Electronic Supplementary Information

Diverse topologies of seven d^{10} coordination polymers constructed from a long ligand and different carboxylates

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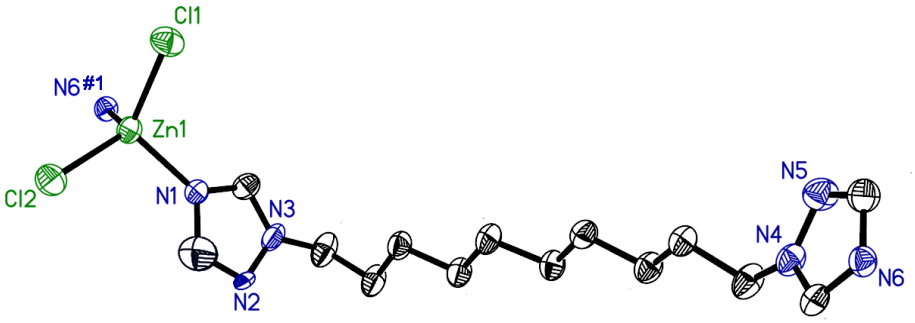
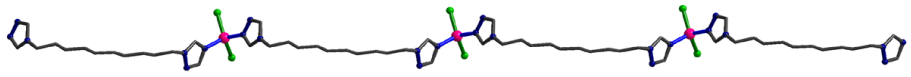
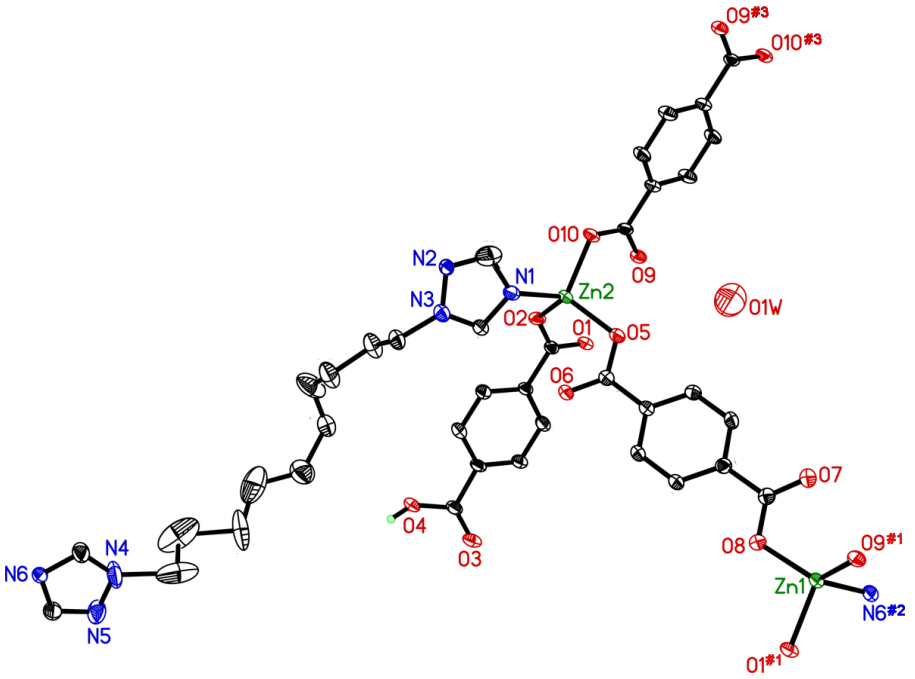


(a)

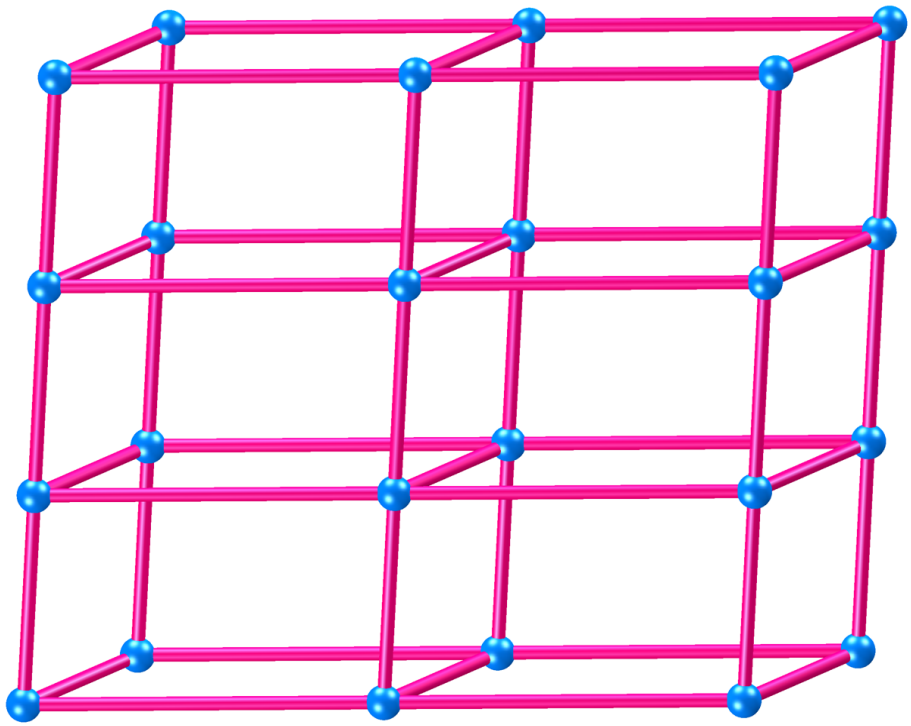


(b)

Fig. S1 (a) The coordination environment of the Zn(II) center in **1**. All H atoms are omitted for clarity. (b) View of 1D polymeric chain of **1**. Symmetry code: $^{\#1}$ x-1, y+1, z.



