	0.187328	-1.744390	0.700789
C	0.755056	4.459911	3.181800
H	0.413861	3.577381	3.715863
C	0.788173	5.831615	1.206179
H	0.474302	6.020739	0.182808
C	1.980339	6.545673	3.185302
H	2.600831	7.273137	3.700736
C	-2.420642	-4.300625	-3.185356
H	-3.266822	-3.917736	-2.620596
C	1.588959	6.766140	1.863583
H	1.899819	7.669516	1.346355
C	1.556970	5.390642	3.844493
H	1.843101	5.217345	4.878176
C	-0.355156	-3.930958	-4.361778
H	0.418732	-3.262311	-4.728482
C	-0.287798	-5.289590	-4.675116
H	0.541564	-5.666265	-5.267279
C	-1.288591	-6.159361	-4.239401
H	-1.240148	-7.216071	-4.486200
C	-2.359455	-5.659341	-3.496466
H	-3.151702	-6.325069	-3.165714

(12) X = Y = ^{n}Bu, isomer P

Zr	-0.380492	-0.312191	0.309021
N	0.354578	-0.300430	-1.670274
C	0.789885	0.875268	-2.401061
H	0.201588	1.012201	-3.327813
H	1.838414	0.790629	-2.737528
C	-2.961178	-0.267717	2.378124
H	-3.051059	-1.357440	2.277331
H	-2.205394	-0.106308	3.164744
C	-2.482578	0.347463	1.050124
H	-2.504741	1.443602	1.166315
H	-3.228535	0.129730	0.267209
C	-4.760684	-0.346256	4.214162
H	-5.718179	0.066246	4.551521
H	-4.025850	-0.171109	5.009199
H	-4.883605	-1.431273	4.115478
C	-4.305095	0.280978	2.891760
H	-5.072167	0.116521	2.122255
H	-4.225774	1.371020	3.010669
C	2.814653	-3.318269	2.521479
C	3.034839	-4.644786	2.119850
H	2.334667	-5.117872	1.436008
C	4.807318	-3.470389	3.916066
H	5.487620	-3.009667	4.626897
N	-0.530141	2.120175	-0.700610
C	-1.251611	-2.467637	0.387310
H	-0.485339	-3.186670	0.053279
H	-1.458494	-2.739147	1.436402
N	0.819858	0.651378	1.754026
N	1.809331	-1.721360	0.759628
C	3.712510	-2.748950	3.437060
H	3.544016	-1.735909	3.792178
C	5.020744	-4.783004	3.492698
H	5.869854	-5.347263	3.867562
C	-2.339568	5.881380	-3.821732
H	-2.489989	6.796093	-4.387931
C	-1.950718	3.505086	-2.352881
C	4.127068	-5.370887	2.595636
H	4.274917	-6.397553	2.272606
C	0.363701	1.906396	2.355307
H	0.921474	2.096387	3.286201
H	-0.688160	1.818563	2.654493
C	-1.441216	3.641659	-3.653027
H	-0.906118	2.812471	-4.107941
C	-2.677179	4.577726	-1.813167
H	-3.108113	4.483618	-0.819606
C	-1.761302	2.221820	-1.557558
H	-2.611258	2.086312	-0.886921
H	-1.746915	1.362556	-2.232211
C	0.834162	-1.546202	-2.272742
H	0.872109	-1.437651	-3.368512
H	0.119356	-2.355863	-2.080516
C	0.705758	2.119175	-1.517239
H	1.546356	2.108486	-0.819593
H	0.786362	3.035652	-2.121379
C	0.517770	3.132045	1.432814
H	0.385486	4.046702	2.027729
H	1.543762	3.176027	1.047291
C	-1.628964	4.818128	-4.380528
H	-1.227868	4.899834	-5.386910
C	-0.509039	3.229254	0.294841
H	-1.507084	3.265499	0.743413
H	-0.364528	4.184949	-0.229976
C	-4.264490	-4.405482	-1.301594
H	-4.579097	-5.455092	-1.290854
H	-4.106435	-4.117727	-2.347963
H	-5.098831	-3.805379	-0.919618
C	2.768764	-0.614644	0.981478
H	2.901925	-0.113273	0.020117
H	3.752161	-0.995713	1.296391
C	2.229633	0.400405	1.987985
H	2.410020	0.058943	3.024744
H	2.838248	1.315515	1.878466
C	1.612154	-2.543696	2.002804
H	0.803009	-3.241249	1.780737
H	1.244494	-1.862830	2.774203
C	-2.518718	-2.719331	-0.450346
H	-3.342407	-2.093476	-0.082319
H	-2.352220	-2.403339	-1.493644
C	2.254039	-2.592397	-0.364395
H	1.597157	-3.468393	-0.360371
H	3.270169	-2.959792	-0.158717
C	2.225436	-1.985174	-1.774795
H	2.928907	-1.147702	-1.860151
H	2.614028	-2.768161	-2.441035
C	-2.868434	5.755771	-2.535849
H	-3.437038	6.571441	-2.098106
C	-2.997420	-4.182807	-0.468197
H	-2.188396	-4.820766	-0.851845
H	-3.174879	-4.509879	0.565841

