Supporting Information

From ladder, net to framework: coordination polymers based on Zn(II)/Cd(II) ions and mixed bicarboxyl- and bipyridine-containing linear ligands

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1. Additional Structural Figures

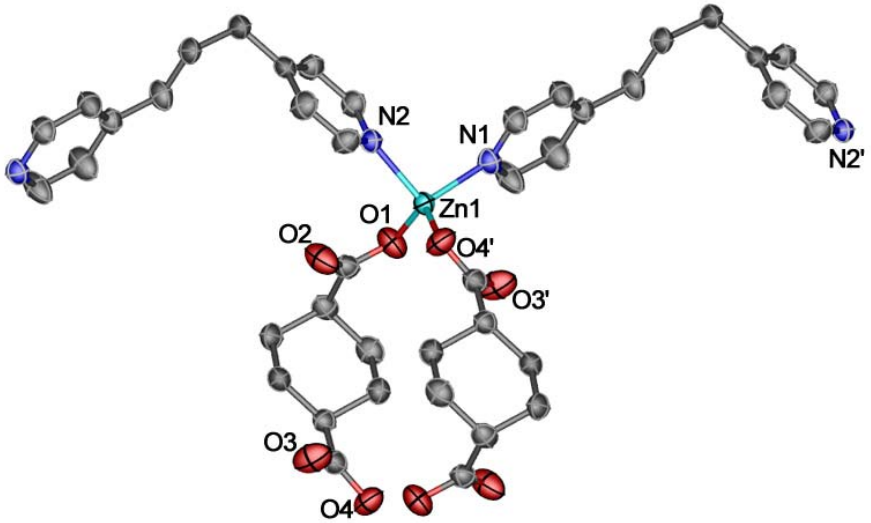

Fig. S1. ORTEP view of the basic unit in compound **1** with thermal ellipsoids of 50%. H atoms are omitted for clarity. The symmetry transformations for O3', O4', and N2' are -x+1,-y+1,-z+1.

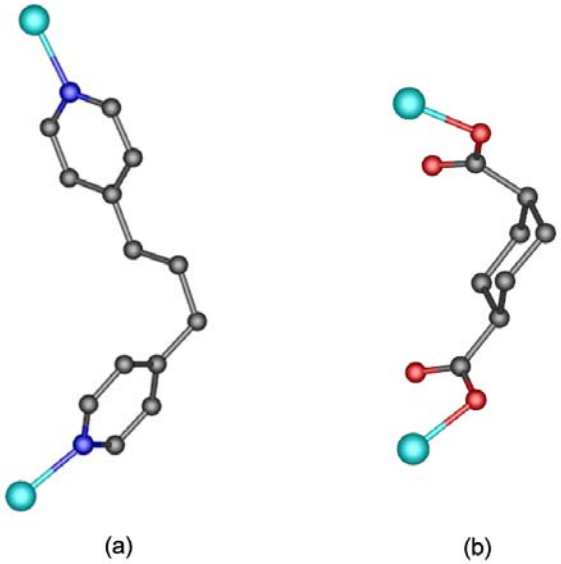

Fig. S2. The coordination modes of organic linear ligands in compound **1**: **(a)** bpp; **(b)** chdc.

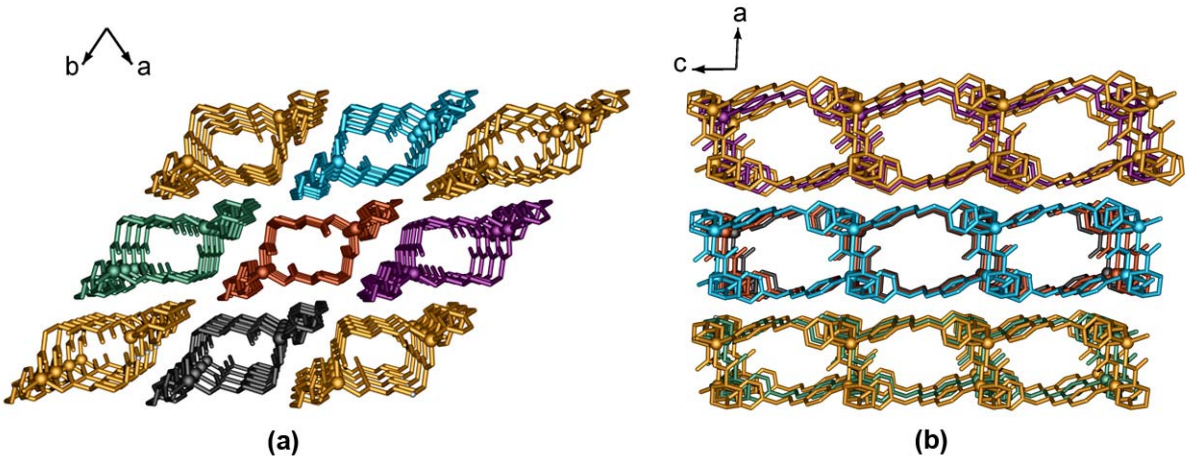

Fig. S3 Packing arrangements of compound **1** viewed along **(a)** *c* axis and **(b)** *b* axis. The solvent water molecules are omitted for clarity.

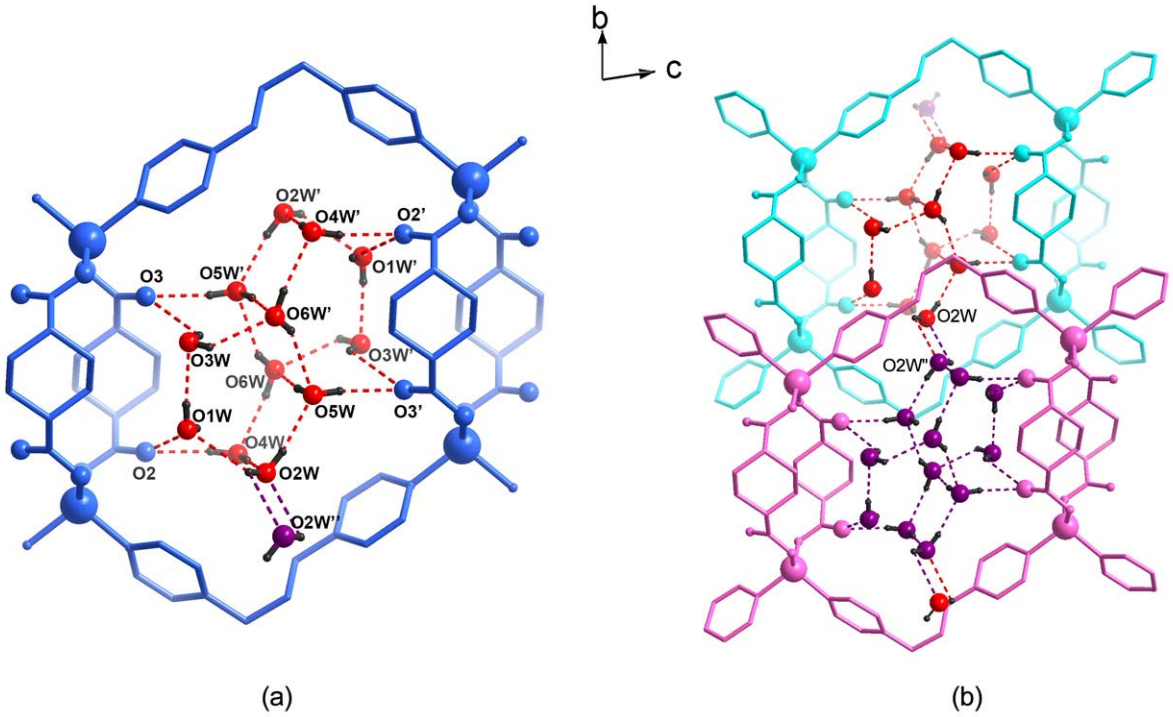

Fig. S4 (a) The hydrogen bonding interactions among $\{H_2O\}_{12}$ clusters and the mesh unit of the 1-D chain in **1**; **(b)** View of the hydrogen bonding interactions between two adjacent $\{H_2O\}_{12}$ clusters.

