

## Supplementary Material

### **Luminescent Functionalized Supramolecular Coordination Polymers Based on an Aromatic Carboxylic Acid Ligand for Sensing of Hg<sup>2+</sup> Ion**

*Xiaojun Sun,<sup>A</sup> Ping Yang,<sup>A</sup> Guangfeng Hou,<sup>B</sup> Jinzhi Wei,<sup>A</sup> Xueliang Wang,<sup>A</sup> Doudou Yang,<sup>A</sup> Xin Zhang,<sup>A</sup> Hong Dong,<sup>A</sup> and Fengming Zhang<sup>A,C</sup>*

<sup>A</sup>Key Laboratory of Green Chemical Engineering and Technology of College of Heilongjiang Province, College of Chemical and Environmental Engineering, Harbin University of Science and Technology, Harbin 150040, China.

<sup>B</sup>Engineering Research Center of Pesticide of Heilongjiang University, Heilongjiang University, Harbin 150080, China.

<sup>C</sup>Corresponding author. Email: zhangfm80@163.com

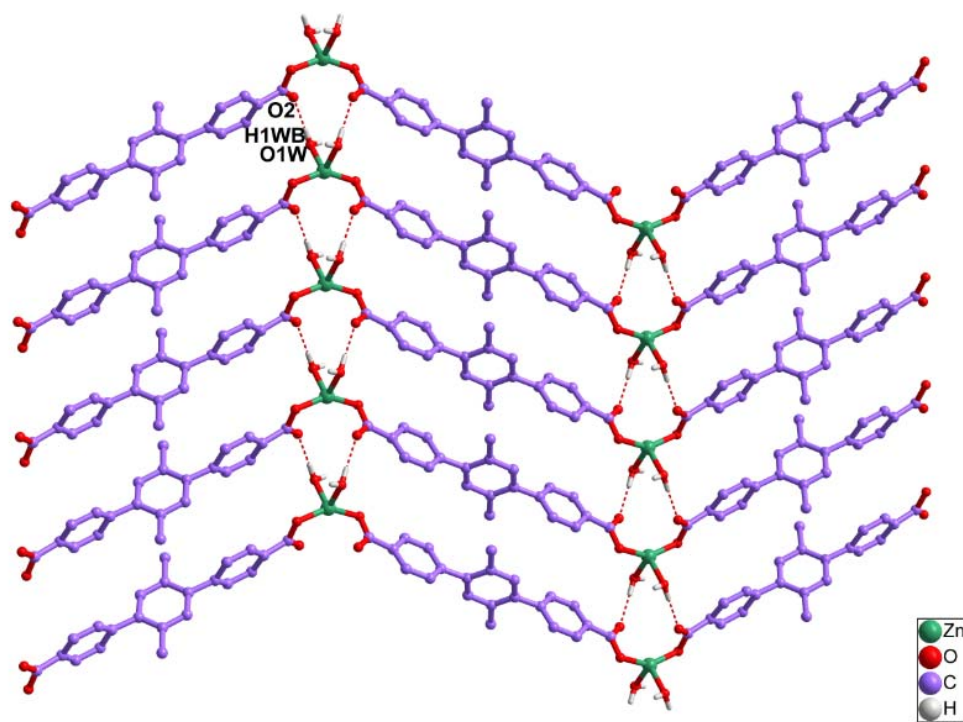


Fig.S1: Connection mode of hydrogen bond in compound 1

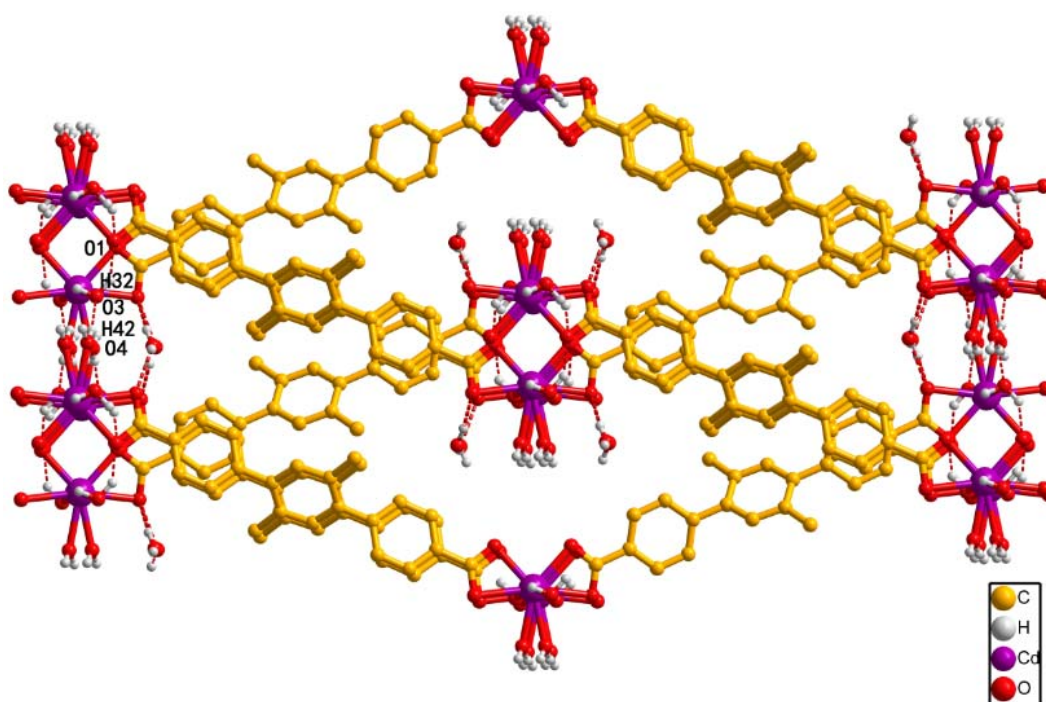


Fig.S2: Connection mode of hydrogen bond in compound 2.

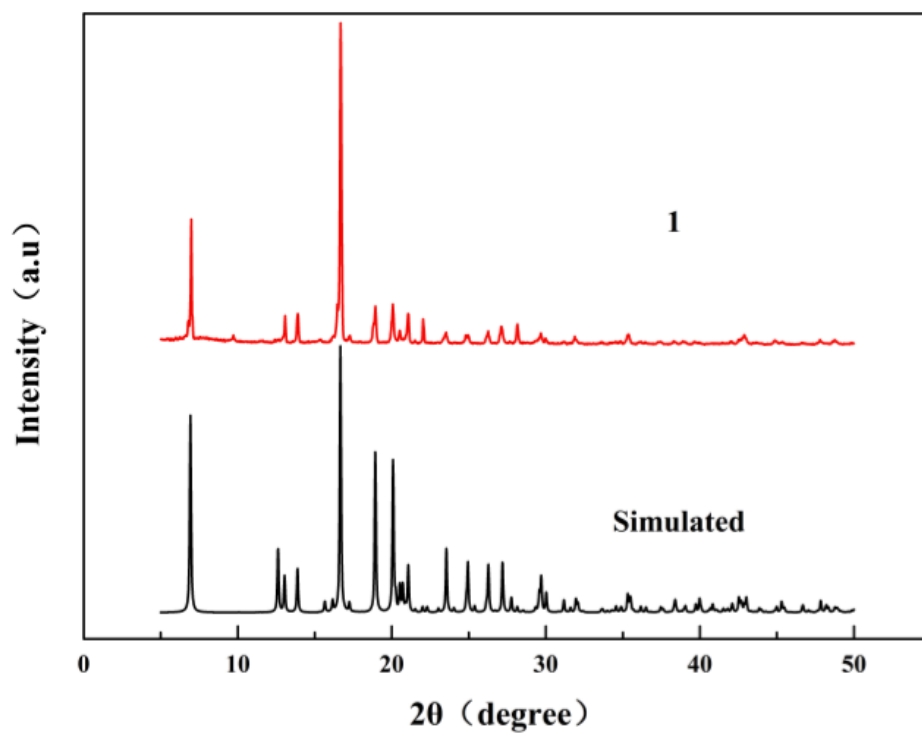


Fig.S3: Powder XRD patterns of simulated and compound 1.

