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Assembly of Zn/Cd coordination polymers containg helixes or polycatenane structures tuned by the tri-pyridyl-bis-amide ligands with different spacer: syntheses, structures, photoluminescent and photocatalytic properties †

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ELECTRONIC SUPPLEMENTARY INFORMATION

Table S1. Selected bond lengths (Å) and angles (°) for complexes **1**–**4**.

1

Zn(1)-O(1)	1.9462(18)	Zn(1)-O(2)	1.9606(17)
Zn(1)-N(5)#1	2.063(2)	Zn(1)-N(1)	2.084(2)
O(1)-Zn(1)-O(2)	102.97(8)	O(1)-Zn(1)-N(5)#1	121.56(9)
O(2)-Zn(1)-N(5)#1	109.48(8)	O(1)-Zn(1)-N(1)	110.07(9)
O(2)-Zn(1)-N(1)	115.04(8)	N(5)#1-Zn(1)-N(1)	98.37(8)

Symmetry transformations used to generate equivalent atoms: #1 $x-1, y, z$

2

Cd(1)-O(1)	2.2476(18)	Cd(1)-O(4)	2.292(2)
Cd(1)-O(3)	2.382(2)	Cd(1)-O(3)#1	2.614(2)
Cd(1)-N(5)	2.431(2)	Cd(1)-N(1)	2.353(2)
O(1)-Cd(1)-O(4)	140.31(8)	O(1)-Cd(1)-N(1)	131.30(7)
O(4)-Cd(1)-N(1)	86.11(7)	O(1)-Cd(1)-O(3)	91.12(7)
O(4)-Cd(1)-O(3)	92.93(7)	N(1)-Cd(1)-O(3)	102.31(8)
O(1)-Cd(1)-N(5)	85.93(8)	O(4)-Cd(1)-N(5)	82.32(8)
N(1)-Cd(1)-N(5)	87.98(8)	O(3)-Cd(1)-N(5)	168.40(7)
O(1)-Cd(1)-O(3)#1	90.75(7)	O(4)-Cd(1)-O(3)#1	53.52(6)
N(1)-Cd(1)-O(3)#1	137.95(7)	O(3)-Cd(1)-O(3)#1	72.18(7)
N(5)-Cd(1)-O(3)#1	96.61(7)		

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

3

Zn(1)-O(1)	1.927(3)	Zn(1)-O(2)	1.969(3)
Zn(1)-N(1)	2.057(3)	Zn(1)-N(5)#1	2.071(3)
O(1)-Zn(1)-O(2)	129.26(13)	O(1)-Zn(1)-N(1)	97.54(13)
O(2)-Zn(1)-N(1)	112.23(13)	O(1)-Zn(1)-N(5)#1	114.77(14)
O(2)-Zn(1)-N(5)#1	92.17(12)	N(1)-Zn(1)-N(5)#1	111.15(13)

Symmetry transformations used to generate equivalent atoms: #1 $-x, -y, -z$

4

Cd(1)-O(1)	2.3021(16)	Cd(1)-O(3)	2.3204(17)
Cd(1)-N(5)	2.3350(19)	Cd(1)-N(1)	2.365(2)
Cd(1)-O(2)	2.4528(16)	Cd(1)-O(4)	2.5283(17)
Cd(1)-N(3)#1	2.6091(19)		
O(1)-Cd(1)-O(3)	139.95(6)	O(1)-Cd(1)-N(5)	123.37(7)
O(3)-Cd(1)-N(5)	86.30(6)	O(1)-Cd(1)-N(1)	88.97(6)
O(3)-Cd(1)-N(1)	87.59(7)	N(1)-Cd(1)-N(1)	132.88(7)
O(1)-Cd(1)-O(2)	54.94(5)	O(3)-Cd(1)-O(2)	110.50(6)
N(5)-Cd(1)-O(2)	83.63(6)	N(1)-Cd(1)-O(2)	141.35(6)
O(1)-Cd(1)-O(4)	86.29(6)	O(3)-Cd(1)-O(4)	53.66(6)
N(5)-Cd(1)-O(4)	126.35(6)	N(1)-Cd(1)-O(4)	84.57(7)
O(2)-Cd(1)-O(4)	80.18(6)	O(1)-Cd(1)-N(3)#1	80.39(6)
O(3)-Cd(1)-N(3)#1	135.51(7)	N(5)-Cd(1)-N(3)#1	79.92(6)
N(1)-Cd(1)-N(3)#1	72.42(7)	O(2)-Cd(1)-N(3)#1	109.70(6)
O(4)-Cd(1)-N(3)#1	153.46(6)		