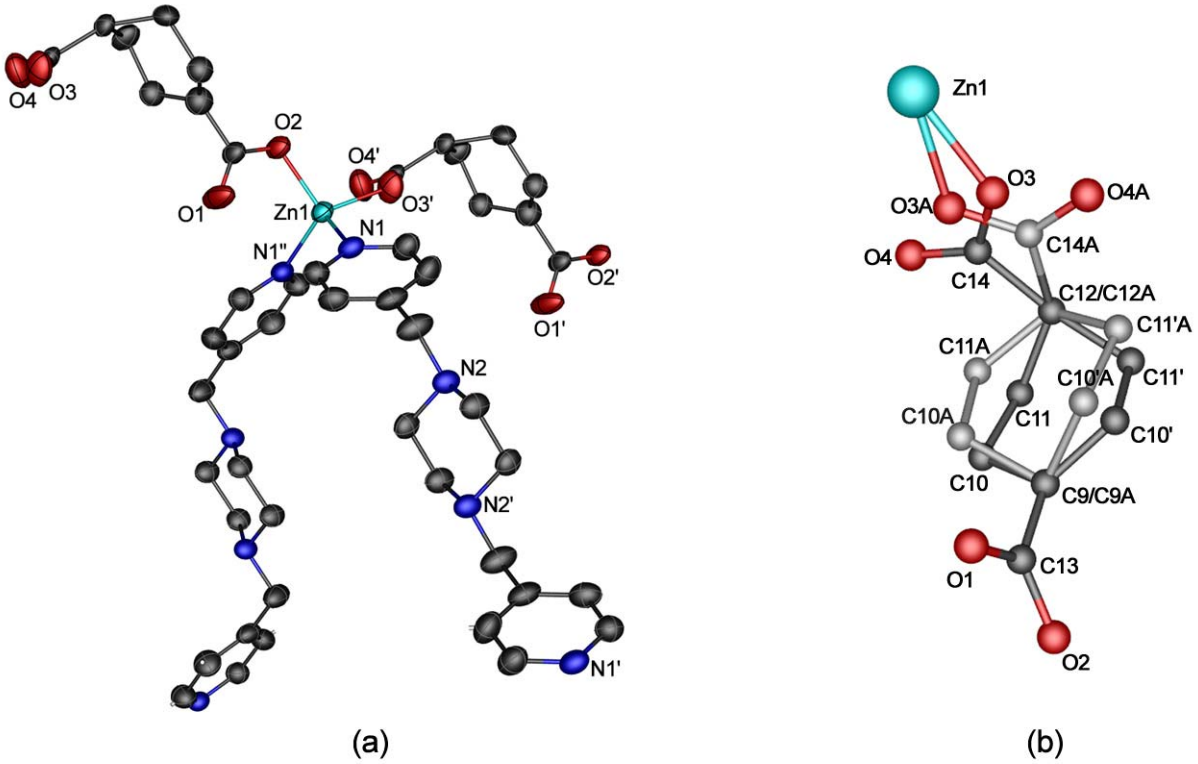

Fig. S5. (a) ORTEP view of the basic unit in compound **2** with thermal ellipsoids of 50%. H atoms are omitted for clarity. The symmetry transformations for O1', O2', O3' and O4' are x, y, z-1, for N1'' is x,-y+1/2,z. (b) The disordered chdc ligand in compound **2**, possessing two possible positions with the occupancies of 50% for each part.

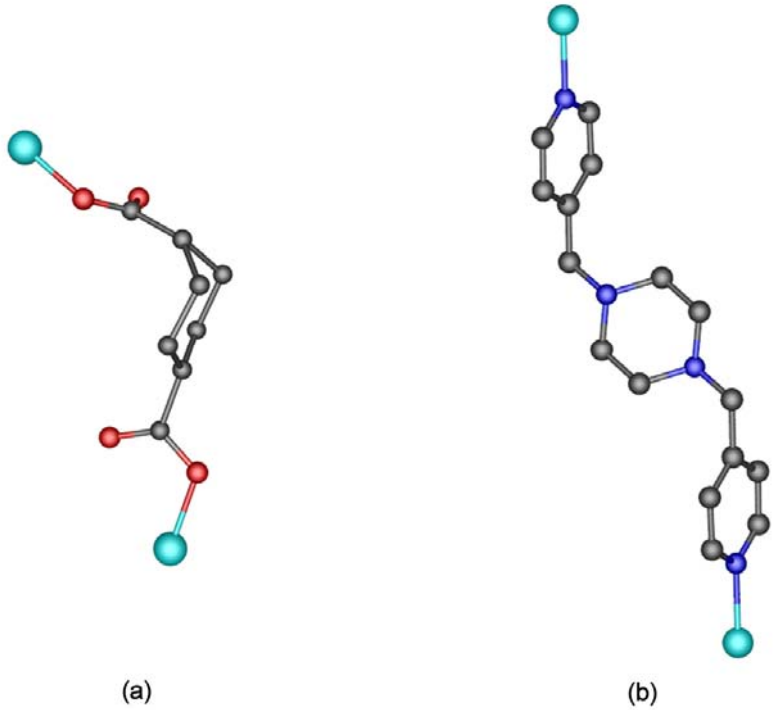

Fig. S6. The coordination modes of organic linear ligands in compound **2**: **(a)** chdc; **(b)** bpmp.

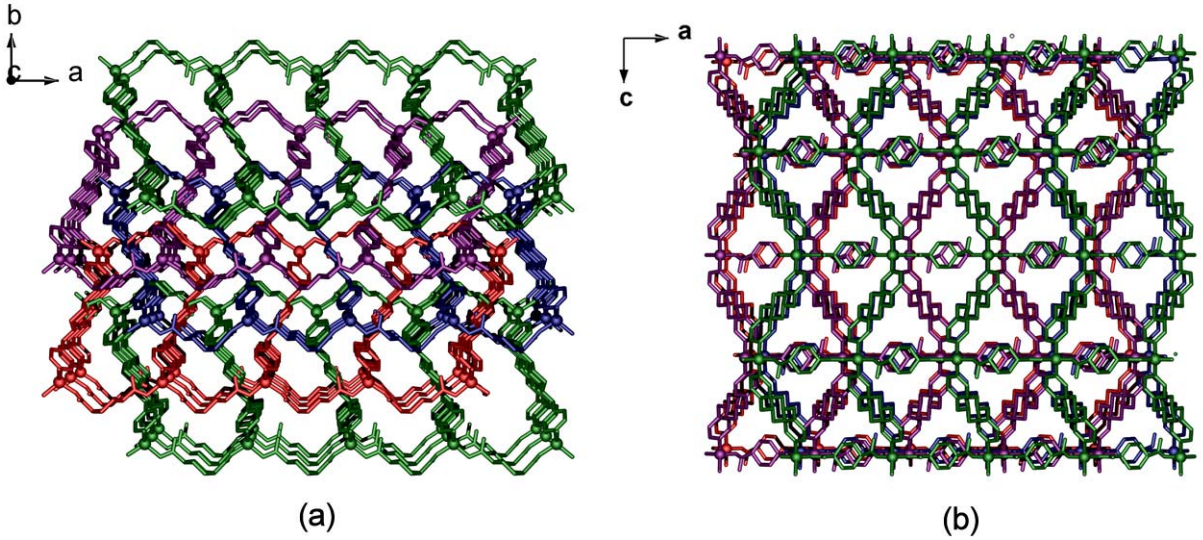

Fig. S7. Packing arrangements of compound **2** viewed along **(a)** *c* axis and **(b)** *b* axis.

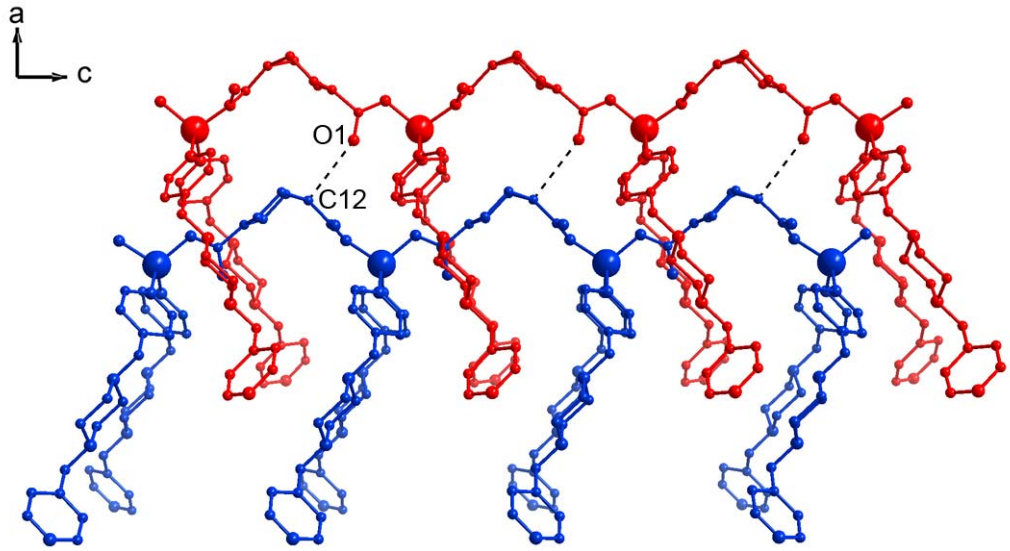

Fig. S8 The weak intermolecular forces between two adjacent layers in **2** with the close distance of O(1)…C(12) 3.26 Å.