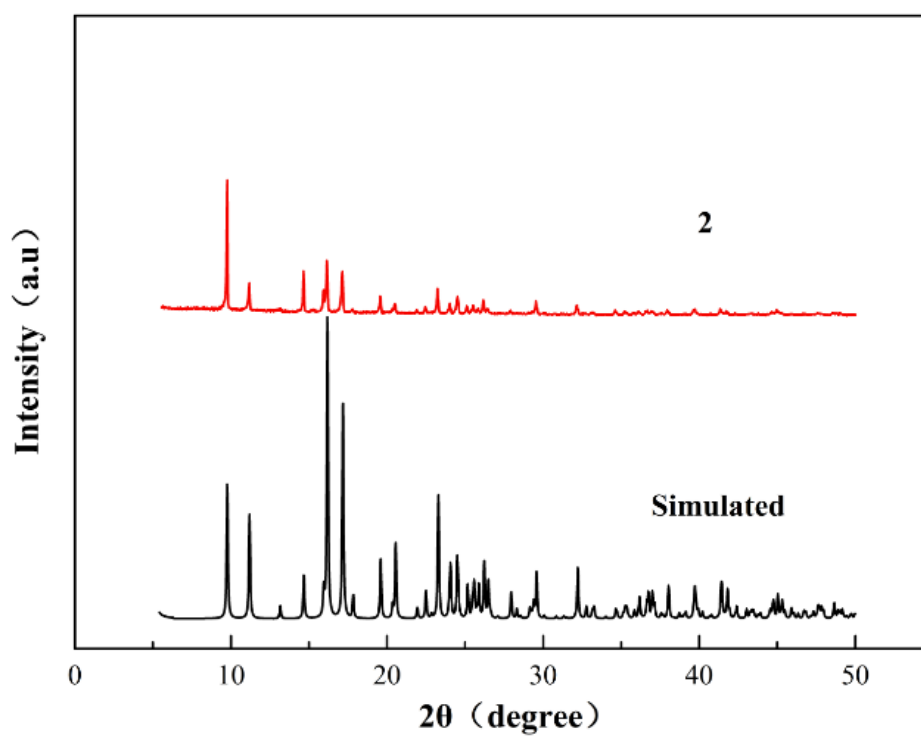


Fig.S4: Powder XRD patterns of simulated and compound 2.

