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[Supporting information]

A series of entangled coordination polymers assembled by a V-shaped bisimidazole ligand and various dicarboxylic acids: synthesis, characterization and luminescent properties

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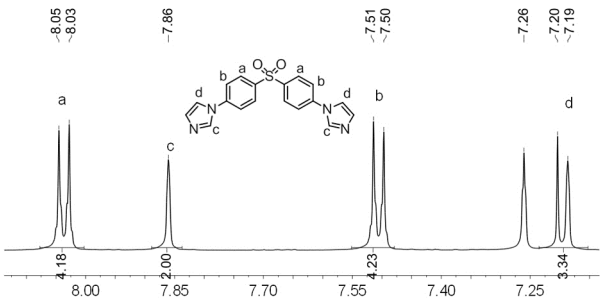

Fig. S1. The ^{1}HNMR spectra of bips.

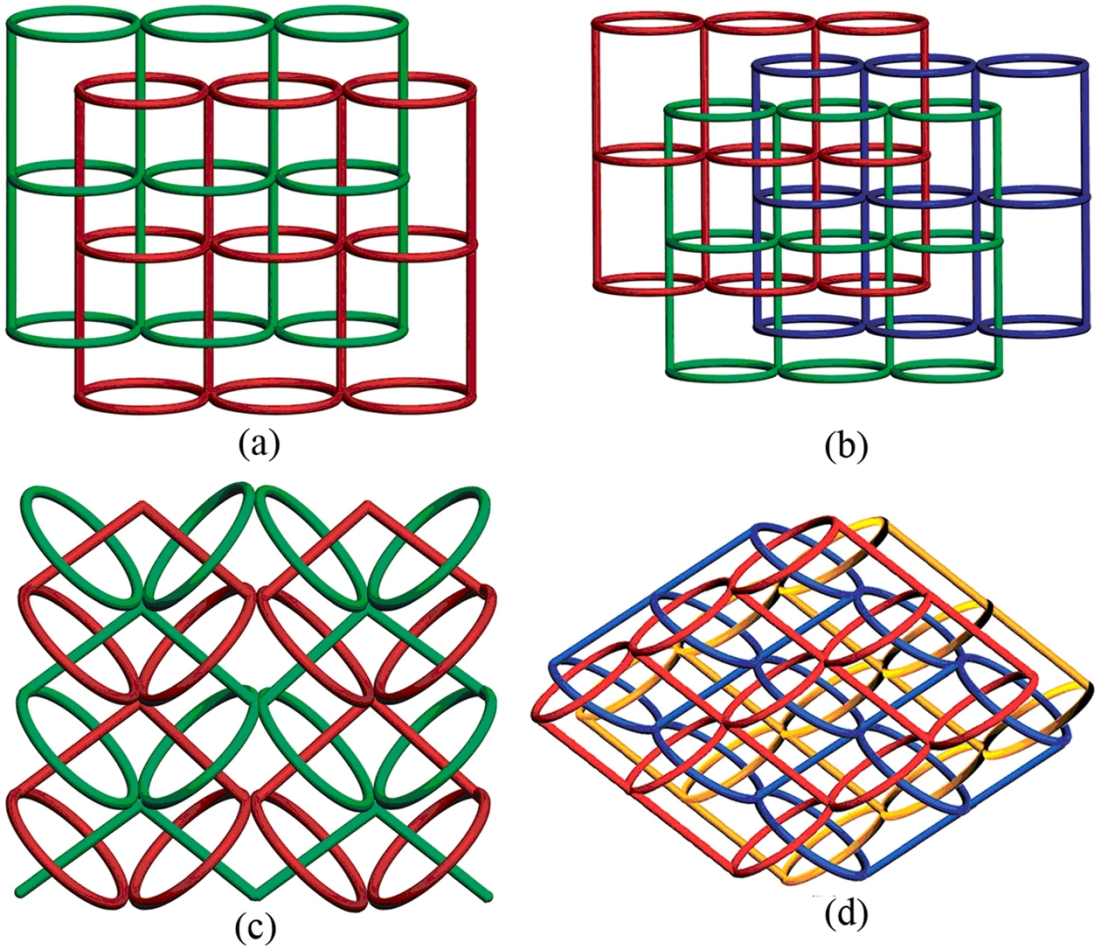

Fig. S2. Four examples of interpenetrated **sql** networks with different type of entanglements involving the 2-membered loops.

