Supporting Information

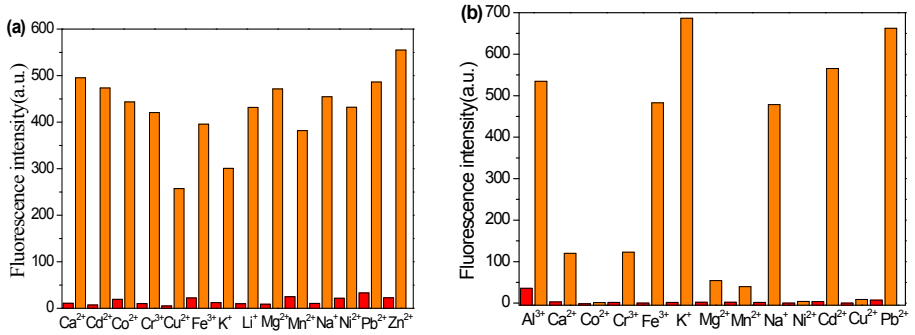
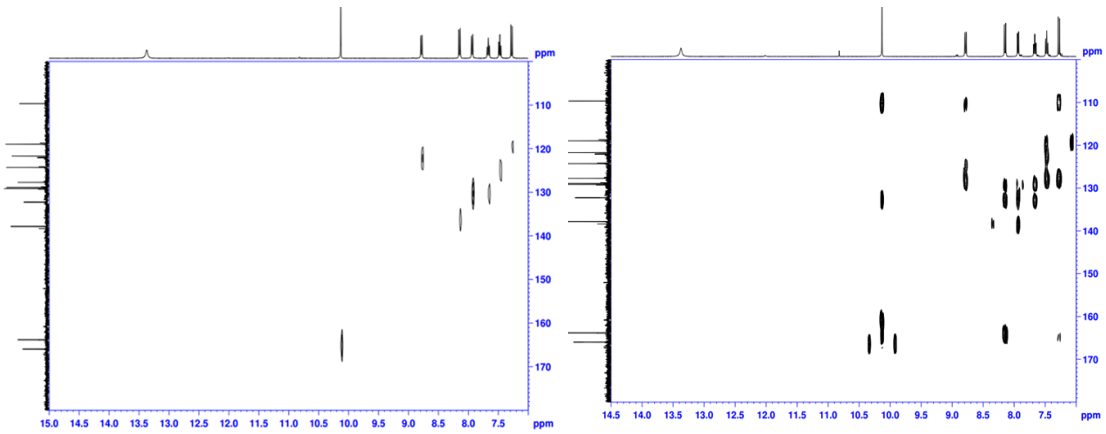
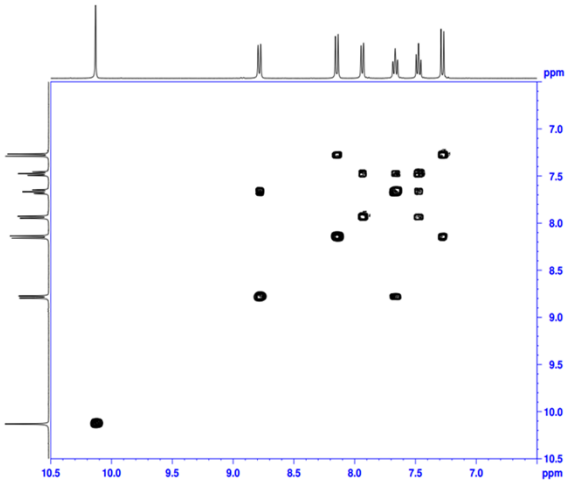


Fig. S1 (a) Fluorescence intensity of complexes of H_2L and Al^{3+} in the presence of various metal ions at 470 nm. Red bars: H_2L (20 μM) with 1.0 equiv of the metal ions stated. Orange bars: Solutions of H_2L (20 μM) with 1.0 equiv of Al^{3+} and 1.0 equiv of the other metal ions stated. (b) Fluorescence intensity of complexes of H_2L and Zn^{2+} in the presence of various metal ions at 480nm. Red bars: H_2L (20 μM) with 1.0 equiv of the metal ions stated. Orange bars: Solutions of H_2L (20 μM) with 1.0 equiv of Zn^{2+} and 1.0 equiv of the other metal ions stated.



