Electronic Supplementary Information for Dalton Transactions

Zn(II), Cd(II) and Pb(II) complexation with pyridinecarboxylate containing ligands

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Supporting Information

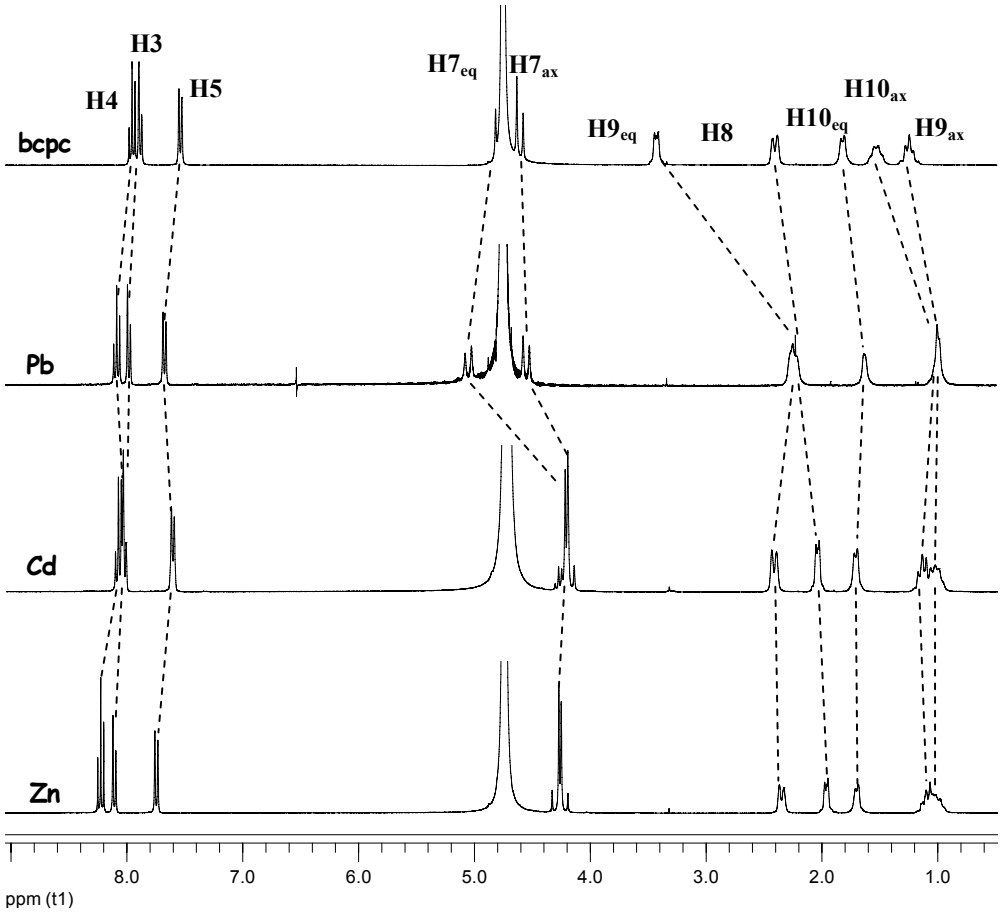

Figure S1. ^{1}H NMR spectra of the [M(bcpc)] complexes (M = Zn, Cd or Pb) recorded from D_2O solutions at 298 K (pD = 7.0).

***tw*-[Pb(bcpe)]** **(0 imaginary frequencies)**

Center Number	Atomic Number		Coordinates (Angstroms) X	Y	Z
1	8	0	-1.486946	-2.032725	-0.722054
2	8	0	1.486755	2.032791	-0.722058
3	8	0	-3.607982	-2.746428	-1.134094
4	7	0	-2.373127	0.339495	0.067936
5	7	0	2.373130	-0.339340	0.068083
6	7	0	0.351137	-1.417613	1.335276
7	1	0	-0.529669	-1.929209	1.269877
8	8	0	3.607756	2.746661	-1.134035
9	6	0	2.695194	-1.506129	0.634898
10	6	0	-2.695044	1.506297	0.634807
11	7	0	-0.351022	1.417451	1.335188
12	1	0	0.529861	1.928915	1.269797
13	6	0	-2.767450	-1.916506	-0.787158
14	6	0	-3.298647	-0.549814	-0.307668
15	6	0	4.657728	0.251468	-0.181620
16	1	0	5.384136	0.991266	-0.498149
17	6	0	-4.029743	1.868896	0.808966
18	1	0	-4.293538	2.810967	1.281117
19	6	0	2.767266	1.916666	-0.787129
20	6	0	-1.488920	2.322299	1.090433
21	1	0	-1.174253	3.023870	0.308055
22	1	0	-1.750576	2.918517	1.977523
23	6	0	-4.657778	-0.251199	-0.181471
24	1	0	-5.384273	-0.990951	-0.497907
25	6	0	3.298566	0.550010	-0.307651
26	6	0	1.489195	-2.322275	1.090613
27	1	0	1.174673	-3.023993	0.308306
28	1	0	1.750955	-2.918364	1.977760
29	6	0	4.029935	-1.868666	0.808869
30	1	0	4.293838	-2.810743	1.280948
31	6	0	-0.479087	0.597887	2.550391
32	1	0	-1.510743	0.235127	2.593515
33	1	0	-0.308162	1.189644	3.462713
34	6	0	-5.018276	0.978064	0.370513
35	1	0	-6.066980	1.238708	0.486977
36	6	0	0.478981	-0.598005	2.550501
37	1	0	1.510649	-0.235301	2.593850
38	1	0	0.307840	-1.189753	3.462787
39	6	0	5.018366	-0.977780	0.370299
40	1	0	6.067099	-1.238377	0.486607
41	82	0	-0.000001	-0.000121	-0.754351

