Electronic Supplementary Material (ESI) for RSC Advances.

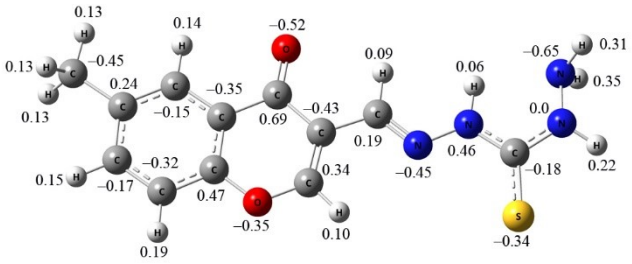

Figure. S1 Electrostatic potential (ESP) charges distributions for ligand predicted using B3LYP/6-31G(d) calculations.

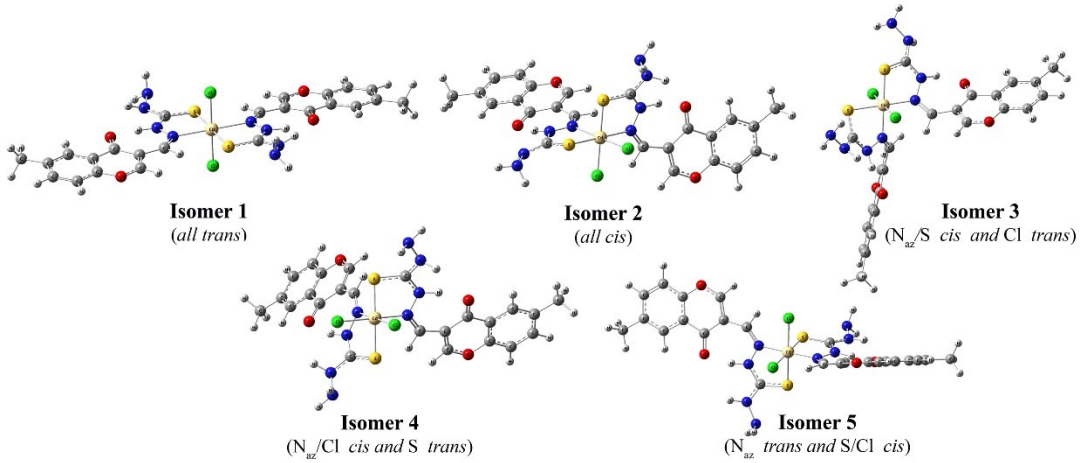

Figure S2. Optimized geometries of the suggested geometrical isomers for $[Cd(MCMT)_2Cl_2]$ complex.

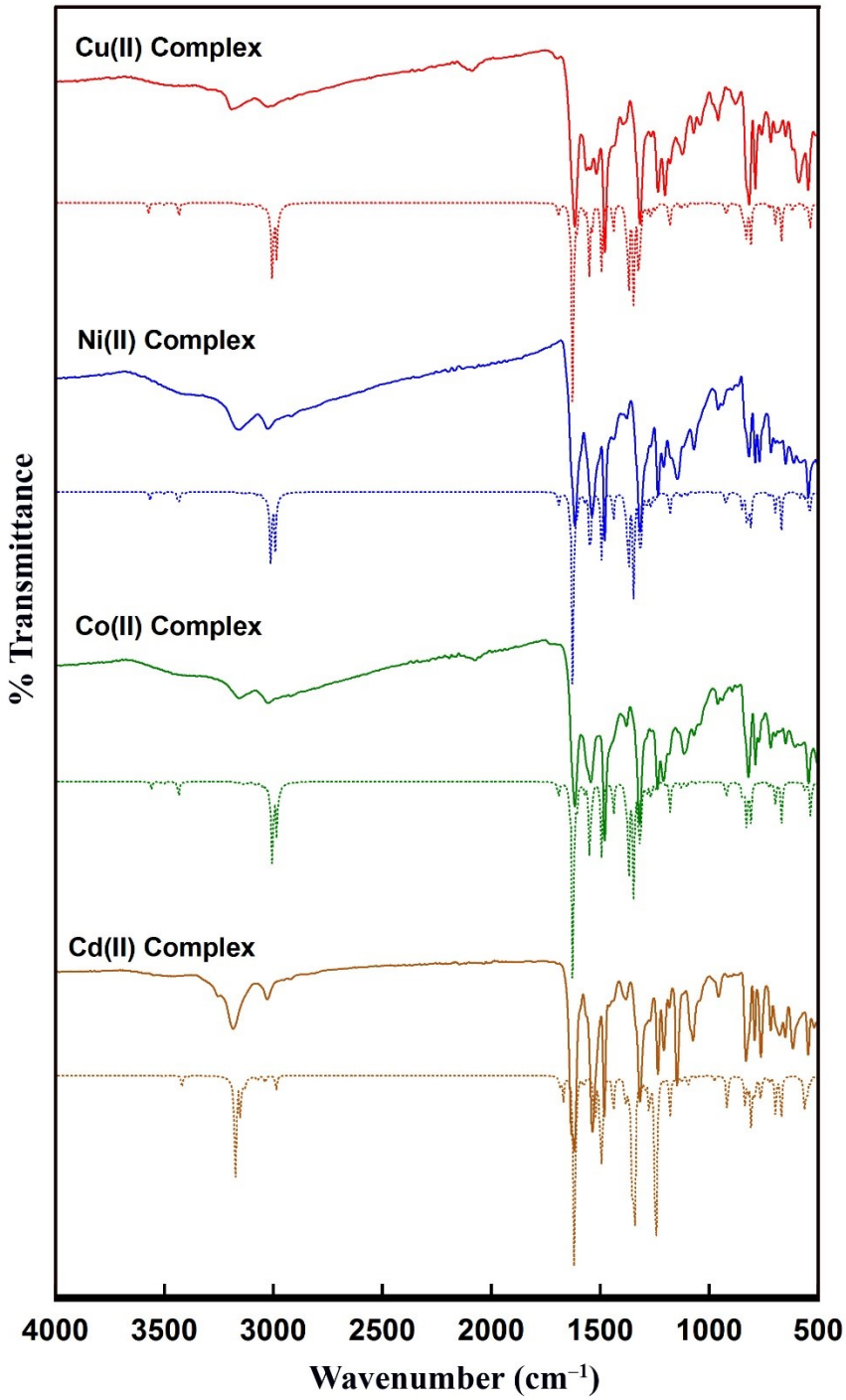

Figure S3. FT-IR spectra of transition metal complexes; experimental (solid line) and calculated. (dashed line).

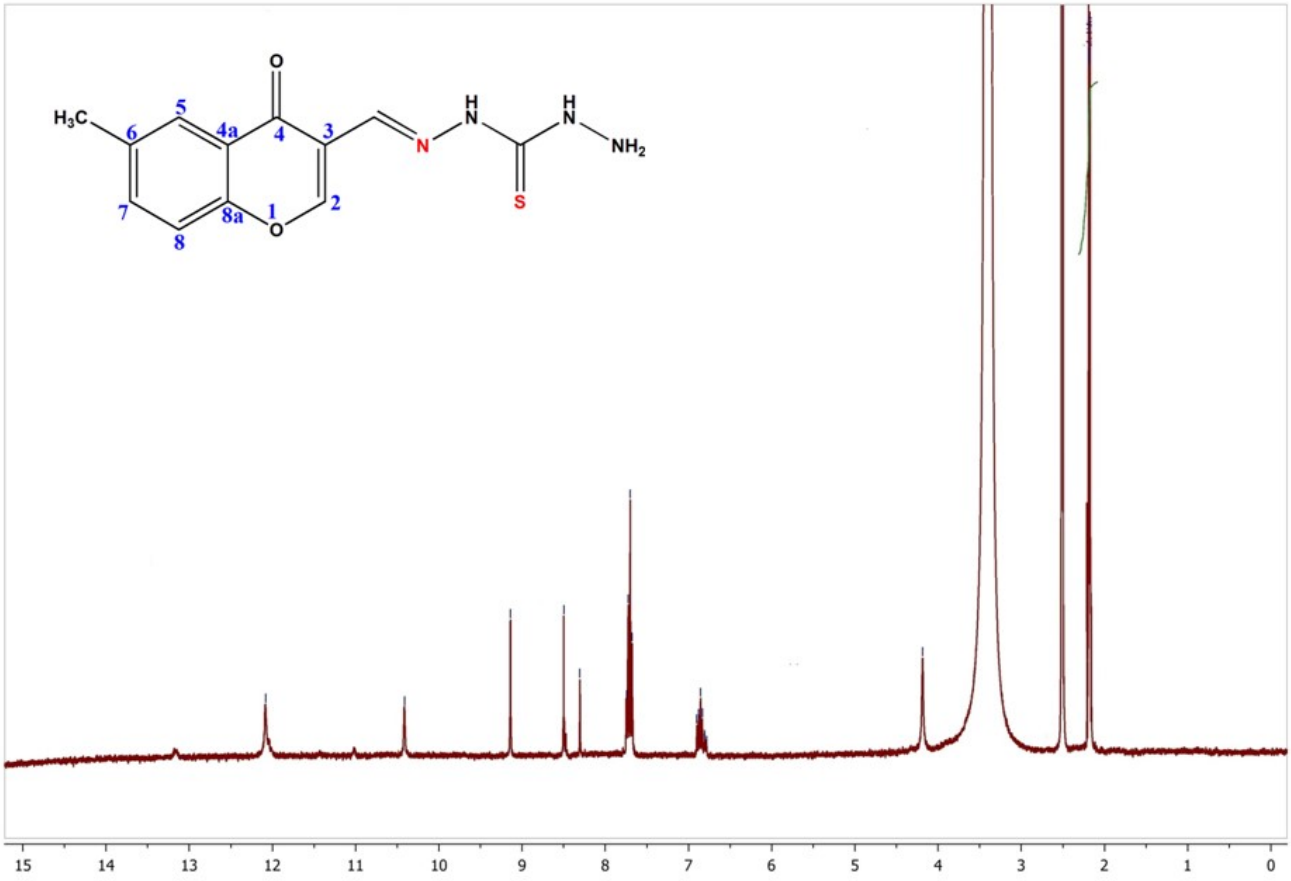

Figure S4. [1]HNMR spectrum of **MCMT** ligand in DMSO-d6.