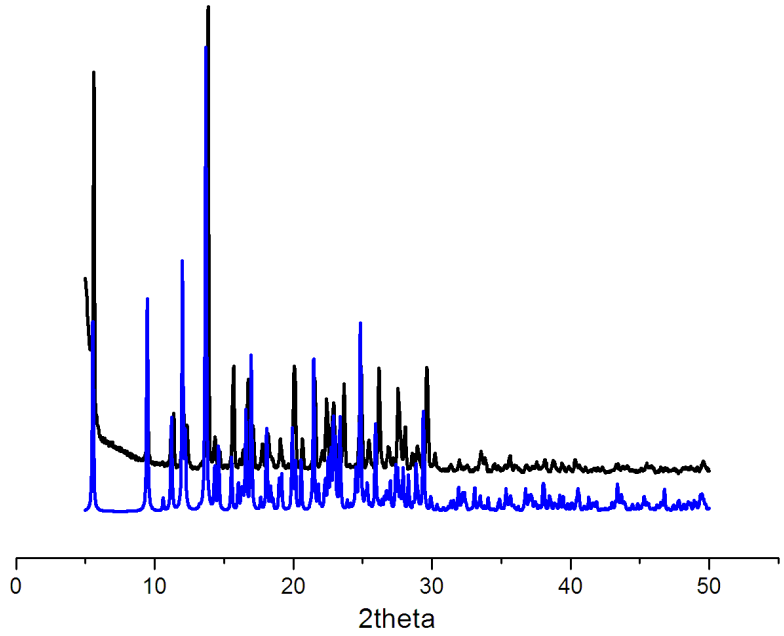

Fig. S3. The simulated(blue) and experimental (black) XRPD patterns for **1**.

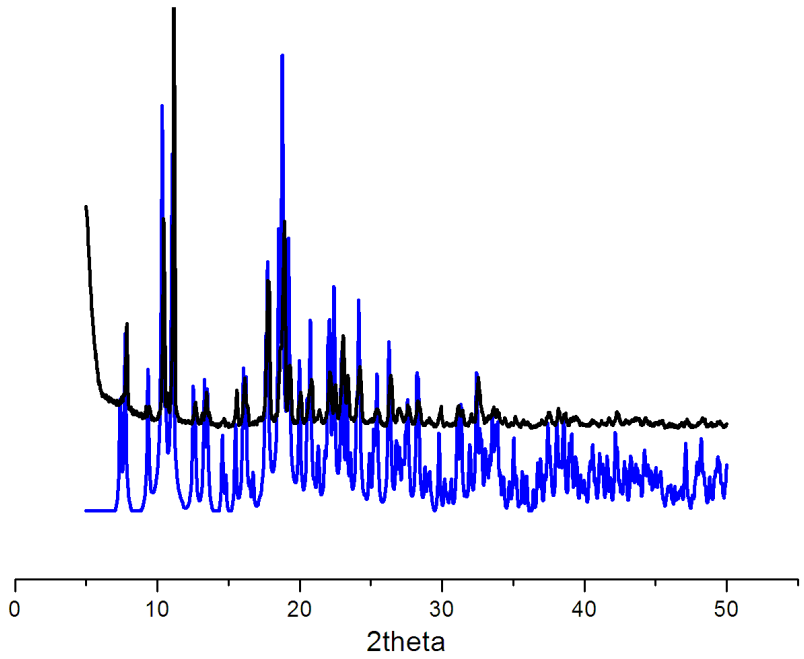

Fig. S4. The simulated (blue) and experimental (black) XRPD patterns for **2**.