(a)



(b)

Fig. S2 (a) The coordination environments of the Zn(II) centers in **2**. (b) A schematic representation of the 5-connected topology of **2**. Symmetry code: $^{\#1}$ x-1,y+1,z; $^{\#2}$ x,y+1,z-1; $^{\#3}$ -x+1,-y,-z+1.

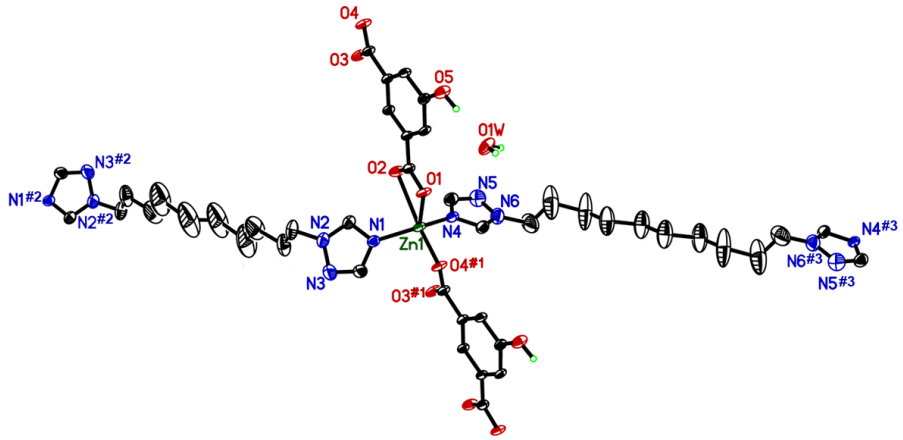
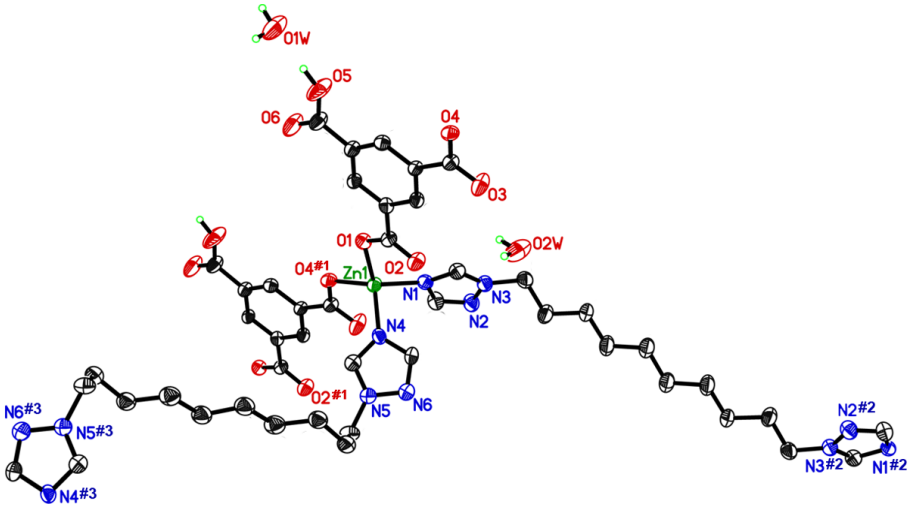


Fig. S3 The coordination environment of the Zn(II) center in **3**. Symmetry code: $^{\#1}$ x, y-1, z; $^{\#2}$ -x+3,-y+1,-z; $^{\#3}$ -x+1,-y,-z+2.

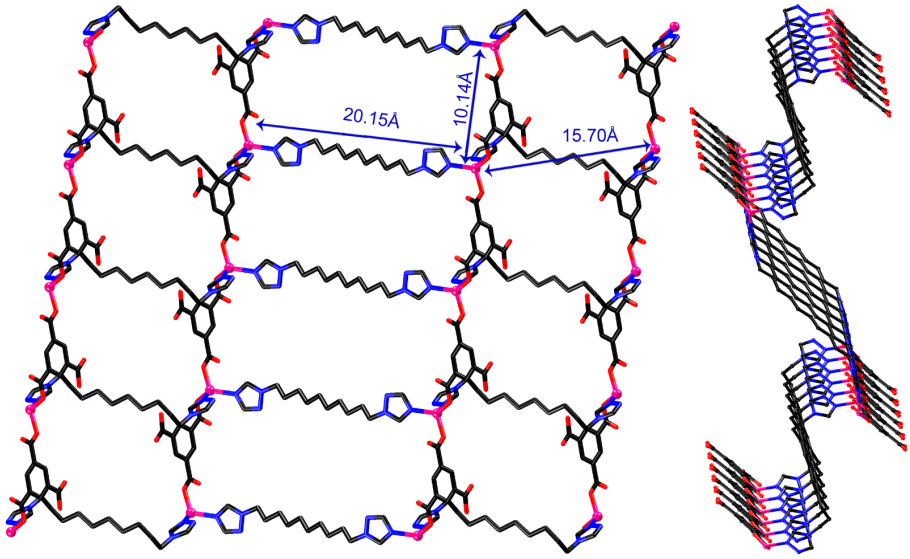
Structure of $[Zn_2(btd)_2(HL3)_2]\cdot 4H_2O$ (4)

The structure of **4** contains one Zn(II) center, two half btd ligands, one HL3 anion and two uncoordinated water molecules (Fig. S1a). The Zn(II) center is four-coordinated by two oxygen atoms from two HL3 anions [Zn1-O1 = 1.973(5) and Zn1-O4$^{\#1}$ =

