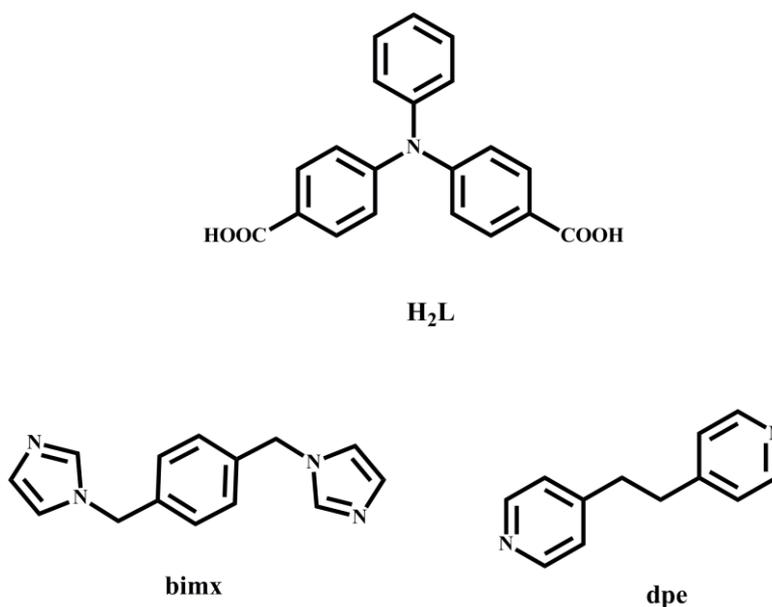## Construction of three metal-organic frameworks based on the sterically hindered V-shaped carboxylate ligand

Ling Qin, Cao Mei, Wei-Juan Zuo, Ya-Guang Wu, Ru-Yong Yan and Yan-Qing Wang

Scheme S1 The N-centered carboxylate H_2L and nitrogen-containing ligands.

Materials and Methods. All chemicals and solvents used in the syntheses were of reagent grade and were used without further purification except H_2L ligand. C, H, and N elemental analyses were performed on a Perkin-Elmer 240C elemental analyzer. Powder X-ray diffraction (PXRD) measurements were carried out with a Bruker D8 Advance X-ray diffractometer using Cu-Kα radiation (1.5418 Å), and the X-ray tube was operated at 40 kV and 40 mA.
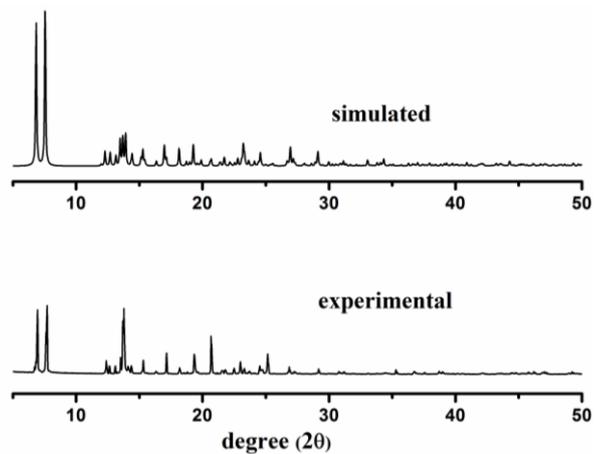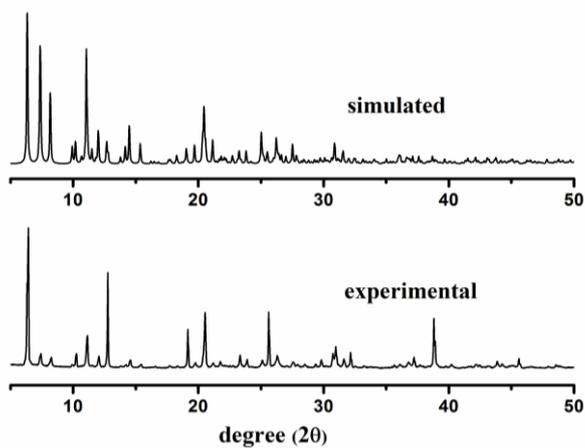
Figure S1 PXRD for compound **1**.
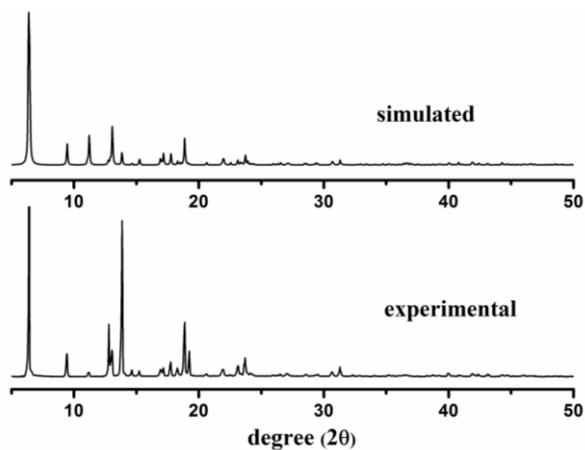

Figure S2 PXRD for compound **2**.