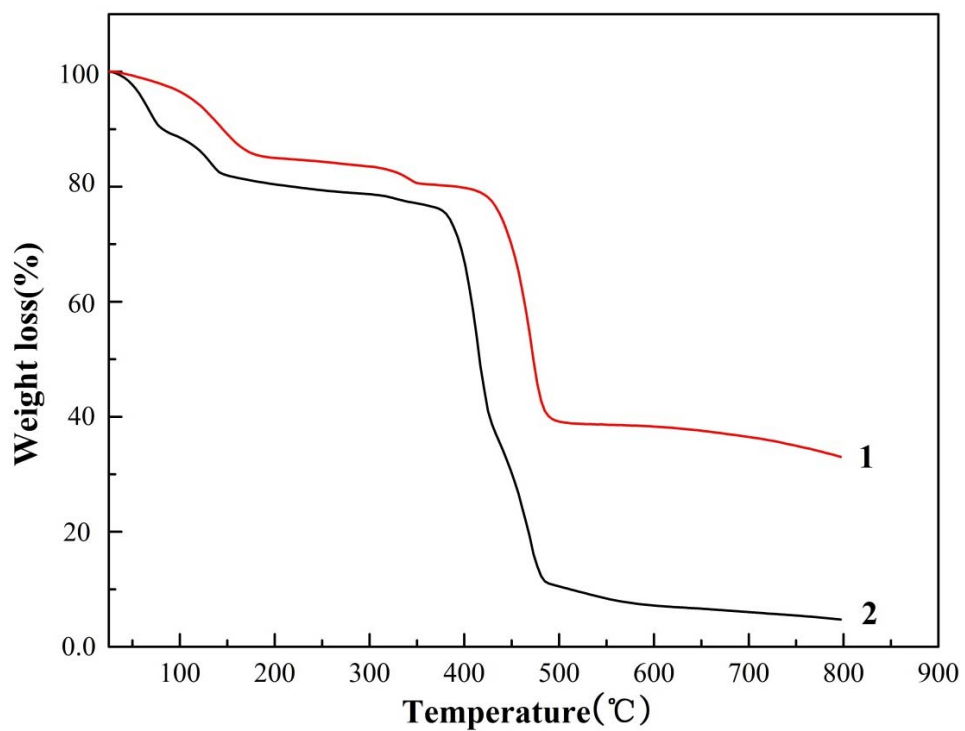


Fig.S5: TGA Plot of compound 1-2 in N<sub>2</sub> atmosphere.

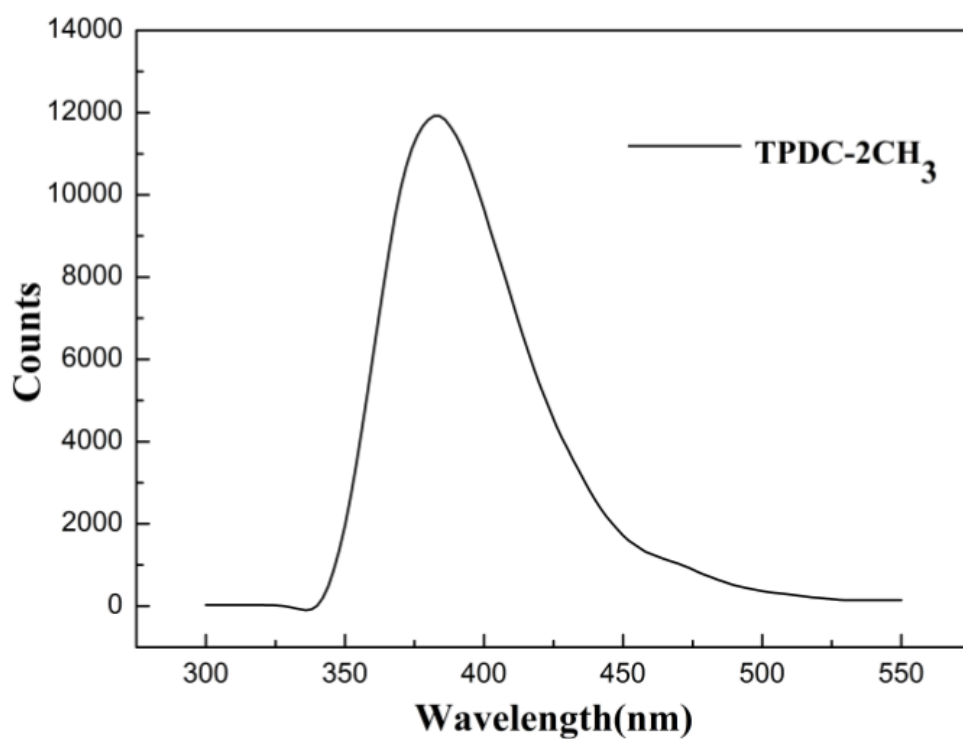


Fig.S6: Emission spectra of TPDC-2CH<sub>3</sub>.

