Supporting Information for

Metal cations- and anions-induced assembly: structures and luminescent properties

Feng Jin,[ab] Hui-Zhen Wang,[a] Ying Zhang,[a] Yang Wang,[a] Jun Zhang,[a] Lin Kong,[a] Fu-Ying Hao,[ab] Jia-Xiang Yang,[a] Jie-Ying Wu,[a] Yu-Peng Tian, [a c d] Hong-Ping Zhou*[a]

[a]School of Chemistry and Chemical Engineering, Anhui University, Hefei 230039, P. R. China

[b]Department of Chemistry, Fuyang Normal College, Fuyang 236041, P. R. China

[c]State Key Laboratory of Coordination Chemistry, Nanjing University, Nanjing 210093, P. R. China

[d] State Key Laboratory of Crystal Materials, Shandong University, Jinan 250100, P. R. China

[*]Corresponding author. *E-mail*: zhpzhp@263.net (H. -P. Zhou).

Contents:

Table S1 Crystal Date and Refinement of Complexes **1-5**

Compound	Complex **1**	Complex **2**	Complex **3**	Complex**4**	Complex **5**
empirical formula	$C_{25}H_{18}Br_2HgN_4$	$C_{27}H_{21}HgI_2N_5$	$C_{27}H_{18}HgN_6S_2$	$C_{52}H_{38}CdN_{10}OS_2$	$C_{53}H_{40}CoN_{10}OS_2$
formula weight	734.84	869.88	691.18	995.44	956.00
crystal system	Monoclinic	Monoclinic	Monoclinic	Orthorhombic	Triclinic
space group	$P2_1/c$	$P2_1/c$	$P2_1/c$	$Fdd2$	$P\bar{1}$
a [Å]	17.794(5)	13.334(5)	13.460(5)	32.440(7)	12.194(5)
b [Å]	18.670(5)	26.776(5)	25.921(5)	38.770(8)	12.533(5)
c [Å]	14.665(5)	7.767(5)	7.340(5)	14.781(3)	15.864(5)
α [°]	90.00	90.00	90.00	90.00	86.325(5)
β [°]	96.751(5)	100.081(5)	95.017(5)	90.00	71.489(5)
γ [°]	90.00	90.00	90.00	90.00	87.781(5)
V [Å^3]	4838(2)	2730(2)	2551(2)	18590(6)	2293.9(15)
Z	8	4	4	16	2
T [K]	298(2)	298(2)	298(2)	298(2)	298(2)
D calcd [g ·cm^{-3}]	2.018	2.116	1.800	1.423	1.384
μ [mm^{-1}]	9.686	7.923	6.225	0.611	0.518
θ range [°]	1.15-25.00	1.52-24.99	1.52-25.00	1.60-27.46	1.36-25.00
total no. data	34120	19252	17956	33289	16421
no.unique data	8517	4809	4497	10303	7994
no. params refined	577	317	326	604	606
R_1	0.0495	0.0243	0.0264	0.0337	0.0392
wR_2	0.0979	0.0554	0.0650	0.0785	0.1297
GOF on F^2	1.019	1.025	1.032	1.072	1.087

Table S2 Selected Bond Lengths (Å) and Angles (°) of Complexes **1-5**

$HgLBr_2$ (**1**)			
Hg(1)–N(5)	2.392(8)	Hg(1)–Br(2)	2.457(2)
Hg(1)–N(6)	2.492(8)	Hg(1)–Br(1)	2.507(1)
Hg(2)–N(1)	2.362(8)	Hg(2)–N(2)	2.419(8)
Hg(2)–Br(4)	2.487(2)	Hg(2)–Br(3)	2.510(1)
N(5)–Hg(1)–Br(2)	114.3(2)	N(5)–Hg(1)–N(6)	69.4(3)
N(5)–Hg(1)–Br(1)	100.0(2)	Br(2)– Hg(1)–N(6)	102.4(2)
N(6)–Hg(1)–Br(1)	117.3 (2)	Br(2)–Hg(1)–Br(1)	134.78(6)
N(1)–Hg(2)–Br(4)	116.4(2)	N(1)–Hg(2)–N(2)	70.2(3)
N(1)–Hg(2)–Br(3)	101.1(2)	N(2)–Hg(2)–Br(4)	103.8(2)
Br(4)–Hg(2)–Br(3)	130.38(5)	N(2)–Hg(2)–Br(3)	119.4(2)