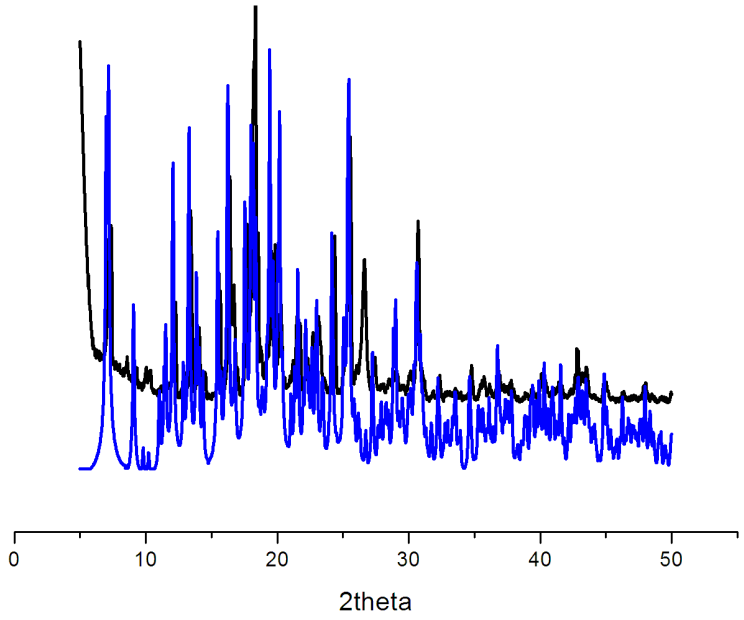

Fig. S5. The simulated (blue) and experimental (black) XRPD patterns for **3**.

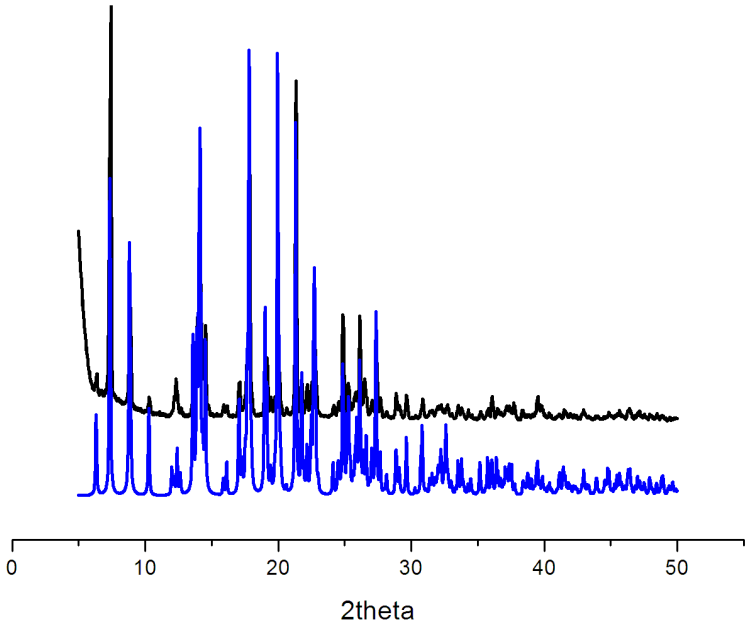

Fig. S6. The simulated (blue) and experimental (black) XRPD patterns for **4**.