(12) X = Y = ^{n}Bu, isomer T

Zr	0.063678	1.260409	-0.195721
N	1.719311	2.569855	1.830023
N	1.991988	1.576327	-0.938556
N	-0.063183	-0.048481	1.427007
C	-2.156074	3.515900	0.861621
C	-1.545225	1.148318	-3.108823
N	0.853898	-1.405675	-1.025057
H	-1.284763	2.216390	-3.173538
H	-2.902010	2.727676	0.674965

C	2.201965	1.443228	2.655811
H	-0.722406	0.615017	-3.611012
H	3.038861	1.752297	3.303239
H	-1.861447	3.397059	1.916514
C	-0.937489	3.318222	-0.056552
C	-1.637177	0.714534	-1.635929
H	2.599881	0.694126	1.967362
H	-1.883605	-0.357172	-1.584998
H	-0.198934	4.110362	0.139946
C	3.140987	2.063806	-0.196990
H	-1.256561	3.486931	-1.099935
H	-2.500655	1.223140	-1.173668
H	3.834319	2.596371	-0.872106
C	-4.066557	5.050691	1.643195
C	-2.700963	1.348858	-5.397433
H	-3.629309	1.173399	-5.952141
H	-4.540605	6.029873	1.513447
H	3.740770	1.244963	0.241563
H	-1.902131	0.795902	-5.906245
H	-3.775865	4.960895	2.696873
C	2.345089	0.876399	-2.165982
H	-2.463708	2.416282	-5.478057
H	-4.827333	4.285931	1.446645
C	-2.826494	0.919182	-3.931741
C	-2.857193	4.879101	0.717521
H	3.002536	1.501992	-2.793591
H	-3.171105	5.005271	-0.327546
H	1.432341	0.732756	-2.759959
H	-3.653490	1.463946	-3.456411
H	-2.127473	5.677526	0.912359
H	-3.096611	-0.144969	-3.880604
C	-0.215413	0.542013	2.750068
H	-0.874661	-0.081245	3.378135
H	-0.739901	1.500912	2.644429
C	2.752237	3.061468	0.892711
H	3.663711	3.376298	1.425944
H	2.335027	3.948201	0.403829
C	1.186384	3.695843	2.648881
H	0.384578	3.299889	3.276497
H	0.720529	4.395033	1.950266
C	2.326729	-1.373510	-0.901922
H	2.751982	-2.390008	-0.927101
H	2.551810	-0.964545	0.085596
C	2.181335	4.451918	3.519691
C	0.211661	-2.119229	0.101118
H	0.577679	-3.155030	0.181455
H	-0.858389	-2.164713	-0.127952
C	0.684045	-3.462376	-2.555921
C	1.108484	0.780963	3.508876
H	0.890877	1.371491	4.407408
H	1.514928	-0.170331	3.873459
C	0.400376	-1.983731	-2.323054
H	0.854309	-1.397531	-3.125173
H	-0.677069	-1.812263	-2.380269
C	3.021552	-0.496739	-1.955511
H	3.080721	-1.007197	-2.924595
H	4.060435	-0.363298	-1.630168
C	0.373266	-1.432256	1.455164
H	-0.234103	-2.012112	2.172787
H	1.415535	-1.539894	1.807982
C	2.459951	4.045807	4.833228
H	1.946782	3.182477	5.248179
C	2.829424	5.596781	3.032144
H	2.607921	5.947086	2.027118
C	4.016481	5.875002	5.120637
H	4.721823	6.423944	5.737925
C	-0.275838	-4.432086	-2.229650
H	-1.232524	-4.117900	-1.819890
C	3.739781	6.301548	3.820535
H	4.226112	7.187735	3.422433
C	3.370153	4.746206	5.626598
H	3.567236	4.415008	6.642409
C	1.895590	-3.896286	-3.114751
H	2.644531	-3.165266	-3.406845
C	2.149260	-5.253330	-3.321006
H	3.094021	-5.565337	-3.757467
C	1.188643	-6.205627	-2.977110
H	1.382908	-7.261872	-3.139878
C	-0.028500	-5.790111	-2.434388
H	-0.788768	-6.522138	-2.176646