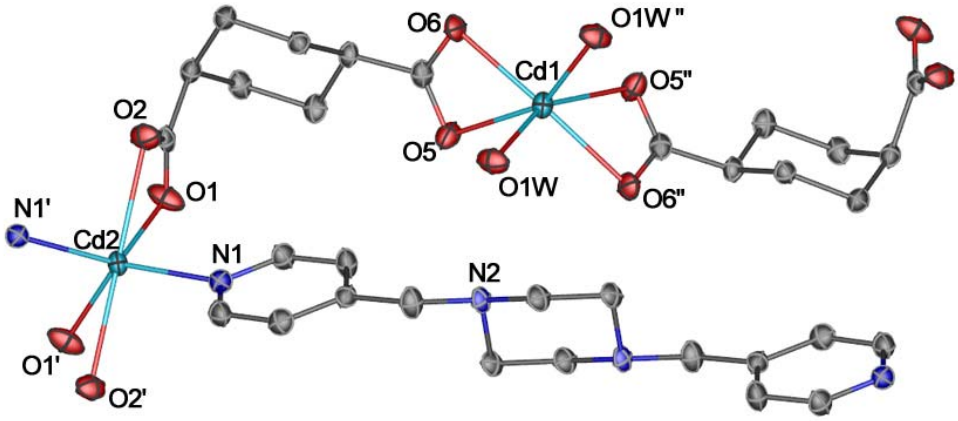

Fig. S9. ORTEP view of the basic unit in compound **3** with thermal ellipsoids of 50%. H atoms are omitted for clarity. The symmetry transformations for N1', O1' and O2' are -x+1,y,-z+1/2, for O5'', O6'' and O1W'' are -x+2,y,-z+1/2.

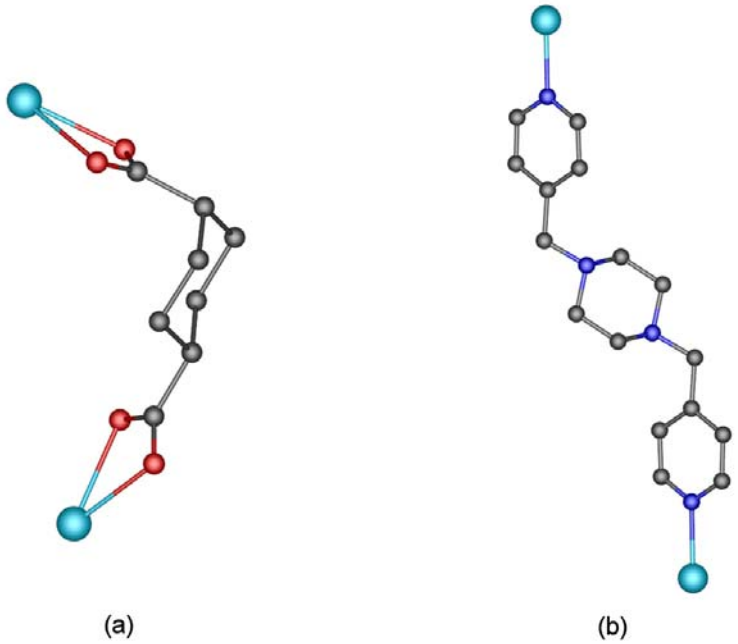

Fig. S10. The coordination modes of organic linear ligands in compound **3**: **(a)** chdc; **(b)** bpmp.

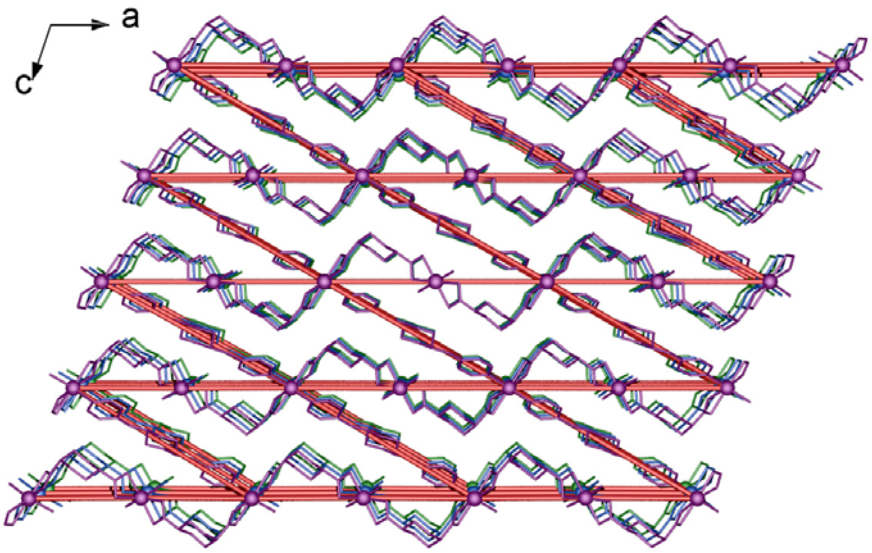

Fig. S11. The packing arrangement of compound **3** viewed along *b* axis.

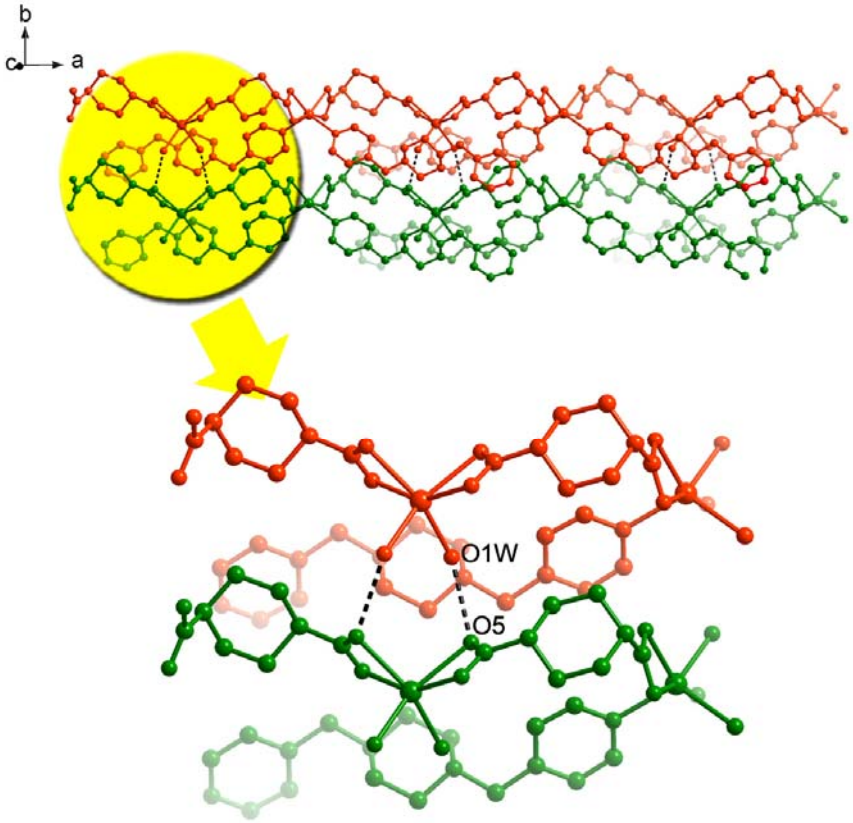

Fig. S12. The hydrogen bonding interactions between two adjacent layers in **3** with the close distance of O(1W)…O(5) 2.81 Å.