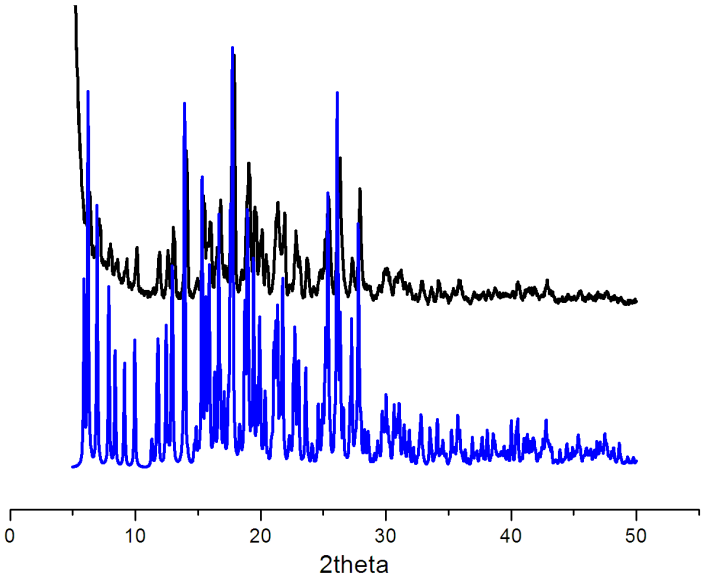

Fig. S7. The simulated (blue) and experimental (black) XRPD patterns for **5**.

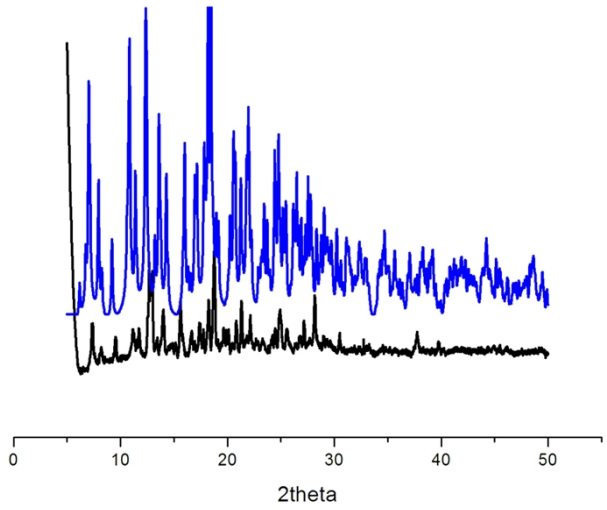

Fig. S8. The simulated (blue) and experimental (black) XRPD patterns for **6**.

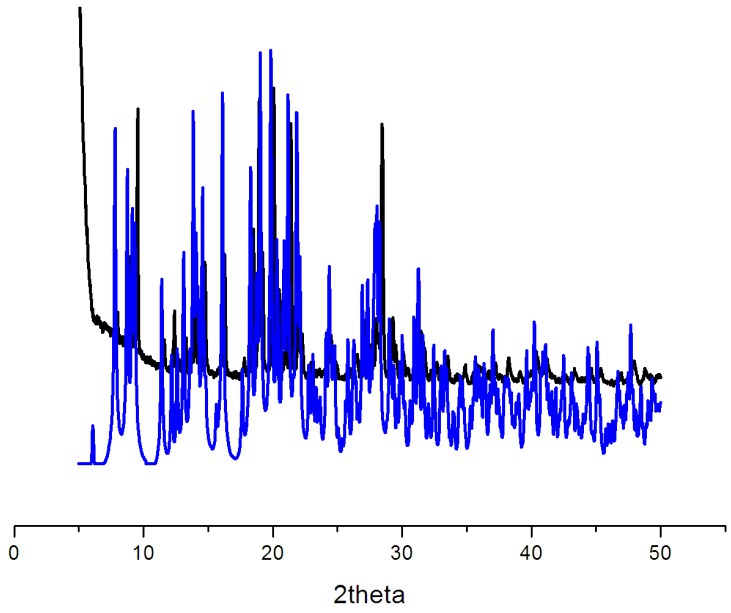

Fig. S9. The simulated (blue) and experimental (black) XRPD patterns for **7**.