HF = -1142.7937235 Hartree
Zero-point correction = 0.315778
Sum of electronic and thermal Enthalpies = -1142.455094
Sum of electronic and thermal Free Energies = -1142.530199

***tf*-[Pb(bcpe)]** **(0 imaginary frequencies)**

Center Number	Atomic Number		Coordinates (Angstroms) X	Y	Z
1	82	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	3.191532
3	6	0	1.521889	0.000000	3.074570
4	6	0	2.333750	0.312926	4.167041
5	1	0	1.867298	0.613982	5.097732
6	6	0	3.714106	0.202230	4.011990
7	1	0	4.382216	0.437501	4.836245
8	6	0	4.233775	-0.245755	2.795241
9	1	0	5.303742	-0.381140	2.661968
10	6	0	3.350683	-0.530611	1.749185
11	6	0	3.837701	-1.046072	0.400858
12	1	0	4.756879	-1.638864	0.566371
13	1	0	4.128653	-0.193559	-0.227587
14	6	0	2.423490	-3.062355	0.270748
15	1	0	2.349875	-2.934736	1.355629
16	1	0	3.184253	-3.845878	0.100233
17	6	0	1.083667	-3.575970	-0.260863
18	1	0	1.100246	-3.576828	-1.359305
19	1	0	0.964743	-4.628138	0.051644
20	6	0	-1.334351	-3.281286	-0.358406
21	1	0	-1.209728	-3.409642	-1.443162
22	1	0	-1.577405	-4.278285	0.044040
23	6	0	-2.498576	-2.340658	-0.114125
24	6	0	-3.794090	-2.811131	0.098351
25	1	0	-3.984601	-3.879146	0.147320
26	6	0	-4.831025	-1.886411	0.248554
27	1	0	-5.847763	-2.231191	0.416243
28	6	0	-4.545753	-0.525949	0.193200
29	1	0	-5.299598	0.244100	0.305992
30	6	0	-3.222081	-0.127390	0.000478
31	6	0	-2.845000	1.360271	-0.040705
32	7	0	2.028768	-0.384279	1.895869
33	7	0	2.791526	-1.773981	-0.314423
34	1	0	3.073545	-1.901611	-1.283317
35	7	0	-0.064706	-2.758248	0.160626
36	1	0	-0.110099	-2.709050	1.179577
37	7	0	-2.239826	-1.026167	-0.160512
38	8	0	-0.495170	0.181149	4.296980
39	8	0	-0.653581	-0.253538	2.092147
40	8	0	-1.577328	1.596554	-0.131622
41	8	0	-3.762938	2.173017	-0.006826

HF = -1142.7997463 Hartree
Zero-point correction = 0.315004
Sum of electronic and thermal Enthalpies = -1142.461577
Sum of electronic and thermal Free Energies = -1142.537585

***tw*-[Pb(bcpc)]** **(0 imaginary frequencies)**

Center Number	Atomic Number		Coordinates (Angstroms) X	Y	Z
1	8	0	-1.480979	-1.219992	2.048639
2	8	0	1.481956	-1.214977	-2.051121
3	8	0	-3.603558	-1.609576	2.771594
4	7	0	-2.367201	-0.426998	-0.320416
5	7	0	2.366421	-0.428799	0.320830
6	7	0	0.339403	0.846326	1.407307
7	1	0	-0.540616	0.774061	1.921267
8	8	0	3.604934	-1.604851	-2.772769
9	6	0	2.683110	0.129308	1.492828
10	6	0	-2.684796	0.133414	-1.491058
11	7	0	-0.340435	0.848786	-1.407179
12	1	0	0.539048	0.776220	-1.922071
13	6	0	-2.762011	-1.273000	1.937959
14	6	0	-3.293482	-0.793105	0.571407
15	6	0	4.651676	-0.660477	-0.270791
16	1	0	5.380591	-0.967143	-1.012296
17	6	0	-4.018474	0.313529	-1.854426
18	1	0	-4.279778	0.779506	-2.800272
19	6	0	2.762792	-1.269499	-1.939223
20	6	0	-1.474938	0.568152	-2.310842
21	1	0	-1.148630	-0.237268	-2.980701
22	1	0	-1.740504	1.424900	-2.945560
23	6	0	-4.652051	-0.659295	0.272666
24	1	0	-5.380414	-0.967361	1.014133
25	6	0	3.293332	-0.793219	-0.571020
26	6	0	1.472562	0.563227	2.311984
27	1	0	1.144690	-0.243262	2.979790
28	1	0	1.737868	1.418558	2.948698
29	6	0	4.016521	0.308283	1.857709
30	1	0	4.277151	0.772375	2.804666
31	6	0	-5.009359	-0.112165	-0.959685
32	1	0	-6.057444	0.009409	-1.220636
33	6	0	5.008053	-0.116013	0.963006
34	1	0	6.055944	0.004686	1.225137
35	82	0	-0.000280	-1.239676	-0.001649
36	6	0	0.466179	2.092248	0.619361
37	6	0	-0.465225	2.093761	-0.617443
38	6	0	0.221786	3.365312	1.456209
39	1	0	1.499839	2.111654	0.250904
40	6	0	-0.218944	3.367565	-1.452627
41	6	0	0.438315	4.644612	0.633390
42	1	0	-0.808606	3.341022	1.841049

