

## Electronic supplementary information

### Syntheses, structures, and photoluminescent properties of Zn(II) and Cd(II) coordination polymers with flexible tripodal triazole-containing ligands

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**Table S1.** Selected bond distances (Å) and angles (°) for compounds **1-7**.

<b>1</b>			
Zn(1)-O(2)	1.963(5)	Zn(1)-O(3) <sup>#1</sup>	2.006(4)
Zn(1)-N(3)	2.041(5)	Zn(1)-N(6) <sup>#2</sup>	2.049(5)
Zn(1)-O(4) <sup>#1</sup>	2.484(5)		
O(2)-Zn(1)-O(3) <sup>#1</sup>	103.4(2)	O(2)-Zn(1)-N(3)	115.6(2)
O(3) <sup>#1</sup> -Zn(1)-N(3)	112.47(19)	O(2)-Zn(1)-N(6) <sup>#2</sup>	94.8(2)
O(3) <sup>#1</sup> -Zn(1)-N(6) <sup>#2</sup>	119.2(2)	N(3)-Zn(1)-N(6) <sup>#2</sup>	110.2(2)
O(2)-Zn(1)-O(4) <sup>#1</sup>	154.15(16)	O(3) <sup>#1</sup> -Zn(1)-O(4) <sup>#1</sup>	57.08(17)
N(3)-Zn(1)-O(4) <sup>#1</sup>	89.1(2)	N(6) <sup>#2</sup> -Zn(1)-O(4) <sup>#1</sup>	82.9(2)
<b>2</b>			
Cd(1)-O(1)	2.283(5)	Cd(1)-N(1)	2.304(5)
Cd(1)-N(9) <sup>#1</sup>	2.304(5)	Cd(1)-N(4) <sup>#2</sup>	2.334(5)
Cd(1)-O(4) <sup>#3</sup>	2.364(4)	Cd(1)-O(3) <sup>#3</sup>	2.575(5)
Cd(1)-O(1W)	2.608(11)		
O(1)-Cd(1)-N(1)	82.64(19)	O(1)-Cd(1)-N(9) <sup>#1</sup>	99.5(2)

N(1)-Cd(1)-N(9) <sup>#1</sup>	89.3(2)	O(1)-Cd(1)-N(4) <sup>#2</sup>	82.1(2)
N(1)-Cd(1)-N(4) <sup>#2</sup>	95.3(2)	N(9) <sup>#1</sup> -Cd(1)-N(4) <sup>#2</sup>	175.32(19)
O(1)-Cd(1)-O(4) <sup>#3</sup>	145.38(19)	N(1)-Cd(1)-O(4) <sup>#3</sup>	131.39(16)
N(9) <sup>#1</sup> -Cd(1)-O(4) <sup>#3</sup>	88.55(19)	N(4) <sup>#2</sup> -Cd(1)-O(4) <sup>#3</sup>	87.68(18)
O(1)-Cd(1)-O(3) <sup>#3</sup>	158.06(19)	N(1)-Cd(1)-O(3) <sup>#3</sup>	79.41(16)
N(9) <sup>#1</sup> -Cd(1)-O(3) <sup>#3</sup>	92.77(19)	N(4) <sup>#2</sup> -Cd(1)-O(3) <sup>#3</sup>	87.10(18)
O(4) <sup>#3</sup> -Cd(1)-O(3) <sup>#3</sup>	52.23(14)	O(1)-Cd(1)-O(1W)	70.7(3)
N(1)-Cd(1)-O(1W)	147.5(2)	N(9) <sup>#1</sup> -Cd(1)-O(1W)	77.5(3)
N(4) <sup>#2</sup> -Cd(1)-O(1W)	99.0(3)	O(4) <sup>#3</sup> -Cd(1)-O(1W)	78.5(2)
O(3) <sup>#3</sup> -Cd(1)-O(1W)	130.1(2)		