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

Table S2. The twist degrees of the $\mathbf{L_1}$ and $\mathbf{L_2}$ ligands in complexes **1–4**.

complex	**1**	**2**	**3**	**4**
θ_1	26.02	27.41	63.30	27.66
θ_2	52.92	52.99	10.23	72.15
θ_3	70.82	73.25	73.06	81.61

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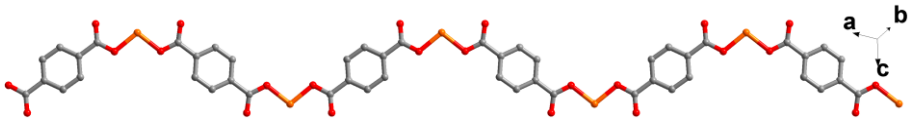

Fig. S1 The 1D zigzag Zn-BDC chain in complex **1**.

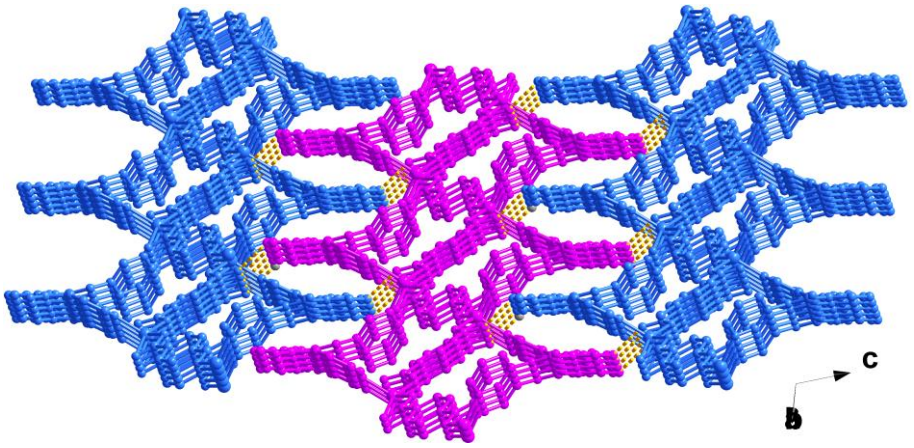

Fig. S2 The 3D supramolecular framework formed by hydrogen-bonding interactions.

