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Supplementary Material

Luminescent Functionalized Supramolecular Coordination Polymers Based on an Aromatic Carboxylic Acid Ligand for Sensing of Hg^{2+} Ion

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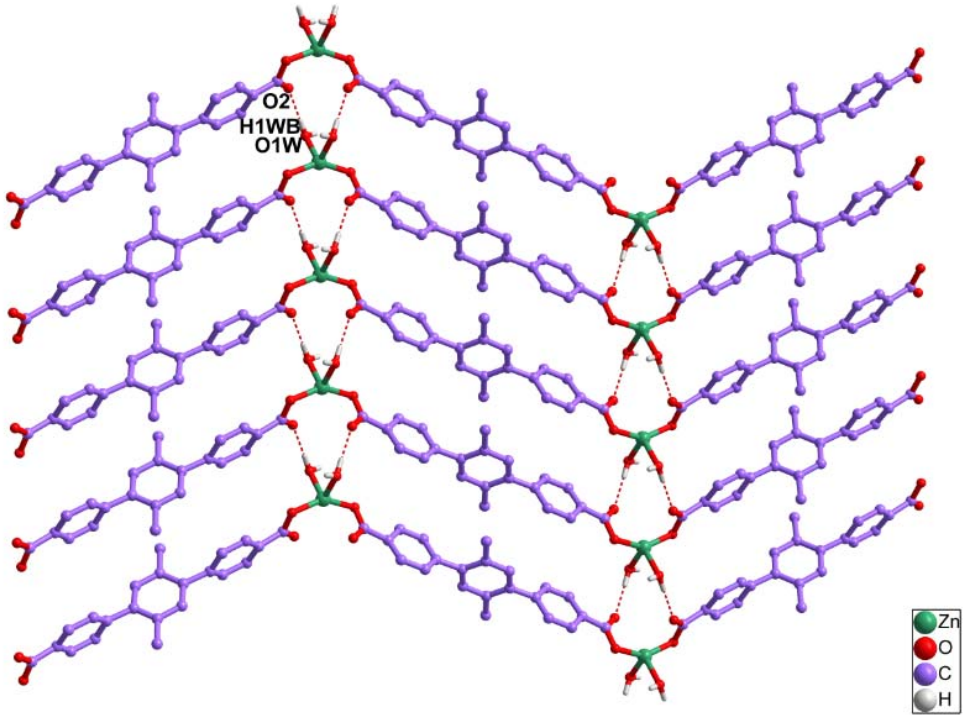