### 3

Zn(1)-O(7) <sup>#1</sup>	1.956(6)	Zn(1)-O(1)	1.980(6)
Zn(1)-N(1)	1.990(8)	Zn(1)-N(6) <sup>#2</sup>	2.054(8)
Zn(2)-O(5)	1.929(6)	Zn(2)-O(3)	1.967(6)
Zn(2)-O(1W)	1.985(8)	Zn(2)-N(9) <sup>#3</sup>	1.989(10)
O(7) <sup>#1</sup> -Zn(1)-O(1)	115.9(3)	O(7) <sup>#1</sup> -Zn(1)-N(1)	113.2(3)
O(1)-Zn(1)-N(1)	120.3(3)	O(7) <sup>#1</sup> -Zn(1)-N(6) <sup>#2</sup>	101.9(3)
O(1)-Zn(1)-N(6) <sup>#2</sup>	93.4(3)	N(1)-Zn(1)-N(6) <sup>#2</sup>	107.8(3)
O(5)-Zn(2)-O(3)	110.6(3)	O(5)-Zn(2)-O(1W)	103.8(4)
O(3)-Zn(2)-O(1W)	96.6(3)	O(5)-Zn(2)-N(9) <sup>#3</sup>	117.4(3)
O(3)-Zn(2)-N(9) <sup>#3</sup>	119.8(3)	O(1W)-Zn(2)-N(9) <sup>#3</sup>	104.6(4)

### 4

Cd(1)-O(8) <sup>#1</sup>	2.209(4)	Cd(1)-O(6) <sup>#2</sup>	2.226(3)
Cd(1)-O(3)	2.298(3)	Cd(1)-N(5)	2.317(4)
Cd(1)-N(3) <sup>#3</sup>	2.318(5)	Cd(1)-O(4)	2.498(5)
Cd(2)-O(7) <sup>#4</sup>	2.238(3)	Cd(2)-O(5) <sup>#5</sup>	2.250(3)
Cd(2)-N(9) <sup>#5</sup>	2.281(5)	Cd(2)-O(1)	2.334(3)
Cd(2)-N(1)	2.357(4)	Cd(2)-O(2)	2.439(3)
O(8) <sup>#1</sup> -Cd(1)-O(6) <sup>#2</sup>	119.24(14)	O(8) <sup>#1</sup> -Cd(1)-O(3)	96.43(13)
O(6) <sup>#2</sup> -Cd(1)-O(3)	144.30(13)	O(8) <sup>#1</sup> -Cd(1)-N(3) <sup>#3</sup>	100.13(16)
O(6) <sup>#2</sup> -Cd(1)-N(3) <sup>#3</sup>	86.44(15)	O(3)-Cd(1)-N(3) <sup>#3</sup>	88.92(15)
O(8) <sup>#1</sup> -Cd(1)-N(5)	96.29(19)	O(6) <sup>#2</sup> -Cd(1)-N(5)	86.94(17)
O(3)-Cd(1)-N(5)	87.67(17)	N(3) <sup>#3</sup> -Cd(1)-N(5)	163.50(19)
O(8) <sup>#1</sup> -Cd(1)-O(4)	150.71(13)	O(6) <sup>#2</sup> -Cd(1)-O(4)	89.99(12)
O(3)-Cd(1)-O(4)	54.31(11)	N(3) <sup>#3</sup> -Cd(1)-O(4)	82.31(14)

N(5)-Cd(1)-O(4)	82.59(17)	O(7) <sup>#4</sup> -Cd(2)-O(5) <sup>#5</sup>	122.57(13)
O(7) <sup>#4</sup> -Cd(2)-N(9) <sup>#5</sup>	92.37(16)	O(5) <sup>#5</sup> -Cd(2)-N(9) <sup>#5</sup>	88.63(16)
O(7) <sup>#4</sup> -Cd(2)-O(1)	144.38(13)	O(5) <sup>#5</sup> -Cd(2)-O(1)	92.82(13)
N(9) <sup>#5</sup> -Cd(2)-O(1)	92.49(16)	O(7) <sup>#4</sup> -Cd(2)-N(1)	88.59(14)
O(5) <sup>#5</sup> -Cd(2)-N(1)	82.72(14)	N(9) <sup>#5</sup> -Cd(2)-N(1)	170.29(17)
O(1)-Cd(2)-N(1)	92.34(14)	O(7) <sup>#4</sup> -Cd(2)-O(2)	89.95(12)
O(5) <sup>#5</sup> -Cd(2)-O(2)	147.23(12)	N(9) <sup>#5</sup> -Cd(2)-O(2)	94.46(17)
O(1)-Cd(2)-O(2)	54.49(12)	N(1)-Cd(2)-O(2)	95.21(13)