XYZ coordinates and total energies (HF) for all the calculated structures

xyz coordinates of diamino-thione tautomeric structure (T-1)

C	-0.428016	-1.506959	-0.368016
C	-2.723655	-1.124732	-0.089601
C	-2.540963	0.260876	-0.162117
C	-0.122422	-0.184628	-0.454161
H	-4.097519	-2.761167	0.143791
H	0.314407	-2.294019	-0.434049
C	-3.992428	-1.682367	0.091899
C	-3.668476	1.092442	-0.048085
C	-4.943151	0.569334	0.132960
C	-5.083808	-0.834446	0.200828
H	-3.502577	2.164098	-0.107376
H	-6.073112	-1.263354	0.342223

C	-6.154102	1.464027	0.255075
H	-6.885218	1.257028	-0.536298
H	-6.666370	1.314495	1.213617
H	-5.875958	2.519603	0.185562
C	-1.188812	0.825500	-0.354539
O	-0.973384	2.036318	-0.425496
O	-1.667964	-1.998576	-0.192920
C	1.249474	0.279989	-0.644629
H	1.375715	1.366606	-0.694440
N	2.225753	-0.550283	-0.743555
N	3.458247	-0.017694	-0.918700
H	3.590340	0.994128	-0.980289
C	4.578292	-0.785577	-1.038694
S	4.664414	-2.452469	-1.009503
N	5.726471	-0.034784	-1.170273
H	6.551621	-0.571447	-1.414616
N	5.665466	1.348196	-1.420617
H	6.297269	1.833471	-0.787221
H	5.941377	1.552761	-2.381302

HF= -1232.0856376

xyz coordinates of imino-thiol tautomeric structure (T-2)

C	-0.382801	-1.459625	-0.408171
C	-2.681889	-1.112067	-0.109975
C	-2.518467	0.275999	-0.179813
C	-0.093535	-0.134124	-0.492799
H	-4.032146	-2.767503	0.129244
H	0.365628	-2.239712	-0.482221
C	-3.941706	-1.687240	0.079884
C	-3.656153	1.092134	-0.054276
C	-4.922130	0.551461	0.135281
C	-5.043388	-0.854367	0.199992
H	-3.505111	2.166075	-0.111610
H	-6.025744	-1.296854	0.347848
C	-6.143869	1.429455	0.270195
H	-6.880627	1.212138	-0.513116
H	-6.643607	1.273374	1.234316
H	-5.881020	2.488705	0.197440
C	-1.176202	0.859877	-0.381071
O	-0.978861	2.073477	-0.449540
O	-1.615271	-1.970338	-0.224399
C	1.265439	0.361519	-0.692920
H	1.367040	1.449128	-0.744476
N	2.269007	-0.437070	-0.799881

N	3.490091	0.110229	-0.981515
H	3.655256	1.116584	-1.046100
C	4.611614	-0.662855	-1.117739
N	5.785887	1.261341	-1.340466
H	6.444031	1.542733	-0.610869
H	6.265515	1.494583	-2.211997
N	5.805348	-0.207236	-1.300272
S	4.339478	-2.422978	-1.026410
H	5.652423	-2.680659	-1.201816

HF=-1232.0678667

xyz coordinates of imino-thiol tautomeric structure (T-3)

C	-0.447063	-1.529046	-0.511933
C	-2.739151	-1.184866	-0.164070
C	-2.572292	0.203292	-0.206327
C	-0.149663	-0.203734	-0.565411
H	-4.089486	-2.842204	0.061945
H	0.295211	-2.309665	-0.625674
C	-3.996643	-1.761312	0.035233
C	-3.705014	1.019055	-0.043229
C	-4.969487	0.477743	0.156623
C	-5.093969	-0.928494	0.192831
H	-3.551336	2.093543	-0.080169
H	-6.074905	-1.371711	0.347961
C	-6.185986	1.356224	0.330831
H	-6.935508	1.159073	-0.445674
H	-6.671305	1.179900	1.298852
H	-5.920547	2.416006	0.277991
C	-1.230660	0.790536	-0.417634
O	-1.038137	2.004277	-0.464365
O	-1.676394	-2.043264	-0.318990
C	1.211284	0.283839	-0.778954
H	1.329693	1.362171	-0.889095
N	2.224674	-0.510444	-0.834610
C	4.458105	-0.630115	-1.103773
N	5.715138	-0.142238	-1.378273
H	6.478836	-0.702431	-1.009492
N	5.904586	1.242536	-1.498299
H	6.193417	1.650180	-0.609382
H	6.624562	1.406367	-2.195594
N	3.423560	0.140934	-1.049922
S	4.469696	-2.415896	-0.870758
H	3.145005	-2.391960	-0.582206

HF=-1232.0622226

xyz coordinates of structure S-1

C	1.129938	0.537659	0.418257
C	2.881038	1.952482	-0.209604
C	3.730109	0.860558	-0.463193
C	1.861148	-0.628211	0.206491
H	2.599073	4.082944	-0.176087
H	0.099580	0.541961	0.763711
C	3.285395	3.268854	-0.382975
C	5.039672	1.130077	-0.910290
C	5.483695	2.436918	-1.096652
C	4.584085	3.495324	-0.825174
H	5.698155	0.291147	-1.107253
H	4.916463	4.520041	-0.966088
C	6.880886	2.735634	-1.573594
H	6.859622	3.304289	-2.510396
H	7.421181	3.344527	-0.839530
H	7.453734	1.820989	-1.743984
C	3.255155	-0.495124	-0.265008
O	4.002831	-1.478693	-0.487626
O	1.582925	1.743970	0.231797
C	1.118156	-1.829559	0.490015
H	0.097731	-1.659042	0.827106
N	1.406626	-3.107469	0.430291
N	2.660908	-3.525098	0.022138
H	3.367792	-2.694687	-0.239132
C	2.916538	-4.831212	-0.026019
S	1.765240	-6.084960	0.395407
N	4.116743	-5.266221	-0.415392
H	4.862141	-4.624912	-0.683752
N	4.293557	-6.650241	-0.435260
H	4.482434	-6.989343	-1.377654
H	5.017168	-6.943905	0.219658
Cu	0.300160	-4.565793	0.842737

HF=-2871. 8120881

xyz coordinates of structure S-2

C	0.449168	-1.433912	-0.278296
C	2.706222	-1.423704	0.366182
C	2.478936	-0.436807	1.346055
C	0.076164	-0.500747	0.655681

H	4.104413	-2.732642	-0.633298
H	-0.225813	-1.865347	-1.014511
C	3.977909	-1.976038	0.134160
C	3.563833	-0.001316	2.100611
C	4.863841	-0.535948	1.898841
C	5.038377	-1.528280	0.903424
H	3.394536	0.760144	2.856705
H	6.026541	-1.947145	0.740678
C	6.017356	-0.041953	2.711013
H	6.853595	-0.745182	2.706106
H	6.385360	0.909945	2.296109
H	5.722977	0.163348	3.745765
C	1.119139	0.109100	1.543122
O	0.834224	0.978014	2.349306
O	1.686010	-1.882769	-0.422760
C	-1.257286	-0.013925	0.802545
H	-1.367128	0.870969	1.433925
N	-2.306696	-0.568779	0.238313
N	-3.490719	0.106347	0.394356
H	-3.470770	0.977855	0.926739
C	-4.756430	-0.277400	0.020425
S	-6.027322	0.628665	0.636032
N	-5.046604	-1.388893	-0.741998
H	-6.046525	-1.470570	-0.917783
N	-4.214206	-1.994967	-1.760593
H	-4.656380	-2.895590	-1.969252
H	-4.268229	-1.442526	-2.626215
Cu	-2.542081	-2.052289	-0.835139

HF=-2871.7707795

xyz coordinates of structure S-3

C	0.429890	-1.323066	0.016125
C	2.771379	-1.088411	0.046852
C	2.683739	0.319367	-0.002224
C	0.201804	0.024364	-0.034146
H	4.024176	-2.848748	0.132722
H	-0.341945	-2.083371	0.028505
C	4.010086	-1.764494	0.092880
C	3.864827	1.049697	-0.003556
C	5.130848	0.404295	0.040418
C	5.168879	-1.013825	0.090794
H	3.802778	2.133627	-0.039060
H	6.130553	-1.515877	0.129608
C	6.390098	1.206632	0.006310
H	7.230516	0.667645	0.451759
H	6.663304	1.424202	-1.039104

H	6.270238	2.172759	0.506511
C	1.352668	0.967297	-0.045574
O	1.192836	2.179365	-0.088722
O	1.657224	-1.858256	0.054882
C	-1.125174	0.605071	-0.079627
H	-1.151334	1.699387	-0.110967
N	-2.186557	-0.131024	-0.086370
N	-3.373911	0.534776	-0.124413
H	-3.362618	1.556159	-0.176350
C	-4.546692	-0.136452	-0.088317
S	-4.553938	-1.841235	0.087378
N	-5.652251	0.664511	-0.193337
H	-5.573813	1.667224	-0.333550
N	-6.966703	0.129849	-0.137059
H	-7.467894	0.598173	0.626383
H	-7.451384	0.382239	-1.005984
Cu	-6.694761	-1.784454	0.064102

HF=-2871.7888185

xyz coordinates of structure S-4

C	0.460534	-1.293064	0.615744
C	2.790841	-1.023142	0.431706
C	2.654600	0.269935	-0.116499
C	0.184603	-0.057483	0.089456
H	4.101189	-2.616663	1.079125
H	-0.283901	-2.002922	0.956840
C	4.050527	-1.618741	0.655784
C	3.810802	0.968949	-0.437828
C	5.098852	0.402985	-0.224534
C	5.184332	-0.901679	0.325480
H	3.713636	1.964457	-0.861589
H	6.162041	-1.344241	0.488486
C	6.329286	1.181918	-0.555352
H	6.585270	1.845452	0.286775
H	7.191558	0.532477	-0.727051
H	6.179604	1.827039	-1.427031
C	1.301576	0.832564	-0.330512
O	1.095229	1.935675	-0.818009
O	1.702506	-1.756286	0.771812
C	-1.161006	0.450701	-0.066707
H	-1.224537	1.485249	-0.411973
N	-2.185543	-0.297177	0.183257
N	-3.460208	0.293785	0.035854
H	-4.101630	-0.402026	0.437598
C	-3.768179	1.580973	0.766483

S	-2.932380	2.161899	2.024278
N	-4.974247	2.095427	0.328501
H	-5.295537	2.920635	0.831294
N	-5.359023	2.028056	-1.059901
H	-6.358878	1.802148	-1.093112
H	-5.262921	2.962460	-1.476909
Cu	-4.160905	0.666181	-1.706925