1.978(5) Å], and two nitrogen atoms from two btd ligands [Zn1-N1 = 2.048(6) and Zn1-N4 = 2.013(7) Å] in a distorted tetrahedral coordination geometries. The adjacent Zn(II) centers are bridged by HL3 anions to give a 1D chain, and the chains are further linked by btd ligands to yield a wave layer with the HL3 ligand hanged on the both sides of the layer (Fig. S1b). There are two kinds of large windows of $Zn_2(L3)_2(btd)_2$ in the resulting layer, which are composed of two Zn(II) atoms, two L3 anions and two btd ligands with the dimensions of 10.14 ×19.70 $Å^2$ and 10.14 × 20.25 $Å^2$ (based on the Zn···Zn distance) respectively. Further, each net is penetrated by another two adjacent nets to result a 2D → 2D interpenetrating framework (Fig. S1c). Interestingly, each sheet is simultaneously interdigitated by one adjacent non-interpenetrated layer which results the 2D → 2D → 3D entanglement (Fig. S1d).



(a)



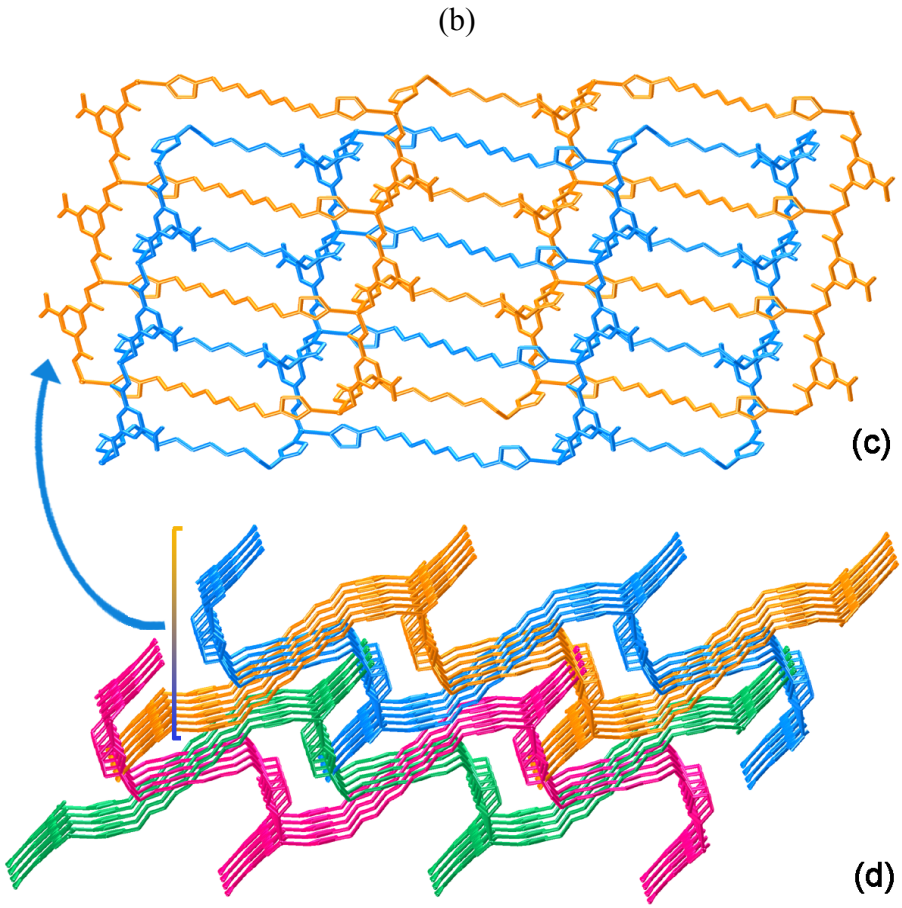


Fig. S4 (a) The coordination environment of the Zn(II) center in **4**. (b) The 2D wave layer in **4**. (c) The 2D → 2D interpenetrating network. (d) The 2D → 2D → 3D interdigitated framework. Symmetry code: #1 x+1, y, z; #2 -x, -y+2, -z; #3 -x+1, -y, -z+2.

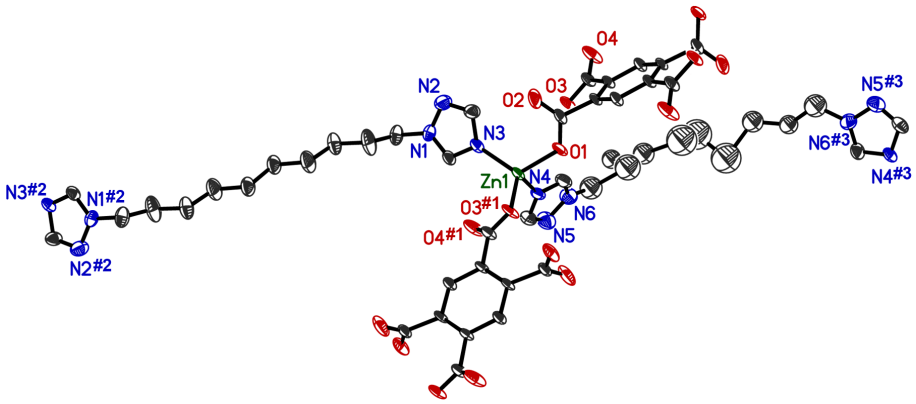


Fig. S5 The coordination environment of the Zn(II) center in **5**. Symmetry code: #1 -x+1/2, y+1/2, -z+3/2; #2 -x+1, -y+1, -z+1; #3 -x, y, -z+3/2.