## 5

Zn(1)-O(3)	1.973(4)	Zn(1)-O(5)	1.974(5)
Zn(1)-N(10)	2.017(6)	Zn(1)-N(17) <sup>#1</sup>	2.062(5)
Zn(2)-O(11)	1.956(4)	Zn(2)-O(9)	1.963(4)
Zn(2)-N(4)	2.018(5)	Zn(2)-N(15) <sup>#2</sup>	2.035(5)
Zn(3)-O(2)	1.959(4)	Zn(3)-O(8) <sup>#3</sup>	1.962(5)
Zn(3)-N(1)	2.020(5)	Zn(3)-N(8) <sup>#4</sup>	2.024(5)
O(3)-Zn(1)-O(5)	106.9(2)	O(3)-Zn(1)-N(10)	113.2(2)
O(5)-Zn(1)-N(10)	120.8(2)	O(3)-Zn(1)-N(17) <sup>#1</sup>	110.7(2)
O(5)-Zn(1)-N(17) <sup>#1</sup>	92.2(2)	N(10)-Zn(1)-N(17) <sup>#1</sup>	111.0(2)
O(11)-Zn(2)-O(9)	106.6(2)	O(11)-Zn(2)-N(4)	109.3(2)
O(9)-Zn(2)-N(4)	114.8(2)	O(11)-Zn(2)-N(15) <sup>#2</sup>	92.0(2)
O(9)-Zn(2)-N(15) <sup>#2</sup>	115.6(2)	N(4)-Zn(2)-N(15) <sup>#2</sup>	115.4(2)
O(2)-Zn(3)-O(8) <sup>#3</sup>	105.4(2)	O(2)-Zn(3)-N(1)	115.8(2)
O(8) <sup>#3</sup> -Zn(3)-N(1)	92.3(2)	O(2)-Zn(3)-N(8) <sup>#4</sup>	110.4(2)
O(8) <sup>#3</sup> -Zn(3)-N(8) <sup>#4</sup>	110.3(2)	N(1)-Zn(3)-N(8) <sup>#4</sup>	120.0(2)

## 6

Zn(1)-O(3) <sup>#1</sup>	1.928(3)	Zn(1)-O(1)	1.936(4)
Zn(1)-N(7) <sup>#2</sup>	2.015(4)	Zn(1)-N(1)	2.028(5)
O(3) <sup>#1</sup> -Zn(1)-O(1)	111.86(16)	O(3) <sup>#1</sup> -Zn(1)-N(7) <sup>#2</sup>	119.02(17)
O(1)-Zn(1)-N(7) <sup>#2</sup>	97.58(17)	O(3) <sup>#1</sup> -Zn(1)-N(1)	109.99(18)
O(1)-Zn(1)-N(1)	109.97(17)	N(7) <sup>#2</sup> -Zn(1)-N(1)	107.67(18)

## 7

Cd(1)-O(1)	2.264(3)	Cd(1)-N(8) <sup>#1</sup>	2.307(3)
Cd(1)-N(5) <sup>#2</sup>	2.336(3)	Cd(1)-O(4) <sup>#3</sup>	2.390(3)
Cd(1)-O(3) <sup>#3</sup>	2.427(3)	Cd(1)-N(1)	2.432(4)
O(1)-Cd(1)-N(8) <sup>#1</sup>	87.08(11)	O(1)-Cd(1)-N(5) <sup>#2</sup>	102.28(11)

N(8) <sup>#1</sup> -Cd(1)-N(5) <sup>#2</sup>	168.36(11)	O(1)-Cd(1)-O(4) <sup>#3</sup>	171.43(10)
N(8) <sup>#1</sup> -Cd(1)-O(4) <sup>#3</sup>	84.44(10)	N(5) <sup>#2</sup> -Cd(1)-O(4) <sup>#3</sup>	86.01(11)
O(1)-Cd(1)-O(3) <sup>#3</sup>	126.37(11)	N(8) <sup>#1</sup> -Cd(1)-O(3) <sup>#3</sup>	87.45(10)
N(5) <sup>#2</sup> -Cd(1)-O(3) <sup>#3</sup>	92.39(11)	O(4) <sup>#3</sup> -Cd(1)-O(3) <sup>#3</sup>	54.45(10)