(a) (b)



(c)

Fig. S2 The ^{1}HSQC (a), ^{1}HMBC (b), and H-H COSY(c) spectra of H_2L in DMSO-d_6.

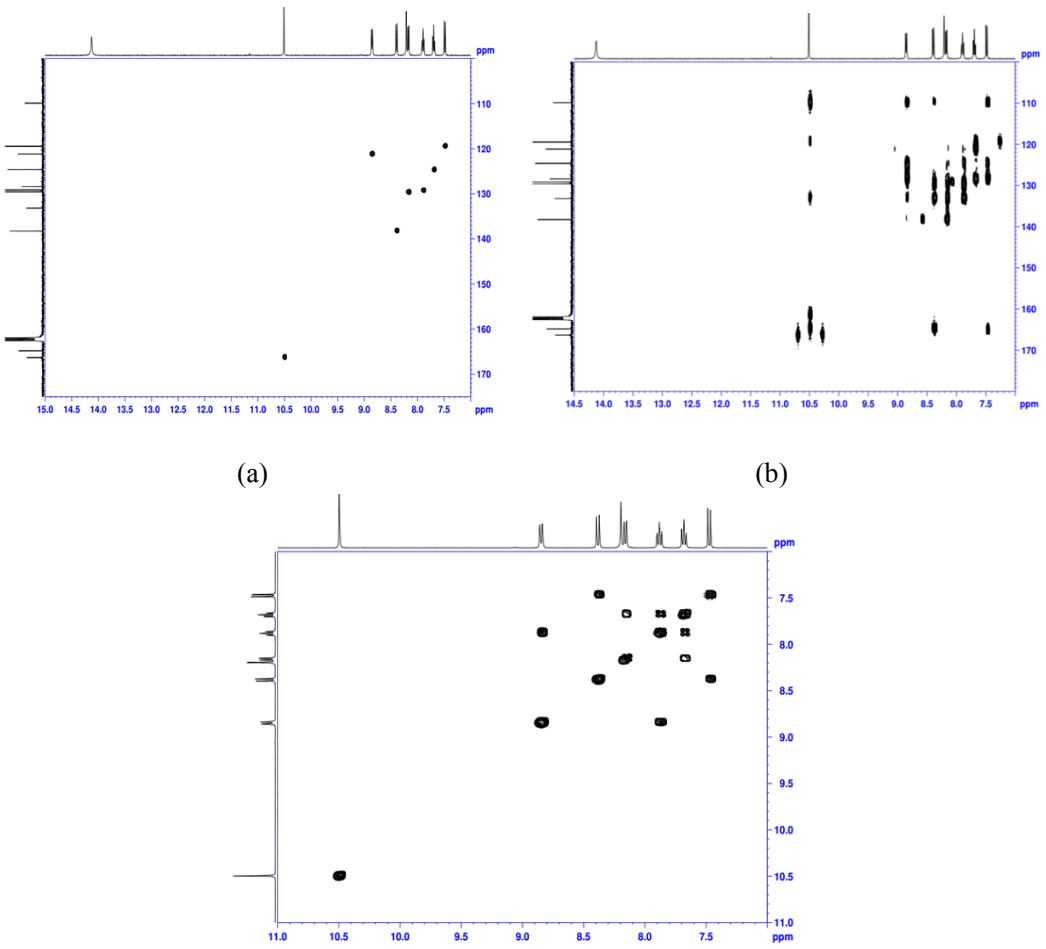


Fig. S3 The ^{1}HSQC (a), ^{1}HMBC (b), and H-H COSY(c) spectra of H_2L in DMF-d_7.