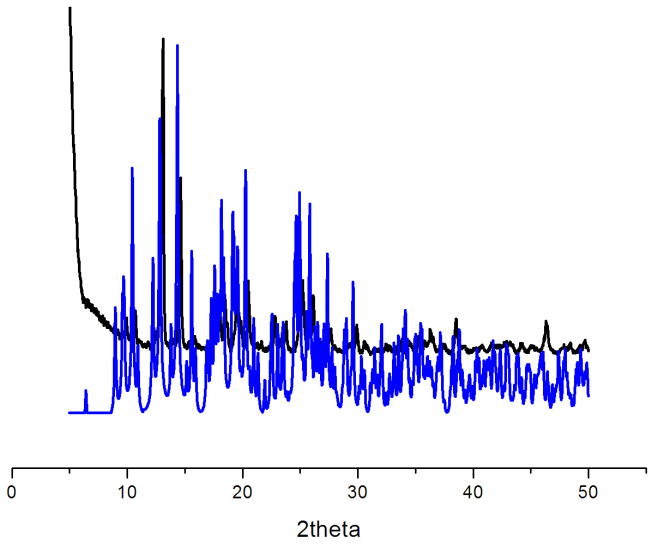

Fig. S10. The simulated (blue) and experimental (black) XRPD patterns for **8**.

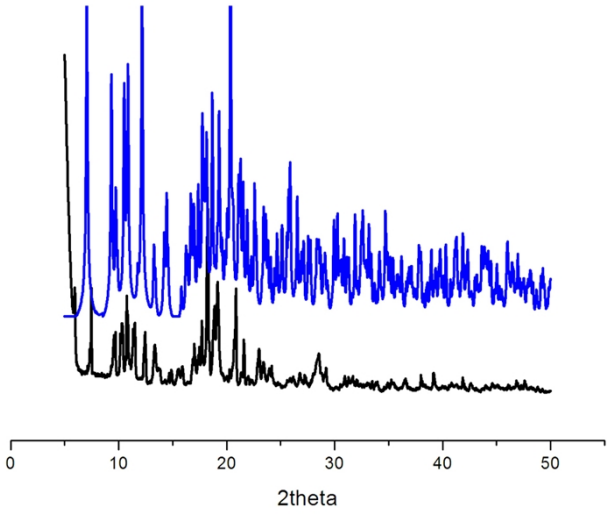

Fig. S11. The simulated (blue) and experimental (black) XRPD patterns for **9**.

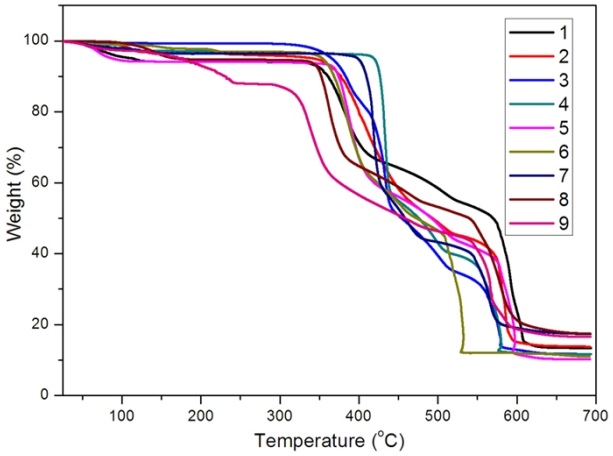

Fig. S12. TGA curves of **1-9**.