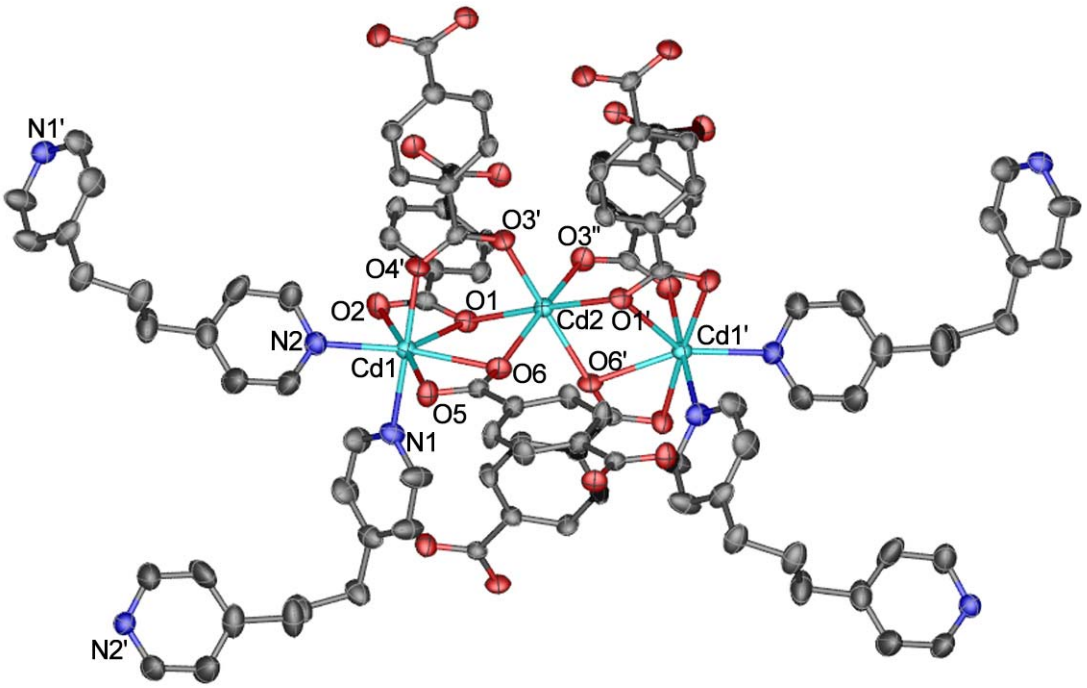

Fig. S13 ORTEP view of the basic unit in compound **4** with thermal ellipsoids of 50%. H atoms are omitted for clarity. The symmetry transformations for O4' and O3' are x,-y+2,z-1/2, for O3'' are -x+1,-y+2,-z+1, and for O1' and O6' are -x+1,y,-z+1/2.

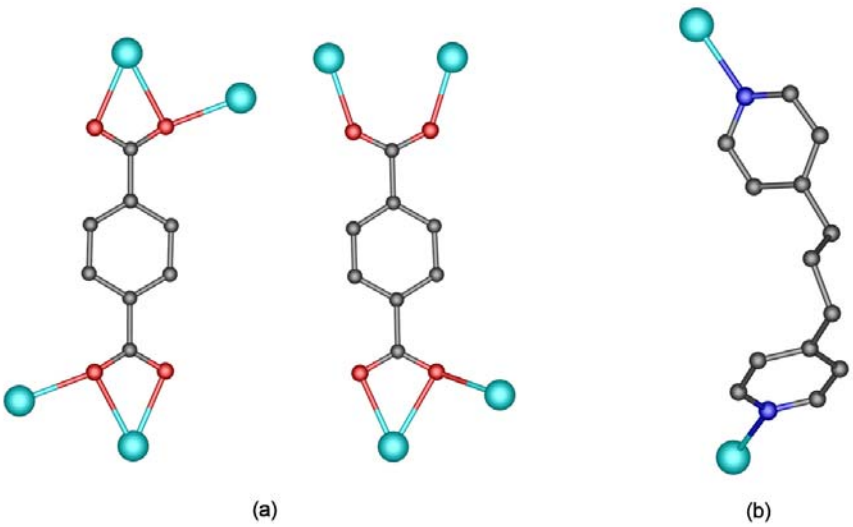

Fig. S14 The coordination modes of organic linear ligands in compound **4**: **(a)** tp; **(b)** bpp.

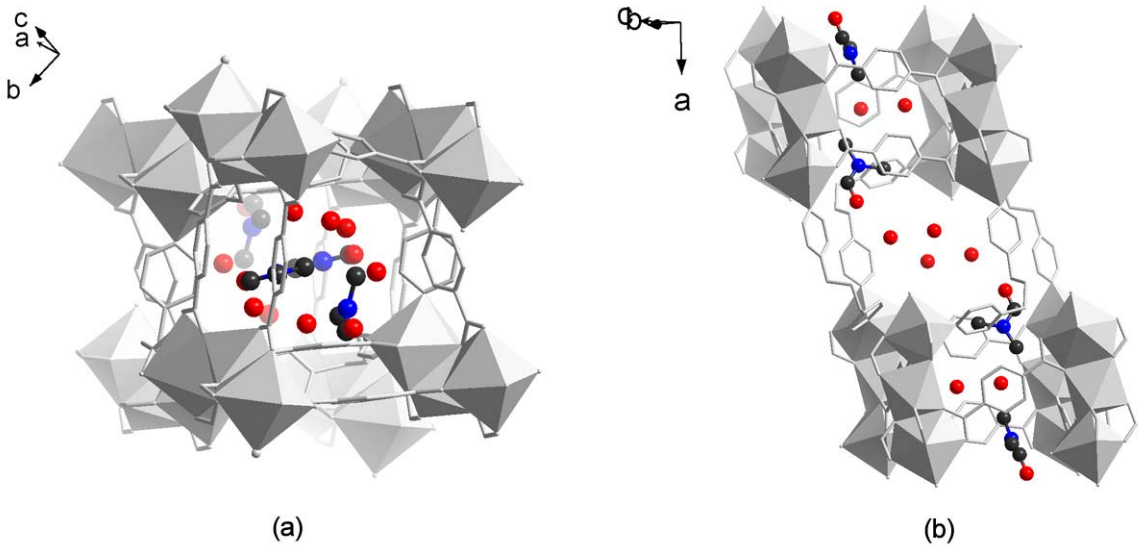

Fig. S15. The arrangement of "guest" solvent DMF and water molecules in one unit of the 3-D open framework of **4**: **(a)** top view and **(b)** side-view of the 3-D open framework unit.

2. Additional Tables of Selected bond lengths and angles as well as H-bonds

Table S1 Selected bond lengths and angles of compounds **1 – 4**

1			
Zn(1)-O(1)	1.950(2)	O(1)-Zn(1)-N(1)	103.64(8)
Zn(1)-O(4)A	1.956(2)	O(4)A-Zn(1)-N(1)	114.59(9)
Zn(1)-N(1)	2.047(2)	O(1)-Zn(1)-N(2)	108.54(9)
Zn(1)-N(2)	2.053(2)	O(4)A-Zn(1)-N(2)	104.56(9)
O(1)-Zn(1)-O(4)A	121.17(9)	N(1)-Zn(1)-N(2)	102.84(8)
2			
Zn(1)-O(3)A	1.920(6)	O(3)B-Zn(1)-O(2)	106.3(2)
Zn(1)-O(3)B	1.920(6)	O(3)A-Zn(1)-N(1)	97.89(19)
Zn(1)-O(2)	1.927(4)	O(3)B-Zn(1)-N(1)	118.7(2)
Zn(1)-N(1)	2.070(3)	O(2)-Zn(1)-N(1)	113.14(10)
Zn(1)-N(1)C	2.070(3)	O(3)A-Zn(1)-N(1)C	118.7(2)
O(3)-Zn(1)E	1.920(6)	O(3)B-Zn(1)-N(1)C	97.89(19)
O(3)A-Zn(1)-O(3)B	24.6(3)	O(2)-Zn(1)-N(1)C	113.14(10)
O(3)A-Zn(1)-O(2)	106.3(2)	N(1)-Zn(1)-N(1)C	106.84(17)
3			
Cd(1)-O(1W)	2.246(2)	O(1W)-Cd(1)-O(5)	95.05(8)
Cd(1)-O(1W)A	2.246(2)	O(1W)A-Cd(1)-O(5)	154.01(7)
Cd(1)-O(6)A	2.264(2)	O(6)A-Cd(1)-O(5)	103.42(8)
Cd(1)-O(6)	2.264(2)	O(6)-Cd(1)-O(5)	56.28(7)
Cd(1)-O(5)A	2.406(2)	O(5)A-Cd(1)-O(5)	96.65(10)
Cd(1)-O(5)	2.406(2)	O(1)B-Cd(2)-O(1)	91.52(11)
Cd(2)-O(1)B	2.290(2)	O(1)B-Cd(2)-N(1)	97.87(8)
Cd(2)-O(1)	2.290(2)	O(1)-Cd(2)-N(1)	126.84(8)
Cd(2)-N(1)	2.295(2)	O(1)B-Cd(2)-N(1)B	126.84(8)
Cd(2)-N(1)B	2.295(2)	O(1)-Cd(2)-N(1)B	97.87(8)
Cd(2)-O(2)B	2.420(2)	N(1)-Cd(2)-N(1)B	116.28(13)

