Electronic Supplementary Information

Synthesis and structures of dinuclear cryptates with Zn(II), Cd(II) and Hg(II): tuning the cascade binding mode with metal ions

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Table S1 Cartesian coordinates of optimized structures (Coordinates are in unit of Å)

$[Zn_2L(OH)(H_2O)]^{3+}$							
Zn	2.948119	0.054974	-0.01082	N	-5.15352	-0.06417	-0.23302
Zn	-2.94619	0.057586	0.07986	N	3.574578	-1.89768	-0.87097
O	1.034546	-0.1771	-0.30267	N	3.064575	0.214141	2.148171
O	-1.09564	0.363026	0.626292	N	-3.30479	-1.90778	1.007618
H	0.849814	-1.10022	-0.5197	N	-2.9146	-0.14397	-2.06015
H	-0.9539	0.229875	1.571974	N	-3.55607	1.979959	0.948882
H	-0.02398	0.164891	0.1523	H	3.058275	-2.61647	-0.35917
N	5.144947	0.289599	0.144918	H	2.360152	0.891286	2.449634
N	3.140734	1.873413	-1.16546	H	-2.68118	-2.53824	0.500022
H	2.587659	1.721661	-2.01112	H	-3.04926	2.051825	1.833856
C	5.465465	1.636342	-0.38218	H	-2.24213	0.541257	-2.41356
H	6.525279	1.708554	-0.67691	C	5.77023	-0.77427	-0.67166
H	5.325469	2.365541	0.428624	C	5.477064	0.158977	1.582146
C	4.566037	1.983734	-1.55398	C	-5.63997	-1.12613	0.673943
H	4.8066	2.992007	-1.92625	C	-5.34318	-0.39178	-1.66365
H	4.739555	1.29294	-2.39249	C	-5.74167	1.254702	0.097351
C	2.619733	3.118607	-0.5343	H	5.574206	-0.91087	1.816138
H	2.928008	3.984796	-1.14731	H	-5.71646	-0.69395	1.682751
H	3.113893	3.243764	0.440851	H	-5.29541	-1.48303	-1.78713
C	1.125579	3.114776	-0.36285	H	-5.67587	1.887917	-0.79917
C	0.273487	2.89164	-1.4516	H	5.771044	-0.44002	-1.71926
H	0.687021	2.707791	-2.44799	C	5.011878	-2.08136	-0.54801
C	0.551182	3.429572	0.87373	C	4.401472	0.783002	2.452189
H	1.194798	3.666917	1.725662	C	-4.6985	-2.31557	0.690856

C	-4.2698	0.274319	-2.50385	C	-1.68168	3.228515	-0.05297
C	-5.0032	1.915927	1.244939	C	-1.03006	-1.6843	-2.60519
H	-5.06383	-3.06876	1.40544	C	1.774833	-2.04159	-2.53648
H	-5.42705	2.914495	1.436098	C	0.391876	-0.64818	3.6219
H	-4.42608	0.044939	-3.56976	C	-0.83104	3.497124	1.023449
H	4.66069	0.654227	3.514961	C	-0.17576	-0.81139	-3.29096
H	5.474212	-2.84442	-1.19323	C	0.917954	-2.97042	-1.92902
H	-4.68788	-2.81013	-0.29125	C	-0.55071	-2.68196	1.984384
H	-5.13037	1.341989	2.174843	H	0.748948	0.127149	4.306128
H	-4.32631	1.369705	-2.40446	H	-1.24981	3.772964	1.995771
H	4.344353	1.867476	2.276007	H	-0.58969	0.016742	-3.87475
H	5.075679	-2.4697	0.479262	H	1.330217	-3.85127	-1.42623
C	2.773143	-1.04767	2.898805	H	-0.89608	-3.5204	1.371711
C	-2.95087	-2.07216	2.452806	C	-0.97982	-0.89314	3.530156
C	-3.16719	3.186727	0.154518	C	-1.10881	2.942869	-1.29646
C	-2.51682	-1.46635	-2.63278	C	1.204317	-0.98184	-3.24916
C	3.257985	-2.13452	-2.31684	C	-0.46477	-2.78513	-1.94978
H	3.114013	-0.93188	3.941726	C	0.815157	-2.43101	2.07143
H	-3.52351	4.092749	0.673418	H	-1.75398	2.804742	-2.17096
H	-2.8857	-1.52459	-3.67205	H	-1.11268	-3.52841	-1.47622
H	3.650355	-3.12066	-2.61765	H	1.850801	-0.27653	-3.77875
H	-3.27241	-3.07288	2.790173	H	1.512275	-3.07576	1.52781
H	3.372483	-1.86021	2.460106	H	-1.67276	-0.30065	4.133856
H	-3.69636	3.148015	-0.80911	H	-6.81581	1.165559	0.328812
H	-3.03458	-2.26286	-2.07737	H	-6.34334	-0.0924	-2.01714
H	3.790183	-1.38244	-2.9165	H	-6.65714	-1.45593	0.402225
H	-3.52958	-1.34247	3.037707	H	6.828158	-0.92162	-0.39728
C	1.307859	-1.38554	2.860002	H	6.456952	0.609801	1.810685
C	-1.47438	-1.8848	2.673129				

$[Zn_2L(F)(H_2O)]^{3+}$

Zn	3.044097	-0.0164	-0.06267	H	3.444286	3.167965	-0.14258
Zn	-3.04254	0.025834	-0.0171	C	1.429772	2.947187	-0.86747
F	1.208842	0.02827	-0.50642	C	0.557749	2.707221	-1.93526
O	-1.06943	0.026167	0.292212	H	0.954865	2.503399	-2.93389
H	-0.77838	0.359617	1.152631	C	0.874692	3.263924	0.377172
H	-0.19466	-0.02393	-0.21937	H	1.531261	3.524368	1.213658
N	5.236141	0.083642	0.106196	N	-5.22995	0.040605	-0.19058
N	3.388182	1.551905	-1.50305	N	3.426859	-2.10049	-0.41756
H	2.826575	1.293067	-2.31644	N	3.103062	0.579964	2.001852
C	5.686038	1.273593	-0.65389	N	-3.43308	-1.58991	1.363052
H	6.74469	1.184693	-0.94778	N	-3.11179	-0.42796	-2.08842
H	5.6298	2.144177	0.015205	N	-3.35525	2.04904	0.643951
C	4.817071	1.506667	-1.87905	H	2.860679	-2.62351	0.253243
H	5.137298	2.427088	-2.39278	H	2.463043	1.372571	2.089763
H	4.942666	0.687318	-2.60254	H	-2.83205	-2.35398	1.046011
C	2.920157	2.900296	-1.07304	H	-2.83624	2.199801	1.511872
H	3.22648	3.648851	-1.82546	H	-2.4509	0.184843	-2.57195

C	5.735533	-1.1788	-0.48089	H	3.224063	-1.36103	2.835078
C	5.51834	0.203157	1.553429	H	-3.38554	2.94269	-1.27174
C	-5.74455	-0.80782	0.908373	H	-3.29878	-2.52732	-1.84359
C	-5.52632	-0.51202	-1.53227	H	3.581893	-2.0253	-2.52501
C	-5.65618	1.451369	-0.05593	H	-3.65669	-0.51403	3.17816
H	5.505986	-0.80484	1.992431	C	1.189847	-0.67917	2.991994
H	-5.79643	-0.18991	1.816354	C	-1.60546	-1.14855	2.961553
H	-5.53571	-1.60907	-1.45752	C	-1.3776	3.040582	-0.50533
H	-5.56547	1.931322	-1.04088	C	-1.24482	-2.05461	-2.29799
H	5.745913	-1.05695	-1.57403	C	1.537272	-2.43989	-1.98847
C	4.855652	-2.35777	-0.09893	C	0.288527	0.310975	3.411584
C	4.483529	1.082309	2.234507	C	-0.50719	3.320444	0.554735
C	-4.84388	-2.0063	1.145888	C	-0.33201	-1.41688	-3.14834
C	-4.48182	-0.0687	-2.54109	C	0.62479	-3.11803	-1.17311
C	-4.80092	2.185856	0.961771	C	-0.70104	-2.15572	2.605044
H	-5.22152	-2.59678	1.994704	H	0.661903	1.268443	3.787615
H	-5.10085	3.244117	1.008242	H	-0.90435	3.621385	1.529683
H	-4.70071	-0.50894	-3.52614	H	-0.69248	-0.78272	-3.96433
H	4.703583	1.155263	3.311118	H	0.979739	-3.82982	-0.42109
H	5.21826	-3.26856	-0.59969	H	-1.06844	-3.14627	2.320148
H	-4.85888	-2.67737	0.274352	C	-1.08921	0.080781	3.394634
H	-4.95925	1.774109	1.969578	C	-0.82136	2.743875	-1.75495
H	-4.5105	1.02318	-2.67454	C	1.037632	-1.6024	-2.98959
H	4.532298	2.107538	1.838042	C	-0.74575	-2.9198	-1.31907
H	4.925701	-2.55525	0.98029	C	0.670656	-1.92153	2.610289
C	2.673303	-0.42643	3.017311	H	-1.47745	2.583462	-2.61606
C	-3.0839	-1.37522	2.804606	H	-1.4397	-3.48237	-0.68701
C	-2.86785	3.093873	-0.31275	H	1.729465	-1.09752	-3.66893
C	-2.71998	-1.82648	-2.46444	H	1.350675	-2.73409	2.340028
C	3.017297	-2.59335	-1.77106	H	-1.76887	0.86413	3.743863
H	2.977279	-0.0771	4.019162	H	-6.72061	1.526576	0.220932
H	-3.17942	4.085629	0.057485	H	-6.53277	-0.22195	-1.8765
H	-3.02559	-2.00476	-3.50938	H	-6.77545	-1.14412	0.70918
H	3.325419	-3.64806	-1.8751	H	6.778904	-1.37958	-0.18524
H	-3.41307	-2.25197	3.387751	H	6.529738	0.601392	1.738348