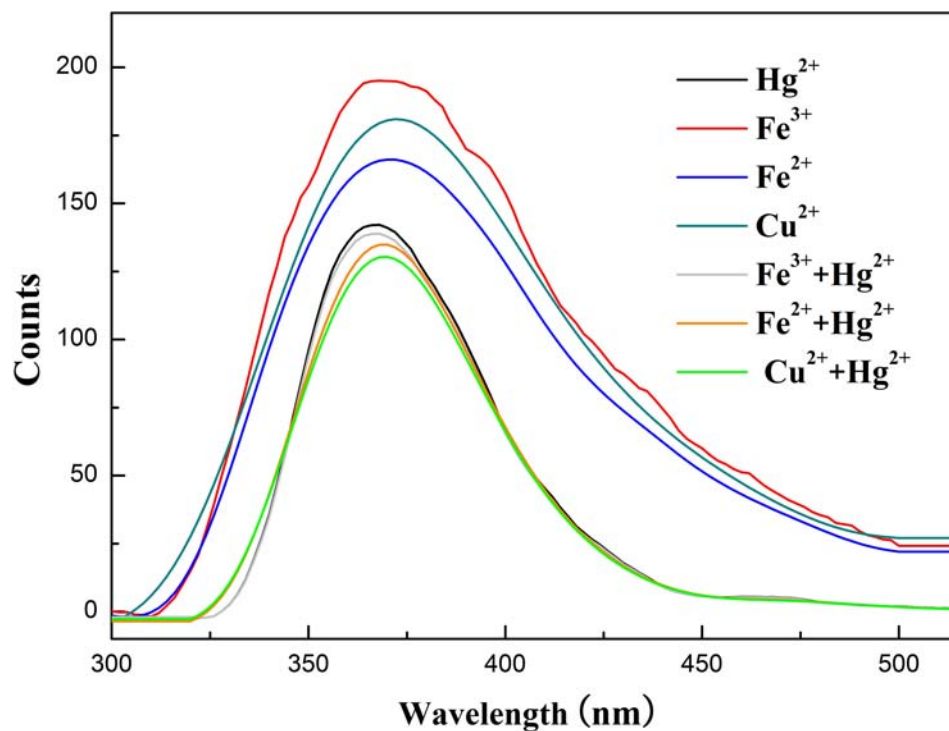


Fig.S7 Emission spectra of **1** in aqueous solutions of  $\text{Hg}^{2+}$ ,  $\text{Fe}^{2+}$ ,  $\text{Fe}^{3+}$ ,  $\text{Cu}^{2+}$ , mixed  $\text{Hg}^{2+}$  and  $\text{Fe}^{2+}$ , mixed  $\text{Hg}^{2+}$  and  $\text{Fe}^{3+}$ , and mixed  $\text{Hg}^{2+}$  and  $\text{Cu}^{2+}$ , respectively.