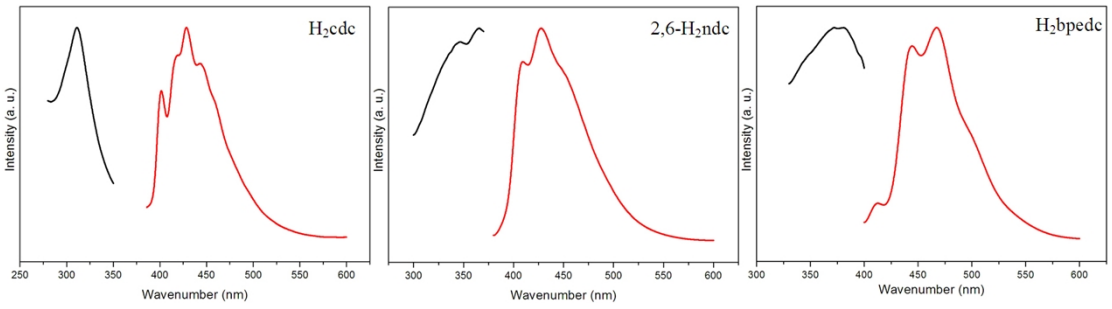

Fig. S13. Excitation (black) and emission (red) spectra of H_2cdc, 2,6-H_2ndc and H_2bpedc.

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

Zn(1)-N(1)	2.038(3)
Zn(1)-N(4)#2	2.005(3)
Zn(1)-O(1)	1.988(2)
Zn(1)-O(4)#1	1.951(2)
O(4)#1-Zn(1)-O(1)	101.74(11)
O(4)#1-Zn(1)-N(4)#2	118.24(12)
O(1)-Zn(1)-N(4)#2	110.72(11)
O(4)#1-Zn(1)-N(1)	102.57(11)
O(1)-Zn(1)-N(1)	107.59(11)
N(4)#2-Zn(1)-N(1)	114.71(12)

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

Table S2. Selected bond distances (Å) and angles (°) for **2**.

Zn(1)-N(1)	2.0119(19)
Zn(1) - O(2)	1.9308(17)
Zn(1) - O(3)	1.9477(19)
Zn(1)-N(4)#1	2.0521(19)
O(2)-Zn(1)-O(3)	115.10(10)
O(2)-Zn(1)-N(1)	124.04(8)
O(3)-Zn(1)-N(1)	111.41(9)
O(2)-Zn(1)-N(4)#1	96.38(8)
O(3)-Zn(1)-N(4)#1	100.44(9)
N(1)-Zn(1)-N(4)#1	104.17(8)

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

Table S3. Selected bond distances (Å) and angles (°) for **3**.

Zn(1)-N(1)	2.072(2)
Zn(1)-O(1)	1.944(2)
Zn(1)-O(3)	2.108(2)
Zn(1)-O(4)	2.267(2)
Zn(1)-N(4)#1	2.032(2)
O(1)-Zn(1)-N(4)#1	124.13(10)
O(1)-Zn(1)-N(1)	108.51(9)
N(4)#1-Zn(1)-N(1)	96.44(9)
O(1)-Zn(1)-O(3)	120.60(9)
N(4)#1-Zn(1)-O(3)	105.98(9)
N(1)-Zn(1)-O(3)	93.92(9)
O(1)-Zn(1)-O(4)	88.26(9)
N(4)#1-Zn(1)-O(4)	90.35(10)
N(1)-Zn(1)-O(4)	153.50(9)
O(3)-Zn(1)-O(4)	59.61(8)

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

Table S4. Selected bond distances (Å) and angles (°) for **4**.

Zn(1)-N(1)	2.031(2)
Zn(1)-O(1)	1.956(2)
Zn(1)-O(5)#1	1.971(2)
Zn(1)-N(4)#2	2.049(2)
O(1)-Zn(1)-O(5)#1	109.20(9)
O(1)-Zn(1)-N(1)	122.29(9)
O(5)#1-Zn(1)-N(1)	97.71(9)
O(1)-Zn(1)-N(4)#2	107.38(9)
O(5)#1-Zn(1)-N(4)#2	121.04(10)
N(1)-Zn(1)-N(4)#2	99.89(9)

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

Table S5. Selected bond distances (Å) and angles (°) for **5**.