$[Zn_2L(\mu\text{-}F)]^{3+}$

Zn	-2.13703	-0.00058	-0.00338	C	-0.11635	3.516129	-0.16902
Zn	2.135381	-0.00731	-0.00438	C	2.585957	2.064304	-2.37289
F	-0.00137	-0.00448	-0.00476	C	4.003889	0.054041	-2.35674
C	-5.04218	1.329974	0.450046	C	5.042332	0.462591	-1.3345
C	-4.00746	1.887109	1.402836	H	-1.97543	2.108204	1.473456
C	-2.58915	3.140074	-0.16797	H	1.971904	0.135609	-2.57349
C	-1.26641	3.115317	-0.85321	H	-2.03789	2.40228	-2.73856
C	-1.14037	2.580428	-2.13926	H	0.205343	1.876164	-3.67313
C	0.113849	2.306286	-2.67111	H	2.035848	3.618928	-0.19765
C	1.263941	2.58932	-1.92976	H	-0.2074	4.034269	0.79037
C	1.138048	3.26448	-0.71195	H	-5.14542	1.986477	-0.42584

H	-3.91241	1.234477	2.284383	H	-4.30027	-2.97849	1.618036
H	-2.7404	4.058203	0.421562	H	-3.41858	-0.75584	3.10958
H	3.410471	2.598006	-1.88224	H	2.732617	1.917885	3.60013
H	3.909428	-1.04248	-2.37867	H	4.288552	2.733485	2.00738
H	6.032724	0.073985	-1.6257	H	5.146895	0.372297	2.003613
H	-6.03426	1.320538	0.931655	N	-2.67579	-1.61808	1.321379
H	-4.30997	2.88029	1.770527	N	2.666437	1.422257	1.528641
H	-3.41387	3.083651	-0.89052	C	-5.03733	-0.275	-1.39524
H	2.737301	2.167246	-3.459	C	-3.9963	0.267053	-2.3501
H	4.302741	0.371451	-3.36805	C	-2.57802	-1.72076	-2.63201
H	5.14936	1.556542	-1.31505	C	-1.25572	-2.30068	-2.26509
N	-4.63188	-0.00503	-0.00831	C	-1.13107	-3.14154	-1.1548
N	-2.6771	1.953081	0.743375	C	0.122512	-3.46537	-0.65037
N	2.67378	0.614481	-2.0009	C	1.272844	-2.96806	-1.26762
N	4.633858	0.00491	0.001054	C	1.148788	-2.25399	-2.4634
C	-5.04285	-1.07077	0.917253	C	-0.10503	-1.91087	-2.955
C	-4.00146	-2.16827	0.934635	C	2.594631	-3.08762	-0.59049
C	-2.59462	-1.41381	2.803946	C	4.009355	-2.06072	1.141304
C	-1.27267	-0.80846	3.126578	C	5.045919	-1.37873	0.275753
C	-1.14555	0.572381	3.304985	H	-1.96115	0.216445	-2.56474
C	0.110022	1.16746	3.334339	H	1.977303	-2.29299	1.177721
C	1.258382	0.381365	3.209057	H	-2.02959	-3.5651	-0.69669
C	1.131719	-1.01079	3.18518	H	0.212735	-4.11293	0.226992
C	-0.12378	-1.60417	3.131779	H	2.047989	-1.98755	-3.02613
C	2.580059	1.026227	2.971478	H	-0.19539	-1.34014	-3.88419
C	3.993096	2.018907	1.223337	H	-5.14669	-1.36103	-1.52519
C	5.036729	0.935338	1.065546	H	-3.90352	1.357002	-2.22813
H	-1.96553	-2.32144	1.097896	H	-2.72979	-1.67512	-3.72196
H	1.957636	2.149687	1.394321	H	3.419155	-2.92918	-1.29823
H	-2.04318	1.181464	3.446612	H	3.912107	-1.53147	2.101944
H	0.203303	2.250198	3.461066	H	6.036534	-1.43293	0.757909
H	2.02977	-1.63345	3.234755	H	-6.02641	0.151522	-1.63244
H	-0.21703	-2.69392	3.100698	H	-4.29162	0.085512	-3.39526
H	-5.1588	-0.64087	1.922588	H	-3.40203	-2.31625	-2.21802
H	-3.9021	-2.61568	-0.06657	H	2.747325	-4.07908	-0.13537
H	-2.74987	-2.38022	3.309727	H	4.311913	-3.09385	1.373327
H	3.404075	0.33487	3.19126	H	5.154031	-1.91042	-0.68074
H	3.897307	2.591737	0.287942	N	-2.66694	-0.33509	-2.06758
H	6.024613	1.386669	0.873831	N	2.680029	-2.03843	0.477112
H	-6.02995	-1.48949	0.659435				

$[Zn_2L(\mu\text{-}Cl)]^{3+}$ (1)							
Zn	2.50591	0.000103	-0.00111	N	2.865995	-0.22164	-2.09269
Zn	-2.50525	-0.00191	0.000588	N	-4.81728	0.001612	0.001814
Cl	0.000683	-0.00324	-0.00094	N	-2.87015	-2.10434	0.067043
N	4.817486	0.003189	-0.00136	N	-2.86625	0.995676	-1.85271
N	2.869547	-1.70477	1.232859	N	-2.8632	1.108718	1.78834
N	2.865216	1.921817	0.858112	C	5.231188	-1.08106	0.911615

C	4.220952	-2.21052	0.876958	H	4.151918	1.43586	-2.22661
C	5.228083	1.336531	0.481437	H	4.52113	0.165558	-3.39883
C	4.215679	1.868443	1.476035	H	-5.30712	-1.71058	-1.11165
C	5.229311	-0.24561	-1.3972	H	-6.23798	-1.56455	0.370835
C	4.214965	0.34405	-2.35645	H	-4.15965	-2.01217	1.724622
C	-5.23267	-1.41371	-0.05545	H	-4.52892	-3.34344	0.622447
C	-4.22097	-2.28697	0.659939	H	-5.30009	1.824009	-0.92522
C	-5.22892	0.760629	-1.19599	H	-6.23478	0.470097	-1.54083
C	-4.21663	0.574329	-2.30871	H	-4.15663	-0.48578	-2.60103
C	-5.22688	0.661068	1.258014	H	-4.52272	1.134061	-3.20605
C	-4.21255	1.716144	1.651196	H	-5.29888	-0.10415	2.044525
C	2.691664	-1.59921	2.719031	H	-6.232	1.106804	1.179323
C	1.313627	-1.11132	3.031851	H	-4.1511	2.497986	0.877923
C	0.22158	-1.97812	2.925012	H	-4.51739	2.21541	2.583947
C	-1.07564	-1.48673	3.023521	H	2.892391	-2.58471	3.16949
C	-1.30798	-0.12293	3.22762	H	3.454188	-0.90925	3.106516
C	-0.21574	0.721765	3.448546	H	0.388899	-3.04743	2.765975
C	1.081372	0.229923	3.352822	H	-1.92355	-2.17714	2.969295
C	-2.68642	0.446467	3.122929	H	-0.38257	1.773481	3.699236
C	2.689442	3.153576	0.019682	H	1.929594	0.891181	3.557356
C	1.310707	3.1826	-0.55738	H	-3.44855	-0.33939	3.219075
C	0.220307	3.520721	0.250282	H	-2.88767	1.186934	3.913946
C	-1.07784	3.361962	-0.22238	H	3.450346	3.139171	-0.773
C	-1.31235	2.858575	-1.50574	H	2.893494	4.038135	0.644459
C	-0.22212	2.629631	-2.35086	H	0.38961	3.914053	1.256926
C	1.075965	2.793173	-1.87995	H	-1.92464	3.658502	0.404899
C	-2.69092	2.482869	-1.94428	H	-0.39153	2.32311	-3.38725
C	2.689709	-1.56486	-2.73731	H	1.922639	2.641166	-2.55715
C	1.309913	-2.0766	-2.47305	H	-2.89431	2.799002	-2.98019
C	0.220906	-1.5426	-3.16921	H	-3.45218	2.957488	-1.3096
C	-1.07823	-1.86993	-2.79696	H	2.894205	-1.46919	-3.81605
C	-1.31578	-2.7323	-1.7222	H	3.449997	-2.24399	-2.32699
C	-0.22708	-3.35474	-1.10345	H	0.392423	-0.86625	-4.01169
C	1.072478	-3.0293	-1.47728	H	-1.92358	-1.47122	-3.36715
C	-2.69544	-2.92273	-1.17874	H	-0.39868	-4.1028	-0.32397
H	5.302195	-0.66945	1.928983	H	1.917479	-3.54291	-1.00737
H	6.237646	-1.46007	0.669655	H	-2.9017	-3.97858	-0.93972
H	4.161713	-2.64353	-0.13412	H	-3.45524	-2.60525	-1.90635
H	4.528654	-3.02381	1.552367	H	2.175406	-2.38606	0.91196
H	5.298344	2.012288	-0.38328	H	2.16952	1.986037	1.607339
H	6.234027	1.318649	0.931776	H	2.168586	0.392443	-2.52359
H	4.156077	1.208257	2.355462	H	-2.17465	-2.4516	0.734122
H	4.52095	2.86036	1.843677	H	-2.16984	0.588638	-2.48412
H	5.303571	-1.3323	-1.54847	H	-2.16617	1.8582	1.749638
H	6.233865	0.156737	-1.60713				