43	1	0	0.882176	3.367702	2.331422
44	6	0	-0.433256	4.646173	-0.628116
45	1	0	-0.879477	3.372123	-2.327729
46	1	0	0.811333	3.342097	-1.837688
47	1	0	0.222927	5.525655	1.249623
48	1	0	1.497173	4.715339	0.345706
49	1	0	-0.216343	5.527633	-1.243219
50	1	0	-1.491991	4.718380	-0.340340
51	1	0	-1.498847	2.114237	-0.248893

HF = -1298.8458105 Hartree
Zero-point correction = 0.409745
Sum of electronic and thermal Enthalpies = -1298.409839
Sum of electronic and thermal Free Energies = -1298.492422

***tf*-[Pb(bcpc)] (0 imaginary frequencies)**

Center Number	Atomic Number		Coordinates (Angstroms) X	Y	Z
1	82	0	0.722691	-0.552363	-0.931517
2	6	0	0.266912	-1.958903	1.903853
3	6	0	-1.067302	-2.390352	1.299781
4	6	0	-1.880391	-3.353745	1.902128
5	1	0	-1.529075	-3.852270	2.798076
6	6	0	-3.122360	-3.614308	1.326423
7	1	0	-3.785992	-4.356358	1.762474
8	6	0	-3.526934	-2.891258	0.199341
9	1	0	-4.507372	-3.048853	-0.241590
10	6	0	-2.649629	-1.949359	-0.344051
11	6	0	-2.994216	-1.088512	-1.550069
12	1	0	-4.092666	-1.045428	-1.649541
13	1	0	-2.621561	-1.577331	-2.460528
14	6	0	-2.824367	1.110874	-0.406407
15	1	0	-2.917366	0.494848	0.497182
16	6	0	-1.807857	2.239495	-0.089646
17	1	0	-1.678895	2.836072	-1.006086
18	6	0	0.562029	2.783270	0.298672
19	1	0	0.536152	3.296303	-0.673711
20	1	0	0.353576	3.551165	1.057312
21	6	0	1.966997	2.264055	0.535182
22	6	0	2.897231	2.996290	1.273636
23	1	0	2.605626	3.932573	1.740156
24	6	0	4.198385	2.503265	1.400686
25	1	0	4.937558	3.058223	1.972058
26	6	0	4.531084	1.293601	0.799880
27	1	0	5.518312	0.851268	0.861192
28	6	0	3.544131	0.602809	0.095120
29	6	0	3.850935	-0.748321	-0.568317
30	7	0	-1.445366	-1.736613	0.197073
31	7	0	-2.340356	0.222722	-1.472883
32	1	0	-2.426931	0.690931	-2.373358
33	7	0	-0.456700	1.720890	0.246825
34	1	0	-0.484769	1.239553	1.147978
35	7	0	2.304193	1.098677	-0.033092
36	8	0	0.588185	-2.426159	2.990090
37	8	0	0.930004	-1.072065	1.218439
38	8	0	2.834748	-1.326223	-1.117272
39	8	0	5.014907	-1.135278	-0.536853
40	6	0	-4.210674	1.716843	-0.730052

41	1	0	-4.123559	2.300532	-1.660286
42	1	0	-4.918426	0.905530	-0.938303
43	6	0	-2.375325	3.157073	1.021548
44	1	0	-2.440786	2.567371	1.948900
45	1	0	-1.676332	3.975758	1.222949
46	6	0	-4.757058	2.620680	0.380661
47	1	0	-4.934401	2.023065	1.286433
48	1	0	-5.727510	3.038506	0.085848
49	6	0	-3.757616	3.737937	0.693359
50	1	0	-4.109117	4.353038	1.530682
51	1	0	-3.676144	4.408732	-0.174466

HF = -1298.8483073 Hartree
Zero-point correction = 0.408874
Sum of electronic and thermal Enthalpies = -1298.412865
Sum of electronic and thermal Free Energies = -1298.496478