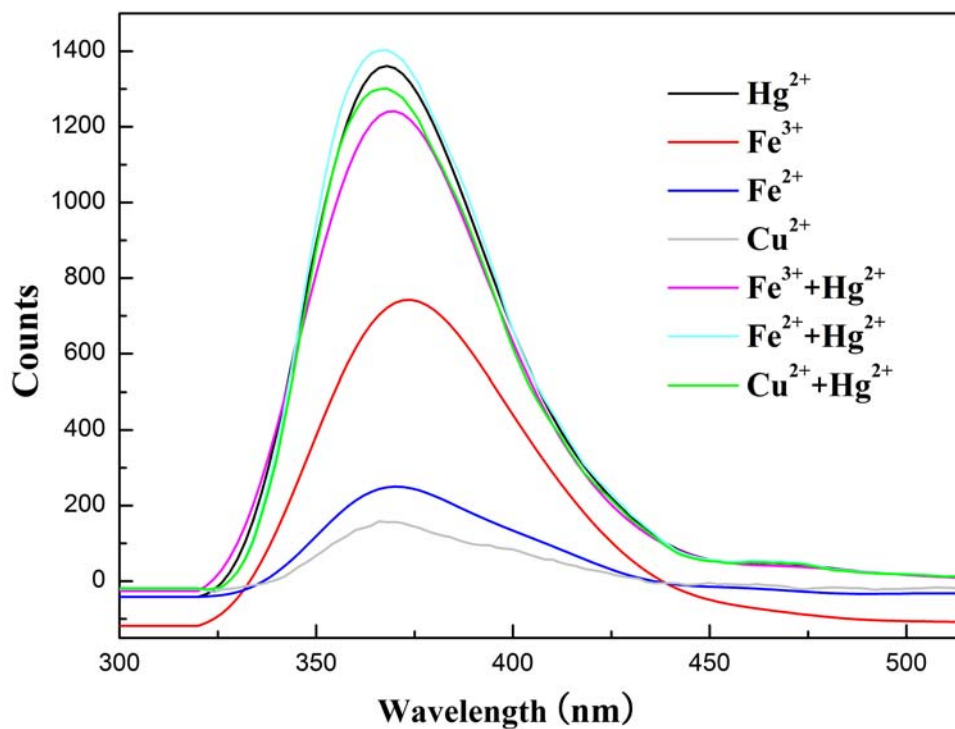


Fig.S8 Emission spectra of **2** in aqueous solutions of  $\text{Hg}^{2+}$ ,  $\text{Fe}^{2+}$ ,  $\text{Fe}^{3+}$ ,  $\text{Cu}^{2+}$ , mixed  $\text{Hg}^{2+}$  and  $\text{Fe}^{2+}$ , mixed  $\text{Hg}^{2+}$  and  $\text{Fe}^{3+}$ , and mixed  $\text{Hg}^{2+}$  and  $\text{Cu}^{2+}$ , respectively.

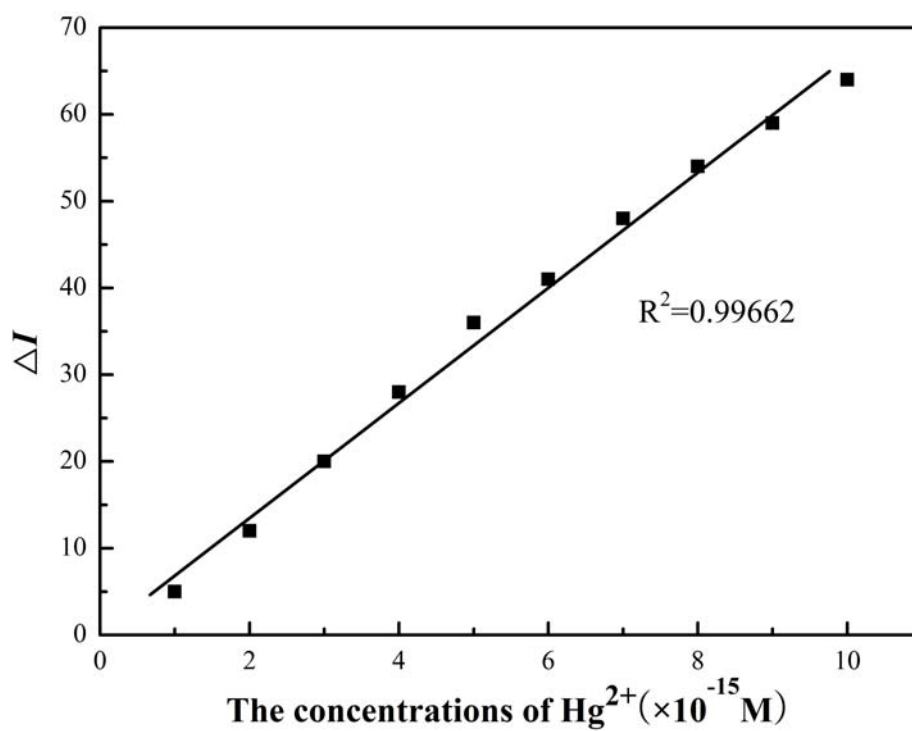


Fig.S9 The luminescence intensity ( $\Delta I$ ) vs  $\text{Hg}^{2+}$  ion with the low concentration t plot.