HF=-2871.7460291

xyz coordinates of structure S-5

C	-1.476083	-2.443683	0.001397
C	-3.423354	-1.154488	0.000948
C	-2.678219	0.041018	0.000075
C	-0.623145	-1.345184	0.000677
H	-5.347745	-2.112273	0.001901
H	-1.124602	-3.471440	0.001921
C	-4.812321	-1.168965	0.001209
C	-3.386555	1.262505	-0.000588
C	-4.776965	1.288347	-0.000372
C	-5.472415	0.052923	0.000548
H	-2.819479	2.186659	-0.001275
H	-6.558849	0.060063	0.000737
C	-5.543072	2.584863	-0.001016
H	-6.191398	2.652850	-0.882244
H	-6.190095	2.654452	0.881052
H	-4.875137	3.449388	-0.002281
C	-1.237309	-0.008374	-0.000034
O	-0.571572	1.076031	-0.000671
O	-2.778014	-2.375704	0.001574
C	0.780837	-1.695193	0.000503
H	0.996048	-2.768408	0.000321
N	1.796776	-0.870904	0.000812
N	3.104595	-1.350975	-0.000338
H	3.761727	-0.580561	0.002578
C	3.628925	-2.608448	-0.001869
S	2.805887	-4.107046	-0.006939
N	4.969572	-2.700964	0.000351
H	5.600823	-1.901698	0.003512
N	5.459926	-4.008055	-0.002558
H	5.986777	-4.219852	-0.849129
H	5.983663	-4.224768	0.844698
Cu	1.246343	0.888071	-0.000098

HF=-2871.7917997

xyz coordinates of Isomer 1 for Co(II) complex

C	-5.039523	-2.098653	-0.190691
C	-7.203976	-1.455716	0.394091
C	-6.843345	-0.105043	0.340794
C	-4.545828	-0.820294	-0.278384
H	-8.735123	-2.921101	0.752538
H	-4.428799	-2.977139	-0.371988
C	-8.497026	-1.863314	0.721375
C	-7.829906	0.858397	0.629077
C	-9.127840	0.489295	0.959099
C	-9.442485	-0.888717	0.999880
H	-7.542160	1.903539	0.585934
H	-10.453329	-1.194114	1.257129
C	-10.187163	1.518605	1.269364
H	-11.031537	1.438719	0.574441
H	-10.587574	1.381207	2.280791
H	-9.789382	2.534668	1.200199
C	-5.473009	0.292722	-0.003232
O	-5.164867	1.497782	-0.051511
O	-6.283532	-2.441597	0.122026
C	-3.117761	-0.776521	-0.638212
H	-2.695138	-1.762564	-0.816983
N	-2.224377	0.148431	-0.756332
N	-2.557977	1.461389	-0.563130
H	-3.559988	1.654684	-0.357966
C	-1.635155	2.462353	-0.467044
S	0.045507	2.322731	-0.716356
N	-2.212748	3.644371	-0.131302
H	-3.188598	3.640927	0.156220
N	-1.454658	4.803402	0.020665
H	-1.883259	5.559809	-0.506232
H	-1.394264	5.056919	1.004930
N	2.199847	-0.147479	-0.601791
S	-0.039712	-2.355642	-0.640167
C	3.090092	0.780045	-0.490332
N	2.547621	-1.459884	-0.441587
C	1.642160	-2.476923	-0.393906
C	4.530184	0.824489	-0.178452
H	2.658942	1.766781	-0.639246
H	3.553987	-1.649507	-0.255616
N	2.235599	-3.661872	-0.094631
C	5.025455	2.103234	-0.111754

C	5.468075	-0.286191	0.067363
O	5.160614	-1.492107	0.036241
H	3.211021	-3.654879	0.193754
N	1.498706	-4.840454	-0.003307
H	4.407818	2.980396	-0.274651
O	6.280084	2.449100	0.154719
C	6.849595	0.114225	0.360838
H	1.942341	-5.562138	-0.565483
H	1.440696	-5.143986	0.966767
C	7.210693	1.465281	0.395535
C	7.847098	-0.847366	0.615864
C	8.515034	1.874834	0.672416
C	9.156214	-0.476254	0.895288
H	7.558645	-1.892820	0.587241
H	8.753232	2.932915	0.690375
C	9.471167	0.902098	0.918669
C	10.227384	-1.503810	1.168779
H	10.490823	1.209180	1.136138
H	11.042657	-1.428742	0.439376
H	10.668833	-1.360174	2.162100
H	9.827036	-2.520180	1.122301
Co	0.003188	-0.000564	-0.678518
Cl	-0.070183	0.036128	1.492430
O	0.067282	-0.032610	-2.574630
H	-0.238107	0.756034	-3.057128
H	-0.255987	-0.821350	-3.045315

HF=-4383.3420226

xyz coordinates of Isomer 2 for Co(II) complex

C	-2.014235	2.703316	0.165596
C	-4.016926	3.899661	0.178372
C	-4.750221	2.715215	0.052752
C	-2.598360	1.468384	0.043041
H	-4.031306	6.042831	0.347538
H	-0.939093	2.839895	0.217226
C	-4.636175	5.147603	0.250733
C	-6.155005	2.804962	-0.001639
C	-6.805723	4.030392	0.066558
C	-6.020150	5.199214	0.194139
H	-6.715297	1.881155	-0.099968
H	-6.513775	6.165991	0.248937
C	-8.310498	4.130219	0.006419
H	-8.712396	4.601458	0.911234
H	-8.632313	4.740825	-0.845560
H	-8.772539	3.144322	-0.093102
C	-4.072148	1.414548	-0.022592

O	-4.737146	0.369991	-0.133467
O	-2.642705	3.873829	0.234715
C	-1.623365	0.364847	-0.017984
H	-0.587734	0.691495	0.027957
N	-1.701883	-0.917775	-0.130948
N	-2.898623	-1.557461	-0.219594
H	-3.741647	-0.953029	-0.189300
C	-3.018920	-2.910360	-0.441274
S	-1.754112	-4.028351	-0.502906
N	-4.322316	-3.259627	-0.616605
H	-5.018550	-2.523061	-0.700908
N	-4.689825	-4.584564	-0.832596
H	-5.410872	-4.854130	-0.168688
H	-5.027006	-4.708253	-1.784795
N	1.452096	-0.822763	-0.103838
S	-0.145508	-2.659851	1.792453
C	2.213350	-0.287843	-1.000335
N	1.816701	-0.830300	1.224014
C	1.148831	-1.574984	2.145786
C	3.528859	0.371346	-0.997124
H	1.764036	-0.400997	-1.986854
N	1.599787	-1.382365	3.409764
C	4.006345	0.633373	-2.258407
C	4.349694	0.794573	0.150432
H	2.361428	-0.726599	3.567454
N	1.090564	-2.129056	4.469953
H	3.460782	0.369123	-3.158518
O	5.161041	1.220560	-2.552897
C	5.623503	1.436401	-0.193962
O	4.021904	0.648560	1.343637
H	1.826941	-2.690409	4.891745
H	0.683122	-1.511642	5.167792
C	5.988585	1.626071	-1.531775
C	6.511949	1.877422	0.806727
C	7.193560	2.230956	-1.889892
C	7.720626	2.482601	0.486843
H	6.220806	1.727467	1.841088
H	7.439168	2.359013	-2.938659
C	8.044386	2.650918	-0.879588
C	8.676038	2.953305	1.556167
H	8.986465	3.122433	-1.146800
H	9.644460	2.446017	1.472029
H	8.867316	4.029481	1.469915
H	8.281480	2.760704	2.557528
H	2.665089	-0.281411	1.476715
O	1.117069	-3.601789	-0.437571
H	1.092042	-4.407057	0.112165
H	1.254066	-3.877495	-1.369459

Co	-0.134956	-2.409623	-0.301380
Cl	-0.123397	-2.152456	-2.445443

HF=-4383.3093483

xyz coordinates of Isomer 3 for Co(II) complex

C	2.609305	1.974291	-1.770315
C	4.569879	3.155776	-1.315136
C	4.910479	2.249495	-0.305008
C	2.827787	0.997594	-0.831318
H	5.078565	4.927180	-2.422063
H	1.731412	1.989995	-2.408577
C	5.378149	4.247395	-1.631606
C	6.107509	2.464104	0.405704
C	6.937526	3.540480	0.117595
C	6.550685	4.426892	-0.914054
H	6.361990	1.757805	1.188983
H	7.189063	5.273752	-1.151813
C	8.222609	3.771578	0.874436
H	9.087982	3.741886	0.201658
H	8.224562	4.754932	1.359277
H	8.372354	3.014311	1.648709
C	4.041996	1.105582	0.001530
O	4.337268	0.317534	0.915983
O	3.406974	3.003570	-2.036471
C	1.756985	-0.010950	-0.764424
H	0.859838	0.268614	-1.311674
N	1.642453	-1.184791	-0.223261
N	2.706487	-1.721978	0.433844
H	3.435788	-1.066480	0.777507
C	2.634820	-3.038041	0.756720
S	1.345727	-3.964066	0.185947
N	3.642204	-3.488772	1.533031
H	4.251592	-2.803908	1.975319
N	3.681043	-4.821377	1.942803
H	4.627201	-5.177301	1.841677
H	3.375718	-4.903166	2.910834
N	-1.454214	-0.898180	-0.510914
S	-1.821549	-3.676422	-0.107467
C	-1.489053	0.239856	0.104137
N	-2.625351	-1.355633	-1.088109
C	-2.904860	-2.672508	-0.940172
C	-2.561345	1.196743	0.416667
H	-0.535138	0.481395	0.562021
N	-4.097404	-3.056445	-1.456350
C	-2.280613	1.996063	1.497011

C	-3.828683	1.419264	-0.299905
H	-4.716480	-2.339300	-1.828193
N	-4.552908	-4.365707	-1.312869
H	-1.366149	1.903457	2.074172
O	-3.065755	2.946739	1.988633
C	-4.676387	2.484022	0.249467
O	-4.181694	0.785499	-1.311581
H	-5.338778	-4.400651	-0.667011
H	-4.831694	-4.733092	-2.218598
C	-4.273035	3.205836	1.378532
C	-5.916960	2.802842	-0.336227
C	-5.061892	4.214796	1.930671
C	-6.728530	3.802271	0.186205
H	-6.220310	2.239743	-1.212769
H	-4.713978	4.749653	2.807879
C	-6.278282	4.500784	1.330297
C	-8.059743	4.144873	-0.436842
H	-6.902054	5.284563	1.751970
H	-8.880140	3.990363	0.274082
H	-8.093488	5.196641	-0.744616
H	-8.258175	3.529647	-1.318552
H	-3.328048	-0.635242	-1.346261
Cl	-0.079926	-2.010159	1.900954
Co	-0.067846	-2.415582	-0.166027
O	-0.057306	-2.797853	-2.115773
H	-0.476632	-3.661585	-2.289651
H	0.826594	-2.849956	-2.520824