Figure S3 PXRD for compound **3**.
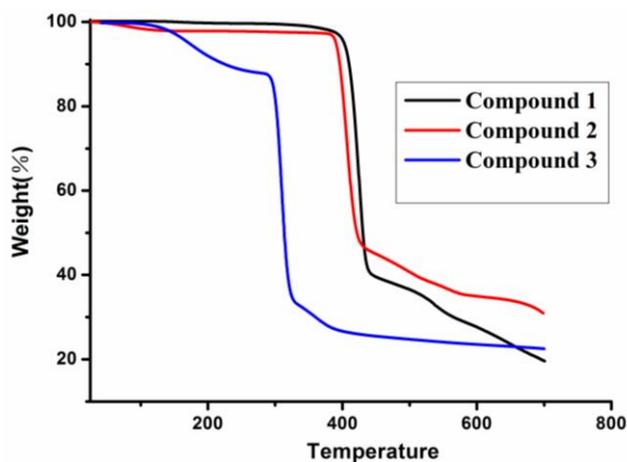
Figure S4 TGA for compounds **1-3**.

Table S1 Bond lengths [Å] and angles [deg] for compounds **1-3**.

Complex **1**

Cd1- N2	2.237(2)	Cd1- O1	2.3445(18)
Cd1- O1a	2.4811(19)	Cd1- O2	2.409(2)
Cd1- O3b	2.217(2)	Cd1- O4c	2.412(2)
N2 - Cd1- O1	86.82(8)	N2 - Cd1- O1a	91.01(9)
N2 - Cd1- O2	146.53(8)	N2 - Cd1- O3	121.78(8)
N2 - Cd1- O4c	82.05(8)	O1 - Cd1- O1a	74.79(7)
O1 - Cd1- O2	101.54(7)	O1 - Cd1- O3b	134.22(8)
O1 - Cd1- O4c	90.39(8)	O1a - Cd1- O2	105.82(9)
O1a - Cd1- O3b	83.81(8)	O1a - Cd1- O4c	160.21(7)
O2 - Cd1- O3b	91.49(8)	O2 - Cd1- O4c	156.21(10)
O3b - Cd1- O4c	115.97(8)		

Complex **2**

Cd1- N1	2.338(7)	Cd1- N2a	2.305(6)
Cd1- O1	2.399(2)	Cd1- O2	2.381(2)
Cd1- O3b	2.259(2)	Cd1- O4c	2.265(2)

N1 - Cd1- N2a	174.8(2)	N1 - Cd1- O1	89.57(19)
N1 - Cd1- O2	86.5(2)	N1 - Cd1- O3b	86.32(18)
N1 - Cd1- O4c	87.39(18)	N2a - Cd1- O1	85.35(15)
N2a - Cd1- O2	91.67(17)	N2a - Cd1- O3b	93.01(16)
N2a - Cd1- O4c	97.55(14)	O1 - Cd1- O2	55.37(5)
O1 - Cd1- O3b	96.65(8)	O1 - Cd1- O4c	146.50(11)
O2 - Cd1- O3b	151.1(2)	O2- Cd1- O4c	91.13(8)
O3b - Cd1- O4c	116.40(6)		

Complex 3

Cu1- N1	2.156(3)	Cu1- O1	1.9631(14)
Cu1- O1a	1.9631(14)	Cu1- O2	1.9629(15)
Cu1- O2b	1.9629(15)	N1 - Cu1- O1	93.35(7)
N1 - Cu1- O1a	93.35(7)	N1 - Cu1- O2	98.92(7)
N1 - Cu1- O2b	98.92(7)	O1 - Cu1- O1a	90.16(10)
O1 - Cu1- O2	88.14(7)	O1 - Cu1- O2b	167.69(7)
O1a - Cu1- O2	91.88(10)	O1a - Cu1- O2b	88.14(7)
O2 - Cu1- O2b	90.93(10)		

Symmetry codes: for **1:** a = 1 - x, -0.5 + y, -0.5 - z; b= 1 + x, 0.5 - y, 0.5 + z; c=1 - x, - y, - z. for **2:** a= -0.5 + x, 1.5 - y, -0.5 + z; b = 1 - x, y, 0.5 - z. for **3:** a = 0.5 - x, 0.5 - y, z; b = 0.5 - x, 0.5 - y, 1 - z.