$[Zn_2L(\mu\text{-}Br)]^{3+}$ (2)

Zn	-2.61169	-0.00219	-0.00108	Zn	2.613676	0.000054	-0.00474

Br	0.002242	0.003529	-0.00144	H	-2.24934	-2.52973	0.403881
N	-4.88832	-0.00344	-0.00529	H	-2.24712	0.92234	-2.39236
N	4.888596	-0.00112	0.008356	H	2.249333	-2.4154	0.853315
N	2.951987	-0.16507	-2.11024	H	-1.82584	-1.14846	-3.58048
N	2.938339	1.910623	0.907608	H	-0.51607	-4.08114	-0.71161
N	-2.94769	0.856695	1.931165	H	-1.83608	-2.53218	2.781054
N	-2.93745	-2.10534	-0.22483	H	-0.5401	1.422643	3.88827
N	-2.93915	1.24538	-1.71002	H	-0.53424	2.668753	-3.17546
N	2.937659	-1.74163	1.201186	H	-3.01964	0.636989	4.044387
C	-1.34895	-0.47752	3.242634	H	-3.47382	-0.80858	3.132411
C	-1.0208	-1.63742	-3.02298	H	1.840079	-3.54903	-1.24646
C	-0.29005	-3.28483	-1.42683	H	1.818553	0.700722	3.698472
C	1.331838	-1.29117	3.013653	H	0.52291	-3.24745	2.56618
C	-1.33244	-2.57469	-2.03249	H	0.529834	-0.59662	-4.09542
C	-1.34368	3.051456	-1.20572	H	-1.83172	3.67149	0.806855
C	-1.03294	-1.8027	2.926106	H	5.368201	-1.31867	-1.55688
C	1.337111	3.261116	-0.38577	H	6.32133	0.157929	-1.58171
C	1.346613	-1.96045	-2.62736	H	2.999804	-2.66246	3.115748
C	-0.31025	0.405525	3.557442	H	3.457078	-0.95469	3.099823
C	-0.30477	2.887529	-2.12845	H	1.823628	2.867237	-2.45532
C	-2.75696	0.023919	3.166518	H	0.527148	3.843551	1.534074
C	1.034937	-2.97772	-1.71926	H	4.24787	-2.6512	-0.16967
C	1.015879	0.002846	3.439914	H	4.603448	-3.05449	1.513266
C	0.293134	-2.20772	2.81686	H	-5.36756	1.936011	-0.65916
C	0.304235	-1.3353	-3.32064	H	-6.30859	0.685975	-1.45922
C	-1.02837	3.437591	0.101006	H	-2.99526	-3.8329	-1.46151
C	5.30898	-0.23343	-1.38938	H	-3.45926	-2.32849	-2.26672
C	2.740361	-1.67965	2.688937	H	-4.25153	2.348419	1.227777
C	1.021288	2.987844	-1.72081	H	-4.61774	1.816526	2.872539
C	0.297704	3.545318	0.506848	H	-5.35519	-1.53878	-1.3619
C	4.295017	-2.23302	0.848067	H	-6.30953	-1.60762	0.112613
C	-5.30058	0.922721	-1.08136	H	4.236715	1.171625	2.386714
C	-2.73996	-2.765	-1.55946	H	4.602714	2.829663	1.898637
C	-4.30416	1.461523	1.878514	H	5.357035	-0.70246	1.934147
C	-5.29841	-1.39791	-0.27276	H	6.309558	-1.46684	0.670499
C	4.292515	1.844585	1.516954	H	-5.3711	-0.40851	2.000324
C	5.298601	-1.0986	0.909857	H	-6.31584	0.904842	1.314968
C	-5.30612	0.463364	1.33332	H	5.36622	2.015363	-0.34502
C	5.300178	1.32691	0.509967	H	6.308374	1.300768	0.954659
C	-4.29476	-2.36485	0.32353	H	-4.24399	-2.24198	1.416788
C	-4.29311	0.896446	-2.21352	H	-4.60479	-3.4046	0.13612
C	2.745173	3.171233	0.113831	H	-4.23813	-0.11043	-2.65648
C	2.754636	-1.48315	-2.80315	H	-4.60368	1.579744	-3.01911
C	4.312399	0.385727	-2.34904	H	3.00534	4.029609	0.754819
C	-2.75074	2.731949	-1.60357	H	3.462641	3.165392	-0.71885
H	2.268581	0.475168	-2.52429	H	3.012511	-1.35933	-3.86774
H	2.24642	1.943641	1.662034	H	3.472593	-2.20131	-2.38264
H	-2.25936	1.612491	1.992179	H	4.263862	1.476143	-2.2037

H	4.628362	0.21948	-3.39052	H	-3.46932	3.117084	-0.86644
H	-3.01265	3.18658	-2.57316				

$[Zn_2L(\mu\text{-}I)]^{3+}$

Zn	-2.94205	0.085601	-0.12964	H	5.378741	-1.10926	-2.22295
Zn	2.888018	-0.06323	-0.14933	C	1.296011	0.367341	3.032972
I	0.06791	-0.00233	-0.66087	C	-5.46525	-1.12753	-1.39558
N	-5.20292	0.025379	-0.50844	H	-6.41841	-1.01021	-1.93652
N	-3.06022	-1.51662	-1.59665	H	-5.56974	-2.03214	-0.77886
H	-2.2624	-1.36473	-2.22304	C	-4.80052	2.441877	-0.59541
C	2.988602	3.032279	-1.10957	H	-5.07291	3.376852	-1.10935
H	3.609422	3.168505	-0.21285	H	-5.04416	2.602341	0.466764
H	3.400779	3.692497	-1.89156	C	0.308994	-3.54637	0.660258
C	-1.39698	-0.45898	3.01573	H	0.680996	-3.63269	1.682862
C	5.782735	0.067279	0.902197	C	-4.95819	-0.88355	1.763039
H	6.778498	0.538966	0.873019	H	-5.43135	-0.95649	2.754562
H	5.94474	-0.9551	1.274009	H	-4.79655	-1.91749	1.418375
N	-3.33232	2.216011	-0.67305	C	5.499551	1.179708	-1.26241
H	-3.07785	2.242462	-1.6672	H	6.482708	1.077959	-1.75076
N	5.179716	-0.01	-0.44575	H	5.572856	2.052275	-0.59729
C	1.080781	3.457852	0.476195	C	0.259845	1.302496	3.08921
H	1.786733	3.466286	1.311478	H	0.504182	2.363962	3.150563
C	-2.66231	3.404676	-0.0472	C	-0.71692	3.513401	-1.64431
H	-3.1802	4.308455	-0.41262	H	-1.40949	3.578008	-2.48895
H	-2.85008	3.356996	1.035056	C	-0.36088	-1.39515	3.067363
C	1.217028	-3.49781	-0.39557	H	-0.60387	-2.45795	3.111508
N	-3.61512	-0.24426	1.870616	C	-0.63372	-3.41696	-1.94951
H	-3.77487	0.711145	2.210798	H	-1.00006	-3.39957	-2.97992
C	-2.81375	-0.93397	2.929115	C	2.683688	-3.42718	-0.12055
H	-3.34203	-0.8131	3.890531	H	3.200871	-4.321	-0.5115
H	-2.84024	-2.0081	2.700148	H	2.875604	-3.40837	0.962101
C	1.555632	3.351504	-0.82977	C	-0.28588	3.529613	0.722787
N	3.343171	-2.21864	-0.71444	H	-0.65577	3.602773	1.746905
H	3.093934	-2.22346	-1.71004	C	4.810243	-2.4289	-0.63177
C	0.969093	-0.99194	3.071476	H	5.104657	-3.33865	-1.17849
H	1.752724	-1.75548	3.10822	H	5.045559	-2.6275	0.425686
N	3.120016	1.611341	-1.58102	C	0.729569	-3.50957	-1.70856
H	2.355052	1.468038	-2.24779	H	1.418258	-3.57367	-2.55611
N	3.525773	0.187205	1.899892	C	-1.53474	-3.31263	-0.88129
H	3.665085	-0.784	2.201767	C	-5.58038	1.290137	-1.16977
C	-5.84873	-0.11848	0.81358	H	-6.66372	1.481389	-1.09024
H	-6.83298	-0.60816	0.733968	H	-5.36627	1.195053	-2.24462
H	-6.04416	0.884981	1.21988	C	2.713701	0.843738	2.968958
C	0.647068	3.450313	-1.89191	H	3.230715	0.696101	3.933189
H	1.008882	3.453884	-2.92397	H	2.7412	1.92424	2.77287
C	-1.19775	3.480256	-0.32949	C	4.405285	1.398412	-2.2817
C	5.580257	-1.24423	-1.14987	H	4.649076	2.252165	-2.933
H	6.665257	-1.4242	-1.06254	H	4.297771	0.521445	-2.93719

C	-1.07059	0.900153	3.075315	H	-4.17788	-0.37743	-2.96672
H	-1.85444	1.663025	3.121455	C	-2.95984	-2.9527	-1.14851
C	4.87724	0.811111	1.853191	H	-3.39158	-3.58404	-1.94316
H	5.325313	0.841165	2.858681	H	-3.58122	-3.09085	-0.25229
H	4.73927	1.859644	1.543495	C	-1.05711	-3.44822	0.420523
C	-4.31038	-1.28522	-2.35885	H	-1.75996	-3.45238	1.258156
H	-4.5001	-2.11168	-3.06108				