HF=-4383.2941792

xyz coordinates of Isomer 4 for Co(II) complex

C	-4.454887	-0.342716	1.658180
C	-6.080446	1.242611	1.122764
C	-5.220207	1.851428	0.202763
C	-3.518921	0.131779	0.769626
H	-8.006639	1.215628	2.076585
H	-4.273862	-1.200576	2.297571
C	-7.370809	1.717952	1.355503
C	-5.686716	2.981855	-0.496431
C	-6.965537	3.483884	-0.289848
C	-7.798500	2.830353	0.647648
H	-5.011872	3.450572	-1.205030
H	-8.802074	3.210228	0.820097
C	-7.470254	4.692394	-1.039830
H	-8.342644	4.439887	-1.654398

H	-7.780875	5.485265	-0.349332
H	-6.701315	5.102749	-1.699997
C	-3.872014	1.319762	-0.027918
O	-3.105213	1.878759	-0.835672
O	-5.674498	0.144043	1.845506
C	-2.266839	-0.639748	0.811570
H	-2.164394	-1.247418	1.703197
N	-1.287151	-0.833772	-0.020887
N	-1.363279	-0.079221	-1.198226
H	-1.936662	0.787498	-1.165377
C	-0.836106	-0.557429	-2.349837
S	0.025779	-2.014343	-2.401674
N	-1.094136	0.226991	-3.430677
H	-1.829119	0.925560	-3.341761
N	-0.663524	-0.157860	-4.702233
H	-1.427409	-0.583713	-5.225467
H	-0.325232	0.661618	-5.198761
N	1.520287	-1.021807	0.013795
S	-0.205320	-2.583256	1.802310
C	2.426561	-0.608073	-0.814220
N	1.657282	-0.721213	1.351568
C	0.885598	-1.364112	2.265676
C	3.678725	0.154641	-0.701442
H	2.192546	-0.919554	-1.829126
N	1.080929	-0.936167	3.538510
C	4.380073	0.194930	-1.883564
C	4.246979	0.869626	0.457202
H	1.823352	-0.262703	3.715255
N	0.437009	-1.556033	4.609316
H	4.028500	-0.287134	-2.790124
O	5.544405	0.796775	-2.084485
C	5.538274	1.524563	0.216706
O	3.702892	0.948514	1.573936
H	1.102495	-2.096652	5.159015
H	0.002850	-0.849872	5.197658
C	6.146798	1.464743	-1.041757
C	6.200444	2.227197	1.242447
C	7.374584	2.073279	-1.299410
C	7.425714	2.844651	1.023003
H	5.721650	2.270333	2.215043
H	7.812331	2.003188	-2.289385
C	7.999619	2.754304	-0.266177
C	8.139787	3.594824	2.120626
H	8.957724	3.231536	-0.454472
H	9.123302	3.154975	2.324224
H	8.306328	4.641622	1.840418
H	7.566481	3.582463	3.051508
H	2.394289	-0.032627	1.611833

O	1.163678	-3.842479	-0.539997
H	1.420567	-4.248752	0.308367
H	0.582105	-4.511397	-0.956131
Co	-0.090831	-2.301907	-0.275603
Cl	-1.857699	-3.689246	-0.590144

HF=-4383.2981814

xyz coordinates of Isomer 5 for Co(II) complex

C	-4.600137	-1.896183	-1.266347
C	-6.879970	-1.507913	-0.961703
C	-6.618182	-0.233603	-0.447607
C	-4.191756	-0.678431	-0.770511
H	-8.337605	-2.996419	-1.491038
H	-3.901251	-2.643458	-1.627448
C	-8.178165	-2.002401	-1.087195
C	-7.712213	0.561583	-0.052172
C	-9.018345	0.102046	-0.162337
C	-9.230528	-1.194193	-0.686741
H	-7.500947	1.549490	0.343323
H	-10.246697	-1.568390	-0.779795
C	-10.192589	0.949519	0.262955
H	-10.889294	1.106338	-0.568909
H	-10.756842	0.466431	1.069633
H	-9.868505	1.930737	0.620237
C	-5.241233	0.256786	-0.324579
O	-5.025071	1.400046	0.123426
O	-5.852118	-2.325252	-1.369108
C	-2.728471	-0.531722	-0.814316
H	-2.225055	-1.353574	-1.312605
N	-1.856095	0.316827	-0.340799
N	-2.397558	1.412054	0.329216
H	-3.434811	1.530827	0.308594
C	-1.579270	2.295961	0.933659
S	0.095194	2.076858	0.868377
N	-2.215030	3.301795	1.581189
H	-3.229964	3.272415	1.646529
N	-1.496965	4.282748	2.263108
H	-1.781353	5.203499	1.938622
H	-1.659643	4.204658	3.264721
N	1.925163	0.006654	-0.049706
S	-0.220714	-0.859621	1.622836
C	2.846411	0.567329	-0.775456
N	2.328623	-0.840679	0.955963
C	1.389838	-1.340213	1.792128
C	4.318364	0.533351	-0.807104

H	2.413033	1.231583	-1.515265
H	3.324799	-1.146786	0.956848
N	1.862196	-2.198720	2.724140
C	4.855695	1.474167	-1.651261
C	5.256059	-0.369196	-0.111198
O	4.915591	-1.282825	0.662128
H	2.841428	-2.470831	2.683955
N	1.000998	-2.813206	3.631490
H	4.244533	2.169041	-2.217628
O	6.146848	1.674555	-1.893606
C	6.677845	-0.137187	-0.393823
H	0.956857	-3.813760	3.449928
H	1.328681	-2.647822	4.579698
C	7.077874	0.876390	-1.270664
C	7.676257	-0.927818	0.208519
C	8.421537	1.120206	-1.555153
C	9.023998	-0.713898	-0.051230
H	7.357100	-1.714207	0.884368
H	8.689517	1.916077	-2.241735
C	9.377608	0.324624	-0.943454
C	10.096086	-1.558150	0.593680
H	10.427855	0.504426	-1.157811
H	10.714078	-2.057641	-0.161741
H	10.767817	-0.944602	1.205917
H	9.663818	-2.328746	1.237686
O	0.273101	1.116350	-1.894528
H	-0.373230	1.805371	-2.125361
H	0.202639	0.420360	-2.580078
Co	0.034534	0.161739	-0.195255
Cl	-0.026911	-1.778198	-1.272670

HF=-4383.3014938

xyz coordinates of Isomer 1 for Ni(II) complex

C	-5.064359	-2.082021	-0.287599
C	-7.233829	-1.440824	0.280587
C	-6.855089	-0.094372	0.307751
C	-4.553998	-0.807388	-0.300116
H	-8.791778	-2.901595	0.524029
H	-4.460048	-2.958240	-0.498918
C	-8.539488	-1.847097	0.555003
C	-7.835773	0.865981	0.624658
C	-9.145906	0.498075	0.904151
C	-9.478995	-0.875536	0.862971
H	-7.533631	1.907771	0.644027

H	-10.499614	-1.180136	1.079331
C	-10.198794	1.524046	1.245708
H	-11.033514	1.485546	0.535832
H	-10.615615	1.345122	2.243979
H	-9.789165	2.537621	1.229177
C	-5.472368	0.302441	0.015428
O	-5.147229	1.503327	0.041376
O	-6.319297	-2.423888	-0.020984
C	-3.118215	-0.763214	-0.625400
H	-2.695219	-1.745768	-0.820206
N	-2.221873	0.161930	-0.703422
N	-2.541497	1.471275	-0.485377
H	-3.539011	1.666837	-0.263193
C	-1.607470	2.463949	-0.379125
S	0.061622	2.322086	-0.669897
N	-2.174679	3.641813	-0.009717
H	-3.142059	3.633942	0.304667
N	-1.405029	4.790382	0.162244
H	-1.840786	5.566126	-0.329321
H	-1.318986	5.011172	1.152590
N	2.201450	-0.161801	-0.582174
S	-0.051900	-2.355991	-0.614476
C	3.094015	0.766526	-0.511435
N	2.535053	-1.470546	-0.388495
C	1.618212	-2.479239	-0.322578
C	4.538213	0.812275	-0.223269
H	2.663989	1.749254	-0.685850
H	3.536869	-1.661355	-0.181660
N	2.199924	-3.658442	0.021609
C	5.046901	2.087448	-0.229070
C	5.466778	-0.294580	0.071231
O	5.144856	-1.496063	0.112608
H	3.165122	-3.645175	0.342128
N	1.450663	-4.826627	0.141810
H	4.435798	2.961843	-0.427707
O	6.308629	2.432514	0.001325
C	6.856625	0.105285	0.323466
H	1.904792	-5.574728	-0.375455
H	1.360740	-5.087622	1.121903
C	7.232553	1.452034	0.280185
C	7.847335	-0.852657	0.615631
C	8.545251	1.860732	0.515211
C	9.164538	-0.482285	0.855478
H	7.547042	-1.894685	0.647445
H	8.795216	2.915388	0.472685
C	9.494560	0.891551	0.799391
C	10.228324	-1.505821	1.169651
H	10.520699	1.198189	0.984614

H	11.041544	-1.469219	0.435136
H	10.674417	-1.322733	2.154438
H	9.819509	-2.519876	1.169063
Ni	0.005247	-0.001067	-0.642375
Cl	-0.052293	0.026056	1.529194
O	0.055502	-0.024756	-2.539024
H	-0.256055	0.748348	-3.040460
H	-0.185643	-0.833450	-3.023332

HF=-4508.8632147

xyz coordinates of Isomer 2 for Ni(II) complex

C	-1.739005	2.722479	0.099152
C	-3.653296	4.054011	0.162742
C	-4.469794	2.920442	0.094184
C	-2.409814	1.528503	0.026648
H	-3.515099	6.195920	0.284923
H	-0.655882	2.785638	0.108670
C	-4.182859	5.342599	0.233637
C	-5.866293	3.105374	0.098754
C	-6.429095	4.373522	0.168838
C	-5.561325	5.488007	0.235944
H	-6.491640	2.220428	0.045500
H	-5.985152	6.487342	0.290858
C	-7.924819	4.574855	0.172522
H	-8.250180	5.107308	1.074024
H	-8.245313	5.172864	-0.688909
H	-8.456295	3.620126	0.135182
C	-3.885177	1.575279	0.018521
O	-4.623826	0.577025	-0.043840
O	-2.282730	3.934815	0.163677
C	-1.514045	0.357950	-0.036086
H	-0.459223	0.618722	0.000275
N	-1.676135	-0.916859	-0.144604
N	-2.920991	-1.462915	-0.224066
H	-3.718170	-0.800529	-0.160616
C	-3.148860	-2.796587	-0.448844
S	-1.972580	-4.007835	-0.562778
N	-4.476905	-3.054297	-0.584940
H	-5.125983	-2.272208	-0.620609
N	-4.936867	-4.347847	-0.812315
H	-5.637596	-4.592708	-0.117755
H	-5.328366	-4.425542	-1.748334
N	1.475619	-1.069701	-0.124427
S	-0.258277	-2.804333	1.748470
C	2.204470	-0.489913	-1.014960