Table S1. Optimized Cartesian Coordinate of the stationary points in DMSO solvent at the (TD-)B3LYP/6-311G level of theory.**

S_0-a

Center Number	Atomic Number	Coordinates(Angstroms) X	Y	Z
1	6	4.234014	-1.835715	0.015136
2	6	4.254961	-0.460164	-0.015212
3	6	3.051055	0.284305	-0.016673
4	6	1.791006	-0.388418	0.011715
5	6	1.807041	-1.804658	0.042321
6	6	2.995942	-2.505808	0.044062
7	1	4.047542	2.202764	-0.070128
8	1	5.158831	-2.400987	0.017166
9	1	5.195667	0.079695	-0.037591
10	6	3.082188	1.708373	-0.046012
11	6	0.573537	0.403234	0.010544
12	1	0.882032	-2.365161	0.066520
13	1	2.972594	-3.589766	0.068561
14	6	0.673173	1.815633	-0.012206
15	6	1.937898	2.452629	-0.042881
16	1	1.963716	3.535437	-0.063301
17	6	-0.715332	-0.218062	0.021618
18	1	-0.775630	-1.303731	0.017598
19	7	-3.320550	-1.445095	-0.122296
20	7	-4.669761	-1.529483	-0.086174
21	7	-5.210664	-0.363379	0.058107
22	7	-4.195260	0.511532	0.119482
23	1	-4.359452	1.505907	0.233387
24	7	-1.818750	0.483551	0.033020
25	6	-3.028513	-0.155977	0.007845
26	8	-0.394952	2.610639	-0.009480
27	1	-1.205052	2.025597	0.011571

S_0-b

Center Number	Atomic Number	Coordinates(Angstroms) X	Y	Z
1	6	-4.252511	-1.832760	0.043363
2	6	-4.258733	-0.449811	0.060296
3	6	-3.054770	0.279561	0.027014

4	6	-1.807374	-0.398914	-0.023267
5	6	-1.830738	-1.807597	-0.043664
6	6	-3.026658	-2.508599	-0.010161
7	1	-4.054418	2.203343	0.086332
8	1	-5.183202	-2.387624	0.070880
9	1	-5.195380	0.096304	0.101023
10	6	-3.082118	1.721425	0.046949
11	6	-0.572047	0.396344	-0.047002
12	1	-0.908810	-2.373618	-0.086231
13	1	-3.006714	-3.592818	-0.025420
14	6	-0.639691	1.867497	-0.030510
15	6	-1.957890	2.472510	0.018998
16	1	-1.995402	3.555709	0.033806
17	6	0.662741	-0.217200	-0.061140
18	1	0.766284	-1.294226	-0.057894
19	7	3.320364	-1.427743	-0.055179
20	7	4.671164	-1.527863	0.023222
21	7	5.227149	-0.369728	0.099765
22	7	4.223379	0.532896	0.074147
23	1	4.407892	1.529379	0.121412
24	7	1.829500	0.465521	-0.068140
25	6	3.058622	-0.131067	-0.025846
26	8	0.385376	2.589249	-0.051459
27	1	1.717578	1.494469	-0.061168

S_0-c

Center Number	Atomic Number	Coordinates(Angstroms) X	Y	Z
1	6	-4.209708	-1.292857	-0.555788
2	6	-3.947178	0.055592	-0.639802
3	6	-2.676818	0.572114	-0.286058
4	6	-1.649975	-0.312392	0.163249
5	6	-1.947531	-1.699117	0.216426
6	6	-3.197031	-2.173391	-0.124453
7	1	-3.179355	2.639086	-0.690996
8	1	-5.184673	-1.680459	-0.828469
9	1	-4.710107	0.747054	-0.981934
10	6	-2.395970	1.963596	-0.364225
11	6	-0.349217	0.211284	0.518983
12	1	-1.179587	-2.406445	0.505965
13	1	-3.397208	-3.237950	-0.072817

14	6	-0.112556	1.585628	0.384010
15	6	-1.159963	2.446737	-0.046354
16	1	-0.934667	3.504746	-0.108828
17	6	0.525671	-0.717386	1.259602
18	1	-0.007106	-1.244806	2.052105
19	7	2.832174	0.558363	-0.301722
20	7	3.922251	0.480378	-1.098163
21	7	4.411560	-0.712211	-1.074438
22	7	3.645154	-1.422501	-0.234208
23	1	3.831749	-2.401666	-0.043364
24	7	1.758186	-1.082098	1.167109
25	6	2.655630	-0.638947	0.240067
26	8	1.034299	2.203992	0.725058
27	1	1.810857	1.689403	0.375682