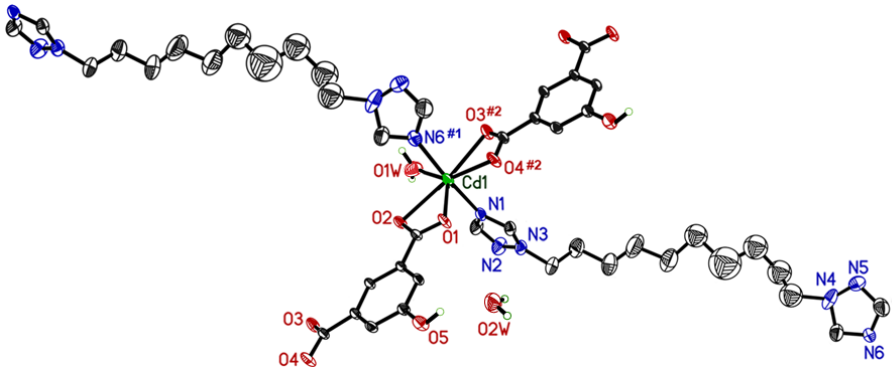
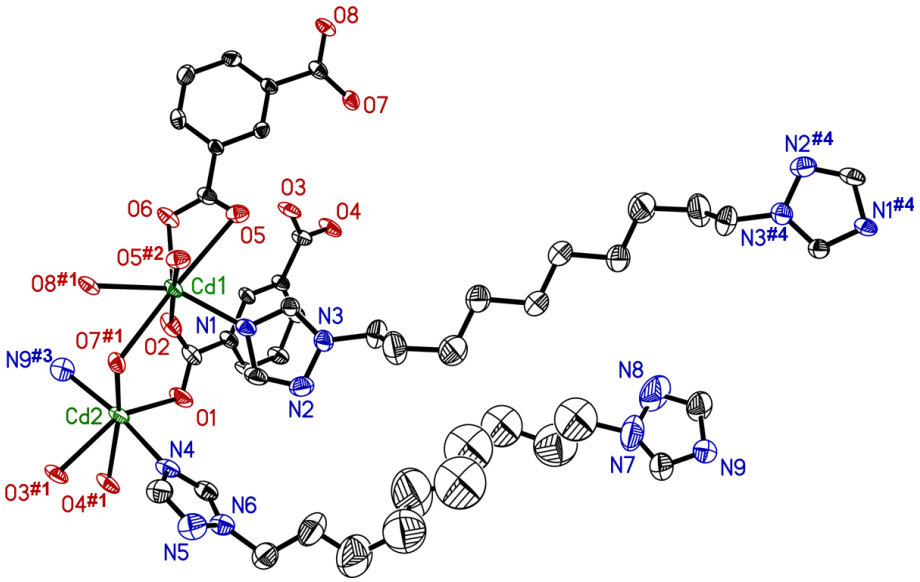
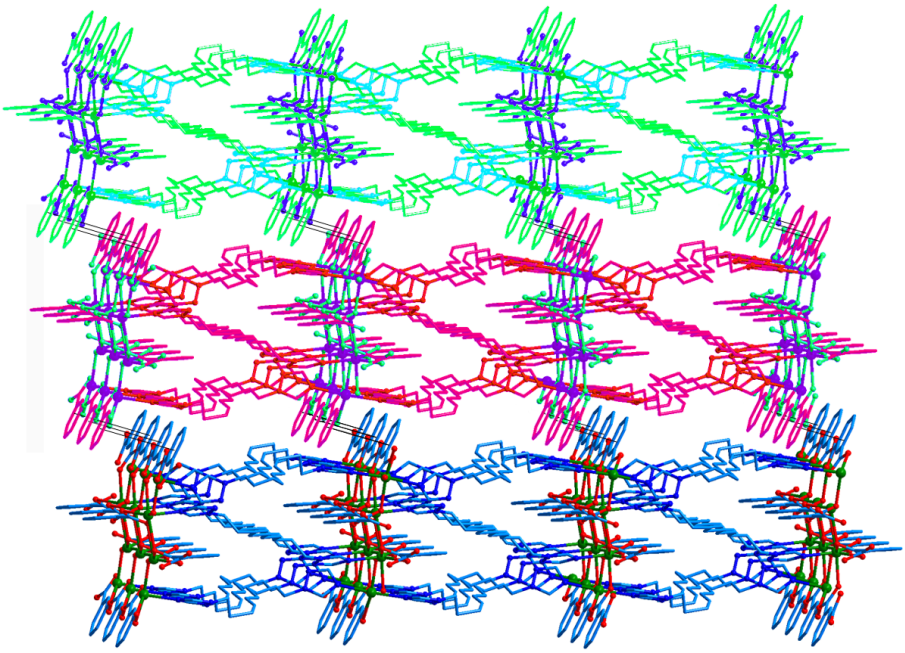


Fig. S6 The coordination environment of the Cd(II) center in **6**. Symmetry code: #1 x,y-1,z-1; #2 x+1,y,z.

