Electronic Supplementary Material for CrystEngComm

Supporting Information

Assembly of two 3-D metal-organic frameworks from Cd(II) and 4,5-imidazoledicarboxylic acid or 2-ethyl-4,5-imidazoledicarboxylic acid

Shuang Wang, Lirong Zhang, Guanghua Li, Qisheng Huo and Yunling Liu*

State Key Laboratory of Inorganic Synthesis and Preparative Chemistry, College of Chemistry, Jilin University, Changchun 130012, P. R. China. E-mail: yunling@jlu.edu.cn

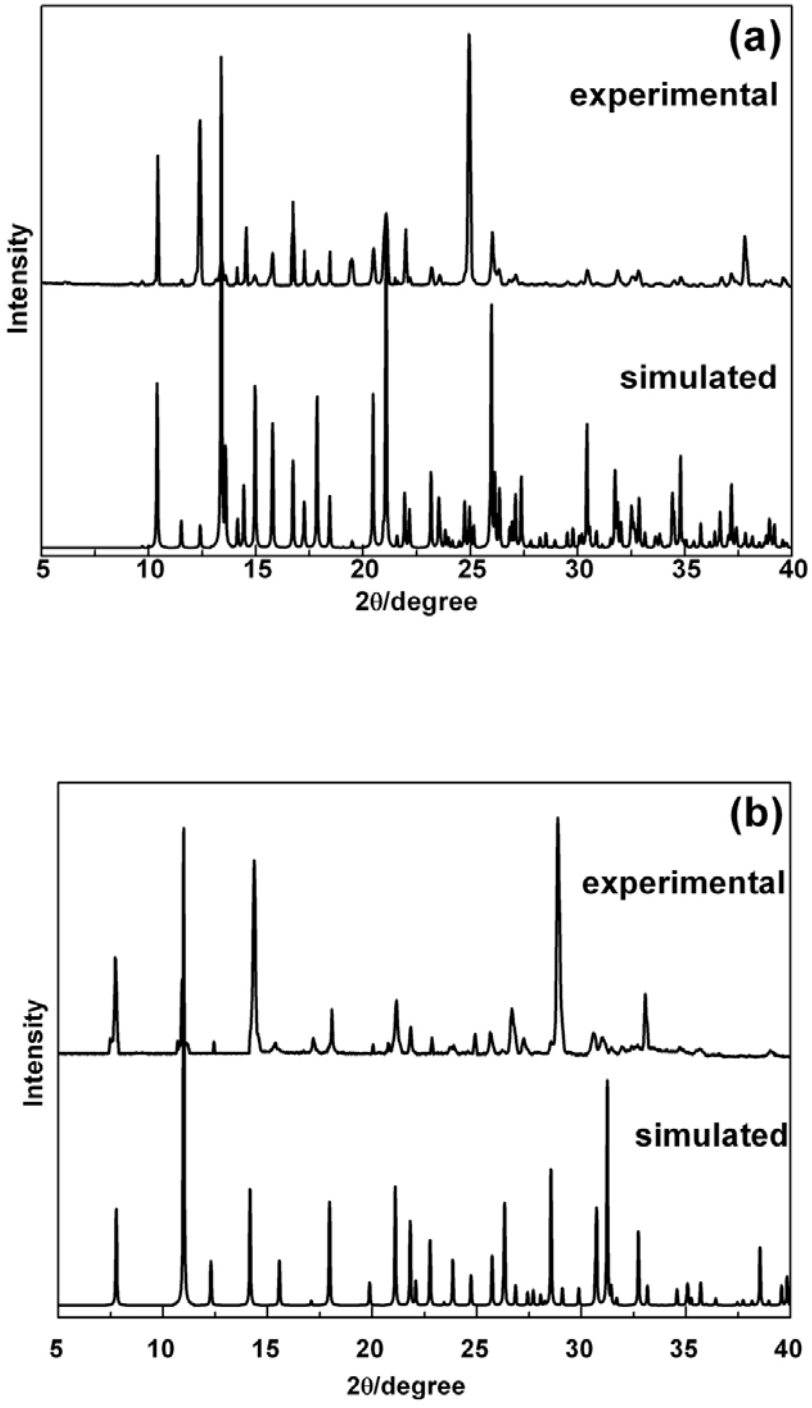

Fig. S1 Simulated and experimental powder X-ray diffraction patterns of **1**(a) and **2**(b).