S_0-a'

Center Number	Atomic Number	Coordinates(Angstroms) X	Y	Z
1	6	4.213555	-1.860477	-0.023933
2	6	4.245353	-0.485250	0.011705
3	6	3.047690	0.268938	0.016529
4	6	1.781837	-0.392909	-0.014031
5	6	1.786971	-1.809206	-0.050712
6	6	2.970140	-2.520126	-0.055542
7	1	4.061286	2.178229	0.077748
8	1	5.133807	-2.433111	-0.027676
9	1	5.190302	0.047031	0.036541
10	6	3.091515	1.692600	0.053252
11	6	0.571260	0.409279	-0.005673
12	1	0.858190	-2.363603	-0.076082
13	1	2.937840	-3.603752	-0.083846
14	6	0.683025	1.821368	0.027821
15	6	1.954017	2.446599	0.057288
16	1	1.989057	3.529024	0.083380
17	6	-0.725257	-0.198226	-0.021656
18	1	-0.781697	-1.284496	-0.048319
19	7	-4.180842	0.673511	-0.128832
20	7	-5.201661	-0.205534	-0.036382
21	7	-4.770199	-1.407989	0.159317
22	7	-3.429317	-1.323712	0.193218
23	1	-2.868353	-2.152015	0.356915

24	7	-1.815085	0.521422	-0.010899
25	6	-3.063857	-0.032843	0.013115
26	8	-0.376803	2.625880	0.033640
27	1	-1.193204	2.045284	0.012786

TSab-S_0

Center Number	Atomic Number	Coordinates(Angstroms) X	Y	Z
1	6	4.360598	-1.687847	0.006807
2	6	4.293577	-0.310063	-0.032979
3	6	3.047594	0.353817	-0.026422
4	6	1.838866	-0.397899	0.017542
5	6	1.938502	-1.805305	0.061535
6	6	3.171077	-2.433725	0.055627
7	1	3.921426	2.333849	-0.098806
8	1	5.319966	-2.192201	0.002408
9	1	5.199341	0.286213	-0.068501
10	6	2.984798	1.786377	-0.061837
11	6	0.572382	0.319789	0.021099
12	1	1.045372	-2.415740	0.105080
13	1	3.215926	-3.516730	0.090616
14	6	0.558740	1.764113	-0.000605
15	6	1.807011	2.465804	-0.047591
16	1	1.773541	3.548571	-0.071611
17	6	-0.664813	-0.339414	0.029442
18	1	-0.740535	-1.421472	0.015820
19	7	-3.367075	-1.454886	-0.145426
20	7	-4.721287	-1.483980	-0.121431
21	7	-5.216380	-0.302656	0.034044
22	7	-4.165945	0.534508	0.119920
23	1	-4.294548	1.532134	0.250491
24	7	-1.785708	0.376762	0.048459
25	6	-3.030504	-0.181606	0.006087
26	8	-0.547279	2.426084	0.014492
27	1	-1.438939	1.536680	0.042912

TSaa-S_0

Center Number	Atomic Number	Coordinates(Angstroms) X	Y	Z

1	6	4.227648	-1.869531	0.007540
2	6	4.257229	-0.494414	0.027840
3	6	3.058217	0.258604	0.015765
4	6	1.793017	-0.405842	-0.017073
5	6	1.801082	-1.823558	-0.038799
6	6	2.984995	-2.531841	-0.026513
7	1	4.067086	2.170551	0.061729
8	1	5.148654	-2.440940	0.017266
9	1	5.201281	0.039455	0.053590
10	6	3.098786	1.682018	0.036927
11	6	0.583410	0.394192	-0.025981
12	1	0.873543	-2.379816	-0.066095
13	1	2.954876	-3.615807	-0.043237
14	6	0.690537	1.802045	-0.004821
15	6	1.958903	2.432659	0.026114
16	1	1.990619	3.515438	0.040761
17	6	-0.715981	-0.222085	-0.053528
18	1	-0.769073	-1.307827	-0.072909
19	7	-3.831913	-0.321314	-1.130876
20	7	-5.007951	-0.786886	-0.637334
21	7	-4.987240	-0.848387	0.650228
22	7	-3.768607	-0.418834	1.023628
23	1	-3.502168	-0.365589	2.000730
24	7	-1.809355	0.478830	-0.057098
25	6	-3.059568	-0.099358	-0.077607
26	8	-0.373344	2.606870	-0.012089
27	1	-1.186739	2.031269	-0.033155