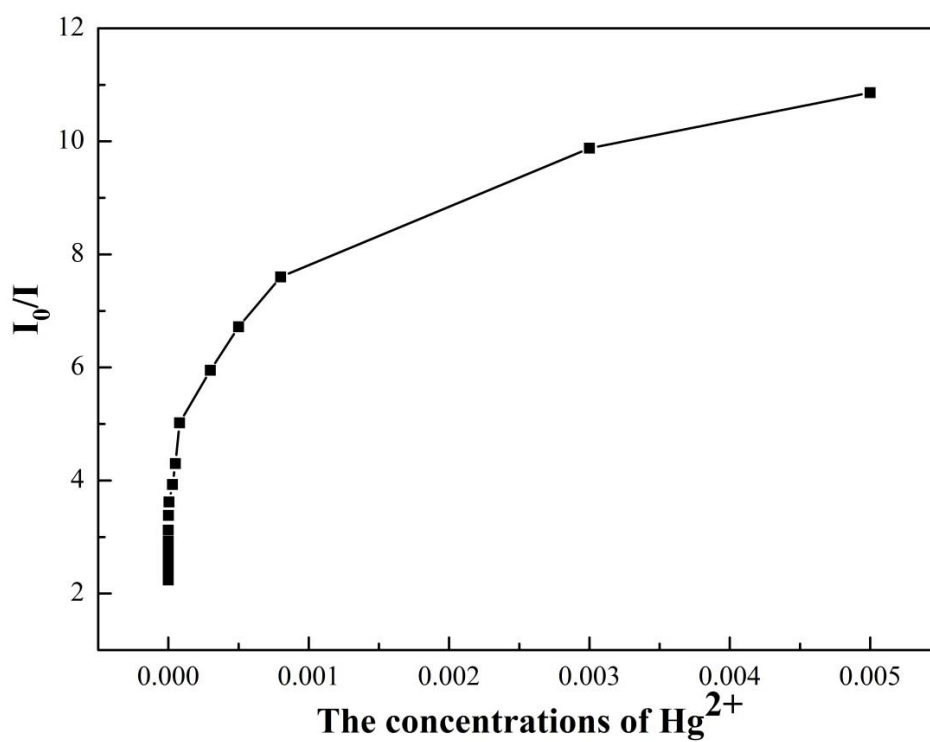


Fig.S10 The luminescence intensity vs  $\text{Hg}^{2+}$  ion concentration plot.

**Table.S1** Selected bond lengths (Å) and angles (deg) for compound **1**

O1-Zn1	1.9736(15)	O1 <sup>#1</sup> -Zn1	1.9736(15)	
O1W-Zn1	2.0253(18)	O1W <sup>#1</sup> -Zn1	2.0252(18)	
Zn1-C1	2.588(2)	Zn1-C1 <sup>#1</sup>	2.588(2)	
O1-C1	1.266(3)	O2-C1	1.243(2)	
C1-C2	1.488(3)	C2-C3	1.366(3)	
C2-C7A	1.365(7)	C2-C7B	1.395(12)	
C3-C4	1.377(3)	C4-C5	1.356(3)	
C5-C8	1.494(3)	C5-C6A	1.430(5)	
C5-C6B	1.348(12)	C8-C9	1.397(3)	
C8-C10 <sup>#2</sup>	1.387(3)	C9-C10	1.394(3)	
C9-C11	1.502(4)	C10-C8 <sup>#2</sup>	1.387(3)	
C6A-C7A	1.385(8)	C6B-C7B	1.382(17)	
O1-Zn1-O1 <sup>#1</sup>	147.64(10)	O1-Zn1-O1W	93.48(7)	
O1-Zn1-O1W <sup>#1</sup>	107.04(8)	O1 <sup>#1</sup> -Zn1-O1W	107.03(8)	
O1 <sup>#1</sup> -Zn1-O1W <sup>#1</sup>	93.48(7)	O1W <sup>#1</sup> -Zn1-O1W	101.23(12)	
O1-Zn1-C1 <sup>#1</sup>	123.07(7)	O1-Zn1-C1	28.35(6)	
O1 <sup>#1</sup> -Zn1-C1 <sup>#1</sup>	28.35(6)	O1 <sup>#1</sup> -Zn1-C1	123.07(7)	
O1W <sup>#1</sup> -Zn1-C1	104.06(7)	O1W <sup>#1</sup> -Zn1-C1 <sup>#1</sup>	121.24(7)	
O1W-Zn1-C1 <sup>#1</sup>	104.06(7)	O1W-Zn1-C1	121.24(7)	
C1-O1-Zn1	103.92(13)	O1-C1-Zn1	47.74(10)	
D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O1W-H1WB...O2	0.87(3)	1.80(3)	2.664(2)	176(2)
O1W-H1WA...O3W	0.77(4)	2.11(4)	2.844(2)	160(4)
O3W-H3W...O1	0.80(3)	2.02(3)	2.758(2)	153(3)