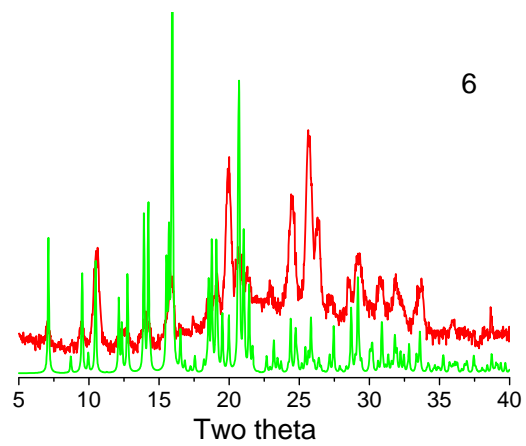
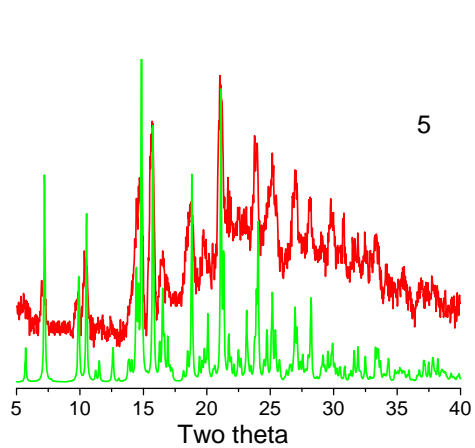
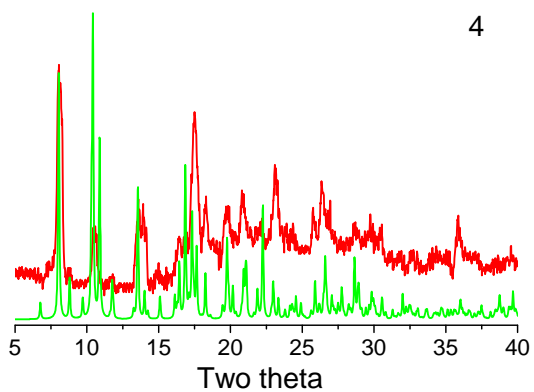
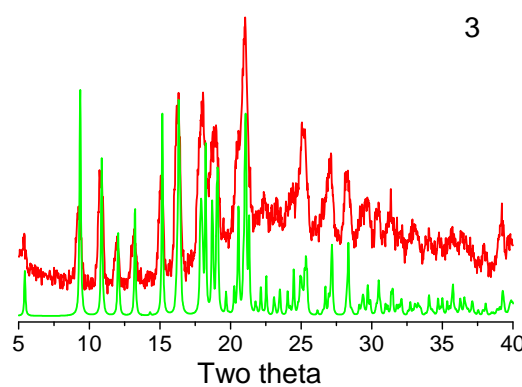
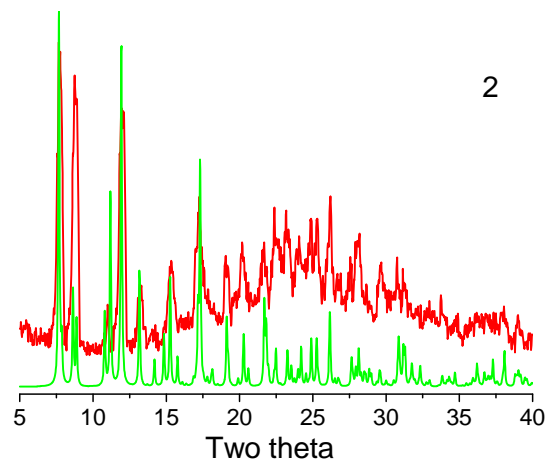
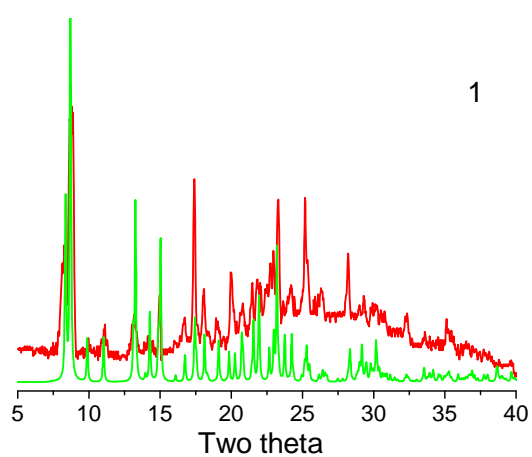
Symmetry codes for **1**: <sup>#1</sup> -x+1, -y+1, -z+1; <sup>#2</sup> x, y+1, z+1. For **2**: <sup>#1</sup> x, -y, z+1/2, <sup>#2</sup> x-1/2, y-1/2, z; <sup>#3</sup> -x+3/2, y+1/2, -z+3/2. For **3**: <sup>#1</sup> -x+2, y-1/2, -z+3/2; <sup>#2</sup> x, y-1, z; <sup>#3</sup> -x+2, -y, -z+1. For **4**: <sup>#1</sup> x+1/2, -y+1/2, z+1/2; <sup>#2</sup> x-1, y, z; <sup>#3</sup> -x-1/2, y-1/2, -z+1/2; <sup>#4</sup> x+1, y, z; <sup>#5</sup> x-1/2, -y+1/2, z-1/2. For **5**: <sup>#1</sup> -x+1, -y+1, -z+1; <sup>#2</sup> -x+2, -y+1, -z+2; <sup>#3</sup> x+1, y, z+1; <sup>#4</sup> -x+3, -y, -z+2. For **6**: <sup>#1</sup> -x+1, -y, -z+1; <sup>#2</sup> x, y, z+1. For **7**: <sup>#1</sup> x-1, y, z; <sup>#2</sup> y+3/2, -x+3/2, z+1/4; <sup>#3</sup> x-1/2, -y+1/2, -z+1/4.