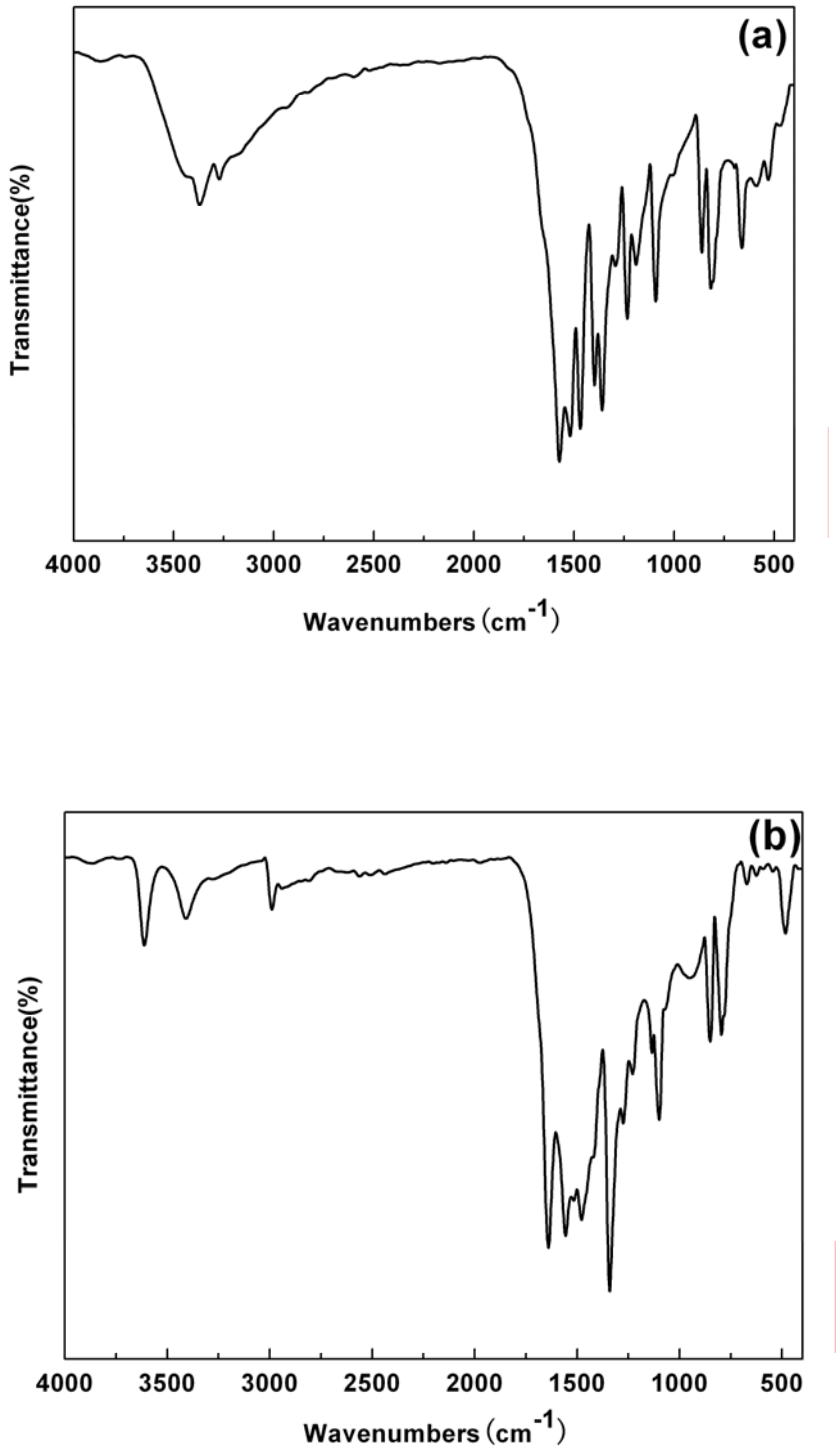

Fig. S2 IR spectra for compound **1(a)** and **2(b)**.