$[Cd_2L(\mu\text{-}OH)]^{3+}$ (3)

Cd	2.198816	0.050926	-0.00792	C	1.103427	-2.2251	-2.53207
Cd	-2.19299	0.046945	0.003812	C	-0.18214	-1.92501	-2.97287
O	0.003906	-0.26029	0.043722	C	-1.29996	-2.38652	-2.26913
N	4.728119	0.02447	0.003258	C	-1.09617	-3.2228	-1.16498
N	2.8821	1.442288	1.825598	C	0.192369	-3.53255	-0.72841
N	-2.8915	-1.70101	1.543876	C	-2.67775	-1.93432	-2.65115
N	-4.73161	0.020637	-0.00634	C	-4.25315	-0.03122	-2.45145
N	2.89258	0.861674	-2.1587	C	-5.17061	-0.47671	-1.32677
N	-2.8987	2.221868	0.707293	H	2.2748	2.263314	1.778423
N	2.886928	-2.27466	0.329584	H	-2.28934	-2.50222	1.341046
N	-2.86808	-0.51111	-2.24831	H	1.962319	-1.79848	3.210977
C	5.177244	0.72512	1.224542	H	-0.3263	-2.7457	3.115248
C	4.274311	1.887191	1.594842	H	-1.96625	1.217307	3.435107
C	2.677089	0.837165	3.172422	H	0.320422	2.169935	3.48168
C	1.29942	0.255328	3.255274	H	5.198421	-0.00163	2.048877
C	1.097692	-1.12823	3.182858	H	4.249806	2.635409	0.788622
C	-0.18824	-1.6611	3.140273	H	2.853113	1.593249	3.955004
C	-1.30389	-0.81746	3.169211	H	-3.4362	-0.61628	3.262504
C	-1.10093	0.560027	3.305054	H	-4.26367	-2.68049	0.304153
C	0.183272	1.092643	3.348832	H	-6.22229	-1.20586	0.914814
C	-2.68446	-1.36665	2.981031	H	6.215286	1.083752	1.119106
C	-4.28454	-2.08984	1.233554	H	4.680996	2.399213	2.481839
C	-5.1818	-0.87611	1.077573	H	3.433644	0.053767	3.314884
C	5.178558	0.731097	-1.2134	H	-2.86573	-2.25658	3.606884
C	4.290465	0.445372	-2.41023	H	-4.69836	-2.74981	2.012765
C	2.662103	2.317958	-2.36958	H	-5.19572	-0.3021	2.014987
C	1.287705	2.668502	-1.88945	H	2.288269	0.370567	-2.82045
C	1.101586	3.271205	-0.63964	H	-2.29607	2.451501	1.499093
C	-0.17802	3.505548	-0.14393	H	1.974835	3.614812	-0.07651
C	-1.30444	3.136178	-0.88859	H	-0.30321	4.019008	0.812866
C	-1.11781	2.570616	-2.15464	H	-1.99074	2.362607	-2.78095
C	0.161981	2.341057	-2.65253	H	0.288305	1.93809	-3.66127
C	-2.67946	3.284915	-0.31365	H	5.178133	1.810322	-1.00347
C	-4.29346	2.151444	1.197035	H	4.277529	-0.63136	-2.63618
C	-5.18685	1.407068	0.223075	H	2.807203	2.575567	-3.43064
C	5.176787	-1.38352	0.003001	H	-3.43806	3.166483	-1.09871
C	4.276685	-2.27593	0.837148	H	-4.27295	1.641907	2.172804
C	2.688098	-3.19164	-0.82886	H	-6.2286	1.431168	0.586392
C	1.30996	-3.00113	-1.38536	H	6.223694	0.476628	-1.45944

H	4.70073	0.946289	-3.30123	H	4.245802	-1.92321	1.878798
H	3.423326	2.871635	-1.80182	H	2.865516	-4.23464	-0.52012
H	-2.83422	4.278789	0.136808	H	-3.43843	-2.54195	-2.14201
H	-4.70409	3.157322	1.376986	H	-4.21505	1.068464	-2.50779
H	-5.19956	1.929301	-0.74387	H	-6.20421	-0.15974	-1.54839
H	2.283398	-2.6197	1.078785	H	6.217141	-1.46967	0.360425
H	-2.25026	0.043308	-2.84464	H	4.692765	-3.29592	0.863956
H	1.969193	-1.8883	-3.11025	H	3.445509	-2.95096	-1.58706
H	-0.31776	-1.32999	-3.87987	H	-2.85608	-2.04424	-3.73368
H	-1.96054	-3.66966	-0.66509	H	-4.65959	-0.37852	-3.41459
H	0.330899	-4.20877	0.120085	H	-5.20156	-1.57475	-1.28591
H	5.190942	-1.74139	-1.0356	H	0.002603	-1.22796	0.13507

$[Cd_2L(\mu\text{-}F)]^{3+}$ (4)

Cd	2.190385	0.00188	0.000206	C	-5.17572	-0.19963	-1.38807
Cd	-2.19113	-0.00019	-0.00051	C	5.172359	0.484967	1.32162
F	-0.00042	0.005359	0.015814	C	4.266505	1.574531	1.863854
N	4.728575	-0.00694	0.001693	C	2.659943	0.293861	3.252946
N	2.876284	1.194994	-1.96091	C	1.29098	-0.31141	3.216908
N	-2.8632	1.999171	1.132152	C	0.159107	0.47246	3.464066
N	-4.72945	0.007545	0.004452	C	-1.11532	-0.0674	3.315426
N	2.86481	-2.29518	-0.06002	C	-1.29114	-1.39711	2.915081
N	-2.8753	-0.01729	-2.29542	C	-0.15928	-2.19601	2.721683
N	2.873038	1.098597	2.0168	C	1.115163	-1.65692	2.873188
N	-2.87555	-1.98167	1.160103	C	-2.6604	-1.93344	2.633954
C	5.175398	0.888168	-1.08456	C	-4.26993	-2.30819	0.784783
C	4.267819	0.818958	-2.29845	C	-5.17403	-1.09379	0.88232
C	2.669662	2.668586	-1.88086	H	6.212944	0.664176	-1.38747
C	1.300024	2.944508	-1.34265	H	5.197969	1.916251	-0.69526
C	0.169775	2.763328	-2.14667	H	4.671207	1.463829	-3.09581
C	-1.10578	2.904558	-1.60729	H	4.244079	-0.20314	-2.70759
C	-1.28417	3.226919	-0.25689	H	2.824784	3.126181	-2.87184
C	-0.15406	3.463302	0.532659	H	3.437449	3.085782	-1.21438
C	1.121489	3.323703	-0.00698	H	0.289026	2.539567	-3.2109
C	-2.65374	3.24861	0.347489	H	-1.98287	2.819831	-2.25671
C	-4.25357	1.840826	1.614773	H	-0.2734	3.787791	1.570662
C	-5.16805	1.319277	0.522129	H	1.998381	3.567038	0.601326
C	5.169044	-1.39735	-0.2302	H	-2.80723	4.129602	0.992317
C	4.254862	-2.40803	0.436147	H	-3.42117	3.291728	-0.4379
C	2.656247	-2.96086	-1.3768	H	-4.65037	2.792672	2.003427
C	1.286071	-2.63196	-1.88235	H	-4.23095	1.142443	2.46587
C	0.15733	-3.24282	-1.32618	H	-6.20449	1.27532	0.899347
C	-1.1191	-2.84782	-1.71641	H	-5.18987	2.031016	-0.31587
C	-1.30002	-1.83516	-2.66582	H	2.265141	0.854779	-2.7062
C	-0.17106	-1.26448	-3.26311	H	-2.24786	2.059118	1.946082
C	1.105424	-1.66076	-2.87423	H	6.205058	-1.55293	0.117521
C	-2.67019	-1.32247	-2.98439	H	5.193193	-1.57559	-1.31503
C	-4.26544	0.482671	-2.39188	H	4.652123	-3.42372	0.277881

H	4.231453	-2.2494	1.525633	H	4.667774	1.943425	2.821654
H	2.810566	-4.04814	-1.27894	H	4.248171	2.438219	1.181008
H	3.422934	-2.59217	-2.07246	H	2.810644	0.924489	4.144683
H	0.278403	-4.05639	-0.60482	H	3.427836	-0.49167	3.285433
H	-1.9948	-3.37154	-1.32023	H	0.276395	1.503799	3.809618
H	-0.29225	-0.52549	-4.06073	H	-1.99293	0.534733	3.570683
H	1.981299	-1.25261	-3.3886	H	-0.2766	-3.25741	2.483612
H	-2.8262	-1.20559	-4.06952	H	1.992781	-2.3045	2.781329
H	-3.43765	-2.02295	-2.62655	H	-2.81053	-2.93472	3.070293
H	-4.66836	0.342864	-3.40798	H	-3.42784	-1.2787	3.070157
H	-4.23886	1.569119	-2.21431	H	-4.67213	-3.1178	1.415096
H	-6.21205	0.151545	-1.53336	H	-4.25256	-2.69585	-0.24563
H	-5.20129	-1.28126	-1.58419	H	-6.21378	-1.38987	0.659182
H	2.249822	-2.76692	0.606328	H	-5.18925	-0.72387	1.917775
H	-2.26225	0.65655	-2.7588	H	2.263175	1.915419	2.090853
H	6.211527	0.855287	1.283118	H	-2.26761	-2.72034	0.800589
H	5.188703	-0.36572	2.018188				