Cd(2)-O(2)	2.420(2)	O(1)B-Cd(2)-O(2)B	55.45(7)
O(1W)-Cd(1)-O(1W)A	84.18(12)	O(1)-Cd(2)-O(2)B	138.21(8)
O(1W)-Cd(1)-O(6)A	98.40(8)	N(1)-Cd(2)-O(2)B	86.28(8)
O(1W)A-Cd(1)-O(6)A	102.38(8)	N(1)B-Cd(2)-O(2)B	85.98(8)
O(1W)-Cd(1)-O(6)	102.38(8)	O(1)B-Cd(2)-O(2)	138.21(8)
O(1W)A-Cd(1)-O(6)	98.40(8)	O(1)-Cd(2)-O(2)	55.45(7)
O(6)A-Cd(1)-O(6)	151.88(11)	N(1)-Cd(2)-O(2)	85.98(8)
O(1W)-Cd(1)-O(5)A	154.01(7)	N(1)B-Cd(2)-O(2)	86.28(8)
O(6)A-Cd(1)-O(5)A	56.28(7)	O(2)B-Cd(2)-O(2)	165.30(11)
O(6)-Cd(1)-O(5)A	103.42(8)		
4			
Cd(1)-O(4)A	2.258(4)	O(4)A-Cd(1)-O(6)	85.09(14)
Cd(1)-N(1)	2.328(5)	N(1)-Cd(1)-O(6)	96.47(15)
Cd(1)-N(2)	2.333(5)	N(2)-Cd(1)-O(6)	143.41(15)
Cd(1)-O(5)	2.346(4)	O(2)-Cd(1)-O(6)	129.73(13)
Cd(1)-O(2)	2.357(4)	O(4)A-Cd(1)-O(1)	89.14(14)
Cd(1)-O(6)	2.483(4)	N(1)-Cd(1)-O(1)	90.68(15)
Cd(1)-O(1)	2.507(4)	N(2)-Cd(1)-O(1)	139.59(15)
Cd(2)-O(3)B	2.211(4)	O(5)-Cd(1)-O(1)	129.76(12)
Cd(2)-O(3)A	2.211(4)	O(6)-Cd(1)-O(1)	76.05(12)
Cd(2)-O(6)C	2.306(4)	O(3)B-Cd(2)-O(3)A	97.9(2)
Cd(2)-O(6)	2.306(4)	O(3)B-Cd(2)-O(6)C	89.40(15)
Cd(2)-O(1)C	2.376(3)	O(3)A-Cd(2)-O(6)C	169.87(14)
Cd(2)-O(1)	2.376(3)	O(3)B-Cd(2)-O(6)	169.87(14)
O(3)-Cd(2)B	2.211(4)	O(3)A-Cd(2)-O(6)	89.40(15)
O(4)-Cd(1)D	2.258(4)	O(6)C-Cd(2)-O(6)	84.3(2)
O(4)A-Cd(1)-N(1)	178.34(16)	O(3)B-Cd(2)-O(1)C	91.14(14)
O(4)A-Cd(1)-N(2)	87.25(16)	O(3)A-Cd(2)-O(1)C	90.72(14)
N(1)-Cd(1)-N(2)	91.82(18)	O(6)C-Cd(2)-O(1)C	82.04(13)

O(4)A-Cd(1)-O(5)	92.32(15)	O(6)-Cd(2)-O(1)C	95.85(13)
N(1)-Cd(1)-O(5)	89.06(15)	O(3)B-Cd(2)-O(1)	90.72(14)
N(2)-Cd(1)-O(5)	90.61(15)	O(3)A-Cd(2)-O(1)	91.14(14)
O(4)A-Cd(1)-O(2)	88.44(15)	O(6)C-Cd(2)-O(1)	95.85(13)
N(1)-Cd(1)-O(2)	90.12(15)	O(6)-Cd(2)-O(1)	82.04(13)
N(2)-Cd(1)-O(2)	85.64(16)	O(1)C-Cd(2)-O(1)	177.17(18)
O(5)-Cd(1)-O(2)	176.13(13)		

a Symmetry codes: A -x+1,-y+1,-z+1 B x,y,z-1 C x,y,z+1 for **1;** A x,y,z-1 B x,-y+1/2,z-1 C x,-y+1/2,z D -x,-y,-z E x,y,z+1 for **2;** A -x+2,y,-z+1/2 B -x+1,y,-z+1/2 C -x,-y,-z for **3**; A x,-y+2,z-1/2 B -x+1,-y+2,-z+1 C -x+1,y,-z+1/2 D x,-y+2,z+1/2 E -x+1,-y+1,-z F -x+3/2,y-1/2,-z+1/2 G -x+3/2,y+1/2,-z+1/2 H -x+1,y,-z+3/2 for **4**

Table S2 Hydrogen bonding interactions of $\{H_2O\}_{12}$ cluster in compound **1**

D-H	**d(D-H) (Å)**	**d(H..A) (Å)**	**<DHA (^{o})**	**d(D..A) (Å)**	**A**	**Symmetry Operation**
O1W-H1AW	0.852	2.477	115.91	2.950	O2	-x+1, -y+1, -z+1
O1W-H1AW	0.852	2.532	155.79	3.328	O4W	
O1W-H1BW	0.846	2.011	169.96	2.848	O3W	
O2W-H2AW	0.831	2.621	119.00	2.830	O2W	-x+1, -y+2, -z
O2W-H2BW	0.834	2.006	170.79	2.832	O5W	-x+1, -y+1, -z
O3W-H3AW	0.845	2.311	116.21	2.789	O6W	
O3W-H3BW	0.856	2.495	111.61	2.921	O3	-x+1, -y+1, -z+1
O3W-H3BW	0.856	2.618	160.44	3.437	O5W	
O4W-H4AW	0.853	2.115	176.96	2.967	O2W	
O4W-H4BW	0.852	2.038	170.80	2.882	O2	-x+1, -y+1, -z+1
O5W-H5AW	0.860	2.026	172.71	2.882	O3	-x+1, -y+1, -z+1
O5W-H5BW	0.853	2.238	165.25	3.070	O6W	
O6W-H6AW	0.837	2.207	146.51	2.942	O5W	-x+1, -y+1, -z
O6W-H6BW	0.839	2.063	160.15	2.866	O4W	-x+1, -y+1, -z

