Electronic supplementary information (ESI)

Functional group effects on structure and topology of cadmium(II) frameworks with mixed organic ligands

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Table S1 Selected bond lengths (Å) and angles (°) for **1 - 4** [a]

1			
Cd(1)-N(1)	2.276(3)	Cd(1)-O(2)	2.477(3)
Cd(1)-N(6)	2.287(3)	Cd(1)-O(1)	2.558(4)
Cd(1)-N(3)#1	2.439(3)	Cd(1)-O(6)	2.579(3)
Cd(1)-O(3)	2.339(3)		
N(1)-Cd(1)-N(6)	95.53(11)	O(3)-Cd(1)-O(2)	90.53(10)
N(6)-Cd(1)-O(3)	135.63(10)	N(1)-Cd(1)-O(1)	100.23(11)
N(1)-Cd(1)-O(6)	97.50(11)	N(1)-Cd(1)-O(2)	84.58(10)
N(1)-Cd(1)-N(3)#1	166.32(10)	O(3)-Cd(1)-O(1)	136.50(10)
O(3)-Cd(1)-N(3)#1	79.76(10)	O(2)-Cd(1)-O(1)	51.93(11)
N(6)-Cd(1)-N(3)#1	96.34(10)	N(6)-Cd(1)-O(6)	83.15(10)
2			
Cd(1)-N(1)	2.267(4)	Cd(1)-O(2)	2.296(4)

Cd(1)-N(5)#1	2.298(4)	Cd(1)-O(4)#2	2.317(3)
Cd(1)-N(3)#3	2.431(4)	Cd(1)-O(1)	2.643(5)
N(1)-Cd(1)-N(5)#1	97.01(17)	N(5)#1-Cd(1)-N(3)#3	164.33(15)
N(1)-Cd(1)-O(2)	122.22(15)	O(4)#2-Cd(1)-N(3)#3	78.07(14)
N(1)-Cd(1)-N(3)#3	88.46(15)	N(3)#3-Cd(1)-O(1)	111.49(15)
N(5)#1-Cd(1)-O(2)	107.45(15)	O(2)-Cd(1)-O(4)#2	100.27(13)
O(2)-Cd(1)-O(1)	51.84(14)	O(4)#2-Cd(1)-O(1)	145.75(12)
N(1)-Cd(1)-O(4)#2	132.97(13)	O(2)-Cd(1)-N(3)#3	81.53(14)

3

Cd(1)-N(5)#1	2.261(2)	Cd(1)-O(2)	2.3494(19)
Cd(1)-N(1)	2.350(2)	Cd(1)-O(4)#2	2.357(2)
Cd(1)-N(3)#3	2.458(2)	Cd(1)-O(3)#2	2.505(2)
N(5)#1-Cd(1)-O(2)	132.52(8)	N(1)-Cd(1)-N(3)#3	161.57(9)
(5)#1-Cd(1)-N(1)	92.50(8)	O(2)-Cd(1)-O(3)#2	138.73(7)
O(2)-Cd(1)-N(1)	87.24(8)	O(4)#2-Cd(1)-O(3)#2	53.65(7)
N(5)#1-Cd(1)-O(4)#2	142.08(8)	O(2)-Cd(1)-O(1)	52.13(7)
O(2)-Cd(1)-O(4)#2	85.11(7)	O(4)#2-Cd(1)-O(1)	136.48(7)
N(5)#1-Cd(1)-N(3)#3	105.24(8)	O(3)#2-Cd(1)-O(1)	166.59(7)

4

Cd(1)-N(1)	2.287(3)	Cd(1)-O(1)	2.300(3)
Cd(1)-N(5)#1	2.351(3)	Cd(1)-O(3)#3	2.416(2)
Cd(1)-N(3)#2	2.363(3)	Cd(1)-O(4)#3	2.474(2)
N(1)-Cd(1)-O(1)	138.77(9)	N(5)#1-Cd(1)-O(3)#3	89.03(9)
N(1)-Cd(1)-N(5)#1	90.31(9)	N(3)#2-Cd(1)-O(3)#3	90.84(9)