**Table S2.** Hydrogen-bonding parameters for **3**, **5** and **6** (in Å and deg)

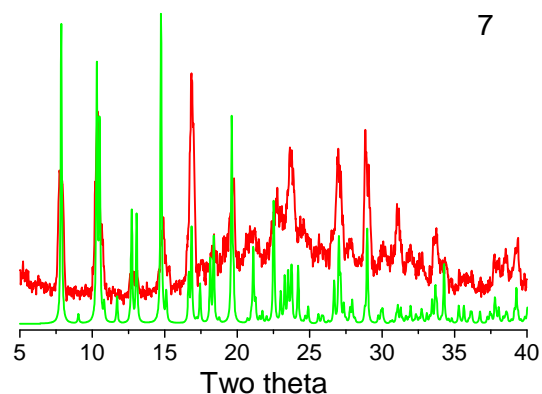
	D-H...A	d(D-H)	d(D...A)	∠(D-H...A)
<b>3</b>				
O(1W)-H(1B)...O(6) <sup>#4</sup>	0.89(2)	1.76(6)	2.616(10)	160(15)
O(1W)-H(1A)...O(8) <sup>#5</sup>	0.89(2)	1.83(5)	2.692(9)	162(15)
<b>5</b>				
O(1W)-H(1B)...O(12)	0.90(2)	2.4(2)	3.032(17)	128(21)
O(1W)-H(1A)...O(1) <sup>#5</sup>	0.91(2)	2.5(3)	3.11(2)	124(25)
<b>6</b>				
O(1W)-H(1B)...O(2)	0.87(2)	2.05(12)	2.836(11)	150(21)
O(1W)-H(1A)...N(4) <sup>#3</sup>	0.87(2)	2.27(19)	2.99(2)	140(25)

Symmetry codes for **3**: <sup>#4</sup> -x+3, -y, -z+2; <sup>#5</sup> x, -y+1/2, z-1/2. For **5**: <sup>#5</sup> -x+2, -y, -z+2.