3. Physical Measurements

Infrared spectrum of 1-4

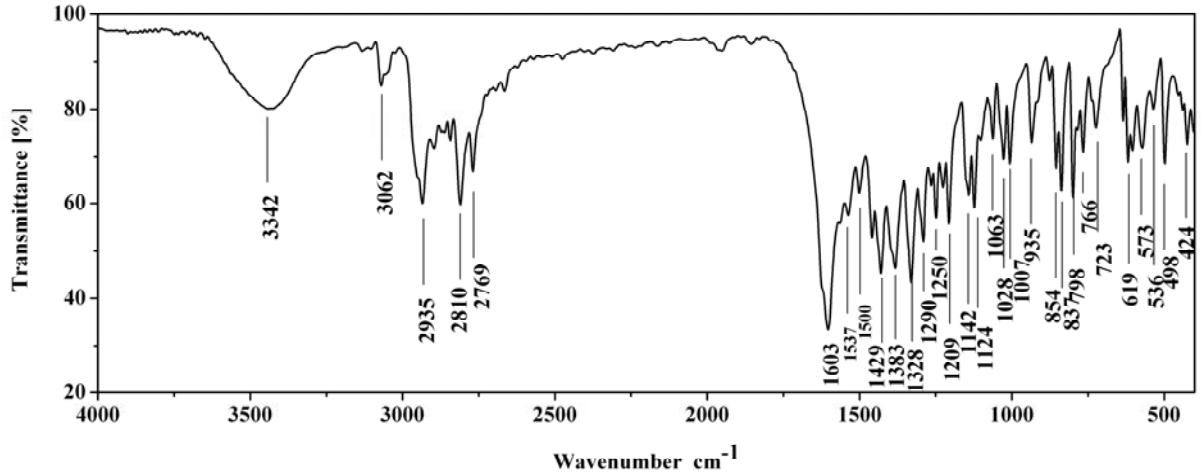

Fig. S16 IR spectra of **1**

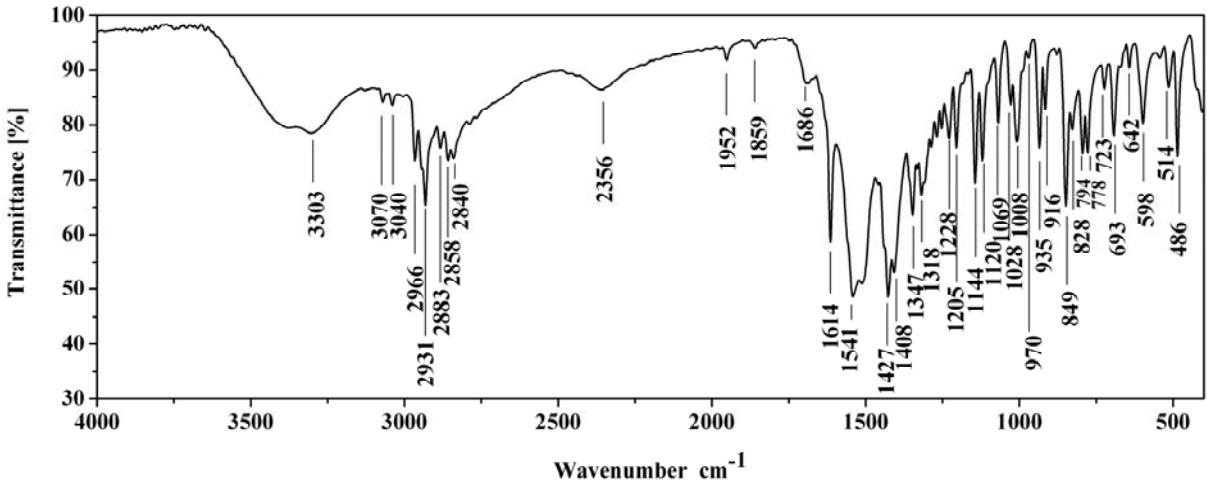

Fig. S17 IR spectra of **2**

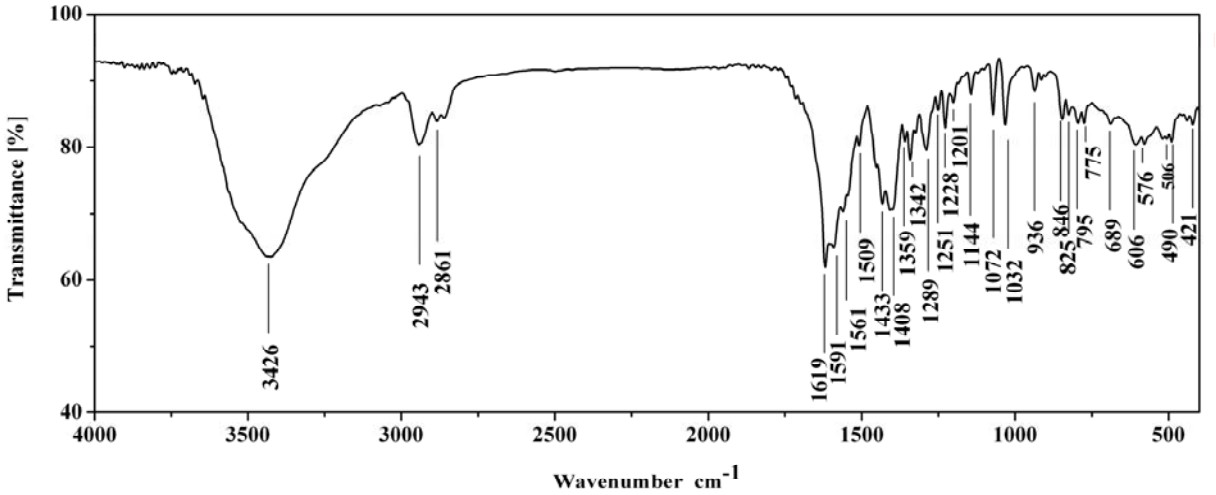

Fig. S18 IR spectra of **3**

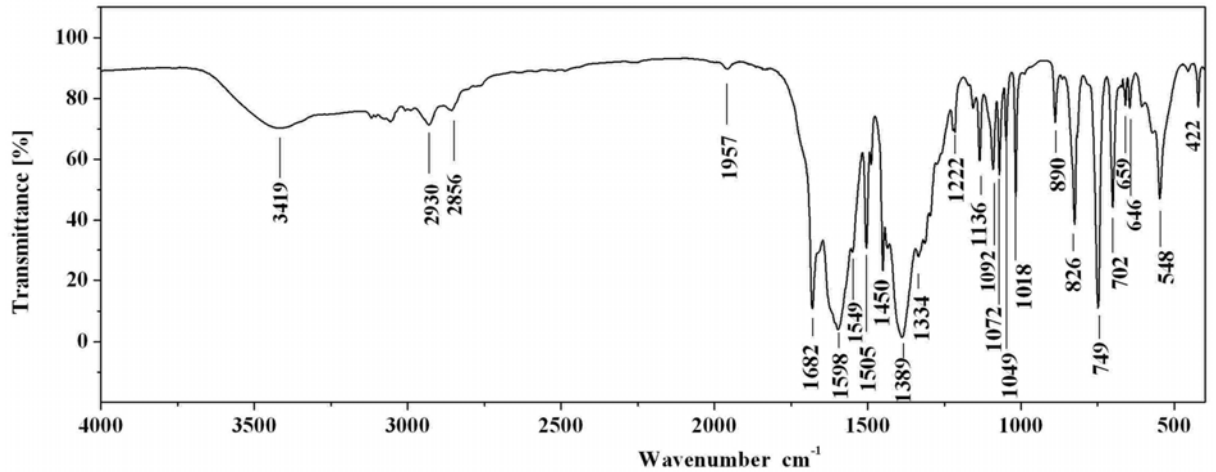

Fig. S19 IR spectra of **4**

Thermogravimetric (TG) analyses of 1–4

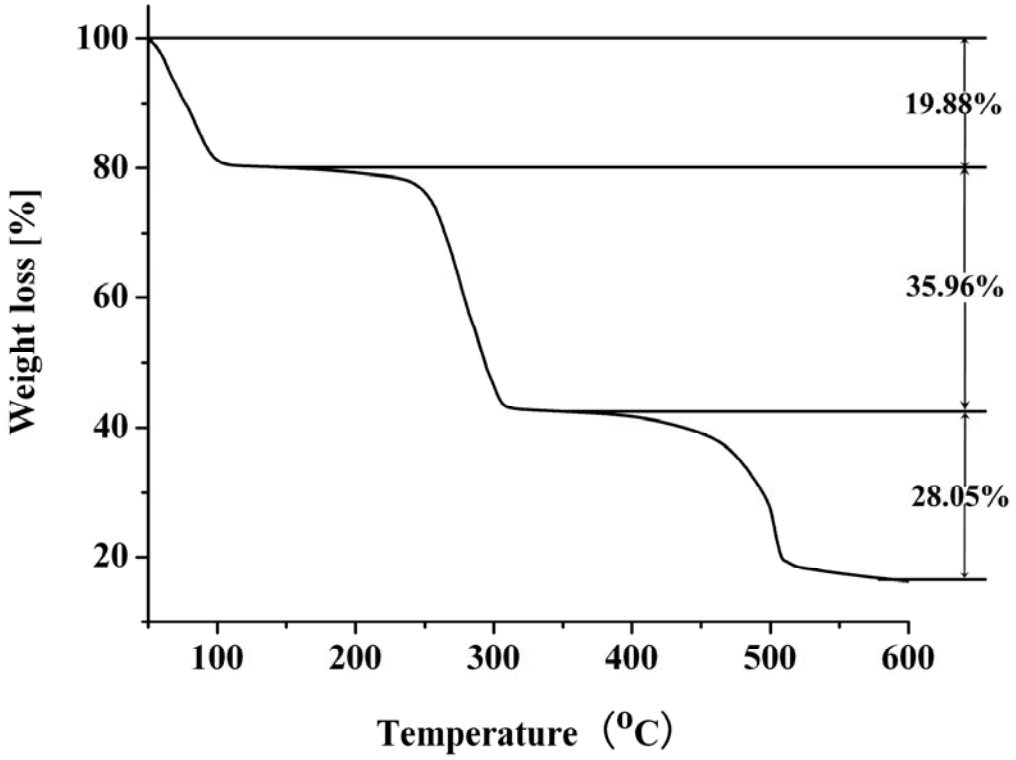

Fig. S20 TGA curve of **1**

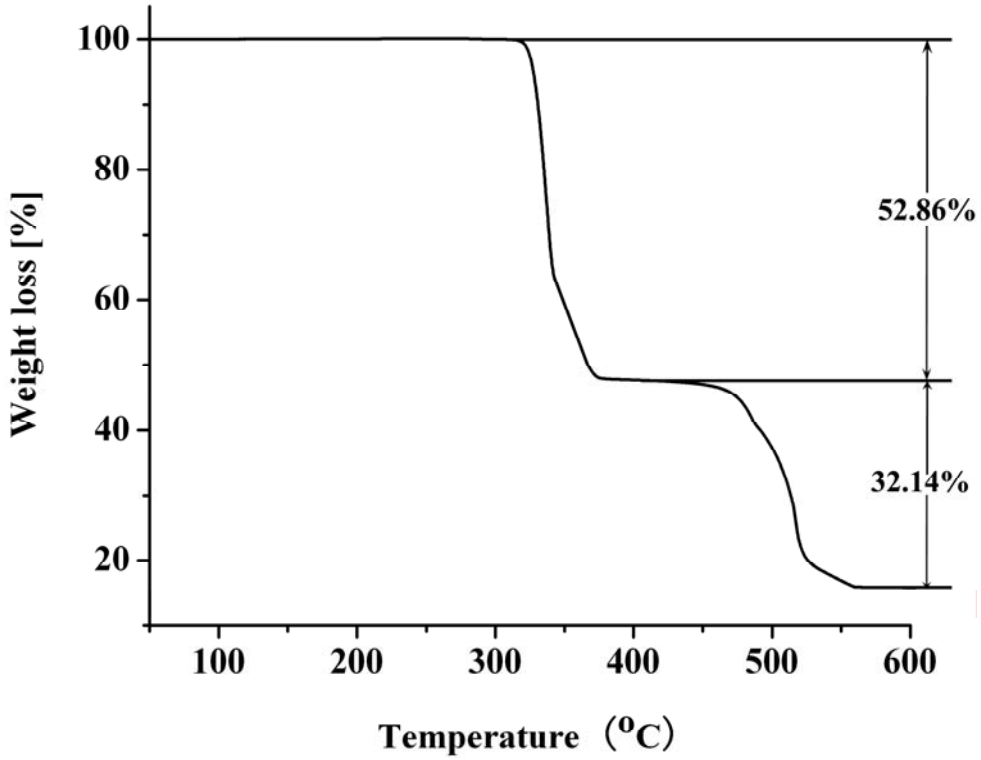