Zn(1)-N(1)	2.023(3)
Zn(1)-N(4)#1	2.040(3)
Zn(1)-O(2)	1.958(2)
Zn(1)-O(11)#2	2.054(3)
Zn(2)-O(6)	1.969(3)
Zn(2)-O(7)	1.985(2)
Zn(2)-N(5)	2.004(3)
Zn(2)-N(8)#3	2.038(3)
O(2)-Zn(1)-N(1)	111.88(12)
O(2)-Zn(1)-N(4)#1	116.26(11)
N(1)-Zn(1)-N(4)#1	100.29(12)
O(2)-Zn(1)-O(11)#2	107.71(11)
N(1)-Zn(1)-O(11)#2	126.29(12)
N(4)#1-Zn(1)-O(11)#2	93.03(12)
O(6)-Zn(2)-O(7)	99.03(11)
O(6)-Zn(2)-N(5)	128.20(14)
O(7)-Zn(2)-N(5)	111.07(11)
O(6)-Zn(2)-N(8)#3	98.70(14)
O(7)-Zn(2)-N(8)#3	112.39(11)
N(5)-Zn(2)-N(8)#3	106.78(12)

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

Table S6. Selected bond distances (Å) and angles (°) for **6**.

Co(1)-N(5)	2.165(3)
Co(1)-N(8)#4	2.137(3)
Co(1)-O(2)	2.093(2)
Co(1)-OW1	2.156(2)
Co(1)-O(10)#3	2.069(2)
Co(1)-O(4)#1	2.085(2)
Co(2) - N(1)	2.127(3)
Co(2)-N(4)#2	2.177(3)
Co(2)-O(3)	2.079(2)
Co(2)-O(7)	2.105(3)
Co(2)-O(9)#4	2.040(2)
Co(2)-OW1#2	2.146(2)
O(10)#3-Co(1)-O(4)#1	95.70(10)
O(10)#3-Co(1)-O(2)	86.76(10)
O(4)#1-Co(1)-O(2)	176.27(10)
O(10)#3-Co(1)-N(8)#4	91.07(10)
O(4)#1-Co(1)-N(8)#4	97.45(10)
O(2)-Co(1)-N(8)#4	85.28(10)
O(10)#3-Co(1)-OW1	90.66(9)
O(4)#1-Co(1)-OW1	90.06(9)
O(2)-Co(1)-OW1	87.10(9)
N(8)#4-Co(1)-OW1	172.08(9)
O(10)#3-Co(1)-N(5)	174.69(10)
O(4)#1-Co(1)-N(5)	89.46(10)
O(2)-Co(1)-N(5)	88.02(10)

N(8)#4-Co(1)-N(5)	89.50(11)
OW1-Co(1)-N(5)	88.07(10)
O(9)#4-Co(2)-O(3)	94.45(11)
O(9)#4-Co(2)-O(7)	179.17(11)
O(3)-Co(2)-O(7)	86.36(12)
O(9)#4-Co(2)-N(1)	94.20(10)
O(3)-Co(2)-N(1)	92.29(10)
O(7)-Co(2)-N(1)	85.62(10)
O(9)#4-Co(2)-OW1#2	91.46(9)
O(3)-Co(2)-OW1#2	89.95(9)
O(7)-Co(2)-OW1#2	88.69(9)
N(1)-Co(2)-OW1#2	173.74(10)
O(9)#4-Co(2)-N(4)#2	89.17(10)
O(3)-Co(2)-N(4)#2	174.59(11)
O(7)-Co(2)-N(4)#2	90.03(11)
N(1)-Co(2)-N(4)#2	91.45(10)
OW1#2-Co(2)-N(4)#2	85.93(9)

Symmetry transformations used to generate equivalent atoms: #1 x,y,z-1; #2 x,y,z+1; #3 x,y+1,z-1; #4 x,y+1,z.

Table S7. Selected bond distances (Å) and angles (°) for **7**.