N	1.802006	-1.074958	1.205866
C	1.092438	-1.812731	2.114791
C	3.472624	0.256299	-0.997581
H	1.764285	-0.631007	-2.003096
N	1.578159	-1.672343	3.374062
C	3.915008	0.598830	-2.251723
C	4.287865	0.665953	0.158764
H	2.394531	-1.083504	3.523270
N	1.017380	-2.362698	4.445834
H	3.372994	0.340509	-3.155773
O	5.028584	1.265136	-2.533214
C	5.515581	1.399436	-0.172057
O	3.993645	0.434890	1.346437
H	1.703991	-2.991407	4.856120
H	0.686543	-1.705777	5.148176
C	5.846780	1.672742	-1.504197
C	6.392874	1.844458	0.836261
C	7.007908	2.364186	-1.849460
C	7.558646	2.534929	0.529240
H	6.128447	1.628238	1.866075
H	7.228706	2.555225	-2.894154
C	7.849135	2.786229	-0.831731
C	8.502951	3.009300	1.606745
H	8.757382	3.324818	-1.089050
H	9.493670	2.553552	1.492274
H	8.640874	4.096042	1.561864
H	8.130599	2.757742	2.603499
H	2.646623	-0.532187	1.477744
O	0.923296	-3.808580	-0.498687
H	0.947066	-4.591166	0.083069
H	1.068120	-4.100211	-1.423900
Ni	-0.231230	-2.524165	-0.341415
Cl	-0.202694	-2.236400	-2.481428

HF=-4508.8297679

xyz coordinates of Isomer 3 for Ni(II) complex

C	-2.358963	1.787075	1.717840
C	-4.327751	3.023931	1.518071
C	-4.622847	2.408181	0.296601
C	-2.535973	1.087991	0.548497
H	-4.898303	4.442363	3.029117
H	-1.504118	1.634664	2.368882
C	-5.162280	3.990222	2.079127
C	-5.799949	2.792335	-0.374985

C	-6.654231	3.752344	0.153277
C	-6.313906	4.342508	1.392458
H	-6.019480	2.312723	-1.323236
H	-6.972199	5.094315	1.819818
C	-7.917743	4.164408	-0.561801
H	-8.804407	3.943868	0.044525
H	-7.924816	5.242050	-0.763174
H	-8.024645	3.642616	-1.516578
C	-3.729939	1.386098	-0.261230
O	-3.989784	0.847342	-1.353519
O	-3.185144	2.698459	2.214605
C	-1.439154	0.151040	0.265868
H	-0.545054	0.334721	0.853373
N	-1.324313	-0.911101	-0.466977
N	-2.424270	-1.289940	-1.228082
H	-3.101898	-0.536954	-1.463644
C	-2.757608	-2.601111	-1.128363
S	-1.726259	-3.628214	-0.272745
N	-3.931388	-2.944058	-1.711195
H	-4.541217	-2.199307	-2.041951
N	-4.396964	-4.256936	-1.651507
H	-5.192612	-4.325697	-1.020449
H	-4.663499	-4.568681	-2.581414
N	1.530472	-1.161195	-0.056051
S	1.412603	-3.837983	0.172259
C	1.648746	-0.031244	-0.690293
N	2.604166	-1.601936	0.665751
C	2.620368	-2.930393	0.903105
C	2.730253	0.957190	-0.817006
H	0.767757	0.198750	-1.281133
N	3.603867	-3.390071	1.703899
C	2.591764	1.794309	-1.895788
C	3.864895	1.194305	0.096257
H	4.117818	-2.711286	2.261535
N	3.664684	-4.746410	2.027089
H	1.766643	1.717895	-2.596993
O	3.415624	2.779402	-2.236342
C	4.765802	2.285217	-0.296596
O	4.064782	0.554249	1.143119
H	4.630641	-5.057902	1.986622
H	3.280182	-4.908622	2.956148
C	4.517368	3.036212	-1.450889
C	5.900513	2.604883	0.474128
C	5.357611	4.074710	-1.851503
C	6.760199	3.632226	0.105211
H	6.082550	2.019514	1.369336
H	5.130135	4.633308	-2.753119
C	6.467702	4.359922	-1.071489

C	7.979246	3.975038	0.926289
H	7.130263	5.166532	-1.374245
H	8.897129	3.860002	0.337616
H	7.944682	5.015694	1.269702
H	8.061597	3.332546	1.807065
H	3.257567	-0.888274	1.043691
Ni	-0.004562	-2.323058	-0.157909
Cl	-0.155751	-2.242798	1.950943
O	0.147633	-2.403860	-2.266091
H	1.008734	-2.825671	-2.438436
H	-0.502836	-3.054424	-2.585227

HF=-4508.805617

xyz coordinates of Isomer 4 for Ni(II) complex

C	-4.458372	-0.290243	1.622888
C	-6.050814	1.304712	1.020842
C	-5.176704	1.859395	0.079871
C	-3.510778	0.131888	0.720712
H	-7.978955	1.353959	1.969764
H	-4.295844	-1.126098	2.295501
C	-7.331732	1.814761	1.231296
C	-5.619084	2.970472	-0.664643
C	-6.887763	3.506012	-0.481161
C	-7.735457	2.906903	0.479204
H	-4.933800	3.397350	-1.389482
H	-8.731444	3.313424	0.634035
C	-7.366606	4.694057	-1.279298
H	-8.240269	4.434109	-1.888964
H	-7.666377	5.518012	-0.621188
H	-6.586954	5.065110	-1.950052
C	-3.839079	1.292121	-0.126048
O	-3.061300	1.800924	-0.956128
O	-5.668866	0.227037	1.786837
C	-2.275494	-0.664132	0.794451
H	-2.196919	-1.258751	1.697068
N	-1.285507	-0.882757	-0.014774
N	-1.320464	-0.176431	-1.215414
H	-1.897537	0.688817	-1.234601
C	-0.771831	-0.707121	-2.335975
S	0.095250	-2.155805	-2.308290
N	-1.010707	0.029981	-3.454963
H	-1.757490	0.720335	-3.414565
N	-0.549550	-0.410117	-4.697434
H	-1.299165	-0.862686	-5.218870
H	-0.200972	0.386868	-5.222628
N	1.455771	-1.043989	0.077801

S	-0.180264	-2.495501	1.950194
C	2.396942	-0.712828	-0.750966
N	1.560786	-0.585796	1.375643
C	0.838657	-1.197712	2.341412
C	3.642542	0.065044	-0.660756
H	2.214073	-1.130040	-1.736727
N	1.003654	-0.672291	3.579785
C	4.426588	-0.068724	-1.782700
C	4.124604	0.960763	0.407375
H	1.703694	0.054979	3.709644
N	0.383496	-1.248391	4.688546
H	4.140265	-0.687400	-2.627146
O	5.602739	0.507049	-1.991087
C	5.425346	1.592046	0.156880
O	3.501487	1.205939	1.457412
H	1.071982	-1.709157	5.280745
H	-0.097143	-0.528046	5.220921
C	6.125052	1.341585	-1.028529
C	6.005166	2.463533	1.099679
C	7.365176	1.921897	-1.292246
C	7.238686	3.060665	0.870956
H	5.455016	2.654768	2.014980
H	7.875267	1.700887	-2.223662
C	7.907468	2.772570	-0.341322
C	7.863004	3.994997	1.878197
H	8.873846	3.230428	-0.535517
H	8.840535	3.624336	2.208491
H	8.024414	4.989905	1.446592
H	7.230069	4.110433	2.762146
H	2.249034	0.174958	1.562647
O	1.243856	-3.825350	-0.306938
H	1.550658	-4.118985	0.570321
H	0.647891	-4.545403	-0.604972
Cl	-1.765020	-3.783601	-0.404936
Ni	-0.044539	-2.327937	-0.148101

HF=-4508.8310651

xyz coordinates of Isomer 5 for Ni(II) complex

C	-4.561643	-2.196070	-0.822468
C	-6.851368	-1.776066	-0.675901
C	-6.610518	-0.428386	-0.389184
C	-4.173656	-0.902715	-0.553568
H	-8.285657	-3.347535	-0.981338
H	-3.848781	-2.993087	-1.006643
C	-8.142888	-2.295847	-0.757408

C	-7.719374	0.414866	-0.178684
C	-9.020057	-0.067692	-0.251920
C	-9.210738	-1.437877	-0.545109
H	-7.524659	1.458629	0.044083
H	-10.222129	-1.831153	-0.605391
C	-10.210029	0.832925	-0.027085
H	-10.856908	0.861837	-0.911993
H	-10.823209	0.476632	0.809117
H	-9.899307	1.857215	0.195965
C	-5.239269	0.088216	-0.308829
O	-5.041447	1.290619	-0.050612
O	-5.807589	-2.646405	-0.889445
C	-2.710142	-0.761164	-0.560948
H	-2.182845	-1.684967	-0.777194
N	-1.862105	0.197456	-0.318304
N	-2.404869	1.432533	0.000223
H	-3.444771	1.513094	0.025603
C	-1.586549	2.479135	0.247643
S	0.082228	2.292026	0.128559
N	-2.228980	3.621872	0.592703
H	-3.234535	3.587574	0.742633
N	-1.514308	4.779103	0.896491
H	-1.860921	5.553031	0.335591
H	-1.606452	5.000748	1.885583
N	1.925303	0.040985	0.013229
S	-0.192624	-0.160727	1.917518
C	2.814217	0.237974	-0.912029
N	2.348455	-0.324682	1.262708
C	1.423923	-0.469550	2.244170
C	4.282349	0.154520	-0.983902
H	2.350228	0.541326	-1.843317
H	3.356117	-0.559878	1.379904
N	1.933134	-0.853396	3.440377
C	4.779039	0.583291	-2.190631
C	5.253169	-0.335381	0.014623
O	4.952449	-0.768753	1.141206
H	2.913778	-1.118437	3.486708
N	1.090267	-1.100105	4.522503
H	4.141574	0.948280	-2.989047
O	6.056745	0.619052	-2.553062
C	6.659872	-0.293218	-0.404265
H	1.067587	-2.095840	4.733384
H	1.416712	-0.581635	5.333613
C	7.016989	0.183433	-1.669540
C	7.686477	-0.730881	0.455370
C	8.345168	0.236046	-2.092249
C	9.020086	-0.694176	0.068133
H	7.400619	-1.100411	1.434504