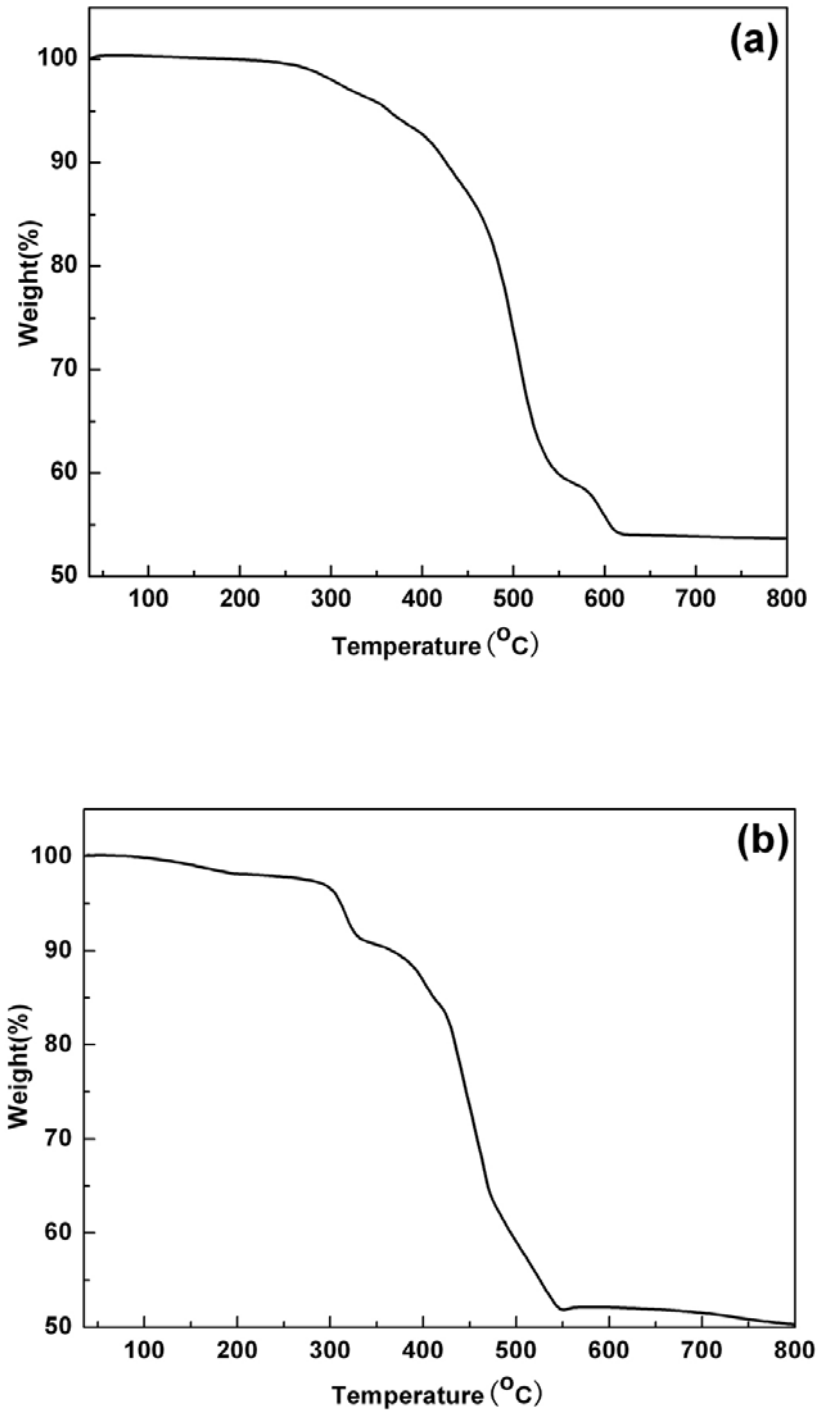

Fig. S3 TG curves for compound **1(a)** and **2(b)**.