TSac-S_0

Center Number	Atomic Number	Coordinates(Angstroms) X	Y	Z
1	6	4.655934	-1.144483	0.148249
2	6	4.317835	0.184741	0.251210
3	6	2.969064	0.601283	0.138239
4	6	1.937437	-0.360243	-0.091556
5	6	2.320247	-1.724432	-0.168106
6	6	3.642707	-2.101086	-0.059651
7	1	3.407286	2.697138	0.441898
8	1	5.689682	-1.458637	0.235005
9	1	5.078391	0.938575	0.424768

10	6	2.618686	1.973583	0.265689
11	6	0.563516	0.087837	-0.203567
12	1	1.575412	-2.498044	-0.298130
13	1	3.902425	-3.151902	-0.125842
14	6	0.281391	1.457259	-0.064801
15	6	1.321861	2.389163	0.169688
16	1	1.055042	3.435259	0.258415
17	6	-0.474416	-0.877404	-0.528125
18	1	-0.132139	-1.805704	-0.992140
19	7	-3.733811	0.475241	-0.620924
20	7	-4.971734	0.315905	-0.096229
21	7	-5.025253	-0.675727	0.718117
22	7	-3.789235	-1.234263	0.717880
23	1	-3.570454	-2.038898	1.292133
24	7	-1.720844	-0.734323	-0.347664
25	6	-2.983846	-0.515499	-0.105248
26	8	-0.939124	2.011850	-0.182201
27	1	-1.615177	1.362844	-0.427817

S_1-a

Center Number	Atomic Number	Coordinates(Angstroms) X	Y	Z
1	6	4.196056	-1.890386	0.035165
2	6	4.231557	-0.489489	0.037344
3	6	3.057269	0.278248	0.007019
4	6	1.787799	-0.392478	-0.025624
5	6	1.788872	-1.814125	-0.031562
6	6	2.971603	-2.550789	-0.000963
7	1	4.081421	2.187416	0.037592
8	1	5.123066	-2.450489	0.061252
9	1	5.187412	0.022005	0.064787
10	6	3.114658	1.698612	0.012903
11	6	0.568461	0.372716	-0.044761
12	1	0.854373	-2.356385	-0.060113
13	1	2.928996	-3.632924	-0.004583
14	6	0.698095	1.830082	-0.039252
15	6	1.949114	2.445875	-0.011277
16	1	1.978568	3.529293	-0.007653
17	6	-0.712745	-0.248918	-0.054428

18	1	-0.796129	-1.328823	-0.058950
19	7	-3.344019	-1.410681	-0.034265
20	7	-4.684283	-1.482528	0.023669
21	7	-5.227577	-0.304608	0.085412
22	7	-4.213445	0.575768	0.067494
23	1	-4.383400	1.573665	0.106271
24	7	-1.834621	0.496958	-0.036709
25	6	-3.031420	-0.097680	-0.011868
26	8	-0.383762	2.605320	-0.060369
27	1	-1.189685	1.997762	-0.055791