$[HgLI_2]CH_3CN$ (**2**)			
Hg(1)–N(2)	2.364(3)	Hg(1)–N(1)	2.456(3)
Hg(1)–I(1)	2.6315(9)	Hg(1)–I(2)	2.671(1)
N(2)–Hg(1)–N(1)	69.0(1)	N(2)–Hg(1)–I(1)	109.92(9)
N(2)–Hg(1)–I(2)	96.67(8)	N(1)–Hg(1)–I(1)	124.03(8)
I(1)–Hg(1)–I(2)	129.59(2)	N(1)–Hg(1)–I(2)	111.97(9)
$HgL(SCN)_2$ (**3**)			
Hg(1)–N(1)	2.350(3)	Hg(1)–N(2)	2.358(3)
Hg(1)–S(2)	2.447(1)	Hg(1)–S(1)	2.456(2)
N(1)–Hg(1)–N(2)	71.1(1)	N(1)–Hg(1)–S(2)	109.22(8)
S(2)–Hg(1)–S(1)	121.07(5)	N(2)–Hg(1)–S(1)	105.70(7)
N(1)–Hg(1)–S(1)	116.49(8)	N(2)–Hg(1)–S(2)	123.38(9)
$[CdL_2(SCN)_2]\cdot H_2O$ (**4**)			
Cd(1)–N(9)	2.316(3)	Cd(1)–N(10)	2.328(3)
Cd(1)–N(5)	2.328(2)	Cd(1)–N(1)	2.343(2)
Cd(1)–N(2)	2.424(3)	Cd(1)–N(6)	2.471(3)
N(9)–Cd(1)–N(10)	98.2(1)	N(9)–Cd(1)–N(5)	89.2(1)
N(2)–Cd(1)–N(6)	81.92(8)	N(1)–Cd(1)–N(6)	117.97(9)
N(9)–Cd(1)–N(6)	154.1(1)	N(1)–Cd(1)–N(2)	69.26(9)
N(5)–Cd(1)–N(2)	119.41(8)	N(10)–Cd(1)–N(2)	150.0(1)
N(9)–Cd(1)–N(2)	97.3(1)	N(10)–Cd(1)–N(1)	86.7(1)
N(5)–Cd(1)–N(1)	170.34(8)	N(9)–Cd(1)–N(1)	85.2(1)
N(10)–Cd(1)–N(5)	86.3(1)	N(10)–Cd(1)–N(6)	94.7(1)
N(5)–Cd(1)–N(6)	69.28(8)		
$[CoL_2(SCN)_2]\cdot CH_3OH$ (**5**)			
Co(1)–N(9)	2.082(2)	Co(1)–N(10)	2.088(2)
Co(1)–N(1)	2.106(2)	Co(1)–N(5)	2.127(2)
Co(1)–N(6)	2.300(2)	Co(1)–N(2)	2.304(2)
N(9)–Co(1)–N(10)	99.33(9)	N(9)–Co(1)–N(1)	87.83(8)
N(1)–Co(1)–N(6)	107.32(7)	N(10)–Co(1)–N(6)	93.58(8)
N(9)–Co(1)–N(6)	159.69(8)	N(1)–Co(1)–N(5)	177.64(7)
N(9)–Co(1)–N(2)	93.87(8)	N(5)–Co(1)–N(6)	74.02(7)
N(10)–Co(1)–N(5)	85.48(8)	N(9)–Co(1)–N(5)	91.34(8)
N(1)–Co(1)–N(2)	74.05(7)	N(10)–Co(1)–N(2)	160.79(8)
N(6)–Co(1)–N(2)	77.97(6)	N(5)–Co(1)–N(2)	108.22(7)
N(10)–Co(1)–N(1)	92.47(8)		

Table S3 The dihedral angles between the neighboring connected aromatic rings in structures of free ligand and the coordinated ligand in complexes **1**, **3** and **4**.

	L	Complex **1**	Complex **3**	Complex **4**
Angle (1-2) [°]	8.29	8.79/12.98	18.83	6.91/15.90
Angle (2-3) [°]	13.88	30.33/3.93	22.73	18.96/9.38
Angle (3-4) [°]	9.85	8.81/28.33	14.18	23.74/9.47