Fig. S21 TGA curve of **2**

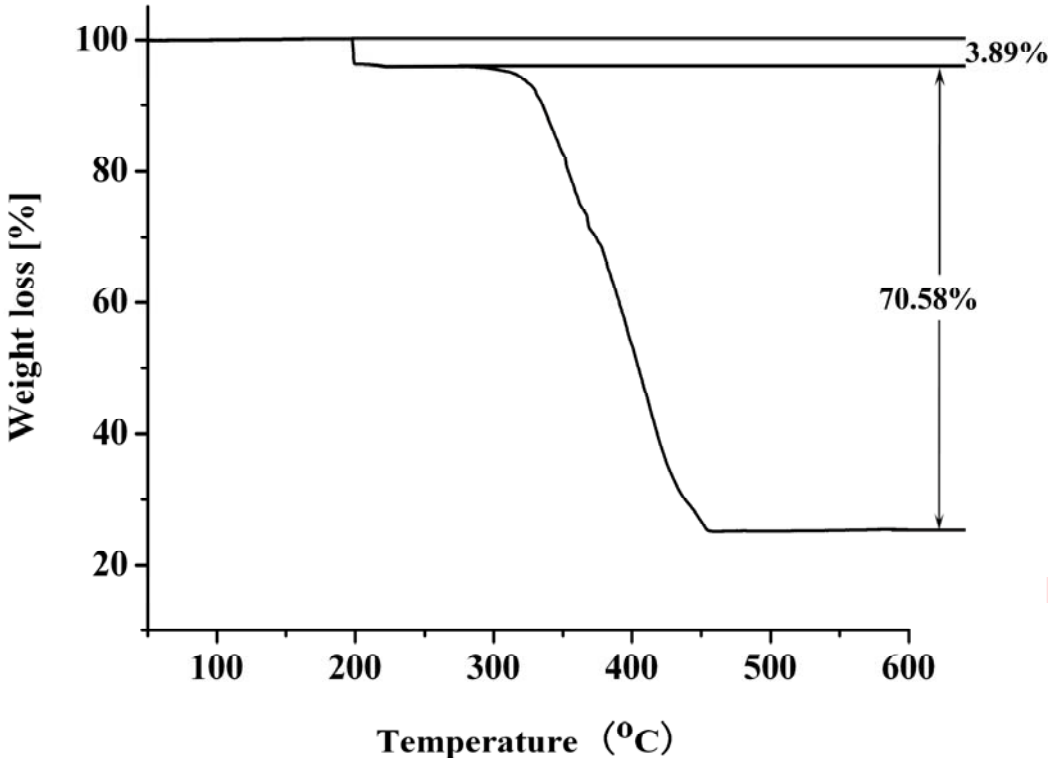

Fig. S22 TGA curve of **3**

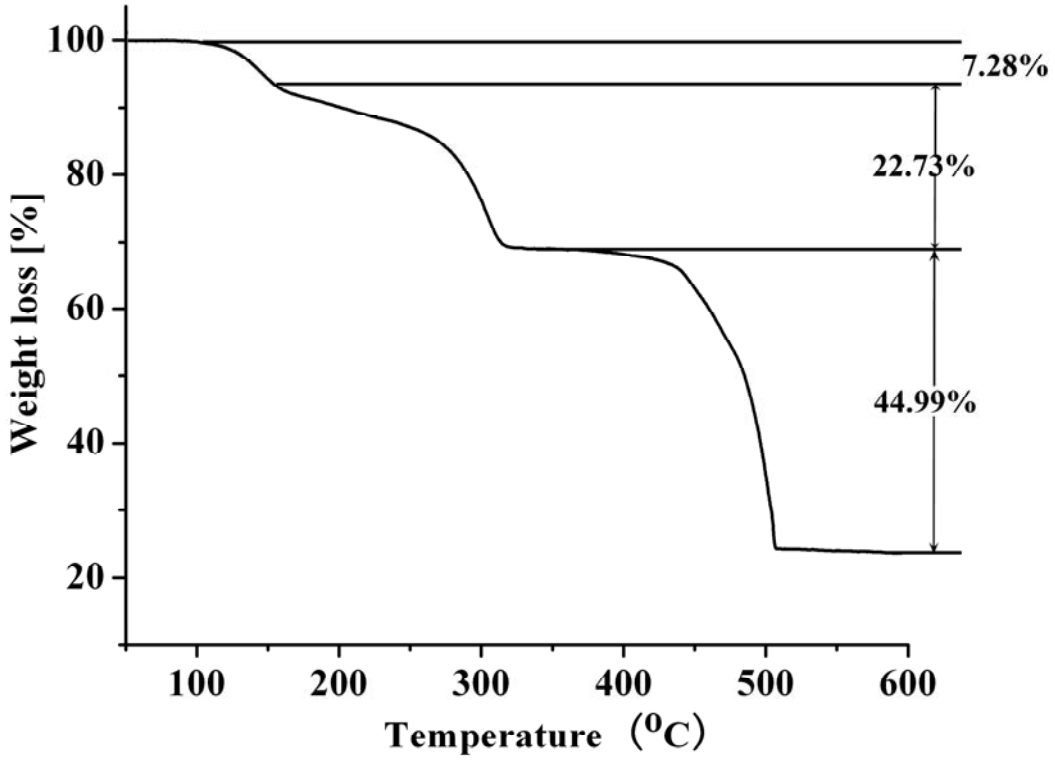

Fig. S23 TGA curve of **4**

Powder X-ray diffraction (PXRD) patterns of 1-4

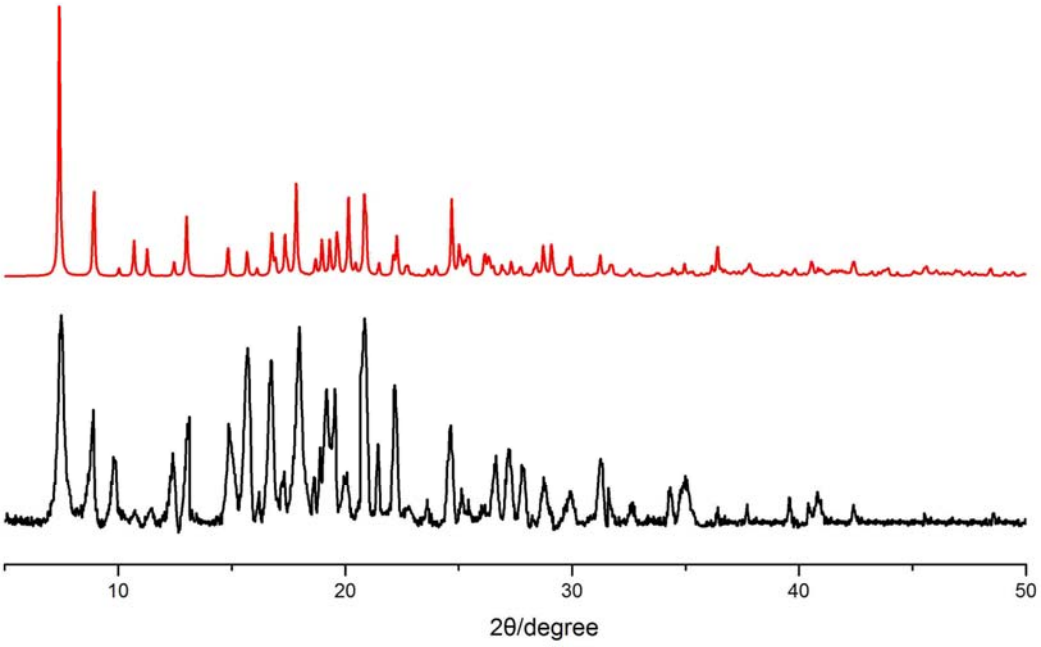

Fig. S24 simulated and experimental patterns of **1**: simulated(red), as-synthesized sample at room temperature(black)

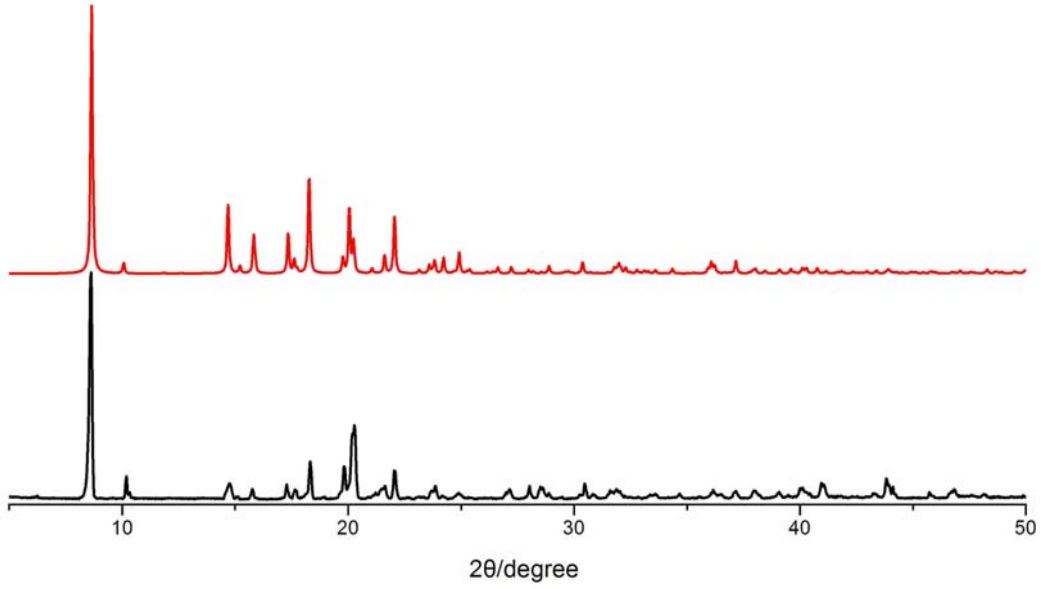