Cd(1)-N(1)	2.230(3)
Cd(1)-N(4)#1	2.256(3)
Cd(1)-O(4)	2.162(3)
Cd(1)-O(5)	2.255(10)
Cd(1)-O(5')	2.246(6)

O(4)-Cd(1)-N(1)	105.14(12)
O(4)-Cd(1)-O(5')	85.24(18)
N(1)-Cd(1)-O(5')	118.56(18)
O(4)-Cd(1)-O(5)	83.4(3)
N(1)-Cd(1)-O(5)	142.2(3)
O(4)-Cd(1)-N(4)#1	124.41(11)
N(1)-Cd(1)-N(4)#1	100.99(11)
O(5')-Cd(1)-N(4)#1	122.44(17)
O(5)-Cd(1)-N(4)#1	103.9(3)

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

Table S8. Selected bond distances (Å) and angles (°) for **8**.

Cd(1)-N(1)	2.344(4)
Cd(1)-N(4)#1	2.294(5)
Cd(1)-O(2)	2.301(4)
Cd(1)-O(3)	2.457(4)
Cd(1)-O(4)	2.287(4)
Cd(1)-OW1	2.300(4)
O(4)-Cd(1)-N(4)#1	141.35(15)
O(4)-Cd(1)-O(2)	96.70(16)
N(4)#1-Cd(1)-O(2)	90.91(16)
O(4)-Cd(1)-OW1	104.45(15)
N(4)#1-Cd(1)-OW1	114.14(16)
O(2)-Cd(1)-OW1	81.71(14)
O(4)-Cd(1)-N(1)	87.06(16)

N(4)#1-Cd(1)-N(1)	92.61(17)
O(2)-Cd(1)-N(1)	168.94(15)
OW1-Cd(1)-N(1)	87.28(15)
O(4)-Cd(1)-O(3)	55.16(13)
N(4)#1-Cd(1)-O(3)	87.08(15)
O(2)-Cd(1)-O(3)	90.39(15)
OW1-Cd(1)-O(3)	157.30(15)

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

Table S9. Selected bond distances (Å) and angles (°) for **9**.

Cd(1)-N(1)	2.266(3)
Cd(1)-N(4)#1	2.251(3)
Cd(1)-O(1)	2.522(3)
Cd(1)-O(2)	2.259(3)
Cd(1)-O(3)#2	2.350(3)
Cd(1)-O(4)#2	2.351(3)
N(4)#1-Cd(1)-O(2)	103.73(12)
N(4)#1-Cd(1)-N(1)	98.04(10)
O(2)-Cd(1)-N(1)	132.39(12)
N(4)#1-Cd(1)-O(3)#2	89.70(10)
O(2)-Cd(1)-O(3)#2	115.03(13)
N(1)-Cd(1)-O(3)#2	106.79(11)
N(4)#1-Cd(1)-O(4)#2	144.50(10)
O(2)-Cd(1)-O(4)#2	91.99(13)
N(1)-Cd(1)-O(4)#2	94.12(12)

O(3)#2-Cd(1)-O(4)#2	54.82(9)
N(4)#1-Cd(1)-O(1)	89.05(11)
O(2)-Cd(1)-O(1)	53.92(12)
N(1)-Cd(1)-O(1)	85.15(9)
O(3)#2-Cd(1)-O(1)	168.05(11)
O(4)#2-Cd(1)-O(1)	125.27(11)

Symmetry transformations used to generate equivalent atoms: #1 x-1/2,-y+5/2,z-1/2; #2 x-1/2,-y+3/2,z+1/2

Table S10. Specified hydrogen bonds of compound **2**

D-H-A	d(D···H)(Å)	d(H···A)(Å)	d(D···A)(Å)	(DHA)(deg)
OW1-HW1B-O(1)	0.90	1.87	2.760(3)	168.9
OW1-HW1A-O(4)#1	0.87	1.95	2.815(4)	172.2

Symmetry codes: #1 -x+2,-y,-z+2

As shown in Table S10, in compound **2**, between the uncoordinated water molecules and carboxylate groups, there exist strong H-bonding (O···O distances range from 2.760(3) to 2.815(4) A°).