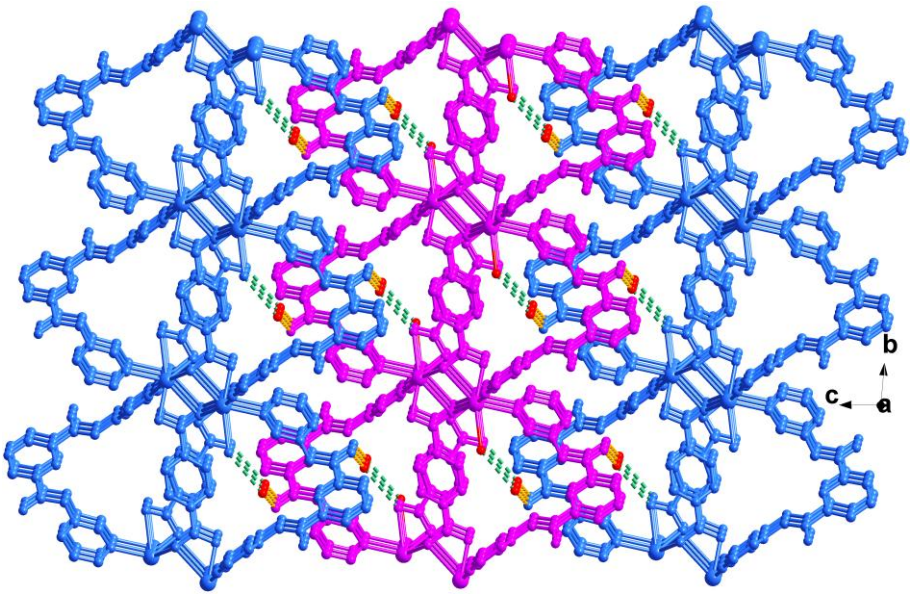

Fig. S3 The 3D supramolecular framework of **2** constructed by hydrogen-bonding interactions.

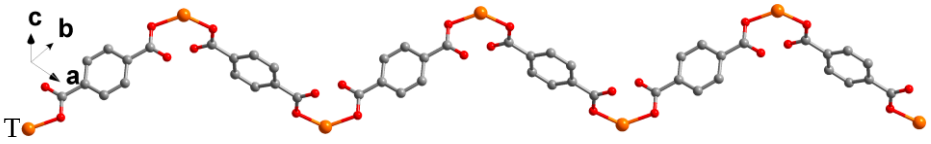

Fig. S4 1D Zn-BDC zigzag chain in complex **3**.

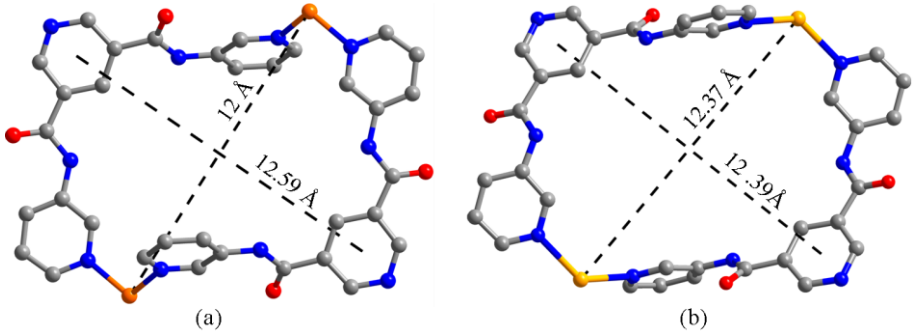

Fig. S5 (a) The special 28-membered loop of **3**. (b) The special 28-membered loop of **4**.