(13) X = Y = NH(Me), isomer P

Zr	-1.292899	1.419918	0.045700
N	0.198869	1.242397	2.255896
C	1.306670	2.713967	4.067169
C	2.665350	3.014569	3.888445
H	3.050283	3.172282	2.884729
C	1.464739	0.784347	1.637124
H	2.274894	0.721782	2.380066
H	1.284174	-0.223055	1.258596
C	-0.849881	-1.709975	-0.452782
H	-1.626363	-2.417162	-0.805286
H	-0.122228	-2.341130	0.090536
N	-1.420607	-0.675817	0.385733
C	-4.027432	2.352757	1.466984
H	-4.312539	3.366597	1.792958
C	0.359172	2.596474	2.881625
H	0.667071	3.274818	2.082938
H	-0.635395	2.920367	3.198038
H	-4.610617	1.643360	2.077813
H	-4.363267	2.239667	0.432304
H	-2.254669	4.638560	-1.920643
H	-2.697039	4.268671	-0.249752
N	-0.837959	0.049166	-2.213082
C	-1.818247	-1.175488	1.700077
H	-2.176785	-2.216243	1.620650
H	-2.662232	-0.583521	2.072992
C	-2.803145	3.925139	-1.282958
H	-3.869922	4.013375	-1.546504
C	-0.021426	0.780420	-3.219852
H	-0.671573	1.557860	-3.638925
H	0.236589	0.102327	-4.047071
N	0.712052	2.021815	-0.338637
C	0.832976	2.558795	5.378894
H	-0.221838	2.353615	5.544339
C	-2.044583	-0.806540	-5.324637
H	-2.070246	0.270353	-5.471950
C	-2.137509	-0.392325	-2.818094
H	-2.675392	0.513234	-3.109975
H	-2.716078	-0.853456	-2.014639
C	-2.029639	-3.566709	-4.971058
H	-2.035922	-4.643344	-4.825530
C	3.041286	2.961137	6.277932
H	3.709257	3.057410	7.129090
C	-2.072590	-1.323578	-4.020305
N	-2.589754	2.112863	1.545013
H	-2.286136	2.244484	2.504462
C	-0.307653	0.265254	3.258205
H	-1.199355	0.717595	3.708615
H	0.430912	0.150090	4.065777
C	1.078317	2.544981	-1.653098
H	2.012633	3.128650	-1.585005
H	0.302910	3.239072	-1.997573
C	-0.097922	-1.095695	-1.634178
H	0.853553	-0.704441	-1.271016
H	0.123669	-1.858910	-2.396409
N	-2.297672	2.561016	-1.401459
H	-2.418170	2.245938	-2.358536
C	3.526387	3.133663	4.980712
H	4.574264	3.369891	4.817807
C	-1.986508	-3.035079	-6.260769
H	-1.954414	-3.694477	-7.123393
C	-0.690116	-1.133595	2.749809
H	0.190885	-1.665817	2.371047
H	-1.009989	-1.692587	3.640911
C	1.688739	2.677018	6.474581
H	1.297731	2.555140	7.480859
C	-1.998482	-1.650078	-6.435062
H	-1.979994	-1.226092	-7.435166
C	1.868162	1.676946	0.462743
H	2.396739	2.582438	0.820437
H	2.629313	1.117409	-0.112369
C	1.267959	1.455901	-2.727618
H	1.992291	0.709984	-2.378885
H	1.721373	1.909716	-3.620553
C	-2.075828	-2.717767	-3.863915
H	-2.130004	-3.143244	-2.865724