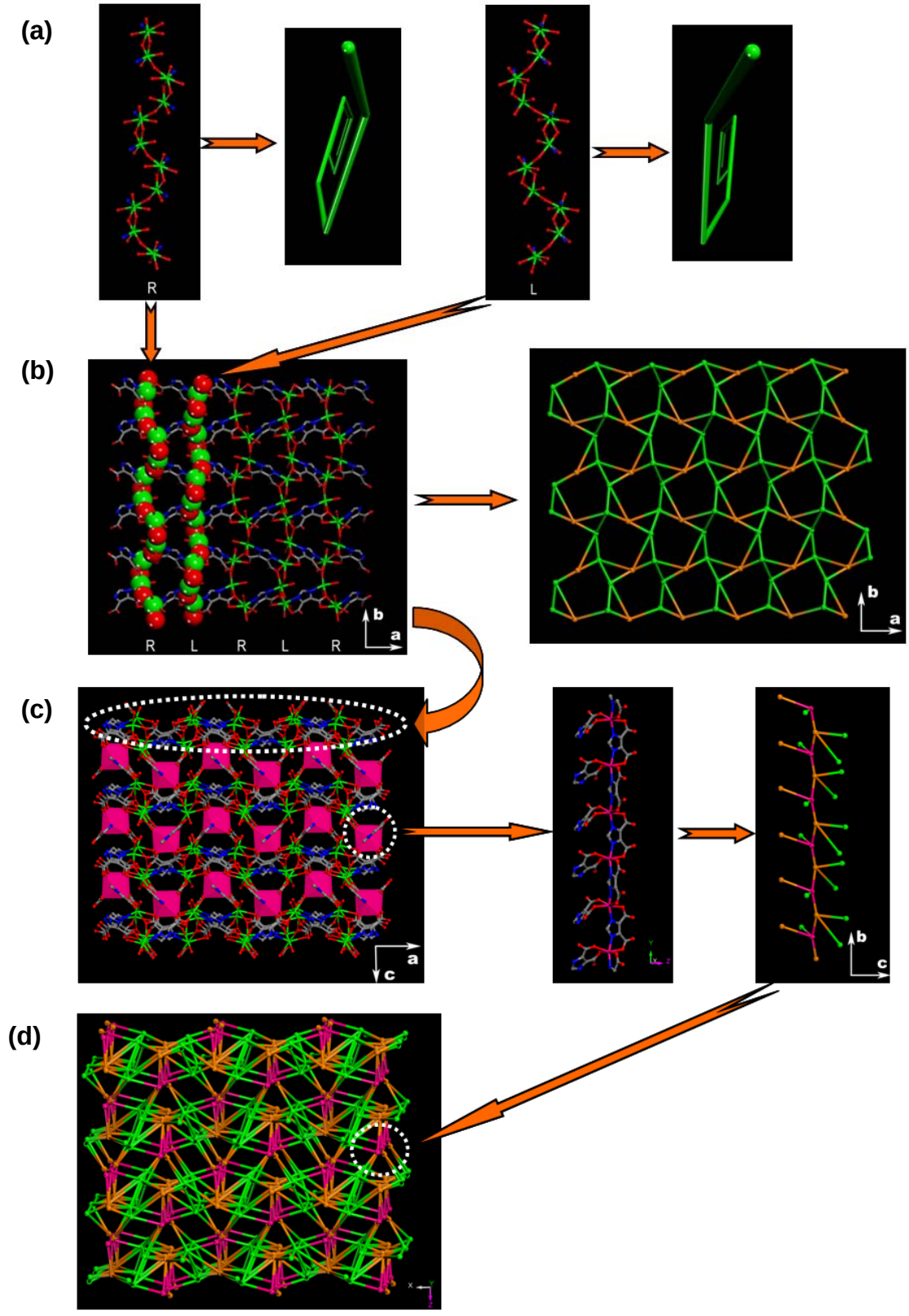

Fig. S4 The 3-D framework structure of **1**: (a) Ball and stick view of right-handed (R) and left-handed (L) helical chains; (b) The 2-D layer viewed along the *c*-axis and the topology of 2-D layer with distorted *Kagomé* net; (c) The 3-D framework of **1** formed by 2-D layers and 1-D chains viewed along the *b*-axis; (d) The framework topology of **1** viewed along the *b*-axis. (Color code: Cd1 and Cd2 atom: green; Cd3 atom: pink; O: red; C: grey, N: blue, the IMDC ligands are denoted by yellow spheres in the topology).

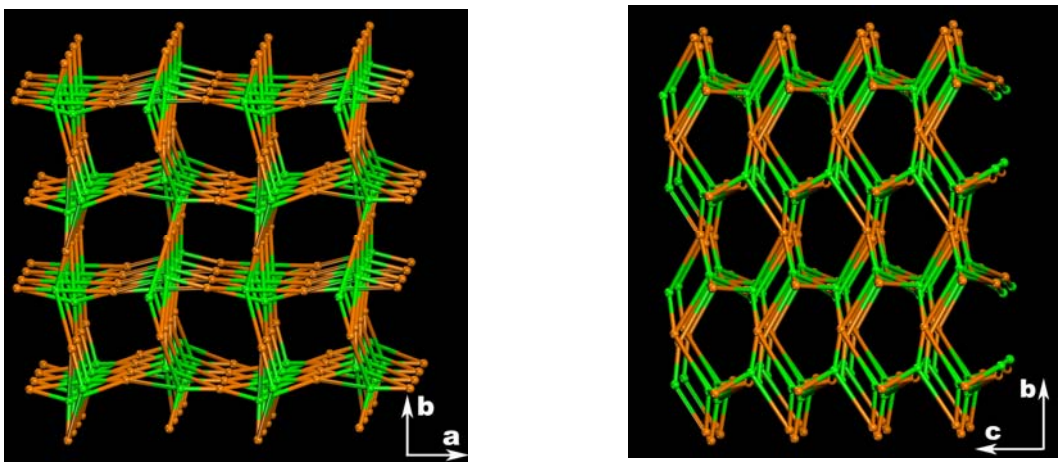

Fig. S5 The topology of the 3D framework of **2** viewed along the *c*-axis and *a*-axis. (Color code: Cd: green; the 2-EtIMDC ligands as 4-connected nodes are denoted by yellow spheres).