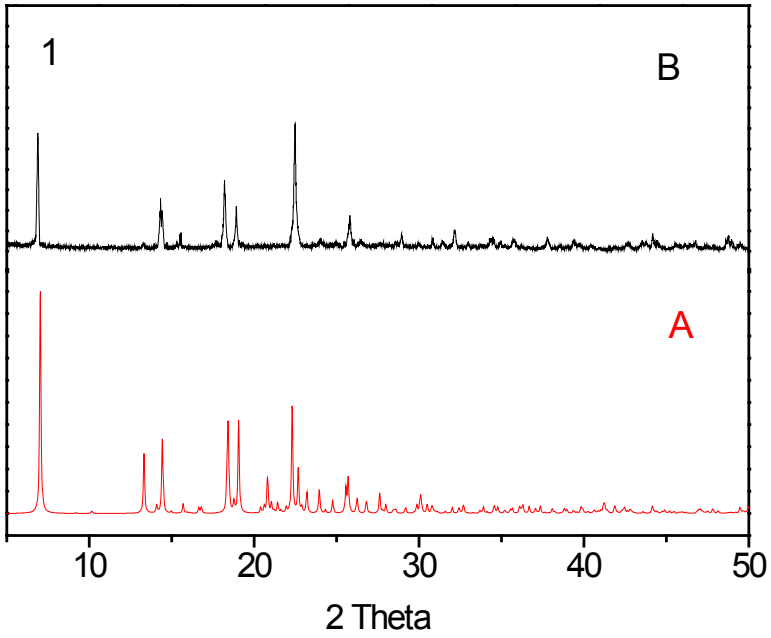


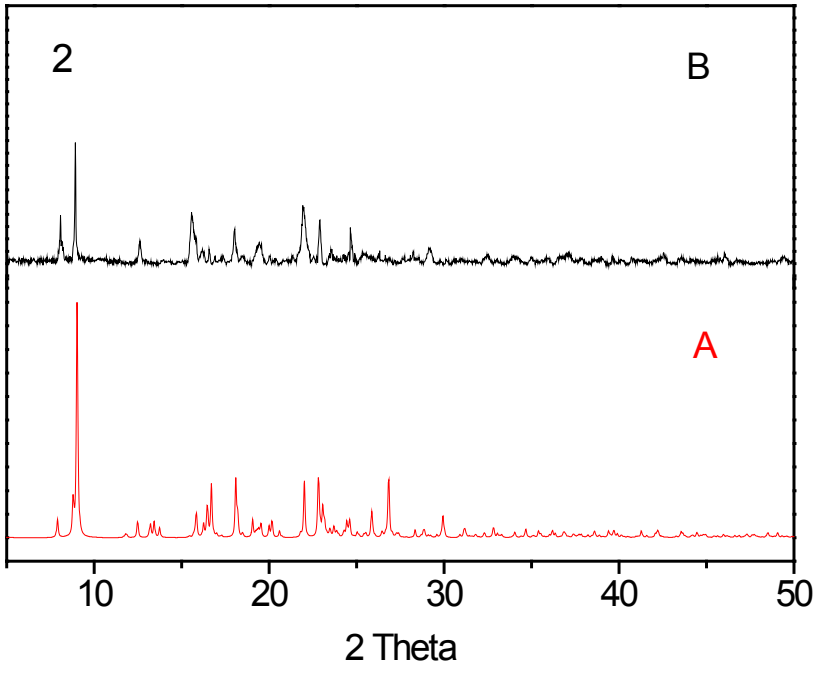
(a)

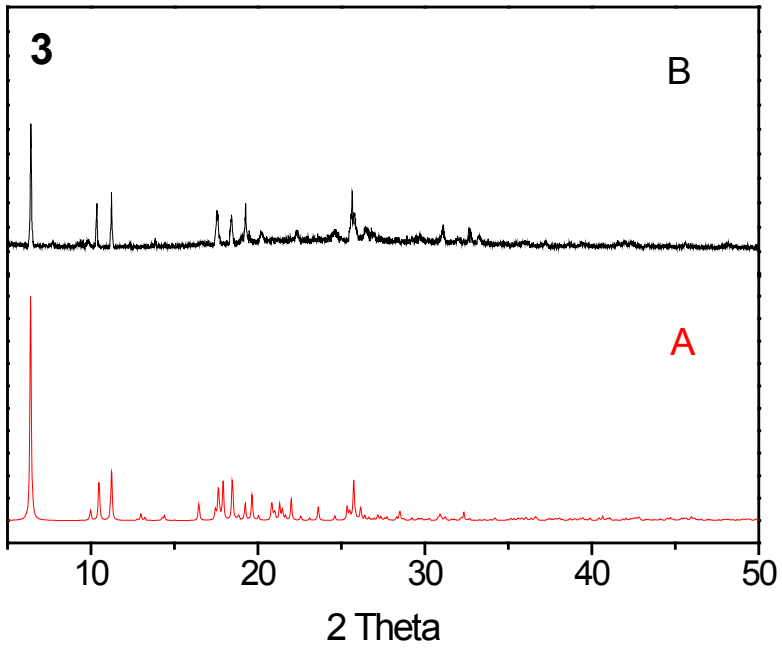


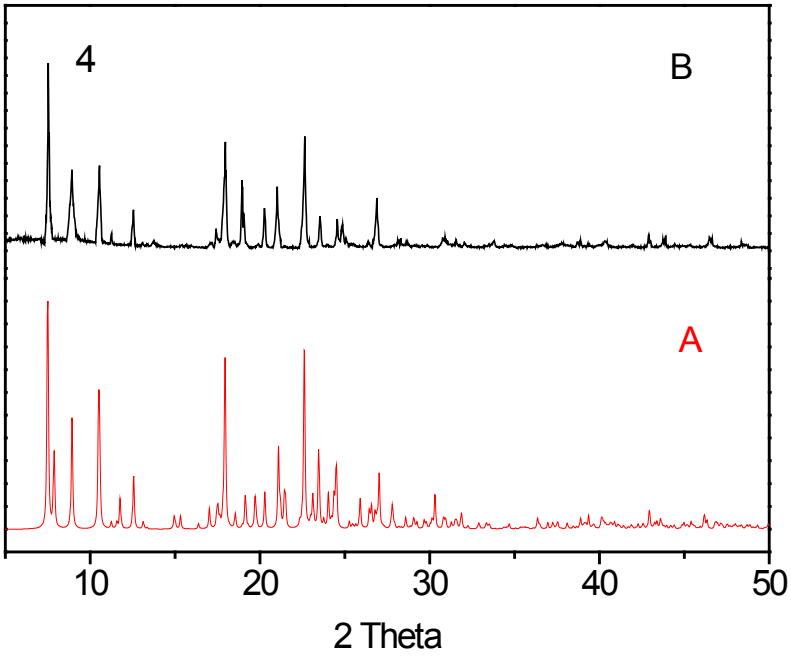
(b)