(13) X = Y = NH(Me), isomer T

Zr	-1.013876	1.255424	-1.009008
N	0.828143	2.687807	0.732473
N	0.864295	1.553034	-1.939567
N	-0.924073	-0.030630	0.672990
N	-0.239408	-1.490646	-1.760620
C	1.395787	1.607206	1.572595
H	2.289185	1.962198	2.112254
H	1.732050	0.826245	0.887946
C	-3.200460	1.577568	-3.366683

C	2.079273	2.087494	-1.359215
H	2.696010	2.581206	-2.132624
H	2.734066	1.302854	-0.933900
N	-2.323358	0.752026	-2.544323
C	1.116186	0.801631	-3.164302
H	1.735791	1.393074	-3.862322
H	0.157078	0.640666	-3.666487
N	-2.111338	2.919235	-0.420618
C	-0.967097	0.615797	1.979938
H	-1.496024	-0.021038	2.712078
H	-1.559489	1.532171	1.888067
C	1.789680	3.140307	-0.295880
H	2.738226	3.474355	0.154724
H	1.336344	4.006584	-0.791234
C	0.351685	3.845815	1.537656
H	-0.422678	3.483438	2.217244
H	-0.135951	4.534617	0.840393
C	1.237771	-1.397669	-1.796159
H	1.694121	-2.401400	-1.807740
H	1.541992	-0.925023	-0.860349
C	1.400424	4.629633	2.318252
C	-0.722277	-2.171032	-0.540045
H	-0.300279	-3.184977	-0.447848
H	-1.808327	-2.272798	-0.647785
C	-0.429605	-3.609517	-3.209440
C	0.416206	0.974579	2.572744
H	0.260916	1.622578	3.444385
H	0.909396	0.074609	2.961637
C	-0.799350	-2.149705	-2.971954
H	-0.512669	-1.551687	-3.840554
H	-1.889730	-2.088678	-2.885742
C	1.807293	-0.566232	-2.955646
H	1.768446	-1.120632	-3.901425
H	2.874882	-0.427767	-2.743369
C	-0.450031	-1.396743	0.745034
H	-0.964181	-1.946875	1.555045
H	0.625515	-1.464359	0.997418
C	-3.558750	3.055810	-0.301031
C	1.735164	4.293355	3.638139
H	1.229503	3.464681	4.125634
C	2.045498	5.731142	1.735429
H	1.783908	6.028333	0.723020
C	3.339416	6.101224	3.744373
H	4.085566	6.667979	4.293880
C	-1.226357	-4.640563	-2.688804
H	-2.117515	-4.390133	-2.118840
C	3.007247	6.459141	2.436681
H	3.491007	7.309589	1.964370
H	-4.043707	2.121034	-0.599278
C	2.696693	5.017763	4.344866
H	2.937530	4.739578	5.367113
H	-4.264502	1.307898	-3.266365
H	-3.878145	3.270856	0.731817
C	0.693951	-3.964951	-3.969900
H	1.311111	-3.187265	-4.410593
C	1.023409	-5.304014	-4.186467
H	1.897233	-5.554788	-4.781392
H	-2.951460	1.514153	-4.438388
H	-3.100951	2.626516	-3.075331
H	-3.971384	3.852854	-0.939940
C	0.227937	-6.317039	-3.649331
H	0.480891	-7.359598	-3.819598
C	-0.902198	-5.980883	-2.901991
H	-1.536153	-6.761554	-2.490930
H	-2.397307	-0.216788	-2.835219
H	-1.656892	3.786430	-0.153959

