

Supporting Information

Synergistic metal and anion effects on formation of coordination assemblies from N,N'-bis(3-pyridylmethyl)naphthalene diimide ligand

5

Hai-Ying Deng, Jian-Rong He, Mei Pan, Lei Li, and Cheng-Yong Su

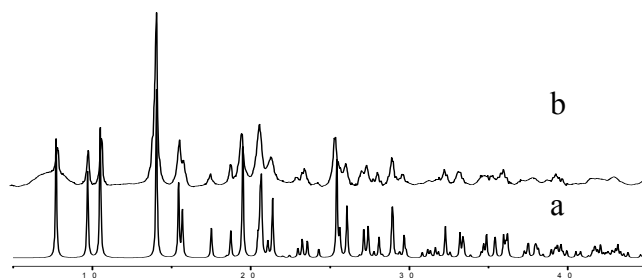


Figure S1 X-Ray powder diffraction of complex 2: (a) simulated, and (b) measured.

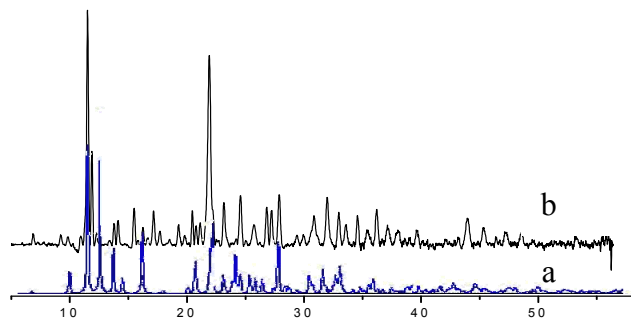


Figure S2 X-Ray powder diffraction of complex 4: (a) simulated, and (b) measured..

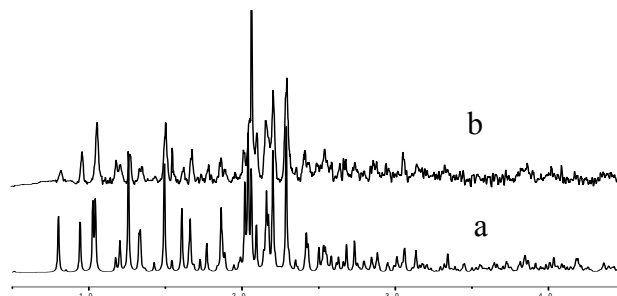


Figure S3 X-Ray powder diffraction of complex 5: (a) simulated, and (b) measured.

10

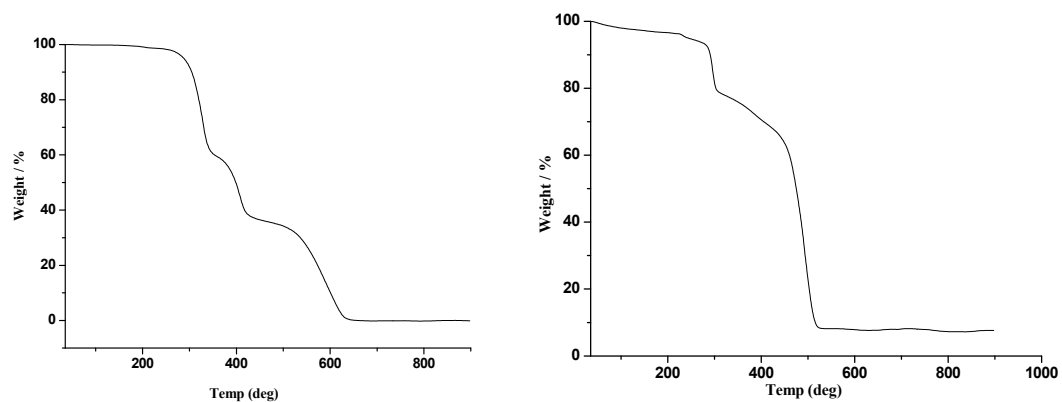


Figure S4 TG curves of complexes **2** (left) and **5** (right).

5

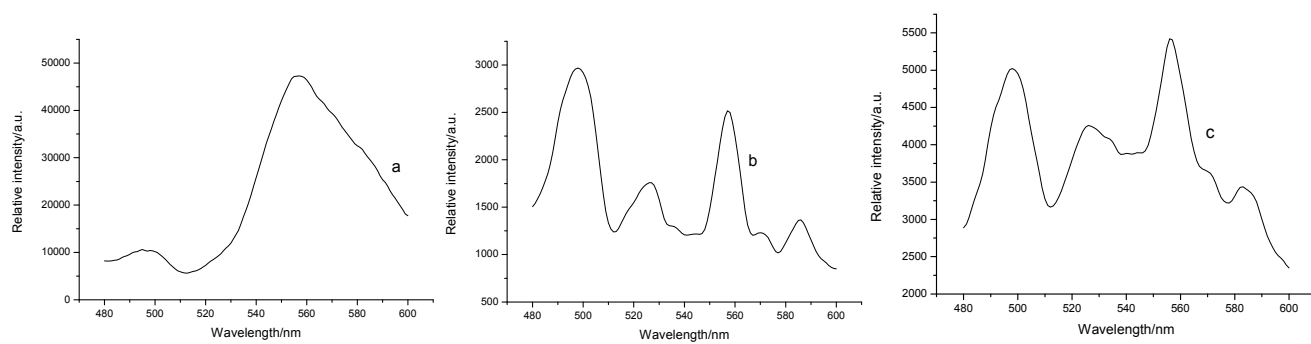


Figure S5 Emission spectra of the ligand (a), complexes **1** (b) and **4** (c) excited at 447 nm.