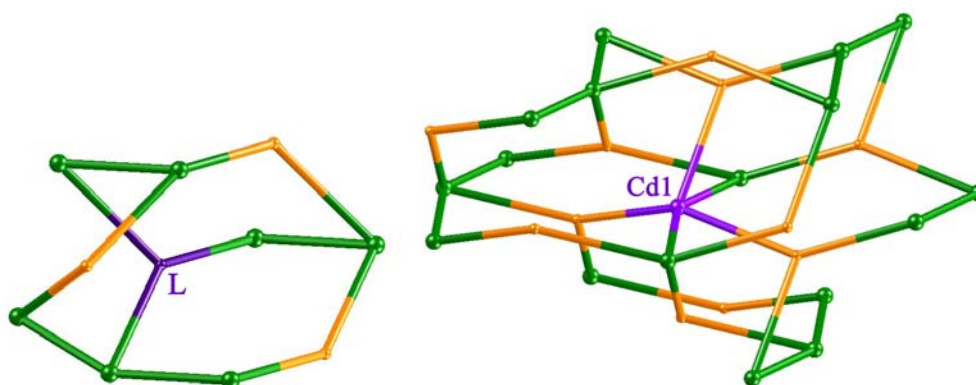
For **6**: <sup>#3</sup> -x, -y+1, -z.



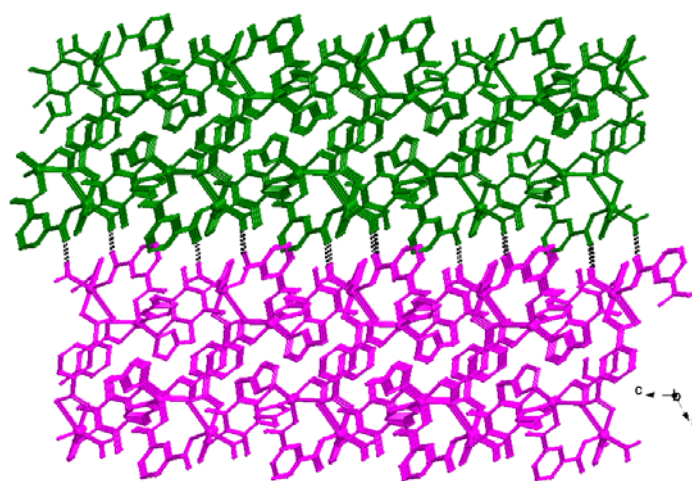
7



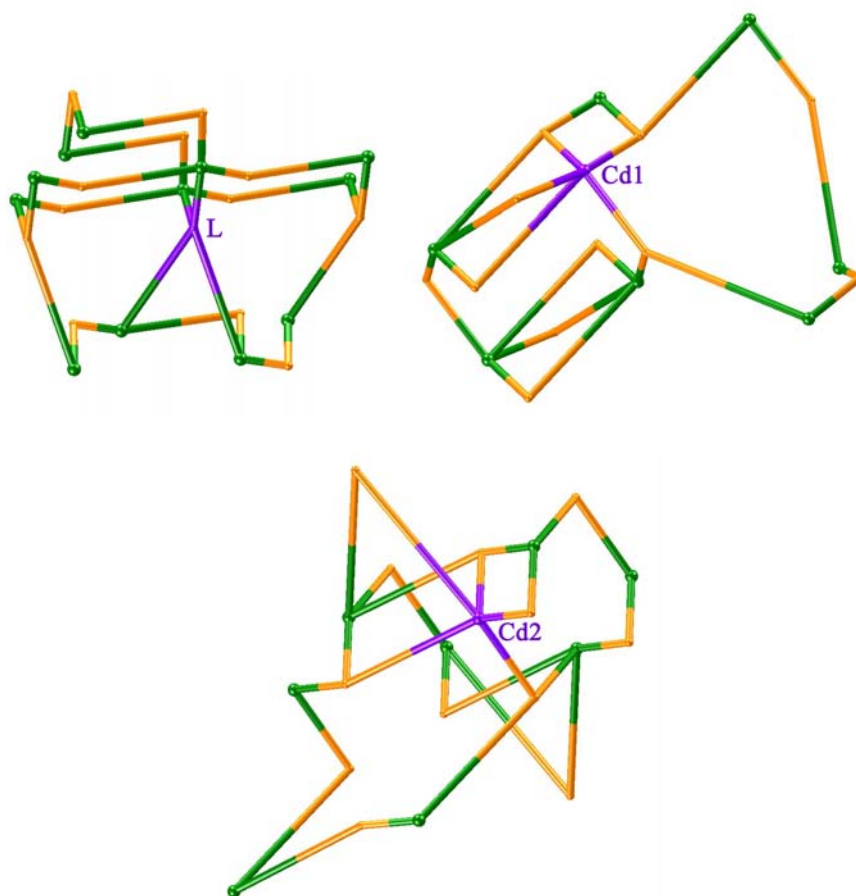
**Fig. S1** The simulated (green) and experimental (red) XRPD patterns for the compounds **1-7** (the diffraction peaks of both simulated and experimental patterns match well in relevant positions, indicating that the phase purities of compounds **1-7** are good).