$[Cd_2L(\mu\text{-}Cl)]^{3+}$ (5)

Cd	2.5325	-0.00108	-0.0016	C	-5.40269	-1.14013	0.841401
Cd	-2.5328	-0.00041	0.002301	C	-4.51929	-2.36412	0.664301
Cl	0.000099	0.014403	-0.0008	C	-5.4045	-0.15433	-1.4042
N	4.9744	0.00083	-0.0033	C	-4.5175	0.606277	-2.3764
N	3.09539	1.77202	-1.4739	C	-5.40191	1.297272	0.572001
N	3.098612	-2.16988	-0.7893	C	-4.51211	1.757177	1.715201
N	3.100597	0.39602	2.267101	C	-2.79119	-2.19321	2.444901
N	-4.9742	0.000475	0.002501	C	-1.35349	-1.84771	2.705101
N	-3.09909	-2.08622	0.988601	C	-0.33179	-2.7123	2.296501
N	-3.0994	0.181585	-2.2943	C	-1.0005	-0.6477	3.333401
N	-3.09601	1.901885	1.301301	C	-2.7951	-1.03011	-3.1116
C	5.401593	1.238533	-0.6923	C	-1.35759	-1.42981	-2.9453
C	4.511291	1.588828	-1.8732	C	-0.3351	-0.6358	-3.4771
C	5.402006	-1.21357	-0.7319	C	-1.00519	-2.5843	-2.2361
C	4.518913	-2.41537	-0.44	C	-2.79692	3.214587	0.655501
C	5.4056	-0.02167	1.411501	C	-1.35802	3.275395	0.232501
C	4.518695	0.826628	2.308401	C	-0.34202	3.345801	1.193201
C	2.797282	3.138418	-0.9513	C	-0.99662	3.235197	-1.119
C	1.358281	3.23861	-0.5362	H	6.448393	1.163239	-1.0337
C	0.342382	3.223104	-1.4993	H	5.384688	2.058633	0.040201
C	0.996981	3.321508	0.813401	H	4.902886	2.49433	-2.3642
C	2.790813	-2.41558	-2.2288	H	4.540795	0.791528	-2.6311
C	1.353211	-2.09629	-2.5205	H	6.451008	-1.46746	-0.5007
C	0.331116	-2.9175	-2.0315	H	5.380405	-0.98877	-1.8081
C	1.000905	-0.96129	-3.2603	H	4.911618	-3.29097	-0.9815
C	2.795704	-0.73378	3.193901	H	4.556915	-2.67377	0.629001
C	1.357906	-1.14609	3.065101	H	6.452798	0.311039	1.513801
C	0.335801	-0.3041	3.518401	H	5.389706	-1.06617	1.755201
C	1.004713	-2.36219	2.468801	H	4.553189	1.882728	2.000601

H	4.910595	0.79463	3.337801	H	-4.909	0.477175	-3.3984
H	3.048078	3.88732	-1.7217	H	-4.55271	1.686677	-2.1698
H	3.462781	3.329822	-0.0971	H	-6.44871	1.253866	0.918901
H	0.597082	3.223806	-2.5633	H	-5.38521	2.044772	-0.2344
H	1.77558	3.412912	1.577201	H	-4.54271	1.034877	2.544801
H	3.031019	-3.46238	-2.4811	H	-4.90382	2.704875	2.118501
H	3.45771	-1.78448	-2.8336	H	-3.03128	-3.21101	2.796501
H	0.578421	-3.84209	-1.5012	H	-3.45789	-1.50712	2.986901
H	1.785101	-0.34669	-3.7136	H	-0.57968	-3.6829	1.856601
H	3.463508	-1.57068	2.942601	H	-1.7843	0.007593	3.726601
H	3.038602	-0.43488	4.227801	H	-3.0377	-0.82861	-4.1689
H	0.583396	0.623406	4.043201	H	-3.46339	-1.83962	-2.7835
H	1.788117	-3.06809	2.175201	H	-0.5822	0.237699	-4.0878
H	2.51399	1.648017	-2.3051	H	-1.78928	-3.25841	-1.8771
H	2.523815	-2.82538	-0.2558	H	-3.46282	3.328183	-0.2121
H	2.523493	1.182717	2.571601	H	-3.04632	4.030685	1.354601
H	-6.45149	-1.41463	0.634101	H	-0.59672	3.442699	2.252701
H	-5.382	-0.81573	1.891901	H	-1.77522	3.258393	-1.888
H	-4.91168	-3.18473	1.286101	H	-2.52399	-2.78881	0.519601
H	-4.55739	-2.72222	-0.3756	H	-2.52211	0.936188	-2.6709
H	-6.4517	0.167566	-1.5378	H	-2.51471	1.854188	2.140501
H	-5.38909	-1.22643	-1.6488				

$[Cd_2L(\mu\text{-}Br)]^{3+}$ (6)

Cd	-2.58803	-0.00994	-0.00123	C	-1.53899	-2.55138	-2.14059
Cd	2.788116	-0.00389	-0.00609	C	-1.21731	-3.25225	-0.97407
Br	0.130953	0.014683	-0.02304	C	0.110862	-3.49404	-0.62983
N	-5.06077	0.008746	-0.01604	C	1.150042	-3.04346	-1.44827
N	-3.17444	-0.72425	-2.182	C	0.825186	-2.40123	-2.64991
N	-3.21421	-1.52608	1.717158	C	-0.49942	-2.15305	-2.98951
N	-3.17301	2.247964	0.456384	C	2.578816	-3.26209	-1.04441
N	5.246204	-0.01382	0.014326	C	-2.99266	-1.02265	3.105609
N	3.416062	-2.03616	-1.16806	C	-1.57045	-0.57802	3.265558
N	3.398149	-0.02657	2.339128	C	-1.23454	0.779201	3.308919
N	3.443959	2.03785	-1.13925	C	0.097692	1.18369	3.344821
C	-5.49019	-0.62204	-1.28223	C	1.128285	0.240133	3.341448
C	-4.56573	-0.28363	-2.4382	C	0.790738	-1.11907	3.357858
C	-5.51321	-0.76192	1.161244	C	-0.53846	-1.52298	3.315084
C	-4.61152	-1.947	1.457083	C	2.559109	0.691423	3.33766
C	-5.48391	1.423536	0.060316	C	-2.93725	3.213022	-0.65848
C	-4.57165	2.25417	0.94496	C	-1.51311	3.137128	-1.11777
C	5.695622	-1.09225	-0.8945	C	-1.17519	2.53438	-2.33272
C	4.822888	-2.32554	-0.80532	C	0.158455	2.372988	-2.70082
C	5.683709	-0.26834	1.405712	C	1.187006	2.81465	-1.86488
C	4.805152	0.427935	2.421701	C	0.846362	3.475909	-0.67784
C	5.712374	1.308554	-0.45918	C	-0.4837	3.630396	-0.3066
C	4.848513	1.858355	-1.57241	C	2.618905	2.586782	-2.25103
C	-2.95577	-2.1772	-2.45378	H	-6.52324	-0.33293	-1.54177

H	-5.51696	-1.71132	-1.13242	H	1.60974	-2.09261	-3.34724
H	-4.95762	-0.73732	-3.36295	H	-0.72778	-1.65819	-3.93797
H	-4.5396	0.80358	-2.61051	H	3.037141	-4.06997	-1.64314
H	-6.55224	-1.11178	1.034588	H	2.632048	-3.59066	0.003936
H	-5.53234	-0.08523	2.027532	H	-3.25815	-1.81272	3.828606
H	-5.01899	-2.51136	2.311487	H	-3.68436	-0.18603	3.279644
H	-4.59342	-2.64307	0.603653	H	-2.02932	1.531094	3.344059
H	-6.52407	1.510008	0.418986	H	0.339221	2.24903	3.371925
H	-5.48651	1.836144	-0.95907	H	1.568123	-1.88677	3.418482
H	-4.96217	3.282725	1.006717	H	-0.77537	-2.59039	3.33988
H	-4.56528	1.863001	1.974056	H	2.617474	1.764681	3.103576
H	6.746966	-1.36278	-0.69506	H	3.011902	0.572383	4.338805
H	5.674502	-0.70302	-1.92405	H	-3.62445	2.961534	-1.47932
H	5.240765	-3.11617	-1.44979	H	-3.20265	4.229445	-0.32113
H	4.818577	-2.74144	0.214956	H	-1.96783	2.205674	-3.01305
H	6.734639	0.036105	1.549803	H	0.402599	1.891261	-3.65078
H	5.657929	-1.35437	1.580722	H	1.62197	3.894631	-0.02907
H	5.213447	0.26499	3.432468	H	-0.72363	4.157591	0.621558
H	4.804764	1.519051	2.269359	H	3.084421	3.520664	-2.61504
H	6.763709	1.258577	-0.79109	H	2.677162	1.871748	-3.08465
H	5.697638	2.004431	0.393293	H	-2.55543	-0.2137	-2.81555
H	5.275904	2.809224	-1.93078	H	-2.61005	-2.34315	1.607947
H	4.838961	1.183439	-2.44343	H	-2.56563	2.539734	1.225423
H	-3.21325	-2.39431	-3.50435	H	3.413579	-1.77551	-2.15911
H	-3.65734	-2.7487	-1.8287	H	3.390431	-1.01709	2.601809
H	-2.02063	-3.63424	-0.33558	H	3.450308	2.746442	-0.39867
H	0.3431	-4.03111	0.293424				