Fig.S1: Connection mode of hydrogen bond in compound **1**

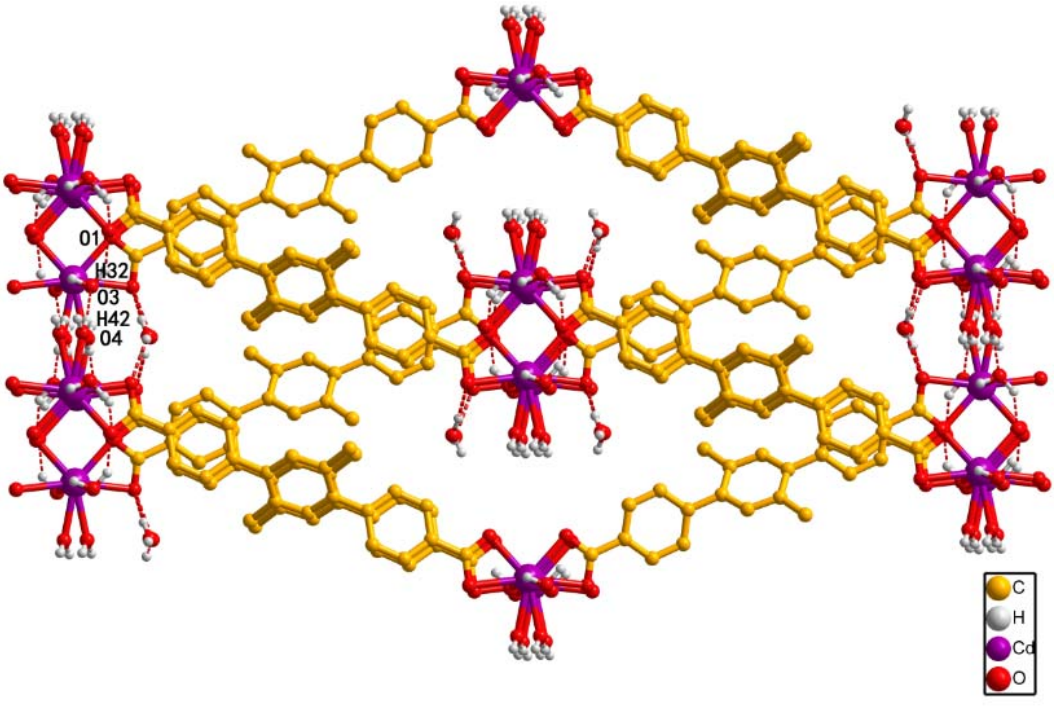

Fig.S2: Connection mode of hydrogen bond in compound **2**.

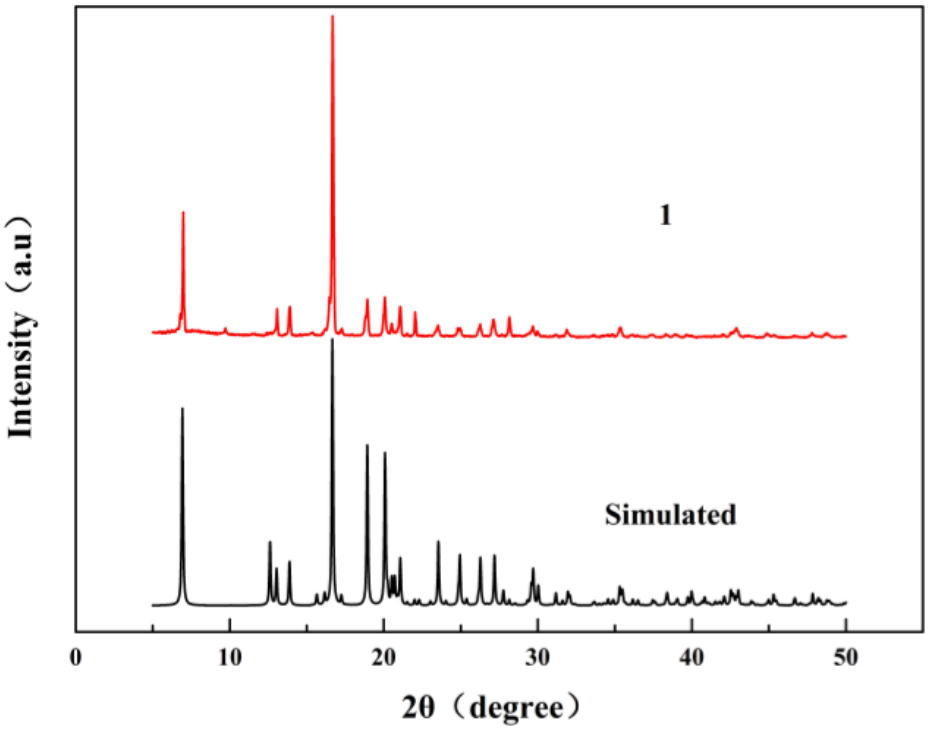

Fig.S3: Powder XRD patterns of simulated and compound **1**.