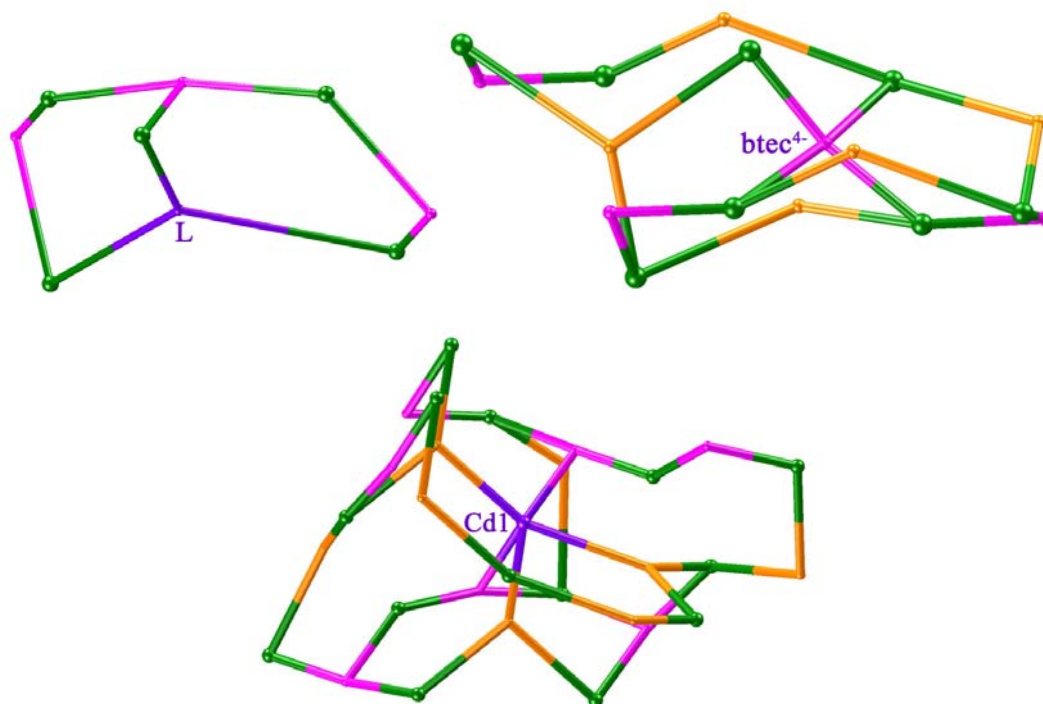
**Fig. S2.** View of the 3- and 5-connected nodes of **2**.



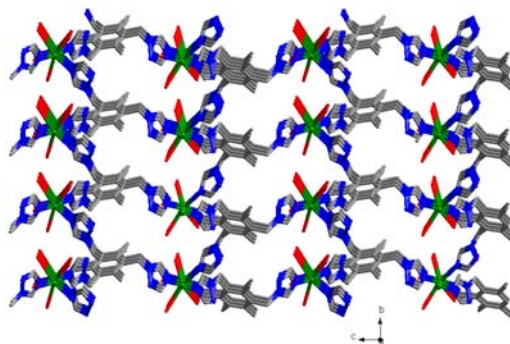
**Fig. S3.** View of the 3D supramolecular architecture of **3** connected by hydrogen bonding interactions of neighboring layers.



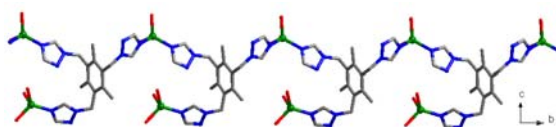
**Fig. S4.** View of the 4-connected and 5-connected nodes of **4**.