S_1-b

Center Number	Atomic Number	Coordinates(Angstroms) X	Y	Z
1	6	-4.252600	-1.815206	0.019799
2	6	-4.273012	-0.428171	0.077044
3	6	-3.089801	0.322536	0.050677
4	6	-1.813026	-0.374978	-0.005714
5	6	-1.841790	-1.808278	-0.096093
6	6	-3.023870	-2.506030	-0.080230
7	1	-4.076824	2.246169	0.110931
8	1	-5.183435	-2.369978	0.040814
9	1	-5.220366	0.096532	0.136511
10	6	-3.116155	1.745189	0.068166
11	6	-0.599063	0.362439	0.027591
12	1	-0.915371	-2.358741	-0.187597
13	1	-3.016494	-3.587246	-0.147657
14	6	-0.659451	1.844853	-0.015555
15	6	-1.949839	2.467595	0.014671
16	1	-1.958192	3.551976	0.018189
17	6	0.660546	-0.299641	0.094279
18	1	0.755764	-1.351089	0.319402
19	7	3.383268	-1.421811	0.221778
20	7	4.733795	-1.461955	0.215827
21	7	5.247721	-0.293693	0.019400
22	7	4.210649	0.557400	-0.115921
23	1	4.357702	1.547493	-0.278242
24	7	1.819689	0.385041	-0.079668
25	6	3.060706	-0.144548	0.013227
26	8	0.399957	2.536135	-0.072717
27	1	1.670003	1.413241	-0.186548

S_1-c

Center Number	Atomic Number	Coordinates(Angstroms) X	Y	Z
1	6	4.503822	-1.158416	0.180972
2	6	4.163257	0.180497	-0.013978
3	6	2.824063	0.594844	-0.028523
4	6	1.790892	-0.386804	0.092017
5	6	2.166811	-1.724839	0.325654
6	6	3.504981	-2.109712	0.377683
7	1	3.248612	2.722224	-0.239863
8	1	5.547610	-1.451397	0.195000
9	1	4.941743	0.924257	-0.144845
10	6	2.468468	1.980549	-0.121873
11	6	0.378342	0.001512	-0.040977
12	1	1.405037	-2.475935	0.491160
13	1	3.759670	-3.145455	0.567251
14	6	0.117265	1.437410	0.229916
15	6	1.152597	2.359511	0.067531
16	1	0.884055	3.407772	0.138347
17	6	-0.471122	-1.011968	-0.569096
18	1	0.100749	-1.849976	-0.948747
19	7	-3.063766	0.340171	0.585011
20	7	-4.387618	0.535486	0.698990
21	7	-5.032371	-0.254476	-0.102300
22	7	-4.115621	-0.978095	-0.745390
23	1	-4.379048	-1.681801	-1.426629
24	7	-1.776709	-1.221206	-0.799557
25	6	-2.865358	-0.615127	-0.337308
26	8	-1.058533	1.943844	0.602306
27	1	-1.804839	1.284288	0.726068

S_1-a'

Center Number	Atomic Number	Coordinates(Angstroms) X	Y	Z
1	6	4.184876	-1.894582	0.013214
2	6	4.227480	-0.494114	0.012557
3	6	3.056991	0.278756	0.002539

4	6	1.782860	-0.385308	-0.006105
5	6	1.777360	-1.808283	-0.009727
6	6	2.956237	-2.549454	0.000640
7	1	4.091818	2.182338	0.010123
8	1	5.109295	-2.459433	0.023047
9	1	5.186101	0.012735	0.021569
10	6	3.121953	1.699116	0.004730
11	6	0.569406	0.385524	-0.004786
12	1	0.840672	-2.347370	-0.020548
13	1	2.909131	-3.631408	-0.000483
14	6	0.705510	1.841801	-0.001471
15	6	1.961440	2.451593	0.001827
16	1	1.995769	3.534838	0.003887
17	6	-0.720038	-0.227863	0.004302
18	1	-0.795387	-1.309034	0.001568
19	7	-4.195819	0.730285	0.170438
20	7	-5.204671	-0.149754	0.186177
21	7	-4.781275	-1.375694	0.105110
22	7	-3.437036	-1.300621	0.035134
23	1	-2.883688	-2.143820	-0.049333
24	7	-1.827584	0.532644	0.036648
25	6	-3.057223	0.012639	0.069019
26	8	-0.370578	2.622695	-0.000558
27	1	-1.181510	2.015956	0.016045