H	8.579437	0.612501	-3.082207
C	9.330001	-0.202035	-1.220710
C	10.121846	-1.165217	0.985901
H	10.368629	-0.166589	-1.538941
H	10.680170	-1.996230	0.538658
H	10.841916	-0.362623	1.184854
H	9.723720	-1.505880	1.945521
O	0.247315	0.388543	-2.144066
H	-0.350866	1.027110	-2.566173
H	0.067308	-0.488512	-2.535978
Ni	0.031599	0.119218	-0.152539
Cl	-0.019687	-2.081747	-0.437279

HF=-4508.8365847

xyz coordinates of Isomer 1 for Cu(II) complex

C	-4.990957	-2.079849	-0.238897
C	-7.096642	-1.458587	0.548914
C	-6.745301	-0.105704	0.492105
C	-4.508937	-0.798462	-0.339827
H	-8.587567	-2.936974	1.009341
H	-4.397716	-2.951678	-0.494836
C	-8.355314	-1.877846	0.979551
C	-7.705259	0.847729	0.884442
C	-8.968563	0.466890	1.318830
C	-9.275159	-0.912925	1.359151
H	-7.424777	1.894678	0.837292
H	-10.259089	-1.227532	1.697059
C	-9.998719	1.485604	1.741830
H	-10.907155	1.405832	1.133120
H	-10.296273	1.336466	2.786611
H	-9.616107	2.505095	1.643521
C	-5.411079	0.304465	0.038332
O	-5.111737	1.511695	-0.013990
O	-6.201796	-2.434800	0.175916
C	-3.120733	-0.737936	-0.833055
H	-2.729385	-1.714974	-1.110245
N	-2.228374	0.184049	-0.974329
N	-2.539403	1.481918	-0.677199
H	-3.524541	1.667595	-0.397728
C	-1.611714	2.476909	-0.592861
S	0.059464	2.338070	-0.886363
N	-2.175963	3.660228	-0.237128
H	-3.158786	3.666707	0.025604
N	-1.401643	4.800913	-0.037578
H	-1.788093	5.572578	-0.574877

H	-1.380799	5.042537	0.951231
N	2.190595	-0.151701	-0.761546
S	-0.067218	-2.339838	-0.847762
C	3.085227	0.766059	-0.621602
N	2.512570	-1.458453	-0.533118
C	1.600010	-2.468123	-0.526687
C	4.499984	0.809262	-0.205430
H	2.680162	1.752198	-0.838309
H	3.501368	-1.652899	-0.272727
N	2.170912	-3.659877	-0.209734
C	5.002078	2.084749	-0.136113
C	5.406760	-0.302494	0.132904
O	5.090680	-1.506424	0.106885
H	3.144552	-3.665905	0.084736
N	1.415382	-4.826486	-0.119157
H	4.406684	2.962345	-0.365756
O	6.238003	2.427260	0.211415
C	6.767342	0.093672	0.516286
H	1.841236	-5.552852	-0.689079
H	1.360147	-5.134325	0.849659
C	7.138369	1.442179	0.544245
C	7.733746	-0.869322	0.867533
C	8.422931	1.847830	0.906472
C	9.022239	-0.502002	1.234080
H	7.437778	-1.912781	0.843286
H	8.669859	2.904019	0.915674
C	9.348437	0.873852	1.246835
C	10.059540	-1.531002	1.612573
H	10.352326	1.177919	1.531531
H	10.933046	-1.473664	0.952302
H	10.418253	-1.372734	2.636582
H	9.656858	-2.545621	1.550507
Cu	-0.003447	0.015001	-0.867194
Cl	-0.106363	0.035694	1.302768
O	0.086440	-0.003073	-2.762441
H	-0.305555	0.758555	-3.223314
H	-0.205193	-0.819188	-3.205056

HF=-4640.9746557

xyz coordinates of Isomer 2 for Cu(II) complex

C	-2.022188	2.691475	0.260840
C	-4.034847	3.870749	0.234228
C	-4.751121	2.685416	0.038677
C	-2.588817	1.456662	0.075614
H	-4.076817	6.006698	0.475204
H	-0.951115	2.835224	0.358311
C	-4.668639	5.110295	0.323897

C	-6.153323	2.765419	-0.069547
C	-6.818150	3.982285	0.014309
C	-6.049689	5.152471	0.213158
H	-6.700107	1.840860	-0.221997
H	-6.554422	6.112698	0.280631
C	-8.320363	4.071184	-0.102093
H	-8.762935	4.501310	0.804269
H	-8.614696	4.713128	-0.940839
H	-8.767592	3.086006	-0.259640
C	-4.058063	1.393437	-0.053780
O	-4.707730	0.348702	-0.231313
O	-2.663748	3.854514	0.344216
C	-1.602468	0.361670	0.013833
H	-0.571854	0.702398	0.085186
N	-1.660250	-0.920254	-0.116989
N	-2.849894	-1.564152	-0.233111
H	-3.698982	-0.968114	-0.242755
C	-2.936548	-2.918764	-0.467612
S	-1.628769	-3.975072	-0.475502
N	-4.221309	-3.294162	-0.706748
H	-4.924164	-2.570135	-0.836438
N	-4.552219	-4.626189	-0.940895
H	-5.317618	-4.900493	-0.330807
H	-4.817478	-4.759113	-1.914508
N	1.400303	-0.812010	-0.062276
S	-0.148457	-2.606780	1.829052
C	2.150098	-0.274433	-0.966403
N	1.788993	-0.788894	1.257313
C	1.132781	-1.525157	2.189367
C	3.465880	0.387603	-0.981470
H	1.694123	-0.394748	-1.948442
N	1.591243	-1.328013	3.448862
C	3.925669	0.636763	-2.251954
C	4.301501	0.824205	0.150069
H	2.351011	-0.667282	3.596996
N	1.083839	-2.060649	4.519821
H	3.367631	0.362593	-3.141455
O	5.075294	1.220647	-2.568291
C	5.570250	1.462784	-0.218242
O	3.989984	0.691395	1.349247
H	1.822562	-2.612998	4.949112
H	0.675034	-1.434042	5.208715
C	5.917154	1.637675	-1.562780
C	6.471907	1.914622	0.765436
C	7.116837	2.238392	-1.944087
C	7.676270	2.516103	0.422478
H	6.194897	1.776163	1.805259
H	7.348192	2.354993	-2.997410

C	7.981326	2.669312	-0.949920
C	8.646050	2.998300	1.473511
H	8.919622	3.137800	-1.235117
H	9.613254	2.490086	1.381560
H	8.835937	4.073451	1.372897
H	8.265208	2.816550	2.482158
H	2.640296	-0.234213	1.491027
O	1.143929	-3.542221	-0.386581
H	1.236690	-4.311106	0.206063
H	1.342162	-3.831075	-1.301061
Cl	-0.089377	-2.107754	-2.409481
Cu	-0.119643	-2.360691	-0.265096

HF=-4640.919524

xyz coordinates of Isomer 3 for Cu(II) complex

C	-2.433774	1.718418	1.754551
C	-4.423530	2.923819	1.571104
C	-4.664938	2.386184	0.301551
C	-2.558110	1.096816	0.535447
H	-5.073638	4.226605	3.152460
H	-1.596513	1.539218	2.421409
C	-5.296522	3.834373	2.166019
C	-5.826500	2.793398	-0.383618
C	-6.717368	3.699972	0.177362
C	-6.431306	4.211092	1.464615
H	-6.003473	2.376086	-1.369477
H	-7.118708	4.920592	1.917687
C	-7.963851	4.137161	-0.552502
H	-8.866315	3.852115	0.001439
H	-7.990119	5.226498	-0.672791
H	-8.023184	3.686930	-1.547048
C	-3.731337	1.422956	-0.291643
O	-3.942025	0.953323	-1.426969
O	-3.297746	2.574891	2.283101
C	-1.424903	0.216607	0.215826
H	-0.537362	0.411083	0.809977
N	-1.271595	-0.810838	-0.559577
N	-2.369691	-1.169973	-1.344073
H	-3.031674	-0.401765	-1.583772
C	-2.747904	-2.460662	-1.222418
S	-1.768310	-3.508979	-0.327239
N	-3.921273	-2.793361	-1.811570
H	-4.522911	-2.042073	-2.142426
N	-4.406768	-4.097907	-1.724121
H	-5.205300	-4.142240	-1.094461

H	-4.673848	-4.427344	-2.647808
N	1.561772	-1.145843	-0.069147
S	1.349111	-3.813106	0.204859
C	1.714692	-0.032911	-0.726562
N	2.599166	-1.610112	0.684023
C	2.545895	-2.930886	0.969400
C	2.817699	0.928826	-0.840451
H	0.851922	0.197317	-1.342964
N	3.446195	-3.389449	1.868370
C	2.728598	1.751064	-1.936286
C	3.929705	1.157074	0.102557
H	3.881659	-2.704346	2.482627
N	3.421559	-4.734242	2.243727
H	1.923358	1.680201	-2.660639
O	3.582795	2.714210	-2.266326
C	4.866251	2.220818	-0.281564
O	4.082760	0.531919	1.166020
H	4.374857	-5.063801	2.362314
H	2.896212	-4.854293	3.108356
C	4.667025	2.958858	-1.453745
C	5.986105	2.527005	0.515939
C	5.541673	3.972037	-1.845860
C	6.878971	3.528797	0.155845
H	6.129906	1.951215	1.424252
H	5.352286	4.521273	-2.761921
C	6.635867	4.244444	-1.039398
C	8.082415	3.857124	1.005362
H	7.325104	5.030948	-1.335428
H	9.012939	3.722030	0.441347
H	8.057017	4.900882	1.340281
H	8.131277	3.220195	1.892678
H	3.258985	-0.907684	1.071167
Cu	-0.007289	-2.259276	-0.190759
Cl	-0.210805	-2.133824	1.911883
O	0.196107	-2.384619	-2.292030
H	1.001171	-2.921290	-2.404752
H	-0.491222	-2.880994	-2.767420

HF=-4640.8930921

xyz coordinates of Isomer 4 for Cu(II) complex

C	-4.489454	-0.654956	1.517845
C	-6.174667	0.915487	1.150842
C	-5.294275	1.730007	0.430043
C	-3.528207	0.026906	0.811602
H	-8.157443	0.609867	1.922519