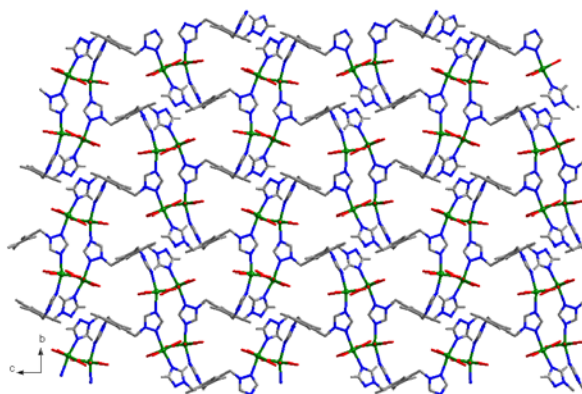
**Fig. S5.** View of the 3-connected, 4-connected and 5-connected nodes of **7**.



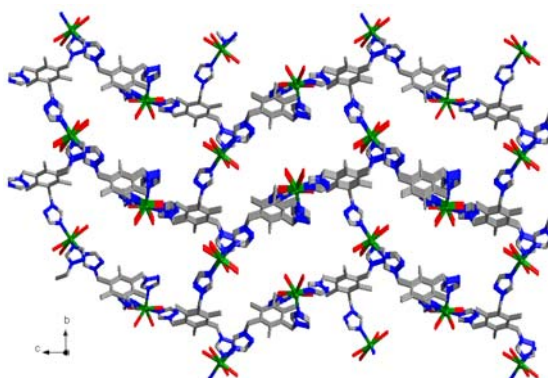
(a)



(b)



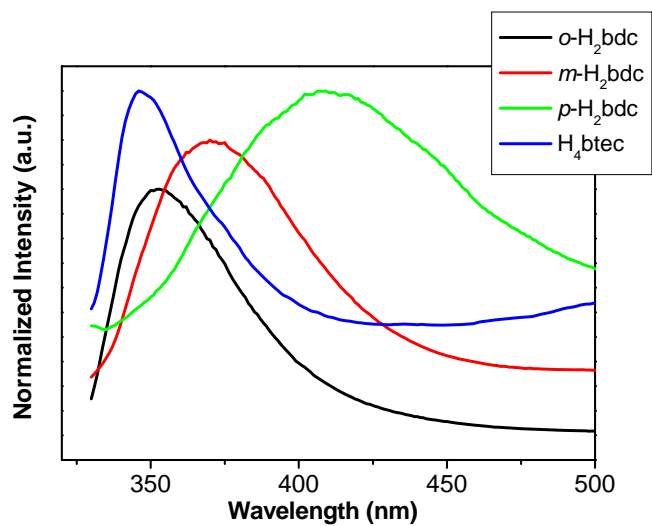
(c)



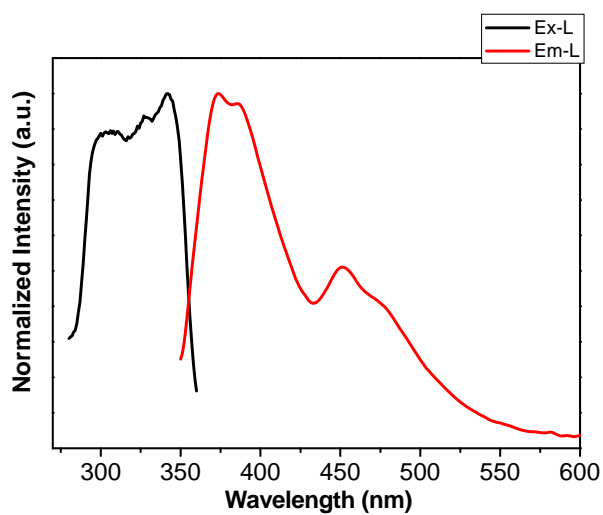
(d)

**Fig. S6.** View of the L connected M(II) structures in **2** (a), **3** (b), **4** (c), and **7** (d).





(a)



(b)

**Fig. S7.** (a) Solid-state emission spectra of free *o*-H<sub>2</sub>bdc, *m*-H<sub>2</sub>bdc, *p*-H<sub>2</sub>bdc, H<sub>4</sub>btcc ligands at room temperature. (b) The excitation and emission spectra of L ligand at room temperature.