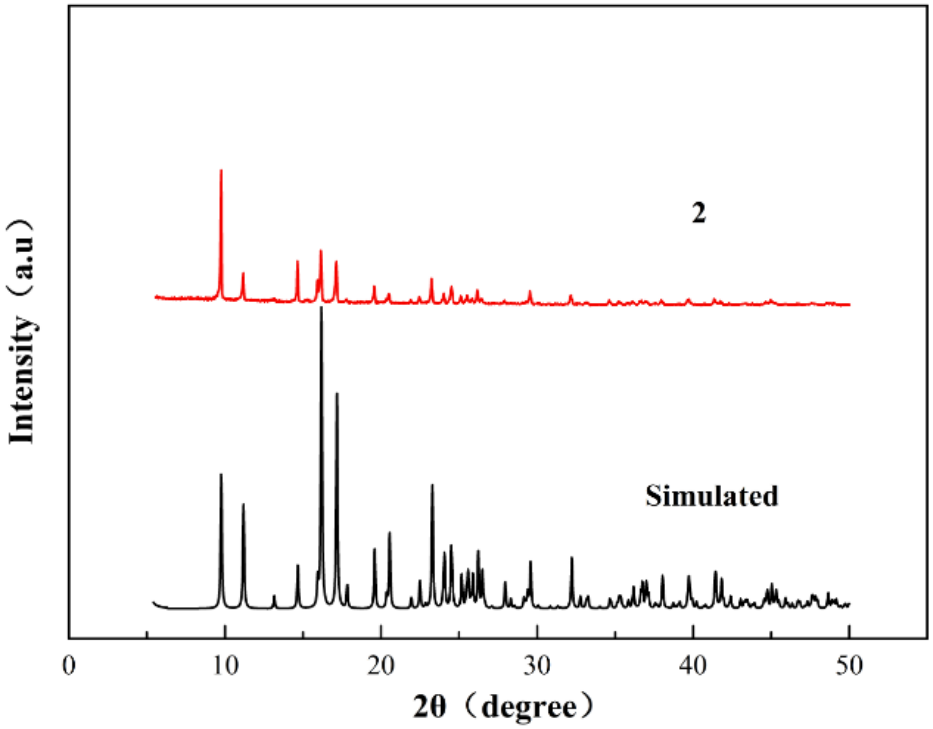

Fig.S4: Powder XRD patterns of simulated and compound **2**.

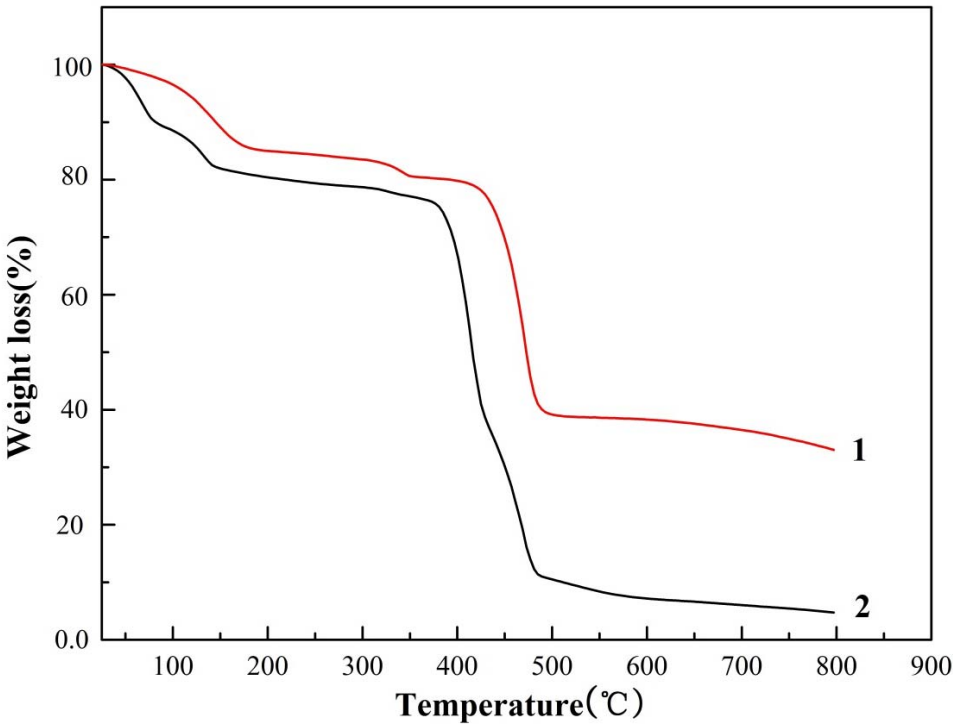

Fig.S5: TGA Plot of compound **1-2** in N_2 atmosphere.