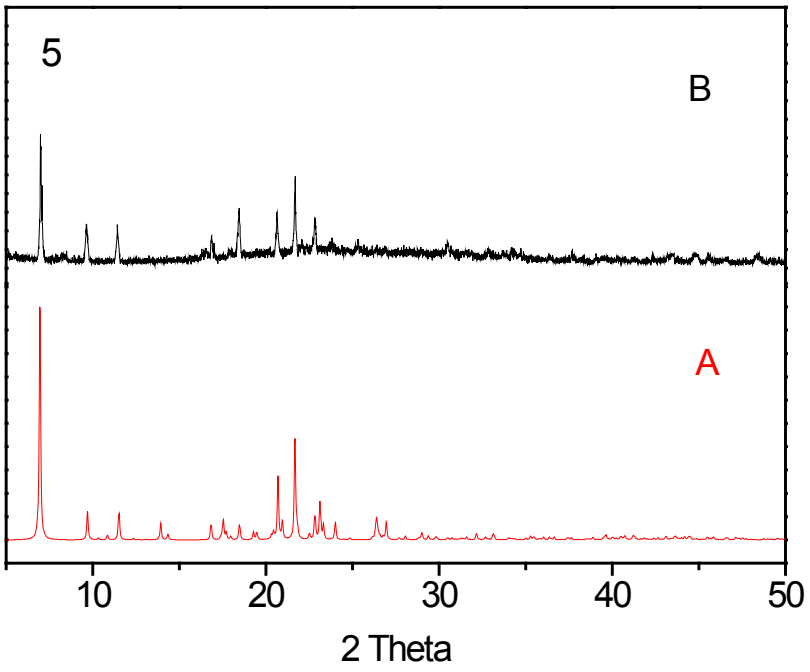
Fig. S7 (a) The coordination environment of the Cd(II) center in **7**, the H atoms and water molecule are omitted for clarity. (b) The 3D superamolecular motif of **7** through strong π-π interaction. Symmetry code: [#1] x-1,y,z; [#2] -x+1,-y+1,-z+2; [#3] x-1,y,z-1; [#4] -x+2,-y+1,-z+3.

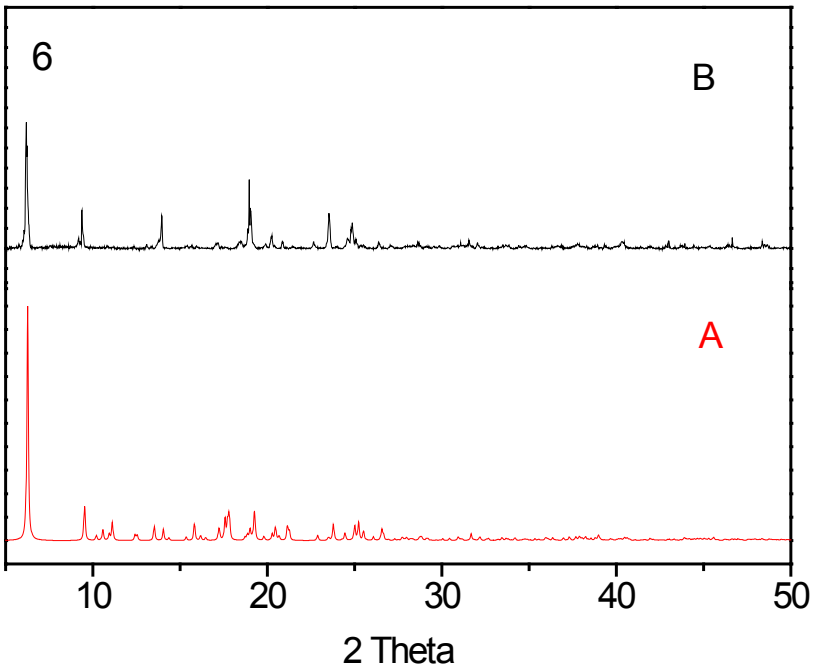












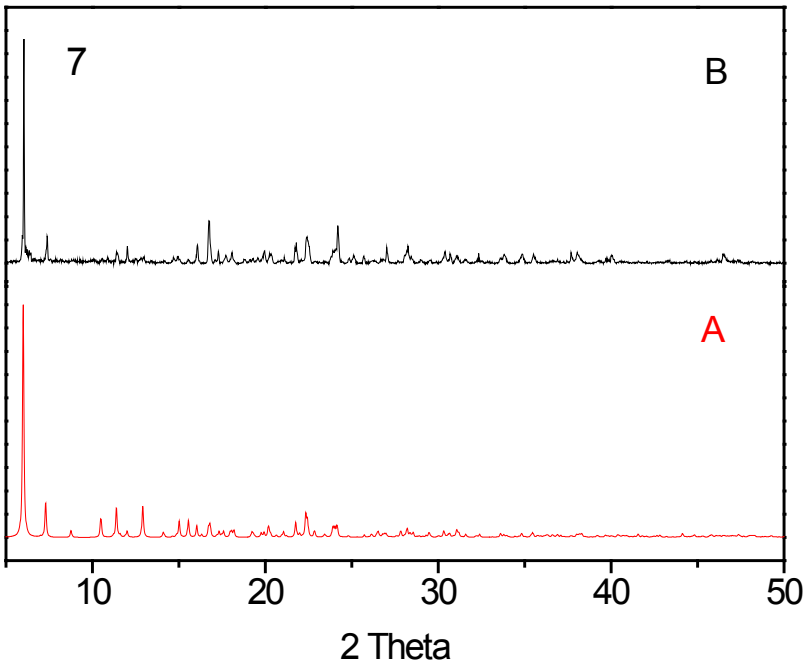


Fig. S8 Simulated A (red) and measured B (black) PXRD patterns of **1-7**.