H	-4.297143	-1.608206	1.999122
C	-7.507524	1.270579	1.358905
C	-5.785602	2.943974	-0.089139
C	-7.106831	3.329633	0.098372
C	-7.958207	2.470178	0.830979
H	-5.095115	3.571755	-0.642599
H	-8.994961	2.757181	0.985955
C	-7.637627	4.627776	-0.459491
H	-8.451582	4.448297	-1.172034
H	-8.040755	5.264990	0.336441
H	-6.855364	5.189921	-0.976786
C	-3.899996	1.323124	0.222373
O	-3.112577	2.065585	-0.398349
O	-5.749200	-0.275078	1.692631
C	-2.226834	-0.663739	0.813278
H	-2.130054	-1.397442	1.606061
N	-1.201871	-0.679460	0.014079
N	-1.272901	0.273373	-1.013293
H	-1.866297	1.110290	-0.835261
C	-0.802745	-0.011050	-2.242929
S	-0.016350	-1.472537	-2.584827
N	-1.037946	0.959397	-3.168022
H	-1.737443	1.663057	-2.940462
N	-0.678006	0.752475	-4.501527
H	-1.489165	0.480756	-5.055341
H	-0.280002	1.609331	-4.875506
N	1.520528	-1.035479	-0.109545
S	-0.150044	-2.767211	1.459606
C	2.439507	-0.550943	-0.883970
N	1.691671	-0.877263	1.249618
C	0.964694	-1.649823	2.082633
C	3.709624	0.167828	-0.687051
H	2.207488	-0.738964	-1.928556
N	1.203688	-1.443999	3.399052
C	4.429172	0.289766	-1.852361
C	4.275168	0.774541	0.532667
H	1.949200	-0.804386	3.664795
N	0.555083	-2.206677	4.369985
H	4.080656	-0.107658	-2.800212
O	5.609119	0.879240	-1.988001
C	5.579004	1.426003	0.362275
O	3.718027	0.770403	1.646427
H	1.216068	-2.827697	4.832630
H	0.125488	-1.591619	5.056187
C	6.206282	1.453389	-0.888069
C	6.234547	2.038734	1.448282
C	7.446738	2.060274	-1.080586
C	7.471204	2.653128	1.294107

H	5.740958	2.016026	2.414134
H	7.898736	2.059278	-2.066618
C	8.064521	2.651773	0.010504
C	8.177644	3.308339	2.455613
H	9.031671	3.128156	-0.126576
H	9.145534	2.830817	2.649328
H	8.375516	4.367171	2.251544
H	7.583157	3.247105	3.371152
H	2.424116	-0.208514	1.573601
O	1.096284	-3.656696	-1.120767
H	1.507504	-4.177157	-0.408573
H	0.413943	-4.252453	-1.492812
Cu	-0.083880	-2.126985	-0.539495
Cl	-1.922449	-3.363007	-1.026561

HF=-4640.9213657

xyz coordinates of Isomer 5 for Cu(II) complex

C	-4.510352	-1.820146	-1.429948
C	-6.767405	-1.604720	-0.881680
C	-6.539896	-0.333251	-0.343986
C	-4.136752	-0.595222	-0.926394
H	-8.169387	-3.173358	-1.322436
H	-3.803008	-2.503363	-1.888267
C	-8.035796	-2.185163	-0.895551
C	-7.637805	0.367734	0.193538
C	-8.914332	-0.179481	0.197744
C	-9.092523	-1.468471	-0.356536
H	-7.453286	1.353989	0.606214
H	-10.085352	-1.910726	-0.361398
C	-10.092203	0.567573	0.774256
H	-10.868974	0.726633	0.016871
H	-10.552918	0.006169	1.595737
H	-9.794232	1.545994	1.160755
C	-5.194341	0.249547	-0.344026
O	-5.008889	1.394190	0.115864
O	-5.735419	-2.332628	-1.425042
C	-2.702899	-0.326143	-1.123846
H	-2.213837	-1.056300	-1.757456
N	-1.835150	0.520599	-0.636984
N	-2.379909	1.519792	0.165020
H	-3.421915	1.593922	0.209832
C	-1.571526	2.413220	0.757589
S	0.105988	2.244775	0.637985
N	-2.200526	3.404148	1.433616
H	-3.216026	3.383791	1.490240
N	-1.471247	4.338751	2.166673

H	-1.718016	5.278799	1.867902
H	-1.659523	4.231258	3.161139
N	1.907019	0.081471	-0.106193
S	-0.367078	-0.653226	1.456136
C	2.883468	0.568957	-0.808886
N	2.209156	-0.735793	0.945562
C	1.196739	-1.181322	1.733353
C	4.353106	0.465710	-0.772240
H	2.513370	1.211976	-1.600199
H	3.190475	-1.074344	1.025759
N	1.588871	-2.037567	2.708111
C	4.969614	1.325493	-1.647327
C	5.214675	-0.431753	0.021562
O	4.797017	-1.278278	0.831916
H	2.549681	-2.371372	2.699495
N	0.658594	-2.610347	3.573542
H	4.416621	2.008172	-2.284064
O	6.277769	1.452603	-1.841323
C	6.657363	-0.280764	-0.207544
H	0.564701	-3.605573	3.380794
H	0.958638	-2.471768	4.534962
C	7.142122	0.655739	-1.126503
C	7.590549	-1.073088	0.489293
C	8.506688	0.821789	-1.362660
C	8.957007	-0.935375	0.279982
H	7.205595	-1.798598	1.198086
H	8.841160	1.559209	-2.084437
C	9.397171	0.026597	-0.658292
C	9.959342	-1.781919	1.026184
H	10.462968	0.146668	-0.834215
H	10.574210	-2.369278	0.333997
H	10.642555	-1.158707	1.615371
H	9.464432	-2.477348	1.709447
O	0.423677	1.219058	-2.130062
H	-0.151632	1.961272	-2.378998
H	0.292858	0.524489	-2.803584
Cu	0.035940	0.301004	-0.371660
Cl	-0.035116	-1.667981	-1.394358

HF=-4640.920911

xyz coordinates of Isomer 1 for Cd(II) complex

C	5.098543	-2.103070	0.173436
C	7.340364	-1.460901	0.181318
C	6.974929	-0.115565	0.076080
C	4.593853	-0.833362	0.070159

H	8.921074	-2.911229	0.321003
H	4.464242	-2.981622	0.219646
C	8.679450	-1.856729	0.239455
C	7.998371	0.851166	0.029465
C	9.338992	0.492674	0.084685
C	9.661076	-0.880021	0.190376
H	7.700140	1.891379	-0.051831
H	10.705623	-1.178586	0.234598
C	10.436360	1.529365	0.033969
H	11.058519	1.495317	0.936834
H	11.101311	1.363288	-0.822524
H	10.025361	2.539352	-0.051617
C	5.557089	0.280362	0.014096
O	5.254642	1.481475	-0.080923
O	6.390516	-2.446910	0.230776
C	3.118171	-0.793153	0.017670
H	2.668154	-1.783220	0.036179
N	2.221891	0.130769	-0.038039
N	2.551922	1.446466	-0.064294
H	3.557943	1.672006	-0.037180
C	1.623800	2.470555	-0.104083
S	-0.039231	2.314578	-0.045215
N	2.283201	3.678390	-0.195353
H	3.236216	3.645736	-0.550084
N	1.564379	4.862839	-0.351691
H	2.012563	5.593564	0.192692
H	1.520430	5.135562	-1.332748
N	-2.206199	-0.147190	-0.031060
S	0.024405	-2.364721	-0.023688
C	-3.096666	0.783230	0.023433
N	-2.553089	-1.459426	-0.055866
C	-1.639945	-2.496605	-0.090082
C	-4.571946	0.835064	0.075871
H	-2.641064	1.770437	0.042524
H	-3.562152	-1.671347	-0.035538
N	-2.316829	-3.694669	-0.181404
C	-5.064803	2.108992	0.186306
C	-5.546062	-0.268919	0.012338
O	-5.255390	-1.472374	-0.089764
H	-3.269130	-3.649007	-0.536530
N	-1.615580	-4.890143	-0.332542
H	-4.422208	2.981196	0.237976
O	-6.353303	2.464818	0.245067
C	-6.960045	0.140336	0.075362
H	-2.074925	-5.612306	0.213951
H	-1.574394	-5.167004	-1.312530
C	-7.312668	1.488391	0.188771
C	-7.992678	-0.816204	0.021614

C	-8.647879	1.896792	0.248388
C	-9.329829	-0.445129	0.077996
H	-7.704440	-1.858697	-0.066190
H	-8.879383	2.953033	0.336449
C	-9.638800	0.929893	0.192270
C	-10.437127	-1.470798	0.019543
H	-10.680476	1.238170	0.237502
H	-11.059648	-1.436757	0.922159
H	-11.099715	-1.292509	-0.836314
H	-10.035869	-2.484117	-0.072516
Cl	-0.010423	-0.019214	-2.207000
Cl	-0.004851	0.000793	2.125450
Cd	-0.007629	-0.009181	-0.034525

HF=-3432.53667

xyz coordinates of Isomer 2 for Cd(II) complex

C	-2.434773	2.762033	0.784822
C	-4.505257	3.821550	0.600727
C	-5.063650	2.673315	0.031005
C	-2.847033	1.567935	0.256681
H	-4.789964	5.848517	1.258744
H	-1.416605	2.934100	1.117011
C	-5.260401	4.977625	0.814556
C	-6.424247	2.702692	-0.331232
C	-7.204474	3.834371	-0.130957
C	-6.597069	4.972042	0.448387
H	-6.843287	1.804615	-0.773531
H	-7.192795	5.866823	0.611371
C	-8.665030	3.864173	-0.514472
H	-9.302173	4.044390	0.360168
H	-8.871285	4.665399	-1.234619
H	-8.976712	2.918240	-0.966381
C	-4.249081	1.464817	-0.187490
O	-4.750249	0.463637	-0.721698
O	-3.184603	3.855370	0.969230
C	-1.779321	0.552756	0.168488
H	-0.785216	0.951289	0.363531
N	-1.738422	-0.717551	-0.054026
N	-2.865202	-1.438989	-0.300722
H	-3.726640	-0.906914	-0.492876
C	-2.834638	-2.805633	-0.565570
S	-1.567815	-3.842168	-0.211303
N	-3.986016	-3.171544	-1.219777
H	-4.339676	-2.480021	-1.880037
N	-4.170571	-4.523778	-1.542915