O(1)-Cd(1)-N(5)#1	93.22(9)	N(1)-Cd(1)-O(4)#3	86.59(9)
N(1)-Cd(1)-N(3)#2	89.12(9)	O(1)-Cd(1)-O(4)#3	134.63(9)
N(5)#1-Cd(1)-N(3)#2	178.94(10)	N(5)#1-Cd(1)-O(4)#3	85.59(9)
O(1)-Cd(1)-O(3)#3	81.08(9)	O(3)#3-Cd(1)-O(4)#3	53.57(8)

[a] Symmetry transformations used to generate equivalent atoms: #1 x-1, y+1, z for **1**; #1 -x+5/2, y+1/2, -z+1/2; #2 x+1/2, -y+1/2, z+1/2; #3 -x+2, -y, -z+1 for **2**; #1 -x, y+1/2, -z-1/2; #2 x, y, z-1 ; #3 -x+1, -y+2, -z for **3**; #1 x-1/2, -y+1/2, -z+2; # 2x+1/2, -y+1/2, -z+2 ; #3 -x+3/2, y-1/2, z for **4**.

Table S2 Hydrogen bonding data for **4**.

Complex **4**		
D–H ··A	d(*D* ··A) (Å)	∠*D*–H ··A (°)
C5–H5A ··O3#1	3.469(4)	175
C12–H12 ··O1#2	3.248(4)	149
Symmetry codes: #1 3/2-x, 1-y, 1/2+z; #2 x, 1/2-y, 1/2+z.		

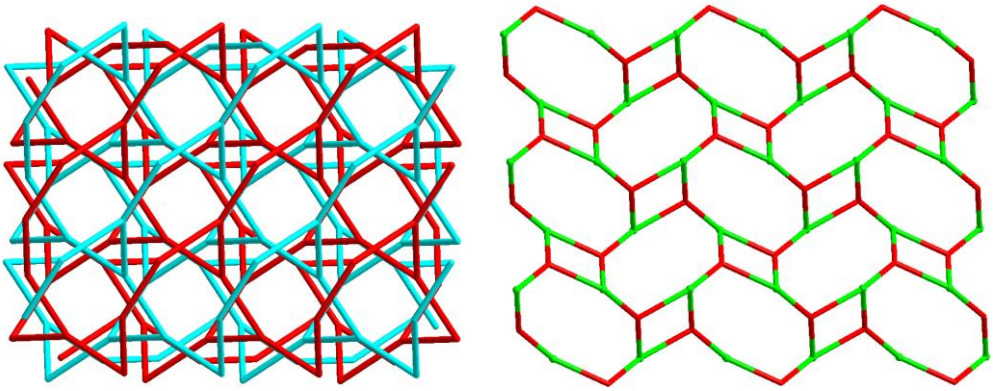
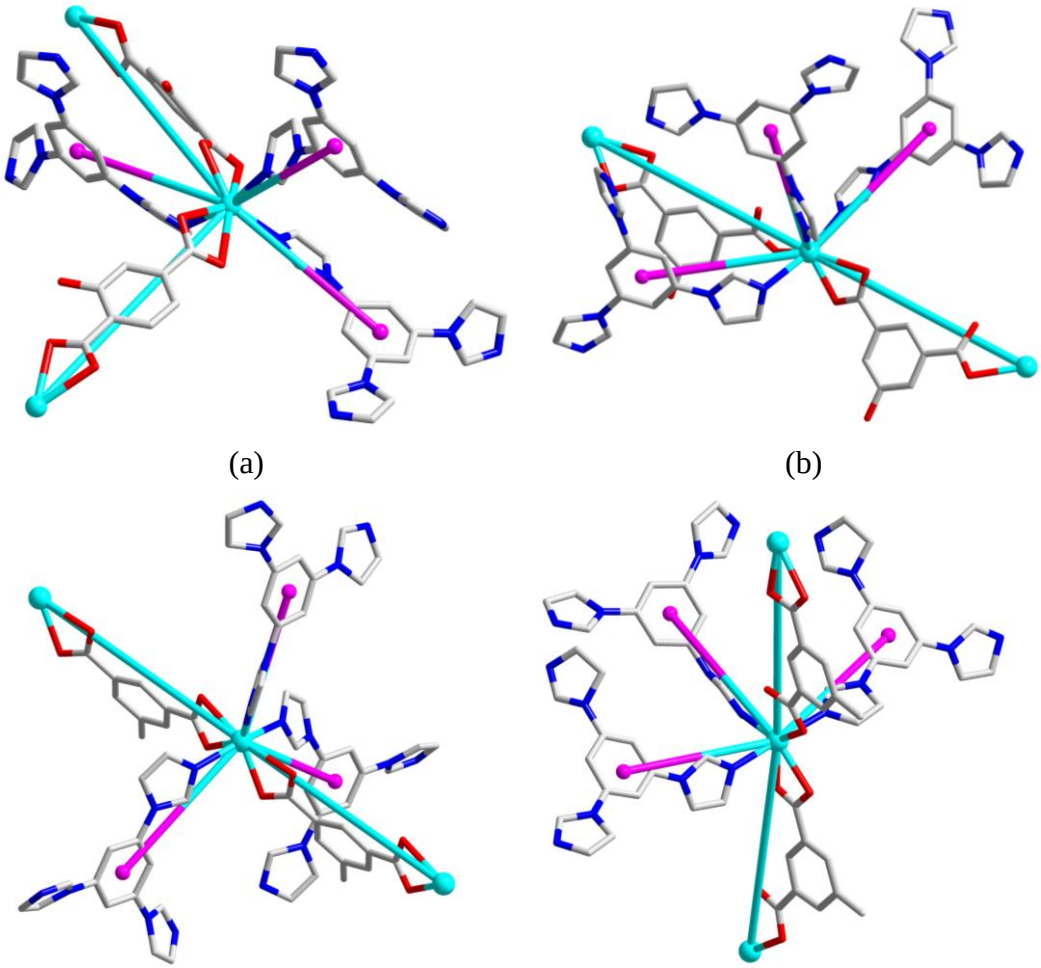