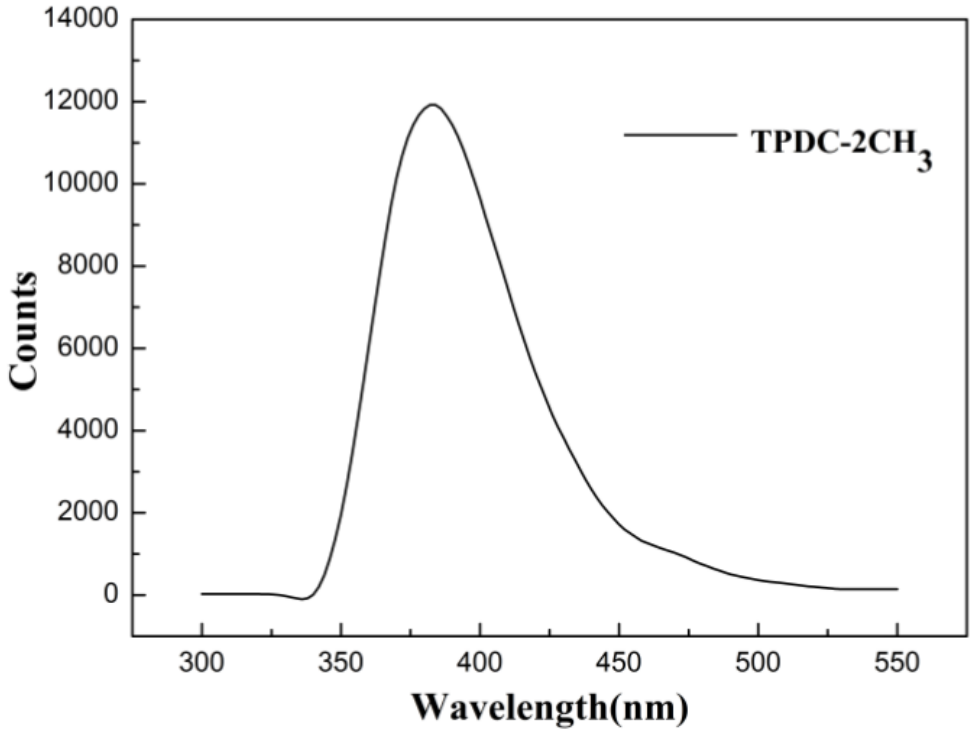

Fig.S6: Emission spectra of TPDC-$2CH_3$.