TSab-S_1

Center Number	Atomic Number	Coordinates(Angstroms) X	Y	Z
1	6	4.283594	-1.805029	0.018690
2	6	4.269310	-0.407241	-0.004661
3	6	3.070027	0.312975	-0.005074
4	6	1.822059	-0.415340	0.011470
5	6	1.876806	-1.845138	0.037575
6	6	3.080221	-2.523822	0.042770
7	1	4.009394	2.265198	-0.036667
8	1	5.231204	-2.330674	0.019941
9	1	5.206778	0.138027	-0.020461
10	6	3.061517	1.739601	-0.018514
11	6	0.587794	0.293885	0.007090
12	1	0.958736	-2.416175	0.056594
13	1	3.091641	-3.606582	0.065129

14	6	0.625368	1.769192	0.013076
15	6	1.873340	2.434772	-0.003627
16	1	1.854501	3.518699	-0.008570
17	6	-0.677866	-0.366640	-0.003492
18	1	-0.780905	-1.441398	-0.055772
19	7	-3.439252	-1.350146	-0.179172
20	7	-4.785667	-1.318428	-0.175416
21	7	-5.238371	-0.114158	-0.025473
22	7	-4.158738	0.682543	0.077388
23	1	-4.253732	1.683478	0.204413
24	7	-1.787384	0.401826	0.041442
25	6	-3.038473	-0.079365	-0.022246
26	8	-0.482825	2.438917	0.031747
27	1	-1.382672	1.558995	0.052095

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Center Number	Atomic Number	Coordinates(Angstroms) X	Y	Z
1	6	4.252242	-1.846426	0.046373
2	6	4.258467	-0.437723	0.034621
3	6	3.074517	0.311227	0.012064
4	6	1.816470	-0.388312	0.002861
5	6	1.848390	-1.812744	0.012132
6	6	3.045900	-2.532196	0.034081
7	1	4.064950	2.238745	0.008152
8	1	5.193237	-2.382865	0.064098
9	1	5.206956	0.087964	0.043765
10	6	3.107570	1.732080	0.000341
11	6	0.585285	0.351777	-0.013796
12	1	0.924121	-2.373075	0.001310
13	1	3.022420	-3.614514	0.041402
14	6	0.687712	1.817184	-0.033961
15	6	1.920457	2.458117	-0.023616
16	1	1.927471	3.541840	-0.037682
17	6	-0.691973	-0.289541	-0.009281
18	1	-0.739558	-1.372843	-0.001673
19	7	-3.844544	-0.424467	-1.050462
20	7	-5.012256	-0.877870	-0.531995
21	7	-4.983211	-0.894380	0.757202
22	7	-3.765034	-0.445583	1.105197
23	1	-3.493799	-0.354076	2.077622

24	7	-1.820013	0.423317	-0.017131
25	6	-3.055922	-0.153474	-0.011597
26	8	-0.417081	2.563503	-0.063737
27	1	-1.207016	1.936281	-0.056605

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Center Number	Atomic Number	Coordinates(Angstroms) X	Y	Z
1	6	4.717393	-1.078182	-0.074132
2	6	4.325750	0.249098	0.081826
3	6	2.969508	0.610752	0.104038
4	6	1.968466	-0.396782	-0.066045
5	6	2.398000	-1.735380	-0.180934
6	6	3.749282	-2.073258	-0.191875
7	1	3.346924	2.724203	0.455152
8	1	5.770709	-1.334155	-0.087110
9	1	5.073265	1.026735	0.195606
10	6	2.580160	1.970843	0.322421
11	6	0.548884	-0.027320	-0.115473
12	1	1.676929	-2.538372	-0.242015
13	1	4.038919	-3.113326	-0.283412
14	6	0.230469	1.365965	0.220001
15	6	1.241617	2.306855	0.399167
16	1	0.938590	3.328977	0.595810
17	6	-0.395199	-0.994728	-0.520522
18	1	-0.001298	-1.941009	-0.876762
19	7	-3.598218	0.517929	-0.094637
20	7	-4.903337	0.318935	-0.164230
21	7	-5.178751	-0.916815	-0.531408
22	7	-4.015897	-1.530766	-0.691956
23	1	-3.973603	-2.499670	-0.987793
24	7	-1.717579	-0.886860	-0.489572
25	6	-2.971994	-0.653397	-0.432083
26	8	-1.022208	1.848452	0.329068
27	1	-1.723848	1.195942	0.176445