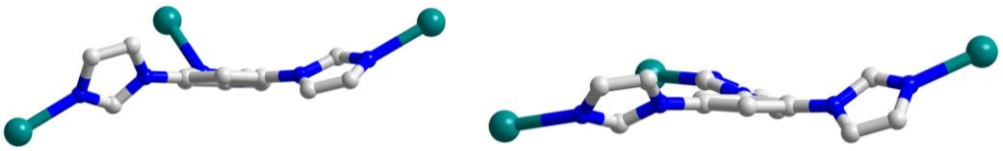
Fig. S1 (a) The schematic representation of 2-fold interpenetrating framework of Cd(II)-tib in **1**. (b) Topology of the Cd(II)-tib 2D network in **2**.



(a) (b)

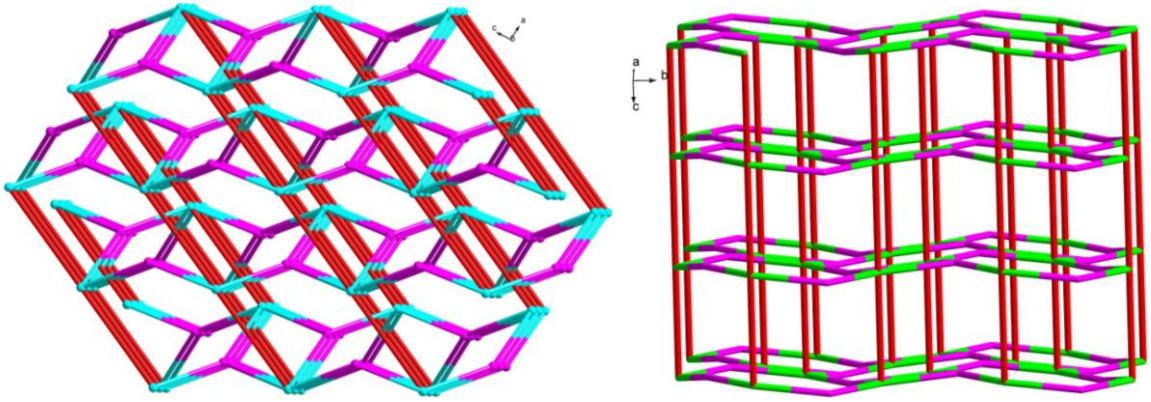
(c) (d)

Fig. S2 The 5-connected node of Cd building unit in **1** (a) - **4** (d).