(14) X = Y = NH(CF_3), isomer P

Zr	-1.160396	1.316806	0.036602
N	0.206048	1.243572	2.205950
C	1.195748	2.848565	3.976683
C	2.542099	3.212964	3.827951
H	2.952560	3.351839	2.831648
C	1.522210	0.780252	1.698528
H	2.283014	0.799760	2.491845
H	1.391596	-0.256232	1.386035
C	-0.770669	-1.783427	-0.472984
H	-1.575564	-2.473357	-0.788181
H	-0.024954	-2.423575	0.031944
N	-1.288792	-0.746542	0.398597
C	-3.960786	1.647374	1.328063
F	-4.575373	0.899533	2.307118
C	0.297756	2.637923	2.767271
H	0.610288	3.287513	1.946829
H	-0.718212	2.932688	3.038095
F	-4.127910	0.931266	0.166346
F	-4.738328	2.758898	1.212242
F	-1.532495	4.769434	-2.174640
F	-1.352704	4.275520	-0.051756
N	-0.828946	0.037546	-2.158125
C	-1.714450	-1.260733	1.704406
H	-1.986381	-2.323513	1.610878
H	-2.617294	-0.739823	2.036585
C	-2.090682	3.998139	-1.180443
F	-3.322577	4.540804	-0.980683
C	-0.053752	0.779624	-3.198348
H	-0.699086	1.596215	-3.536780
H	0.116138	0.114525	-4.056135
N	0.819992	1.888597	-0.356700
C	0.683921	2.724769	5.277463
H	-0.364393	2.473745	5.418202
C	-2.228167	-0.695442	-5.217488
H	-2.210803	0.384456	-5.340801
C	-2.181373	-0.342002	-2.700998
H	-2.689438	0.593025	-2.946311
H	-2.733922	-0.801682	-1.878540
C	-2.329395	-3.461990	-4.924808
H	-2.381999	-4.540125	-4.802665
C	2.837127	3.278633	6.227980
H	3.469294	3.445974	7.095188
C	-2.216847	-1.243308	-3.925500
N	-2.625749	1.876023	1.543734
H	-2.510647	2.476706	2.351448
C	-0.334237	0.309951	3.240629
H	-1.265684	0.757211	3.600798
H	0.364791	0.273461	4.087486
C	1.201529	2.441789	-1.660199
H	2.177177	2.944753	-1.575228
H	0.485733	3.209780	-1.968413
C	-0.083220	-1.155180	-1.682611
H	0.905586	-0.807931	-1.380392
H	0.049799	-1.888886	-2.490610
N	-2.066985	2.649265	-1.425286
H	-2.699935	2.427371	-2.184569
C	3.357738	3.422081	4.941161
H	4.396730	3.707067	4.802143
C	-2.321882	-2.901526	-6.202893
H	-2.363204	-3.540557	-7.080194
C	-0.637643	-1.127847	2.794538
H	0.277257	-1.646874	2.483884
H	-0.982091	-1.650197	3.697940
C	1.494602	2.933625	6.393530
H	1.075474	2.835372	7.390840
C	-2.276191	-1.513714	-6.346444
H	-2.286686	-1.067084	-7.336574
C	1.961606	1.603541	0.490002
H	2.462051	2.537419	0.807290
H	2.741680	1.024022	-0.036106
C	1.291723	1.381232	-2.769497
H	2.004005	0.597651	-2.484041
H	1.708880	1.846729	-3.673310
C	-2.281622	-2.638778	-3.798585
H	-2.311990	-3.085484	-2.808637