10

Table S1 Selected bond distances (Å) and angles (°) for complexes **1-5**.

Complex 1			
Cd(1)-N(1)	2.313(7)	N(1)-Cd(1)-I(1)	105.2(2)
Cd(1)-N(4) ^a	2.309(6)	N(4) ^a -Cd(1)-I(1)	103.0(2)
Cd(1)-I(1)	2.708(1)	N(1)-Cd(1)-I(2)	99.5(2)
Cd(1)-I(2)	2.712(1)	N(4) ^a -Cd(1)-I(2)	102.1(2)
		I(1)-Cd(1)-I(2)	134.6(3)
		N(1)-Cd(1)-N(4)	112.0(2)
Complex 2			
Hg(1)-Cl(1)	2.359(3)	Cl(1)-Hg(1)-N(1)	101.6(3)
Hg(1)-Cl(3)	2.359(3)	Cl(1)-Hg(1)-N(1)	96.3(3)
Hg(1)-N(1)	2.422(11)	Cl(1)-Hg(1)-N(1)	101.6(3)
Hg(1)-N(1)	2.422(11)	N(1)-Hg(1)-N(1)	93.4(5)
		Cl(1)-Hg(1)-Cl(1)	153.9(2)
Complex 3			
Zn(1)-N(5) ^a	2.074(2)	N(5) ^a -Zn(1)-N(5)	180.0(1)
Zn(1)-N(5)	2.074(2)	N(1) ^a -Zn(1)-N(1)	180.0(1)
Zn(1)-N(1) ^a	2.229(2)	N(5) ^a -Zn(1)-N(1) ^b	89.5(1)
Zn(1)-N(1)	2.229(2)	N(5) ^a -Zn(1)-N(1) ^c	89.5(1)
Zn(1)-N(4) ^b	2.258(2)	N(5) ^a -Zn(1)-N(4) ^c	89.7(1)
Zn(1)-N(4) ^c	2.258(2)	N(5) ^a -Zn(1)-N(1) ^c	90.5(1)
		N(1)-Zn(1)-N(4)	93.6(1)
		N(4)-Zn(1)-N(5)	89.7(1)
		N(4) ^b -Zn(1)-N(4) ^c	180.0(1)
Complex 4			
Cd(1)-N(1) ^a	2.395(2)	O(6) ^a -Cd(1)-O(6)	180.0(1)
Cd(1)-N(1)	2.395(2)	N(1) ^a -Cd(1)-N(3)	87.3(1)
Cd(1)-O(6) ^a	2.334(2)	N(1)-Cd(1)-N(3)	92.7(1)
Cd(1)-O(6)	2.334(2)	O(6) ^a -Cd(1)-N(1)	96.0(1)
Cd(1)-N(3)	2.308(2)	O(6)-Cd(1)-N(1)	84.0(1)
Cd(1)-N(3) ^a	2.308(2)	N(1) ^a -Cd(1)-N(3) ^a	92.7(1)
		N(1)-Cd(1)-N(3) ^a	87.3(1)
		N(1)-Cd(1)-N(1) ^a	180.0(1)
		N(3) ^a -Cd(1)-N(3)	180.0(1)
		N(3) ^a -Cd(1)-O(6) ^a	82.9(1)
		N(3)-Cd(1)-O(6) ^a	97.2(1)
Complex 5			
Co(1)-N(1)	2.146(3)	N(1)-Co(1)-O(5)	87.0(1)
Co(1)-N(4) ^a	2.158(3)	N(4) ^a -Co(1)-O(5)	93.0(1)
Co(1)-N(5)	2.164(3)	N(5)-Co(1)-O(5)	86.0(1)
Co(1)-O(11)	2.191(3)	O(11)-Co(1)-O(5)	170.8(1)
Co(1)-O(5)	2.194(4)	N(1)-Co(1)-O(9)	142.2(1)
Co(1)-O(9)	2.197(3)	N(4) ^a -Co(1)-O(9)	91.3(1)
Co(1)-O(6)	2.287(5)	N(5)-Co(1)-O(9)	85.8(1)
		O(11)-Co(1)-O(9)	58.1(1)
		O(5)-Co(1)-O(9)	130.0(1)
		N(1)-Co(1)-O(6)	142.5(2)
		N(4) ^a -Co(1)-O(6)	81.9(2)
		N(5)-Co(1)-O(6)	93.8(1)
		O(11)-Co(1)-O(6)	132.7(1)
		O(5)-Co(1)-O(6)	56.2 (2)
		O(9)-Co(1)-O(6)	75.2(2)
		N(1)-Co(1)-N(4) ^a	94.3(1)
		N(1)-Co(1)-N(5)	90.3(1)
		N(4) ^a -Co(1)-N(5)	175.3(1)
		N(1)-Co(1)-O(11)	84.4(1)
		N(4) ^a -Co(1)-O(11)	91.1(1)
		N(5)-Co(1)-O(11)	90.6(1)

^a Symmetry transformations used to generate equivalent atoms: 1: a, -x,-y+1,-z+1; 3: a, -x+1,-y,-z+1; b, -x,y-1/2,-z+1/2; c, x+1,-y+1/2,z+1/2; d, -x,y+1/2,-z+1/2; 4: a, -x+2,-y+1,-z+1; 5: a, -x+2,y-1/2,-z+3/2