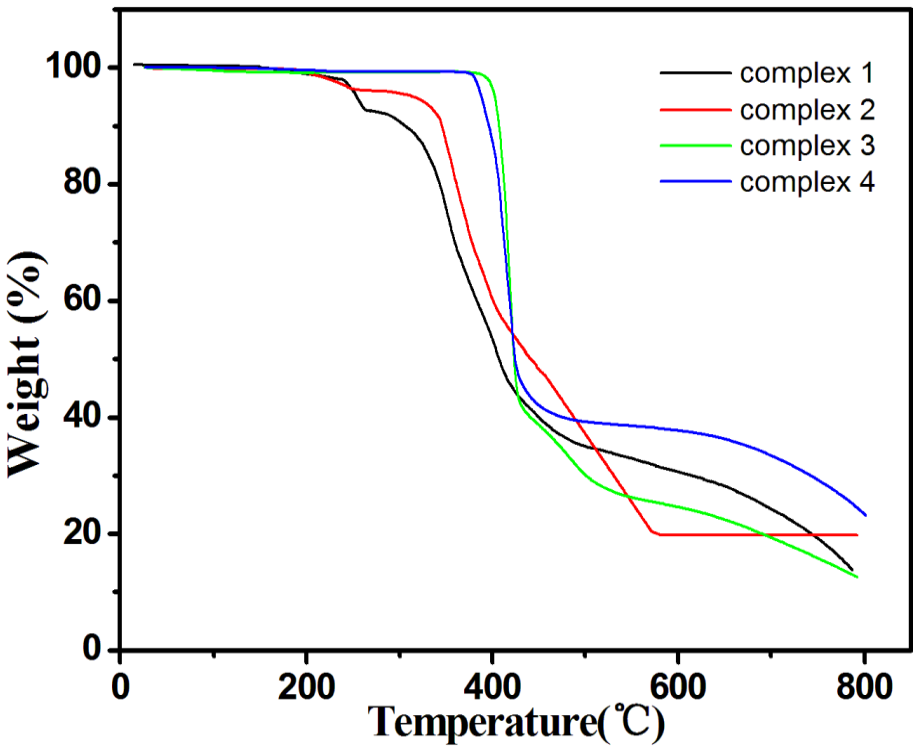

Fig. S6 The TG curves of complexes **1**–**4**.

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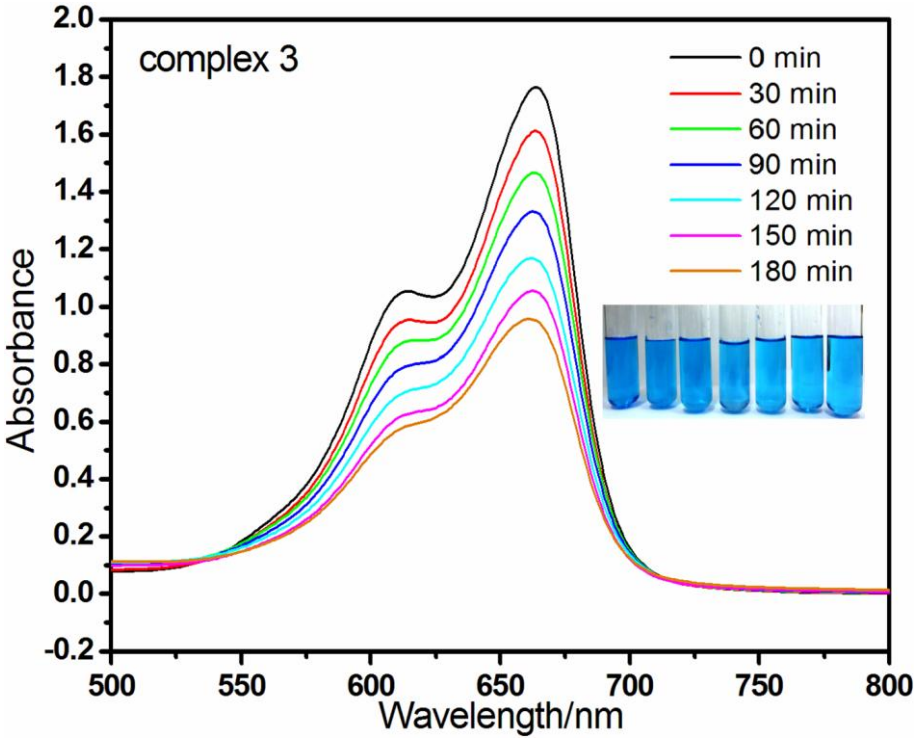

Fig. S7 Absorption spectra of the MB solution during the decomposition reaction under UV irradiation with the presence of complex **3**.