$[Cd_2L(\mu\text{-}I)]^{3+}$

Cd	-2.73648	0.097906	-0.04902	H	-3.1927	4.499537	-0.46251
Cd	2.739256	-0.05623	-0.07543	H	-2.96456	3.593438	1.034935
I	0.008316	0.120196	-1.08067	C	1.241727	-3.50302	-0.716
N	-5.20921	0.044538	-0.3185	N	-3.61719	-0.35014	2.123261
N	-3.21513	-1.65002	-1.68691	H	-3.72324	0.572618	2.556539
H	-2.53503	-1.49234	-2.4355	C	-2.78972	-1.17245	3.035142
C	3.00723	3.284584	-0.8904	H	-3.22632	-1.15786	4.049941
H	3.583176	3.376851	0.042197	H	-2.86384	-2.2169	2.698015
H	3.406347	4.037868	-1.59146	C	1.544558	3.499151	-0.64471
C	-1.35569	-0.73337	3.07103	N	3.382907	-2.25558	-0.98866
C	5.795828	-0.13636	1.031064	H	3.16182	-2.15199	-1.98519
H	6.818402	0.276791	1.058352	C	0.993333	-1.28714	3.330566
H	5.901325	-1.20865	1.252121	H	1.759069	-2.04775	3.511607
N	-3.38705	2.392296	-0.63597	N	3.235169	1.922167	-1.46021
H	-3.18296	2.420912	-1.64106	H	2.576364	1.832258	-2.23839
N	5.200046	0.010281	-0.3155	N	3.592177	-0.07519	2.152865
C	1.002617	3.372492	0.634211	H	3.70295	-1.07425	2.357738
H	1.673679	3.23884	1.488227	C	-5.80905	-0.04408	1.030324
C	-2.72608	3.59305	-0.03888	H	-6.84142	-0.43046	0.982066

H	-5.88867	0.971385	1.445811	H	2.988535	-3.66087	0.520007
C	0.680557	3.758741	-1.71739	C	-0.37486	3.430161	0.830288
H	1.087603	3.922046	-2.71912	H	-0.78536	3.355288	1.840121
C	-1.24267	3.608334	-0.24843	C	4.852707	-2.39056	-0.8712
C	5.589606	-1.11104	-1.19846	H	5.227525	-3.20029	-1.51832
H	6.678073	-1.29096	-1.15067	H	5.062815	-2.71534	0.159916
H	5.377607	-0.8181	-2.23747	C	0.66224	-3.60002	-1.98866
C	1.350923	0.062329	3.202403	H	1.291724	-3.75762	-2.86892
C	-5.56999	-1.13832	-1.13021	C	-1.55095	-3.32094	-1.03479
H	-6.58038	-1.02636	-1.56032	C	-5.59864	1.296258	-1.00359
H	-5.62045	-2.01042	-0.46229	H	-6.68613	1.46967	-0.92191
C	-4.85613	2.506607	-0.48149	H	-5.39314	1.173417	-2.0779
H	-5.23417	3.408418	-0.99031	C	2.781185	0.505741	3.257713
H	-5.05639	2.667015	0.589763	H	3.245119	0.247798	4.225116
C	0.403108	-3.38968	0.393986	H	2.843744	1.598973	3.164978
H	0.839298	-3.37467	1.395066	C	4.60202	1.745144	-1.99385
C	-4.98251	-0.90282	1.962732	H	4.968751	2.674681	-2.45869
H	-5.49019	-0.9884	2.936978	H	4.555525	0.997549	-2.79907
H	-4.87795	-1.93036	1.578536	C	-0.99964	0.615461	2.970832
C	5.571368	1.312283	-0.91332	H	-1.76515	1.39147	2.868326
H	6.596718	1.276579	-1.32078	C	4.951779	0.514471	2.104542
H	5.589345	2.062875	-0.1091	H	5.45624	0.419751	3.0797
C	0.334363	1.005072	3.041631	H	4.831464	1.594593	1.921521
H	0.588478	2.064606	3.011461	C	-4.56488	-1.39921	-2.23276
C	-0.69435	3.813555	-1.52197	H	-4.90837	-2.24829	-2.84619
H	-1.34686	4.027434	-2.37319	H	-4.4969	-0.53569	-2.91105
C	-0.33978	-1.67688	3.266659	C	-3.01288	-3.06171	-1.23972
H	-0.59844	-2.73222	3.386919	H	-3.43464	-3.74479	-1.99721
C	-0.71575	-3.50937	-2.14489	H	-3.57938	-3.22345	-0.30998
H	-1.14924	-3.59009	-3.14563	C	-0.97687	-3.29384	0.23745
C	2.7288	-3.52202	-0.54	H	-1.61676	-3.19931	1.120212
H	3.179737	-4.36826	-1.08666				

$[Hg_2L(\mu\text{-}OH)]^{3+}$ (7)

Hg	-2.23253	0.07814	0.040512	C	-1.3157	-2.39812	-2.3584
Hg	2.231993	0.058563	0.023473	C	-1.04657	-3.26265	-1.28984
O	-0.00241	-0.29412	-0.02356	C	0.266444	-3.55517	-0.91778
N	-4.79881	-0.02073	0.007408	C	1.344761	-2.97536	-1.60018
N	-2.94815	-0.57699	-2.29567	C	1.073358	-2.15436	-2.70174
N	2.986003	-2.3673	0.10794	C	-0.23672	-1.87515	-3.08132
N	4.802642	0.039605	-0.02539	C	2.751215	-3.17243	-1.11757
N	-3.04111	2.290477	0.717164	C	4.388887	-2.36171	0.558099
N	2.944202	1.080052	-2.13576	C	5.237615	-1.35958	-0.2072
N	-2.94306	-1.77538	1.59229	C	-5.28314	1.362732	0.178231
N	3.009799	1.336895	1.981318	C	-4.44687	2.179684	1.148836
C	-5.22164	-0.57815	-1.29292	C	-2.79662	3.30174	-0.34376
C	-4.34297	-0.13025	-2.44907	C	-1.39139	3.171108	-0.85031
C	-2.72087	-1.99073	-2.68838	C	-1.12961	2.642029	-2.12015

C	0.178331	2.463007	-2.56323	H	-2.47067	2.54848	1.523444
C	1.259703	2.800273	-1.74168	H	2.354747	0.627827	-2.83585
C	0.997813	3.348688	-0.48034	H	-1.96383	2.421809	-2.79337
C	-0.30982	3.537559	-0.04046	H	0.358753	2.092141	-3.57631
C	2.666545	2.536189	-2.18797	H	1.832707	3.686202	0.141768
C	4.350273	0.722351	-2.39166	H	-0.48953	4.010762	0.929449
C	5.220769	0.889088	-1.15715	H	-5.28503	1.848414	-0.8082
C	-5.21807	-0.88051	1.131046	H	-4.44782	1.720505	2.148786
C	-4.3488	-2.11532	1.310796	H	-2.99724	4.313379	0.048123
C	-2.66677	-1.47004	3.018521	H	3.381637	3.04404	-1.52517
C	-1.26791	-0.95054	3.164539	H	4.369596	-0.31988	-2.74392
C	-1.02939	0.424266	3.277652	H	6.272137	0.688421	-1.42822
C	0.268284	0.924252	3.329535	H	-6.3341	1.370441	0.516297
C	1.365499	0.057174	3.26326	H	-4.90538	3.175579	1.262869
C	1.127564	-1.31959	3.179866	H	-3.51657	3.12731	-1.15579
C	-0.17236	-1.81913	3.133903	H	2.848232	2.920989	-3.20628
C	2.762314	0.602261	3.248945	H	4.773701	1.331414	-3.20721
C	4.413615	1.735365	1.775399	H	5.193249	1.936713	-0.82474
C	5.267971	0.586789	1.263212	H	-2.35303	-2.56676	1.330752
H	-2.35172	0.004532	-2.88551	H	2.428274	2.175533	1.99182
H	2.408374	-2.76489	0.85052	H	-1.87858	1.107426	3.380437
H	-1.87743	-3.74131	-0.7627	H	0.428058	1.998384	3.463295
H	0.452075	-4.25295	-0.09586	H	1.973588	-2.01383	3.200358
H	1.905127	-1.75612	-3.29083	H	-0.33522	-2.90073	3.106033
H	-0.42253	-1.251	-3.9602	H	-5.19382	-0.27582	2.049369
H	-5.20946	-1.67461	-1.21878	H	-4.36712	-2.74047	0.405026
H	-4.33134	0.968541	-2.51617	H	-2.83386	-2.36684	3.6391
H	-2.93717	-2.12359	-3.76286	H	3.494013	-0.21523	3.317668
H	3.466002	-2.84352	-1.88472	H	4.418357	2.57511	1.064158
H	4.390703	-2.12848	1.633842	H	6.316655	0.924145	1.189933
H	6.294141	-1.47928	0.089648	H	-6.26925	-1.19568	1.008512
H	-6.26974	-0.30732	-1.50896	H	-4.77889	-2.73345	2.116279
H	-4.78142	-0.49686	-3.39224	H	-3.39372	-0.71568	3.352665
H	-3.43964	-2.61879	-2.14352	H	2.949243	1.267863	4.109131
H	2.965973	-4.23688	-0.91988	H	4.858164	2.118614	2.708709
H	4.845915	-3.36049	0.458264	H	5.269053	-0.22992	1.999444
H	5.20145	-1.59038	-1.28125	H	-0.00877	-1.22827	-0.28705