Table S1. Selected Bond Lengths [Å] and Angles [deg] for **1**–**7**. [a]

		Compound **1**	
Zn(1)-N(1)	2.017(2)	Zn(1)-N(6)$^{\#1}$	2.016(2)
Zn(1)-Cl(1)	2.2145(9)	Zn(1)-Cl(2)	2.2146(10)
N(6)$^{\#1}$-Zn(1)-N(1)	103.66(8)	N(6)$^{\#1}$-Zn(1)-Cl(1)	103.92(8)
N(1)-Zn(1)-Cl(1)	110.72(8)	N(6)$^{\#1}$-Zn(1)-Cl(2)	110.80(7)
N(1)-Zn(1)-Cl(2)	105.85(8)	Cl(1)-Zn(1)-Cl(2)	120.70(4)
		Compound **2**	
Zn(1)-O(1)$^{\#1}$	1.991(2)	Zn(1)-O(8)	1.929(2)
Zn(1)-O(9)$^{\#1}$	1.956(2)	Zn(1)-N(6)$^{\#2}$	2.002(3)
Zn(2)-O(5)	1.934(2)	Zn(2)-O(10)	1.9534(19)
Zn(2)-O(2)	1.961(2)	Zn(2)-N(1)	1.989(3)
O(8)-Zn(1)-O(9)$^{\#1}$	118.82(9)	O(8)-Zn(1)-O(1)$^{\#1}$	101.45(10)
O(9)$^{\#1}$-Zn(1)-O(1)$^{\#1}$	116.05(9)	O(8)-Zn(1)-N(6)$^{\#2}$	118.90(10)
O(9)$^{\#1}$-Zn(1)-N(6)$^{\#2}$	102.87(10)	O(1)$^{\#1}$-Zn(1)-N(6)$^{\#2}$	97.27(10)
O(5)-Zn(2)-O(10)	105.44(9)	O(5)-Zn(2)-O(2)	112.37(9)

O(10)-Zn(2)-O(2)	113.75(9)	O(5)-Zn(2)-N(1)	115.81(10)
O(10)-Zn(2)-N(1)	107.02(10)	O(2)-Zn(2)-N(1)	102.62(11)
		Compound **3**	
Zn(1)-O(1)	1.9971(17)	Zn(1)-O(4)$^{\#1}$	1.988(3)
Zn(1)-O(2)	2.4760(19)	Zn(1)-N(1)	2.014(2)
Zn(1)-N(4)	2.014(2)	O(4)$^{\#1}$-Zn(1)-O(1)	100.86(9)
O(4)$^{\#1}$-Zn(1)-N(4)	102.05(10)	O(1)-Zn(1)-N(4)	107.28(8)
O(4)$^{\#1}$-Zn(1)-N(1)	104.11(9)	O(1)-Zn(1)-N(1)	115.42(8)
N(4)-Zn(1)-N(1)	123.60(9)	O(4)$^{\#1}$-Zn(1)-O(2)	158.08(6)
O(1)-Zn(1)-O(2)	57.61(10)	N(4)-Zn(1)-O(2)	89.58(9)
N(1)-Zn(1)-O(2)	84.04(9)		
		Compound **4**	
Zn(1)-O(1)	1.968(4)	Zn(1)-O(4)$^{\#1}$	1.981(5)
Zn(1)-N(1)	2.056(5)	Zn(1)-N(4)	2.016(6)
O(1)-Zn(1)-O(4)$^{\#1}$	96.54(18)	O(1)-Zn(1)-N(4)	117.9(2)
O(4)$^{\#1}$-Zn(1)-N(4)	111.4(2)	O(1)-Zn(1)-N(1)	113.8(2)
O(4)$^{\#1}$-Zn(1)-N(1)	120.0(2)	N(4)-Zn(1)-N(1)	98.5(2)
		Compound **5**	
Zn(1)-O(1)	1.940(3)	Zn(1)-O(3)$^{\#1}$	1.968(4)
Zn(1)-N(3)	2.015(5)	Zn(1)-N(4)	2.034(6)
O(1)-Zn(1)-O(3)$^{\#1}$	106.21(16)	O(1)-Zn(1)-N(3)	118.24(17)
O(3)$^{\#1}$-Zn(1)-N(3)	117.90(18)	O(1)-Zn(1)-N(4)	96.57(19)
O(3)$^{\#1}$-Zn(1)-N(4)	109.33(19)	N(3)-Zn(1)-N(4)	106.2(2)
		Compound **6**	
Cd(1)-O(1)	2.336(2)	Cd(1)-O(2)	2.491(2)
Cd(1)-O(3)$^{\#2}$	2.591(2)	Cd(1)-O(1W)	2.319(2)
Cd(1)-O(4)$^{\#2}$	2.313(2)	Cd(1)-N(1)	2.287(3)
Cd(1)-N(6)$^{\#1}$	2.300(3)	N(1)-Cd(1)-N(6)$^{\#1}$	165.50(11)
N(1)-Cd(1)-O(4)$^{\#2}$	97.72(10)	N(6)$^{\#1}$-Cd(1)-O(4)$^{\#2}$	89.16(10)
N(1)-Cd(1)-O(1W)	85.66(11)	N(6)$^{\#1}$-Cd(1)-O(1W)	81.37(11)
O(4)$^{\#2}$-Cd(1)-O(1W)	144.36(10)	N(1)-Cd(1)-O(1)	90.89(10)
N(6)$^{\#1}$-Cd(1)-O(1)	102.77(11)	O(4)$^{\#2}$-Cd(1)-O(1)	81.65(7)
O(1W)-Cd(1)-O(1)	133.92(9)	N(1)-Cd(1)-O(2)	94.24(9)
N(6)$^{\#1}$-Cd(1)-O(2)	90.12(10)	O(4)$^{\#2}$-Cd(1)-O(2)	133.60(7)
O(1W)-Cd(1)-O(2)	81.00(10)	O(1)-Cd(1)-O(2)	53.41(6)
N(1)-Cd(1)-O(3)#2	88.40(9)	N(6)#1-Cd(1)-O(3)#2	85.69(10)
O(4)#2-Cd(1)-O(3)#2	52.53(7)	O(1W)-Cd(1)-O(3)#2	92.35(9)
O(1)-Cd(1)-O(3)#2	133.54(7)	O(2)-Cd(1)-O(3)#2	172.62(6)
		Compound **7**	
Cd(1)-O(6)	2.272(3)	Cd(1)-O(2)	2.296(4)
Cd(1)-O(8)$^{\#1}$	2.306(4)	Cd(1)-O(5)$^{\#2}$	2.406(4)
Cd(1)-O(7)$^{\#1}$	2.545(3)	Cd(2)-O(1)	2.225(4)
Cd(2)-O(3)$^{\#1}$	2.349(3)	Cd(2)-O(7)$^{\#1}$	2.359(4)
Cd(2)-O(4)$^{\#1}$	2.421(4)	Cd(1)-N(1)	2.266(5)