(a) (b)

Fig. S3 Coordination modes of tib with Cd (II) in **2 (**a**)** and **3 (**b**)**.



(a) (b)

Fig. S4 The illustrations of the 3D nets formed by Cd-tib 2D networks and Cd-*m*-BDC-R 1D chains in **2** (a) and **3** (b). The Cd-*m*-BDC-R 1D chains are indicated by red lines.

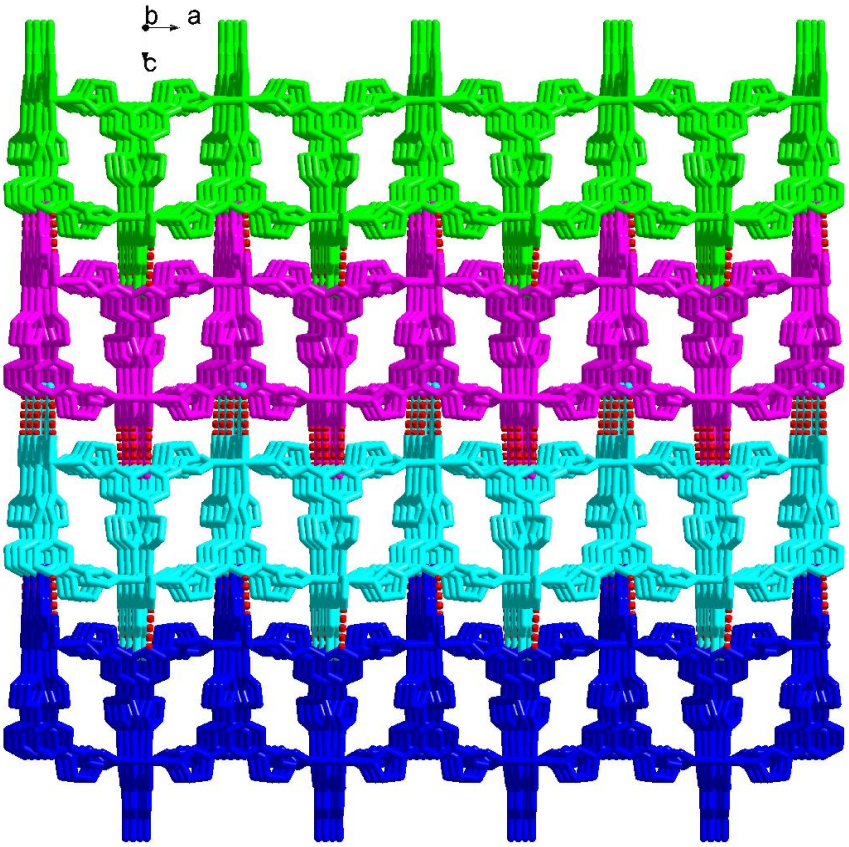


Fig. S5 The 3D supramolecular structure of **4** with 2D layers linked by hydrogen bonds: different color indicates the different layers. The hydrogen bonds are indicated by dashed lines.