$[Hg_2L(\mu\text{-}F)]^{3+}$ (8)

Hg	2.246144	0.017269	-0.01223	N	2.979558	1.769798	-1.58541
Hg	-2.24626	0.016517	0.014471	N	-2.97163	1.821709	1.527226
F	0.000554	0.126289	0.065563	C	5.232652	-1.25017	-0.6909
N	4.827602	0.001607	-0.02627	C	4.354408	-2.43607	-0.32339
N	2.947425	-2.23965	-0.72012	C	2.674432	-2.53408	-2.15104
N	-3.00288	0.408154	-2.30443	C	1.275036	-2.1253	-2.49713
N	-4.82933	0.006198	0.0312	C	1.027853	-0.92364	-3.17152
N	3.001536	0.473371	2.29756	C	-0.27352	-0.49905	-3.42174
N	-2.95238	-2.22157	0.773652	C	-1.36461	-1.26475	-2.99384

C	-1.11729	-2.48351	-2.35131	H	4.771508	-3.34488	-0.78749
C	0.185596	-2.91224	-2.10846	H	3.401863	-1.97695	-2.75793
C	-2.76261	-0.76035	-3.18902	H	-2.9511	-0.4813	-4.24
C	-4.40243	0.871581	-2.27538	H	-4.83755	0.880078	-3.28819
C	-5.27781	0.016284	-1.37298	H	-5.28736	-1.02045	-1.73894
C	5.274929	0.049303	1.377879	H	2.410792	1.245434	2.60955
C	4.402236	0.931912	2.256329	H	-2.3674	-2.85899	0.230957
C	2.759131	-0.67209	3.211346	H	1.959963	-3.05013	2.120727
C	1.362227	-1.18211	3.023984	H	-0.35191	-3.81371	1.682418
C	1.117587	-2.40238	2.383261	H	-1.87394	-0.27306	3.60173
C	-0.1841	-2.83778	2.147091	H	0.438192	0.499988	4.021883
C	-1.27507	-2.0561	2.542429	H	5.280761	-0.97698	1.772177
C	-1.03041	-0.85216	3.213191	H	4.39876	1.967955	1.884857
C	0.270159	-0.42133	3.456484	H	2.943877	-0.36586	4.255297
C	-2.67455	-2.47618	2.210922	H	-3.40077	-1.90386	2.804922
C	-4.36229	-2.42476	0.390768	H	-4.38633	-2.62887	-0.69039
C	-5.23468	-1.22623	0.730764	H	-6.28779	-1.47597	0.51163
C	5.26332	1.192325	-0.77777	H	6.320137	0.3983	1.446643
C	4.378824	1.511998	-1.9728	H	4.837843	0.966143	3.268441
C	2.733772	3.131444	-1.04473	H	3.492799	-1.45663	2.978713
C	1.327506	3.228372	-0.53438	H	-2.84465	-3.54169	2.441249
C	1.061875	3.282978	0.838956	H	-4.77922	-3.31853	0.883304
C	-0.24681	3.297823	1.312962	H	-5.19335	-1.03406	1.812707
C	-1.32554	3.246329	0.423648	H	2.383006	1.65272	-2.40566
C	-1.06015	3.228167	-0.95092	H	-2.36993	1.732779	2.347281
C	0.248509	3.224453	-1.42533	H	1.893668	3.373797	1.544588
C	-2.73052	3.165244	0.940376	H	-0.42992	3.379993	2.388363
C	-4.36807	1.573879	1.930589	H	-1.89269	3.275433	-1.66004
C	-5.26026	1.218499	0.751135	H	0.430959	3.251415	-2.50386
H	2.357356	-2.85821	-0.16141	H	5.272525	2.046853	-0.08639
H	-2.41005	1.171301	-2.63429	H	4.376472	0.676401	-2.68867
H	1.871112	-0.34083	-3.55521	H	2.939267	3.886941	-1.82259
H	-0.44225	0.421531	-3.98821	H	-3.45147	3.315617	0.124174
H	-1.95777	-3.13339	-2.08832	H	-4.35983	0.759874	2.670801
H	0.35591	-3.8854	-1.63903	H	-6.29977	1.115535	1.108881
H	5.198099	-1.08728	-1.77791	H	6.305222	1.079512	-1.12548
H	4.370738	-2.60895	0.763432	H	4.80642	2.376213	-2.50701
H	2.846206	-3.6052	-2.35182	H	3.451489	3.309256	-0.23135
H	-3.49463	-1.53911	-2.93352	H	-2.93424	3.945882	1.693364
H	-4.39544	1.917063	-1.93153	H	-4.79387	2.452942	2.441657
H	-6.3218	0.36691	-1.45129	H	-5.27448	2.052826	0.035519
H	6.283688	-1.49724	-0.45919				

$[Hg_2L(\mu\text{-}Cl)]^{3+}$ (9)

Hg	-2.5591	0.001714	0.002678	N	-3.18698	-1.50511	1.828779
Hg	2.558712	-0.00395	-0.00092	N	-3.1653	-0.84153	-2.21738
Cl	0.000002	-0.0035	0.001616	N	-3.18315	2.34064	0.380519
N	-5.04547	-0.0006	-0.01113	N	5.045471	0.008032	0.007365

N	3.187458	-2.36818	-0.00547	H	-6.51885	1.527299	0.207123
N	3.165982	1.181267	2.056527	H	-5.4136	1.720579	-1.14595
N	3.181197	1.19678	-2.04545	H	-5.03	3.369349	0.67551
C	-5.46702	-0.64071	1.25157	H	-4.67516	2.078171	1.818874
C	-4.61393	-1.84016	1.645535	H	-3.09935	-1.7364	3.940465
C	-5.4539	-0.77629	-1.20027	H	-3.46814	-0.10257	3.375513
C	-4.59035	-0.51581	-2.42812	H	-0.67889	-2.66304	3.154128
C	-5.46218	1.414201	-0.09127	H	-1.73317	1.503216	3.478949
C	-4.61171	2.352667	0.755478	H	-3.0822	-2.56374	-3.46081
C	-2.83849	-0.98226	3.177547	H	-3.4427	-2.87959	-1.75944
C	-1.38252	-0.61633	3.249054	H	-0.66402	-1.40383	-3.87826
C	-0.39517	-1.60701	3.188041	H	-1.70164	-3.77674	-0.43313
C	-0.97877	0.718541	3.366272	H	-3.09451	4.279238	-0.48766
C	-2.81694	-2.27207	-2.42948	H	-3.45364	2.964743	-1.61331
C	-1.35962	-2.51433	-2.15301	H	-0.67599	4.0438	0.737423
C	-0.37635	-1.96261	-2.98277	H	-1.71274	2.270674	-3.05251
C	-0.95055	-3.28462	-1.05859	H	-2.63226	-2.34875	1.677945
C	-2.82974	3.240034	-0.75041	H	-2.60617	-0.29256	-2.8718
C	-1.37172	3.119758	-1.09502	H	-2.63305	2.637725	1.187474
C	-0.38863	3.5553	-0.19848	H	6.522459	-1.53186	-0.01502
C	-0.96194	2.562665	-2.31188	H	5.430855	-1.5018	-1.39219
C	5.468105	-1.37348	-0.30092	H	5.034494	-3.42933	0.12766
C	4.613509	-2.44042	0.371903	H	4.668961	-2.34573	1.466436
C	5.454242	0.433859	1.361576	H	6.50794	0.762818	1.365751
C	4.591619	1.549074	1.939104	H	5.412232	-0.44597	2.019477
C	5.461832	0.96881	-1.03416	H	5.004777	1.837104	2.919543
C	4.608894	0.91253	-2.2953	H	4.648282	2.447622	1.306975
C	2.841348	-3.07207	-1.2701	H	6.517723	0.808825	-1.31327
C	1.384329	-2.89929	-1.59569	H	5.415922	1.977857	-0.60029
C	0.400902	-3.48286	-0.7881	H	5.027039	1.619096	-3.03068
C	0.975231	-2.14562	-2.70191	H	4.669779	-0.08353	-2.75841
C	2.814881	0.441664	3.298526	H	3.107166	-4.13971	-1.17835
C	1.358677	0.069582	3.305383	H	3.468458	-2.659	-2.07358
C	0.371369	1.057522	3.401938	H	0.688523	-4.12411	0.050428
C	0.955038	-1.26679	3.207151	H	1.726291	-1.73273	-3.38238
C	2.83004	2.642258	-2.02137	H	3.074402	1.058153	4.176889
C	1.372644	2.833341	-1.70814	H	3.443742	-0.45909	3.34905
C	0.389672	2.429163	-2.61913	H	0.654718	2.105975	3.534452
C	0.96294	3.405715	-0.49832	H	1.709342	-2.05949	3.191862
H	-6.52212	-0.9601	1.194254	H	3.093936	3.098541	-2.99146
H	-5.42614	0.119265	2.044999	H	3.455626	3.13351	-1.26185
H	-5.0348	-2.2804	2.564237	H	0.677646	2.028115	-3.5955
H	-4.67182	-2.62454	0.876493	H	1.713929	3.784333	0.201851
H	-6.50733	-0.5701	-1.45772	H	2.632423	-2.79215	0.739138
H	-5.41255	-1.84308	-0.93783	H	2.607197	2.035505	2.044824
H	-5.00375	-1.09086	-3.27271	H	2.628683	0.762299	-2.78586
H	-4.64595	0.542899	-2.72182				