(14) X = Y = NH(CF_3), isomer T

Zr	-0.800639	1.153350	-0.884280
N	0.889252	2.546430	0.907102
N	1.013818	1.521478	-1.830524
N	-0.737175	-0.092250	0.778241
N	-0.008374	-1.401720	-1.729922
C	1.506937	1.521876	1.777985
H	2.353677	1.943329	2.342743
H	1.922739	0.756186	1.118365
C	-2.938036	0.879760	-3.133758
C	2.202726	2.051658	-1.178979
H	2.831485	2.580102	-1.915781
H	2.848394	1.257416	-0.762823
N	-2.529555	0.397738	-1.919550
C	1.296955	0.852708	-3.095188
H	1.899771	1.507285	-3.745961
H	0.352455	0.703988	-3.629941
N	-1.645389	3.129901	-0.800774
C	-0.838008	0.493989	2.109804
H	-1.381001	-0.187284	2.785439
H	-1.458200	1.394787	2.047052
C	1.848751	3.063115	-0.093882
H	2.772088	3.426260	0.383247
H	1.369729	3.921013	-0.575888

C	0.301562	3.681613	1.684326
H	-0.403920	3.260179	2.402852
H	-0.293640	4.260683	0.977175
C	1.470399	-1.376086	-1.804762
H	1.877451	-2.395928	-1.889684
H	1.830777	-0.974860	-0.854174
C	1.280808	4.590477	2.412408
C	-0.482213	-2.156074	-0.547094
H	-0.050651	-3.168176	-0.517962
H	-1.565719	-2.264624	-0.657934
C	-0.417637	-3.441426	-3.237667
C	0.522761	0.848117	2.747709
H	0.339386	1.475169	3.628539
H	1.012762	-0.057308	3.125981
C	-0.634302	-1.959260	-2.970328
H	-0.264636	-1.378570	-3.817723
H	-1.700968	-1.745235	-2.896197
C	2.022214	-0.502704	-2.942672
H	1.981351	-1.029124	-3.903634
H	3.087996	-0.344030	-2.738583
C	-0.212983	-1.449346	0.777288
H	-0.707681	-2.045449	1.563198
H	0.864153	-1.487390	1.019140
C	-2.831738	3.406487	-0.176524
C	1.725554	4.299859	3.711001
H	1.354083	3.414528	4.219793
C	1.744832	5.767485	1.805741
H	1.389436	6.030202	0.812516
C	3.084458	6.300716	3.747121
H	3.777754	6.959791	4.261710
C	-1.375727	-4.382129	-2.830487
H	-2.278068	-4.039663	-2.330200
C	2.639318	6.613994	2.461614
H	2.980932	7.521962	1.972571
F	-3.186694	2.323349	0.601503
C	2.620771	5.142298	4.372372
H	2.948200	4.898170	5.379131
F	-4.037729	1.678952	-3.125362
F	-2.791242	4.480550	0.680368
C	0.717919	-3.909615	-3.916169
H	1.459284	-3.201217	-4.275431
C	0.902098	-5.271835	-4.158948
H	1.787878	-5.610512	-4.689088
F	-3.225001	-0.087214	-4.067090
F	-1.916536	1.631125	-3.678634
F	-3.893280	3.659978	-0.986457
C	-0.054130	-6.194885	-3.732876
H	0.085430	-7.254847	-3.924825
C	-1.198047	-5.744943	-3.071245
H	-1.956312	-6.453505	-2.749952
H	-3.259448	-0.134874	-1.459147
H	-1.353364	3.886832	-1.409133