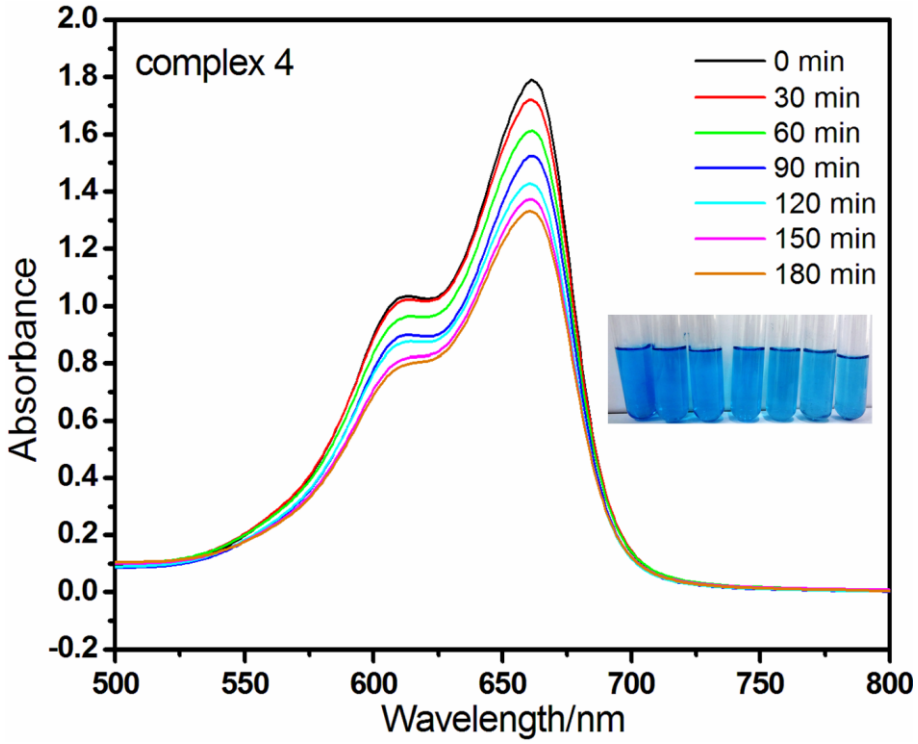

Fig. S8 Absorption spectra of the MB solution during the decomposition reaction under UV irradiation with the presence of complex **4**.

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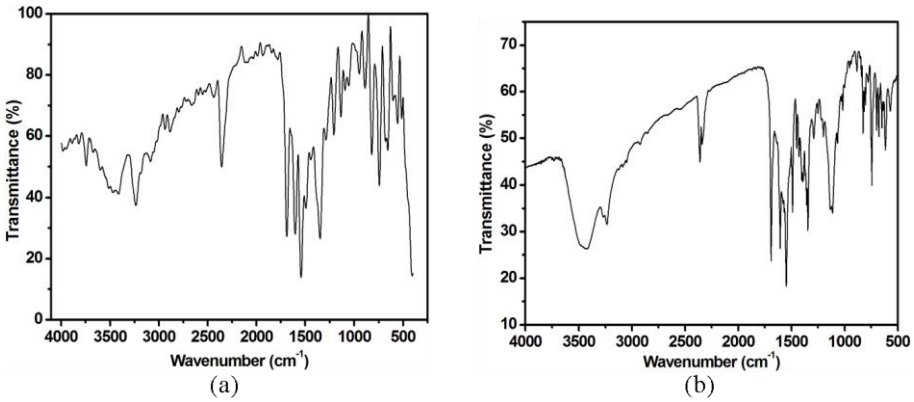

Fig. S9 (a) The IR spectrum of complex **1**. (b) The IR spectrum of complex **1** after a photocatalysis process.