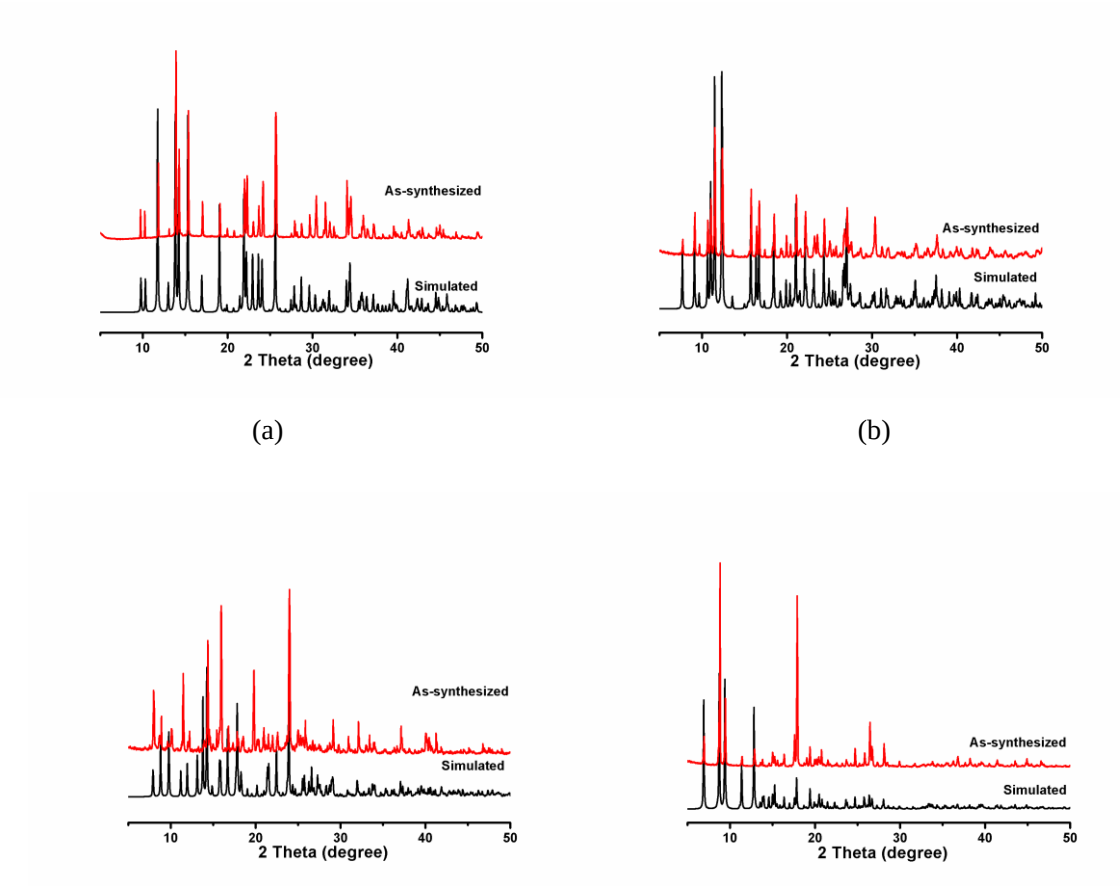


Fig. S6 The PXRD patterns of **1** (a) - **4** (d).

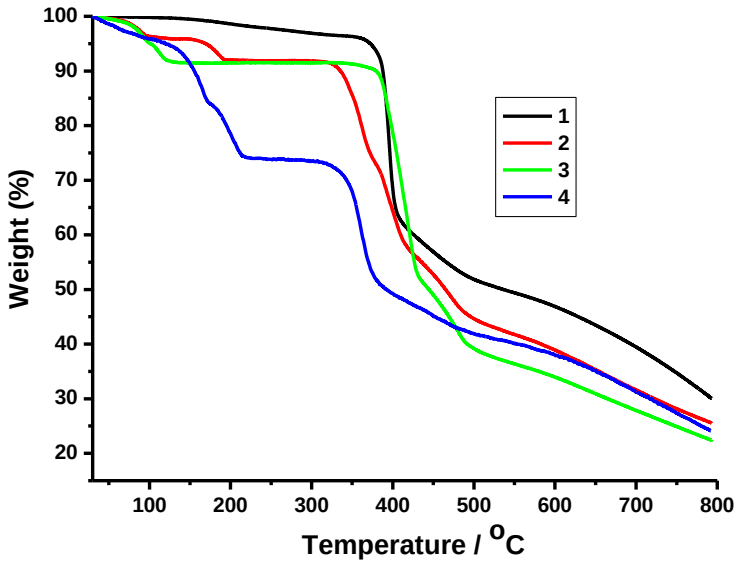


Fig. S7 The TGA curves of **1** - **4**.