H	-5.160382	-4.670990	-1.715448
H	-3.631528	-4.768675	-2.374625
N	1.399919	-0.399991	0.030476
S	-0.114784	-2.212370	2.016197
C	2.102798	0.124319	-0.914205
N	1.780996	-0.366505	1.347331
C	1.230145	-1.231107	2.279637
C	3.413484	0.792515	-0.998071
H	1.622774	-0.056440	-1.876058
N	2.004168	-1.264950	3.415910
C	3.821223	1.018225	-2.287329
C	4.310185	1.216229	0.089537
H	3.005382	-1.164458	3.249446
N	1.615143	-2.116810	4.461835
H	3.228155	0.724667	-3.146618
O	4.965507	1.596073	-2.668641
C	5.562962	1.856382	-0.348417
O	4.076159	1.074369	1.301385
H	1.896276	-3.077802	4.261571
H	2.072206	-1.794952	5.309787
C	5.846791	2.019626	-1.707897
C	6.509093	2.312855	0.589661
C	7.032568	2.616699	-2.144321
C	7.697639	2.910456	0.190396
H	6.275690	2.178153	1.640938
H	7.216549	2.722480	-3.208263
C	7.942194	3.054119	-1.194747
C	8.714178	3.395965	1.196563
H	8.868196	3.518326	-1.525134
H	9.673809	2.878993	1.073236
H	8.908811	4.469247	1.080502
H	8.371734	3.225758	2.221309
H	2.651170	0.141972	1.567899
Cl	-0.021515	-1.991825	-2.245266
Cl	1.576903	-3.471011	-0.123941
Cd	-0.069143	-2.103967	-0.089317

HF=-3432.4547438

xyz coordinates of Isomer 3 for Cd(II) complex

C	3.189907	1.422953	-2.159895
C	5.175246	2.549232	-1.663744
C	5.020117	2.283524	-0.298688
C	2.939665	1.064754	-0.866359
H	6.356466	3.452945	-3.215893
H	2.539731	1.148823	-2.984470
C	6.270046	3.267744	-2.150389

C	5.998977	2.763462	0.591056
C	7.100494	3.480637	0.140199
C	7.217832	3.723698	-1.247189
H	5.861651	2.549801	1.646431
H	8.073618	4.282628	-1.617778
C	8.153878	3.992235	1.094127
H	9.141306	3.578679	0.855042
H	8.240556	5.084575	1.042790
H	7.918895	3.722556	2.127696
C	3.857336	1.519056	0.189051
O	3.679141	1.315499	1.398571
O	4.248892	2.120033	-2.584621
C	1.694957	0.308872	-0.650207
H	0.873785	0.541673	-1.324165
N	1.426841	-0.669966	0.150549
N	2.449776	-1.081229	0.997662
H	2.916857	-0.338329	1.528875
C	2.378768	-2.394031	1.367510
S	1.525116	-3.414371	0.354009
N	2.980261	-2.682508	2.558601
H	2.811249	-1.954940	3.253892
N	2.866617	-4.009760	3.018436
H	3.528153	-4.124592	3.780724
H	1.915622	-4.165441	3.359269
N	-1.419774	-0.669384	-0.375765
S	-1.597344	-3.349144	-0.227812
C	-1.582344	0.420146	0.309668
N	-2.523587	-1.112442	-1.081385
C	-2.619917	-2.460064	-1.187833
C	-2.770374	1.248107	0.580587
H	-0.697552	0.697108	0.874882
N	-3.486640	-2.906511	-2.153433
C	-2.811396	1.779137	1.840062
C	-3.839323	1.589316	-0.367117
H	-3.473693	-2.331516	-2.995922
N	-3.575832	-4.297105	-2.338314
H	-2.055039	1.569589	2.589607
O	-3.770465	2.578182	2.319157
C	-4.877772	2.484204	0.173515
O	-3.884180	1.190474	-1.542079
H	-4.450622	-4.493577	-2.814673
H	-2.790252	-4.633158	-2.896323
C	-4.808405	2.938680	1.495153
C	-5.964559	2.898436	-0.619461
C	-5.785595	3.780326	2.032805
C	-6.952626	3.735353	-0.115997
H	-6.003117	2.536583	-1.642087
H	-5.698072	4.110120	3.062658

C	-6.843073	4.168458	1.225127
C	-8.121747	4.176701	-0.964450
H	-7.608182	4.822786	1.635741
H	-9.073616	3.839761	-0.535653
H	-8.170201	5.270077	-1.037895
H	-8.050902	3.774887	-1.979243
H	-3.122627	-0.405392	-1.526664
Cl	0.209231	-2.200374	-2.120849
Cd	-0.031617	-1.962671	-0.031881
Cl	-0.305821	-1.693035	2.337109

HF=-3432.3534938

xyz coordinates of Isomer 4 for Cd(II) complex

C	-2.786430	1.896315	1.962974
C	-4.694913	3.129047	1.429958
C	-4.990383	2.256417	0.378717
C	-2.924654	0.989933	0.944885
H	-5.245232	4.877968	2.552892
H	-1.973097	1.850679	2.679632
C	-5.507316	4.225851	1.726389
C	-6.144317	2.503627	-0.388865
C	-6.973868	3.586286	-0.123249
C	-6.634084	4.443009	0.948533
H	-6.363461	1.814666	-1.198255
H	-7.273413	5.293716	1.171116
C	-8.211795	3.852386	-0.946585
H	-9.116311	3.814168	-0.327140
H	-8.177545	4.847432	-1.406826
H	-8.323234	3.115624	-1.747176
C	-4.119652	1.102490	0.086781
O	-4.423638	0.298788	-0.806151
O	-3.590603	2.931349	2.222540
C	-1.875245	-0.046323	0.940283
H	-1.363004	-0.151586	1.891506
N	-1.400921	-0.863981	0.049864
N	-1.973066	-0.769425	-1.223389
H	-2.965360	-0.491499	-1.246287
C	-1.482368	-1.587936	-2.225196
S	0.074543	-2.193522	-2.149601
N	-2.446362	-1.931371	-3.135647
H	-3.340123	-2.153756	-2.694036
N	-2.049866	-2.779121	-4.190043
H	-1.904256	-3.724355	-3.828344
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N	1.345290	-0.767358	0.093340
S	-0.137479	-2.199724	2.093734
C	1.819766	0.034860	-0.808779
N	1.939227	-0.763349	1.338951
C	1.409757	-1.606713	2.289746
C	2.931092	1.001871	-0.870997
H	1.260986	-0.043639	-1.737492
N	2.317314	-1.967631	3.248668
C	2.854779	1.843542	-1.950056
C	4.115158	1.116224	0.001723
H	3.251671	-2.139107	2.874376
N	1.872457	-2.847664	4.254659
H	2.046185	1.795659	-2.671732
O	3.721521	2.808490	-2.271545
C	5.057915	2.189691	-0.363062
O	4.356578	0.377892	0.968142
H	1.774729	-3.789336	3.869692
H	2.575053	-2.849873	4.988353
C	4.827992	2.996676	-1.481130
C	6.217273	2.423643	0.400956
C	5.710127	4.016200	-1.846714
C	7.115571	3.429537	0.066764
H	6.385069	1.786096	1.262985
H	5.497330	4.618637	-2.723538
C	6.840420	4.221928	-1.071169
C	8.359737	3.680660	0.885342
H	7.533914	5.012173	-1.347888
H	9.265679	3.549738	0.280892
H	8.378513	4.705025	1.277176
H	8.422357	2.994847	1.735019
H	2.920971	-0.449049	1.388303
Cl	-1.614023	-3.818937	-0.114393
Cd	-0.032108	-2.197586	-0.003136
Cl	1.546907	-3.735087	-0.062744

HF=-3432.3501245

xyz coordinates of Isomer 5 for Cd(II) complex

C	-4.442194	-2.129339	1.069154
C	-6.741394	-1.991027	0.704717
C	-6.574719	-0.809591	-0.023023
C	-4.127690	-0.972697	0.399881
H	-8.087591	-3.477537	1.478488
H	-3.687478	-2.754116	1.534164
C	-8.001950	-2.558090	0.909032

C	-7.720602	-0.189657	-0.557805
C	-8.988872	-0.725482	-0.373498
C	-9.108844	-1.921812	0.369964
H	-7.576608	0.726038	-1.122076
H	-10.094052	-2.355595	0.522651
C	-10.217662	-0.059464	-0.946373
H	-10.750102	-0.729358	-1.632697
H	-10.924463	0.220217	-0.155353
H	-9.956839	0.847886	-1.498649
C	-5.235193	-0.229400	-0.227908
O	-5.110157	0.808452	-0.899208
O	-5.663012	-2.643799	1.243799
C	-2.675051	-0.714258	0.406064
H	-2.085473	-1.529409	0.820596
N	-1.892323	0.244941	0.014995
N	-2.498477	1.355672	-0.539304
H	-3.505186	1.298053	-0.761106
C	-1.721641	2.389451	-0.976188
S	-0.090123	2.400461	-0.673686
N	-2.443467	3.322893	-1.680374
H	-3.282544	2.968748	-2.137095
N	-1.771448	4.389814	-2.286456
H	-1.475830	4.141584	-3.230455
H	-2.399822	5.186681	-2.319263
N	1.909835	0.374375	-0.063378
S	-0.001748	0.916014	1.987281
C	2.741889	-0.144436	-0.913248
N	2.461392	0.819236	1.128837
C	1.632030	1.150114	2.158874
C	4.172532	-0.505436	-0.893321
H	2.216214	-0.450767	-1.814046
H	3.486063	0.938416	1.170813
N	2.307495	1.662716	3.239073
C	4.491150	-1.396680	-1.886886
C	5.264263	-0.031571	-0.027020
O	5.139309	0.805235	0.884826
H	3.317056	1.531558	3.246384
N	1.649323	1.851269	4.454245
H	3.751901	-1.780484	-2.581454
O	5.698185	-1.913952	-2.134603
C	6.588607	-0.609283	-0.315699
H	1.875644	1.104940	5.109618
H	1.920468	2.748906	4.844195
C	6.757046	-1.531799	-1.352546
C	7.717527	-0.249887	0.445831
C	8.002616	-2.096530	-1.639536
C	8.970028	-0.792150	0.188122
H	7.573000	0.469342	1.245534

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H        8.090528   -2.808879   -2.453057
C        9.092109   -1.723140   -0.868834
C       10.179304   -0.409662    1.008554
H       10.065265   -2.157389   -1.084541
H       10.594521   -1.278384    1.534483
H       10.977978   -0.003607    0.375877
H        9.927915    0.346456    1.757861
Cl       0.109041   -1.808100    0.633678
Cl       0.019743   -0.322378   -2.121185
Cd       0.008738    0.309756   -0.024220

HF=-3432.335477
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