Table S1. Hydrogen bonds for **1** [Å and deg.].

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(9)-H(9A)···N(4)#7	0.96(8)	2.43(4)	3.333(7)	157(8)
O(9)-H(9B)···O(6)#2	0.96(6)	2.18(3)	3.123(7)	169(9)
O(10)-H(10A)···O(1W)#8	0.99(10)	2.10(10)	2.949(11)	143(8)
O(10)-H(10A)···O(4)#8	0.99(10)	2.53(10)	3.250(9)	130(7)
O(10)-H(10B)···O(1W)#9	1.00(10)	1.98(10)	2.896(10)	152(8)
O(10)-H(10B)···O(10)#10	1.00(10)	2.38(10)	3.000(11)	119(7)
O(1W)-H(1A)···O(8)#7	0.86(10)	2.31(11)	3.031(9)	141(9)
O(1W)-H(1B)···O(4)	0.86(11)	2.07(11)	2.885(8)	157(10)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1/2, y-1/2, z #2 -x, y-1/2, -z+1/2 #3 -x+1/2, -y+1, z-1/2 #4 -x+1/2, y+1/2, z #5 -x, y+1/2, -z+1/2 #6 -x+1/2, -y+1, z+1/2 #7 x-1/2, y, -z+1/2 #8 -x, -y+1, -z #9 x, y-1, z #10 -x, -y, -z