Symmetry transformations used to generate equivalent atoms: #1: -3/2-x,+y,3/2-z;

#2:-x,-2-y,1-z

**Table.S2** Selected bond lengths (Å) and angles (deg) for compound **2**

Cd(1)-O(3)	2.295(5)		Cd(1)-O(4) <sup>#2</sup>	2.346(7)
Cd(1)-O(3) <sup>#2</sup>	2.295(5)		Cd(1)-O(4)	2.346(7)
Cd(1)-O(1)	2.310(4)		Cd(1)-O(2)	2.465(4)
Cd(1)-O(1) <sup>#2</sup>	2.310(4)		Cd(1)-O(2) <sup>#2</sup>	2.465(4)
O(3)-Cd(1)-O(3) <sup>#2</sup>	164.1(2)		O(4) <sup>#2</sup> -Cd(1)-O(4)	23.1(3)
O(3)-Cd(1)-O(1)	90.79(16)		O(3)-Cd(1)-O(2)	86.8(2)
O(3) <sup>#2</sup> -Cd(1)-O(1)	100.96(19)		O(3) <sup>#2</sup> -Cd(1)-O(2)	91.47(19)
O(3)-Cd(1)-O(1) <sup>#2</sup>	100.96(19)		O(1)-Cd(1)-O(2)	54.11(14)
O(3) <sup>#2</sup> -Cd(1)-O(1) <sup>#2</sup>	90.79(16)		O(1) <sup>#2</sup> -Cd(1)-O(2)	138.65(14)
O(1)-Cd(1)-O(1) <sup>#2</sup>	85.0(2)		O(4) <sup>#2</sup> -Cd(1)-O(2)	73.5(2)
O(3)-Cd(1)-O(4) <sup>#2</sup>	76.3(3)		O(4)-Cd(1)-O(2)	93.75(19)
O(3) <sup>#2</sup> -Cd(1)-O(4) <sup>#2</sup>	88.1(2)		O(3)-Cd(1)-O(2) <sup>#2</sup>	91.47(19)
O(1)-Cd(1)-O(4) <sup>#2</sup>	126.77(18)		O(3) <sup>#2</sup> -Cd(1)-O(2) <sup>#2</sup>	86.8(2)
O(1) <sup>#2</sup> -Cd(1)-O(4) <sup>#2</sup>	147.8(2)		O(1)-Cd(1)-O(2) <sup>#2</sup>	138.65(14)
O(3)-Cd(1)-O(4)	88.1(2)		O(1) <sup>#2</sup> -Cd(1)-O(2) <sup>#2</sup>	54.11(14)
O(3) <sup>#2</sup> -Cd(1)-O(4)	76.3(3)		O(4) <sup>#2</sup> -Cd(1)-O(2) <sup>#2</sup>	93.75(19)
O(1)-Cd(1)-O(4)	147.8(2)		O(4)-Cd(1)-O(2) <sup>#2</sup>	73.5(2)
O(1) <sup>#2</sup> -Cd(1)-O(4)	126.77(18)		O(2)-Cd(1)-O(2) <sup>#2</sup>	167.2(2)
D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(3)-H(32)...O(1) <sup>#4</sup>	0.8500	2.06	2.691(6)	103.1
O(4)-H(41)...O(3) <sup>#5</sup>	0.8500	2.00	2.798(9)	156.8
O(4)-H(42)...O(3) <sup>#6</sup>	0.8500	1.81	2.651(9)	167.7
O(5)-H(51)...O(2)	0.8500	2.13	2.962(7)	165.4
O(5)-H(52)...O(2) <sup>#3</sup>	0.8500	2.13	2.738(7)	128.1

Symmetry transformations used to generate equivalent atoms:#2:-x,y,-z+1/2;

#3:x,-y,z-1/2; #4:x,-y+1,z-1/2; #5:x,-y,z+1/2; #6:-x,-y,-z.