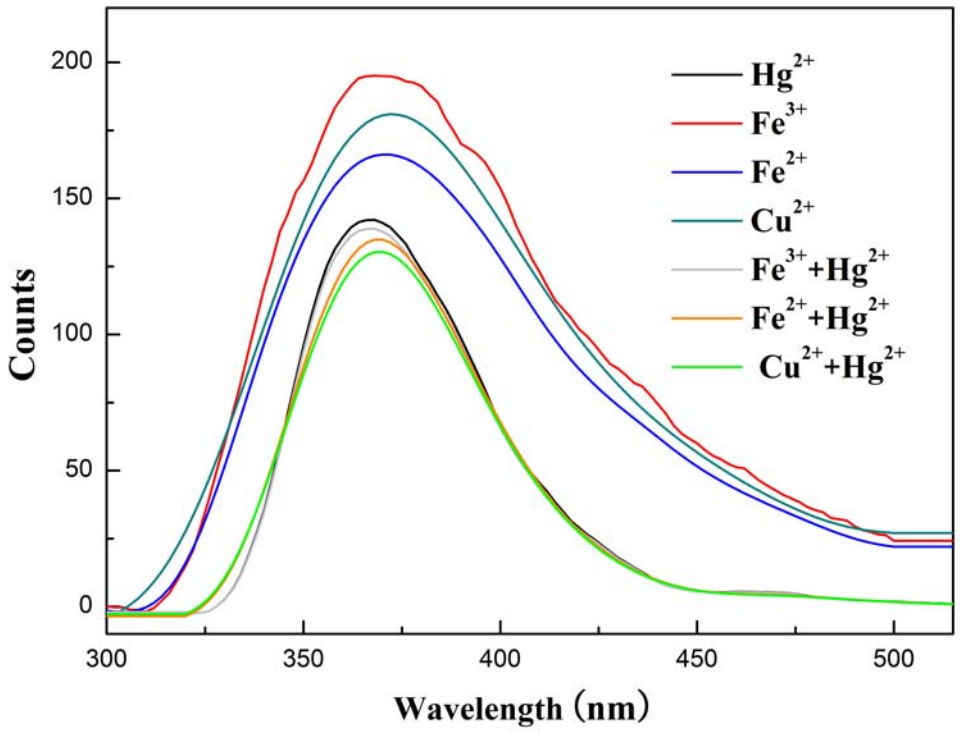

Fig.S7 Emission spectra of **1** in aqueous solutions of Hg^{2+}, Fe^{2+}, Fe^{3+},Cu^{2+}, mixed Hg^{2+} and Fe^{2+}, mixed Hg^{2+} and Fe^{3+}, and mixed Hg^{2+} and Cu^{2+}, respectively.

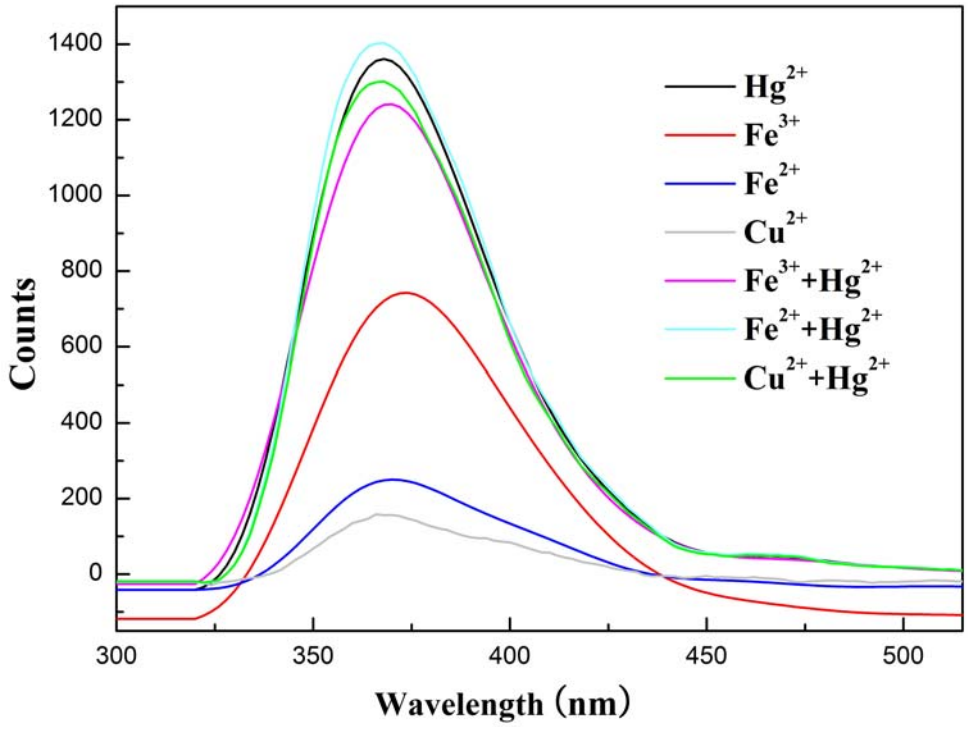

Fig.S8 Emission spectra of **2** in aqueous solutions of Hg^{2+}, Fe^{2+}, Fe^{3+},Cu^{2+}, mixed Hg^{2+} and Fe^{2+}, mixed Hg^{2+} and Fe^{3+}, and mixed Hg^{2+} and Cu^{2+}, respectively.