Cd(2)-N(9)$^{\#3}$	2.302(6)	Cd(2)-N(4)	2.320(5)
N(1)-Cd(1)-O(6)	123.82(14)	N(1)-Cd(1)-O(2)	89.59(15)
O(6)-Cd(1)-O(2)	86.87(15)	N(1)-Cd(1)-O(8)$^{\#1}$	145.16(14)
O(6)-Cd(1)-O(8)$^{\#1}$	90.39(13)	O(2)-Cd(1)-O(8)$^{\#1}$	99.63(14)
N(1)-Cd(1)-O(5)$^{\#2}$	85.00(15)	O(6)-Cd(1)-O(5)$^{\#2}$	101.77(13)
O(2)-Cd(1)-O(5)$^{\#2}$	171.34(14)	O(8)$^{\#1}$-Cd(1)-O(5)$^{\#2}$	81.23(14)
N(1)-Cd(1)-O(7)$^{\#1}$	96.67(14)	O(6)-Cd(1)-O(7)$^{\#1}$	136.51(13)
O(2)-Cd(1)-O(7)$^{\#1}$	77.45(12)	O(8)$^{\#1}$-Cd(1)-O(7)$^{\#1}$	53.75(12)
O(5)$^{\#2}$-Cd(1)-O(7)$^{\#1}$	96.43(11)	O(1)-Cd(2)-N(9)$^{\#3}$	99.62(19)
O(1)-Cd(2)-N(4)	89.35(17)	N(9)$^{\#3}$-Cd(2)-N(4)	170.94(19)
O(1)-Cd(2)-O(3)$^{\#1}$	141.68(14)	N(9)$^{\#3}$-Cd(2)-O(3)$^{\#1}$	85.94(19)
N(4)-Cd(2)-O(3)$^{\#1}$	86.17(16)	O(1)-Cd(2)-O(7)$^{\#1}$	110.38(14)
N(9)$^{\#3}$-Cd(2)-O(7)$^{\#1}$	90.95(16)	N(4)-Cd(2)-O(7)$^{\#1}$	87.16(15)
O(3)$^{\#1}$-Cd(2)-O(7)$^{\#1}$	107.38(12)	O(1)-Cd(2)-O(4)$^{\#1}$	86.47(14)
N(9)$^{\#3}$-Cd(2)-O(4)$^{\#1}$	95.29(17)	N(4)-Cd(2)-O(4)$^{\#1}$	83.84(15)
O(3)$^{\#1}$-Cd(2)-O(4)$^{\#1}$	55.21(12)	O(7)$^{\#1}$-Cd(2)-O(4)$^{\#1}$	160.82(11)
O(1)-Cd(2)-C(8)$^{\#1}$	113.87(16)	N(9)$^{\#3}$-Cd(2)-C(8)$^{\#1}$	92.6(2)
N(4)-Cd(2)-C(8)$^{\#1}$	82.42(17)	O(3)$^{\#1}$-Cd(2)-C(8)$^{\#1}$	27.83(13)
O(7)$^{\#1}$-Cd(2)-C(8)$^{\#1}$	134.27(14)	O(4)$^{\#1}$-Cd(2)-C(8)$^{\#1}$	27.50(13)

[a] Symmetry operations: for **1**: $^{\#1}$ x-1,y+1,z; for **2**: $^{\#1}$ x-1,y+1,z $^{\#2}$ x,y+1,z-1; for **3**: $^{\#1}$ x,y-1,z; for **4**: $^{\#1}$ x+1,y,z; for **5**: $^{\#1}$ -x+1/2,y+1/2,-z+3/2; for **6**: $^{\#1}$ x,y-1,z-1 #2 x+1,y,z; for **7**: $^{\#1}$ x-1,y,z #2 -x+1,-y+1,-z+2 #3 x-1,y,z-1.