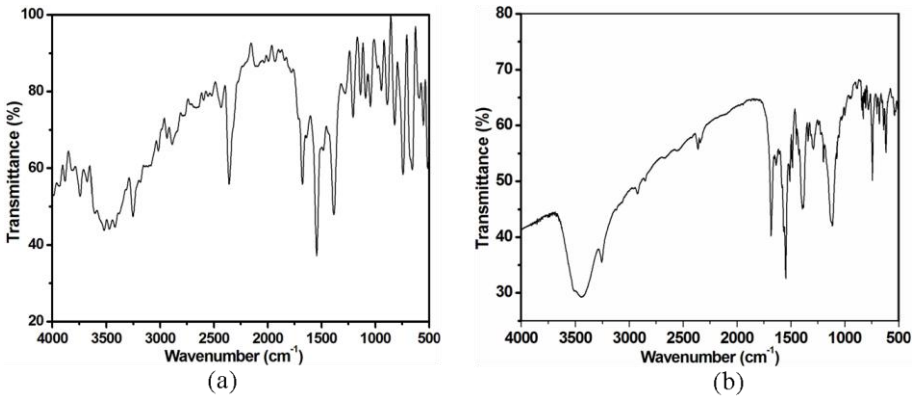

Fig. S10 (a) The IR spectrum of complex **2**. (b) The IR spectrum of complex **2** after a photocatalysis process.

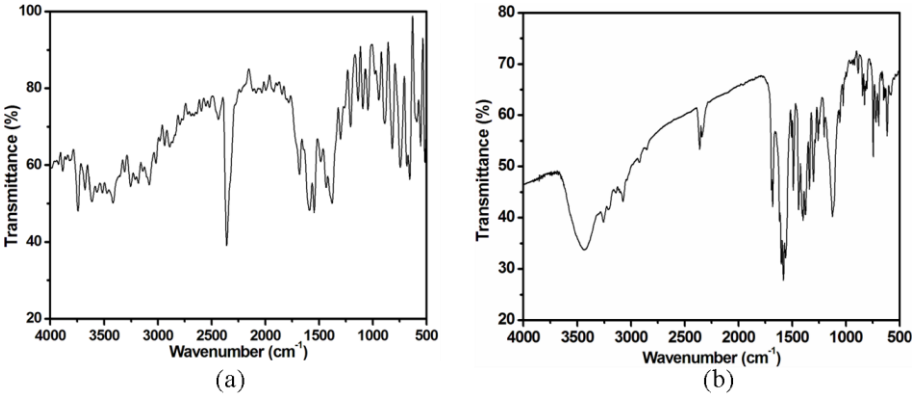

Fig. S11 (a) The IR spectrum of complex **3**. (b) The IR spectrum of complex **3** after a photocatalysis process.

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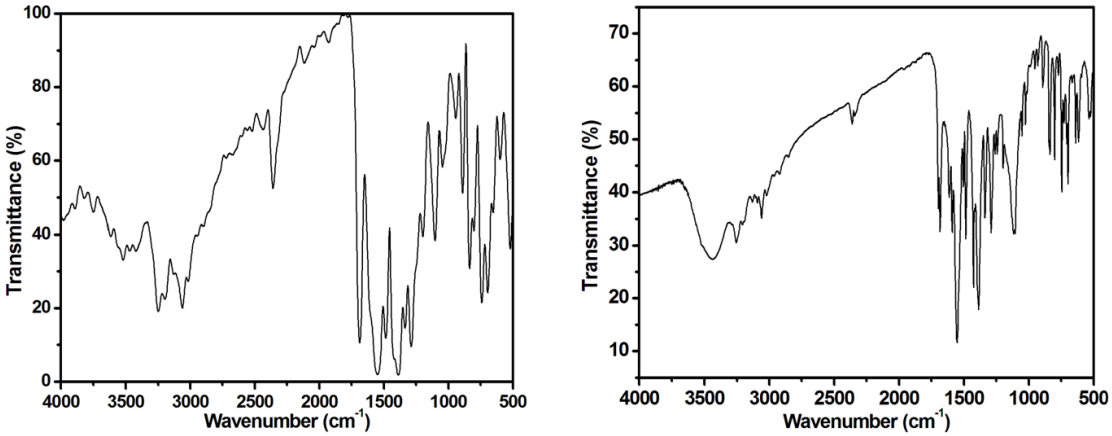

Fig. S12 (a) The IR spectrum of complex **4**. (b) The IR spectrum of complex **4** after a photocatalysis process.