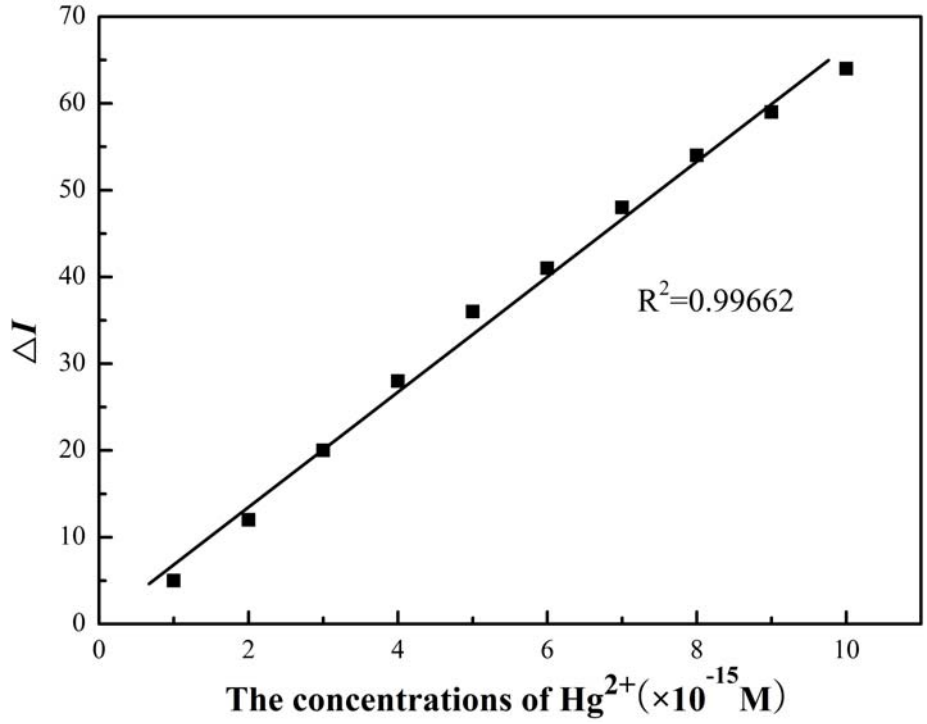

Fig.S9 The luminescence intensity (ΔI) vs Hg^{2+} ion with the low concentration t plot.

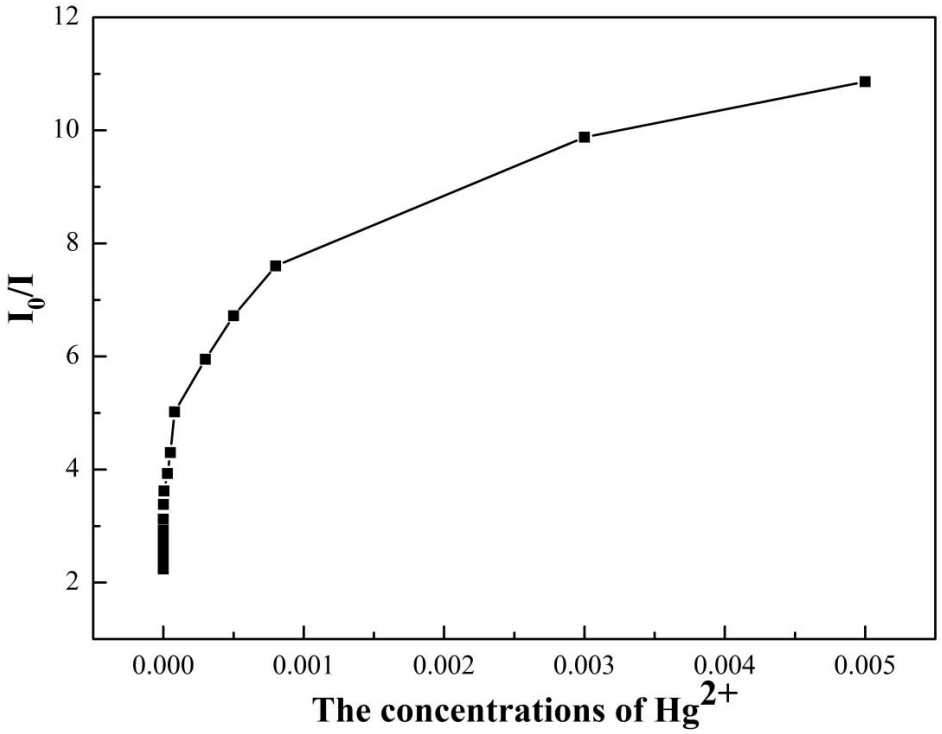

Fig.S10 The luminescence intensity vs Hg^{2+} ion concentration plot.