Fig. S25 simulated and experimental patterns of **2**: simulated(red), as-synthesized sample at room temperature(black)

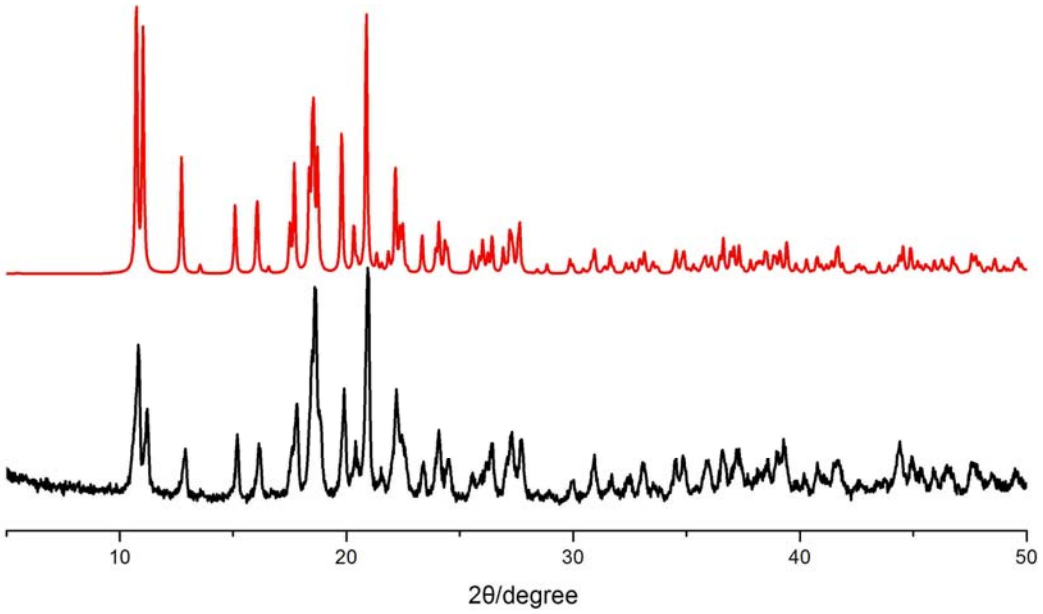

Fig. S26 simulated and experimental patterns of **3**: simulated(red), as-synthesized sample at room temperature(black)

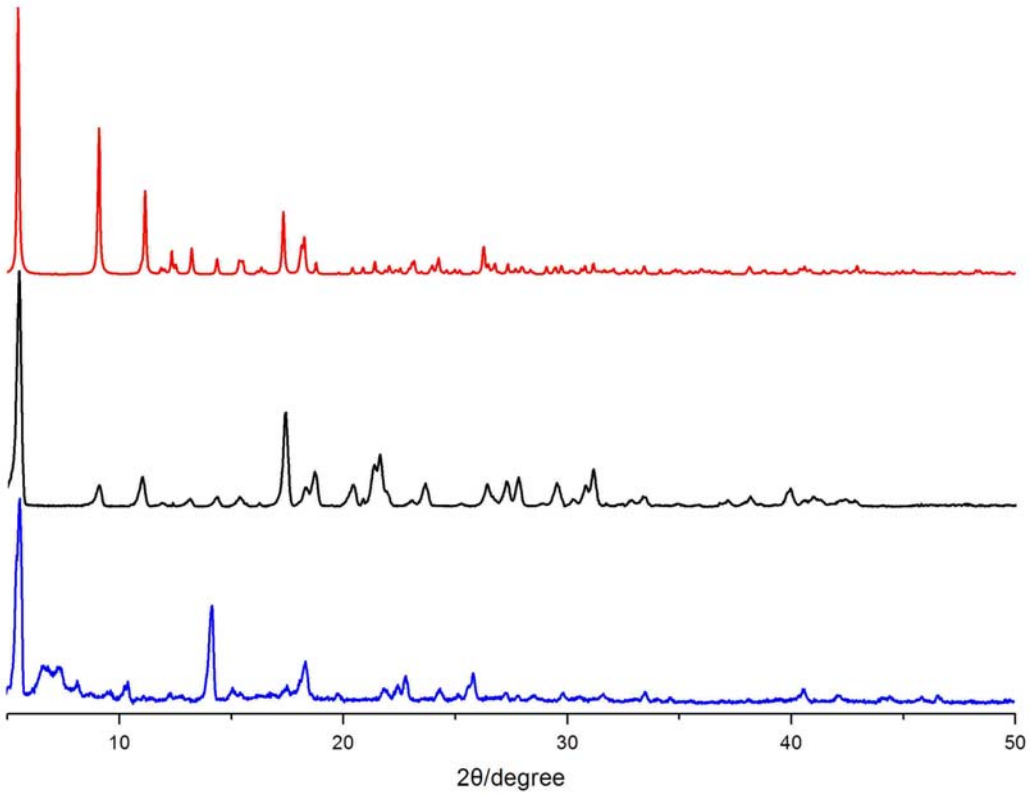

Fig. S27 simulated and experimental patterns of **4**: simulated(red), as-synthesized sample at room temperature(black), desolvated sample(blue) of **4** (heated at 140°C for 12 h under vacuum).