$[Hg_2L(\mu\text{-}Br)]^{3+}$ (10)							
Hg	-2.76948	0.009085	-0.01011	H	-6.78817	-1.10582	-0.97369
Hg	2.626711	0.002273	-0.00945	H	-5.71253	-2.02716	0.069995
Br	-0.11038	0.000723	-0.03047	H	-5.35783	-2.45839	-2.36241
N	-5.27275	0.023409	0.013087	H	-4.8809	-0.78635	-2.61991
N	-3.49064	-1.87323	-1.50597	H	-6.76293	-0.24525	1.512986
N	-3.45137	-0.40176	2.372959	H	-5.65164	1.092821	1.780178
N	-3.45623	2.278506	-0.83073	H	-5.3067	-0.83433	3.337853
N	5.142467	-0.00526	-0.00808	H	-4.87467	-1.87715	1.989851
N	3.26159	-2.3598	-0.15009	H	-6.76591	1.462464	-0.47871
N	3.284456	1.040321	2.119737	H	-5.67837	1.018137	-1.78937
N	3.279346	1.334036	-1.96387	H	-5.31236	3.331174	-0.91322
C	-5.73355	-1.20789	-0.66398	H	-4.85683	2.689771	0.659639
C	-4.89263	-1.59	-1.86672	H	6.60258	-1.56042	-0.07864
C	-5.70323	0.051925	1.427425	H	5.521528	-1.46791	-1.46079
C	-4.86129	-0.82926	2.328964	H	5.092875	-3.44037	0.008582
C	-5.71072	1.235738	-0.71134	H	4.704509	-2.37908	1.360983
C	-4.86012	2.456385	-0.41683	H	6.617334	0.709424	1.358145
C	5.552253	-1.37776	-0.36541	H	5.546915	-0.53717	1.978651
C	4.676252	-2.4523	0.263945	H	5.122912	1.70819	2.970402
C	5.567604	0.368068	1.355433	H	4.725483	2.366977	1.38593
C	4.698379	1.446178	1.987466	H	6.613755	0.811702	-1.32005
C	5.5676	0.986887	-1.01444	H	5.557339	1.978729	-0.53995
C	4.689097	1.005818	-2.25782	H	5.115044	1.723889	-2.97771
C	-2.668	-2.17916	-2.70294	H	4.702462	0.024854	-2.75624
C	-1.21959	-2.42364	-2.38838	H	-3.10573	-3.04617	-3.23127
C	-0.22748	-1.7769	-3.13026	H	-2.76374	-1.32557	-3.38928
C	1.121208	-1.98094	-2.84752	H	-0.51172	-1.10317	-3.94229
C	1.515052	-2.83617	-1.81426	H	1.880715	-1.48426	-3.45974
C	0.521805	-3.51359	-1.09529	H	0.800933	-4.22875	-0.31562
C	-0.82412	-3.31346	-1.38113	H	-1.56798	-3.88195	-0.81461
C	2.962162	-3.00575	-1.45764	H	3.242853	-4.07223	-1.40627
C	-2.61985	-1.32853	3.179203	H	3.605335	-2.54574	-2.22135
C	-1.17427	-0.92645	3.24093	H	-2.71453	-2.32857	2.731136
C	-0.17335	-1.87525	3.014389	H	-3.04647	-1.40743	4.196459
C	1.171681	-1.51522	3.064161	H	-0.44787	-2.9109	2.798634
C	1.55133	-0.19848	3.341129	H	1.940434	-2.28052	2.916714
C	0.548867	0.74436	3.60223	H	0.819378	1.768899	3.87375
C	-0.79326	0.384042	3.555813	H	-1.54628	1.140574	3.796175
C	2.992937	0.214181	3.323489	H	3.25988	0.787511	4.228386
C	-2.62267	3.44795	-0.45177	H	3.649132	-0.66743	3.302252
C	-1.17595	3.298755	-0.82609	H	-2.71809	3.577704	0.635901
C	-0.78844	2.935272	-2.12241	H	-3.05188	4.360133	-0.90656
C	0.555048	2.789474	-2.44965	H	-1.53722	2.783757	-2.90542
C	1.552802	3.015394	-1.49232	H	0.829108	2.523522	-3.47489
C	1.167098	3.419482	-0.21103	H	1.931895	3.655249	0.535525
C	-0.17952	3.554177	0.119909	H	-0.45856	3.866033	1.129244
C	2.99591	2.789978	-1.83375	H	3.273064	3.299564	-2.77331

H	3.649754	3.196341	-1.04865	H	2.683681	-2.82112	0.554721
H	-3.48335	-2.69892	-0.90031	H	2.705552	1.879464	2.183207
H	-3.41505	0.519643	2.817836	H	2.693223	0.978535	-2.721
H	-3.43787	2.199824	-1.85148				

$[Hg_2L(\mu\text{-}I)]^{3+}$ (11)

Hg	-2.63344	0.074915	-0.01871	C	-1.00564	0.620128	3.090673
Hg	2.631077	-0.05191	-0.03375	C	4.943604	0.497042	2.147625
I	0.0103	0.157541	-1.27858	C	-4.5868	-1.47024	-2.19805
N	-5.19345	0.024589	-0.2884	C	-3.0056	-3.13308	-1.23844
N	-3.22638	-1.73944	-1.7079	C	-0.95333	-3.22249	0.227243
N	-3.39287	2.436873	-0.65718	H	-2.56421	-1.57509	-2.46949
N	5.183463	0.014777	-0.28366	H	3.577931	3.415179	0.072052
N	-3.61577	-0.34884	2.20204	H	3.40397	4.121098	-1.54323
N	3.389111	-2.31366	-0.99906	H	6.798806	0.246381	1.091043
N	3.248432	2.001728	-1.46438	H	5.863418	-1.22985	1.269728
N	3.590316	-0.08851	2.226822	H	-3.18616	2.449019	-1.66106
C	3.009421	3.342201	-0.86714	H	1.64009	3.074548	1.475163
C	-1.35933	-0.73236	3.154115	H	-3.19262	4.543489	-0.48354
C	5.771028	-0.15437	1.059657	H	-2.98453	3.632294	1.014974
C	0.981483	3.296579	0.629608	H	-3.71159	0.585054	2.611376
C	-2.73794	3.631543	-0.0573	H	-3.23296	-1.14426	4.130136
C	1.256092	-3.54856	-0.7164	H	-2.87047	-2.21511	2.786406
C	-2.7936	-1.16851	3.116084	H	3.16085	-2.19349	-1.9911
C	1.541324	3.532679	-0.62663	H	1.761814	-2.05216	3.513661
C	0.993405	-1.28727	3.365011	H	2.604129	1.914053	-2.25333
C	-5.78373	-0.03439	1.062577	H	3.68969	-1.09104	2.415757
C	0.691496	3.877992	-1.6856	H	-6.82117	-0.40903	1.022442
C	-1.25147	3.634964	-0.25397	H	-5.84965	0.988287	1.461715
C	5.559428	-1.09372	-1.1846	H	1.112358	4.118422	-2.66578
C	1.348827	0.065217	3.270694	H	6.651364	-1.25978	-1.15914
C	-5.55707	-1.17381	-1.06957	H	5.323787	-0.7889	-2.21502
C	-4.85636	2.500442	-0.49041	H	-6.57626	-1.07076	-1.48216
C	0.426195	-3.32041	0.383892	H	-5.59427	-2.03094	-0.38205
C	-4.97481	-0.89129	2.014683	H	-5.27396	3.381646	-1.00594
C	5.558378	1.324434	-0.85607	H	-5.05444	2.666038	0.580375
C	0.328397	1.011982	3.152769	H	0.868447	-3.22965	1.378041
C	-0.68671	3.927353	-1.50265	H	-5.50496	-0.9643	2.978372
C	-0.33933	-1.67935	3.305532	H	-4.86939	-1.92235	1.640842
C	-0.71282	-3.64972	-2.12875	H	6.589671	1.288493	-1.24975
C	2.744803	-3.57601	-0.5469	H	5.570765	2.060888	-0.03897
C	-0.39756	3.351511	0.814258	H	0.5787	2.073873	3.149767
C	4.854603	-2.39744	-0.86874	H	-1.32783	4.213418	-2.34111
C	0.667172	-3.73837	-1.97356	H	-0.59314	-2.73883	3.395563
C	-1.53853	-3.36598	-1.03289	H	-1.15419	-3.81038	-3.11604
C	-5.57048	1.263641	-0.99811	H	3.187882	-4.42676	-1.09386
C	2.780681	0.503599	3.321198	H	3.00957	-3.71269	0.512419
C	4.62052	1.795242	-1.95198	H	-0.82183	3.194794	1.808501

H	5.266389	-3.18654	-1.52012
H	5.068643	-2.72496	0.160677
H	1.289997	-3.97347	-2.84093
H	-6.66118	1.428172	-0.93792
H	-5.34478	1.122662	-2.06593
H	3.241574	0.248862	4.291693
H	2.849677	1.595906	3.223198
H	5.02985	2.721275	-2.38938
H	4.580489	1.062658	-2.77084
H	-1.77553	1.39499	3.024118
H	5.469147	0.3985	3.111556
H	4.821247	1.577509	1.969146
H	-4.97429	-2.32258	-2.78084
H	-4.52986	-0.62126	-2.89477
H	-3.41944	-3.84143	-1.97758
H	-3.56499	-3.28151	-0.30205
H	-1.58827	-3.03798	1.099815