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

O1-Zn1	1.9736(15)	$O1^{\#1}$- Zn1	1.9736(15)
O1W-Zn1	2.0253(18)	$O1W^{\#1}$-Zn1	2.0252(18)
Zn1-C1	2.588(2)	Zn1-$C1^{\#1}$	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 -$C10^{\#2}$	1.387(3)	C9-C10	1.394(3)
C9-C11	1.502(4)	C10-$C8^{\#2}$	1.387(3)
C6A-C7A	1.385(8)	C6B-C7B	1.382(17)
O1-Zn1-$O1^{\#1}$	147.64(10)	O1-Zn1-O1W	93.48(7)
O1-Zn1-$O1W^{\#1}$	107.04(8)	$O1^{\#1}$-Zn1-O1W	107.03(8)
$O1^{\#1}$-Zn1-$O1W^{\#1}$	93.48(7)	$O1W^{\#1}$-Zn1-O1W	101.23(12)
O1-Zn1-$C1^{\#1}$	123.07(7)	O1-Zn1-C1	28.35(6)
$O1^{\#1}$-Zn1-$C1^{\#1}$	28.35(6)	$O1^{\#1}$-Zn1-C1	123.07(7)
$O1W^{\#1}$-Zn1-C1	104.06(7)	$O1W^{\#1}$-Zn1-$C1^{\#1}$	121.24(7)
O1W-Zn1-$C1^{\#1}$	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)$^{\#2}$	2.346(7)
Cd(1)-O(3)$^{\#2}$	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)$^{\#2}$	2.310(4)	Cd(1)-O(2)$^{\#2}$	2.465(4)
O(3)-Cd(1)-O(3)$^{\#2}$	164.1(2)	O(4)$^{\#2}$-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)$^{\#2}$-Cd(1)-O(1)	100.96(19)	O(3)$^{\#2}$-Cd(1)-O(2)	91.47(19)
O(3)-Cd(1)-O(1)$^{\#2}$	100.96(19)	O(1)-Cd(1)-O(2)	54.11(14)
O(3)$^{\#2}$-Cd(1)-O(1)$^{\#2}$	90.79(16)	O(1)$^{\#2}$-Cd(1)-O(2)	138.65(14)
O(1)-Cd(1)-O(1)$^{\#2}$	85.0(2)	O(4)$^{\#2}$-Cd(1)-O(2)	73.5(2)
O(3)-Cd(1)-O(4)$^{\#2}$	76.3(3)	O(4)-Cd(1)-O(2)	93.75(19)
O(3)$^{\#2}$-Cd(1)-O(4)$^{\#2}$	88.1(2)	O(3)-Cd(1)-O(2)$^{\#2}$	91.47(19)
O(1)-Cd(1)-O(4)$^{\#2}$	126.77(18)	O(3)$^{\#2}$-Cd(1)-O(2)$^{\#2}$	86.8(2)
O(1)$^{\#2}$-Cd(1)-O(4)$^{\#2}$	147.8(2)	O(1)-Cd(1)-O(2)$^{\#2}$	138.65(14)
O(3)-Cd(1)-O(4)	88.1(2)	O(1)$^{\#2}$-Cd(1)-O(2)$^{\#2}$	54.11(14)
O(3)$^{\#2}$-Cd(1)-O(4)	76.3(3)	O(4)$^{\#2}$-Cd(1)-O(2)$^{\#2}$	93.75(19)
O(1)-Cd(1)-O(4)	147.8(2)	O(4)-Cd(1)-O(2)$^{\#2}$	73.5(2)
O(1)$^{\#2}$-Cd(1)-O(4)	126.77(18)	O(2)-Cd(1)-O(2)$^{\#2}$	167.2(2)

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(3)-H(32)...O(1)$^{\#4}$	0.8500	2.06	2.691(6)	103.1
O(4)-H(41)...O(3)$^{\#5}$	0.8500	2.00	2.798(9)	156.8
O(4)-H(42)...O(3)$^{\#6}$	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)$^{\#3}$	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.