Electronic Supplementary Material (ESI) for CrystEngComm

Supporting Information

Auxiliary Ligands-Assisted Structural Diversity of Three Metal-Organic Frameworks Assembled by Potassium 1*H*–1,2,3–Triazole–4,5–Dicarboxylic Acid: Syntheses, Crystal Structures and Luminescence Properties

Ji-Yong Zou,[a] Hong-Ling Gao,*[a] Wei Shi,[b] Jian-Zhong Cui*[a] and Peng Cheng [b]

1. Thermogravimetric analysis

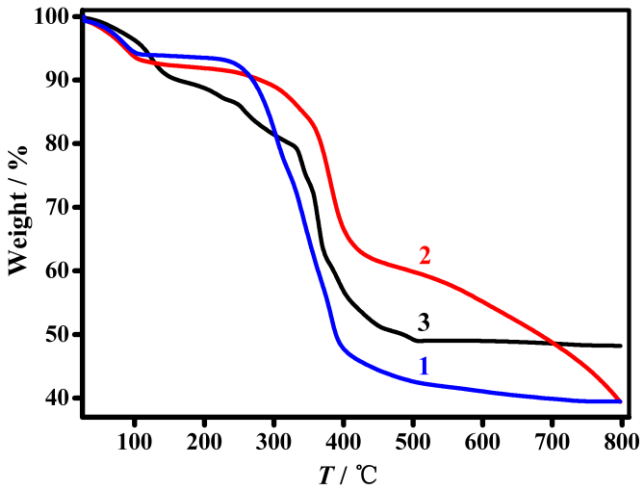

Fig. S1 The thermal gravimetric analysis (TGA) data of **1-3.**

2. Power X-Ray diffraction

Powder X-ray diffraction measurements were recorded on a D/Max-2500 X-ray diffractometer using Cu/Kα radiation.

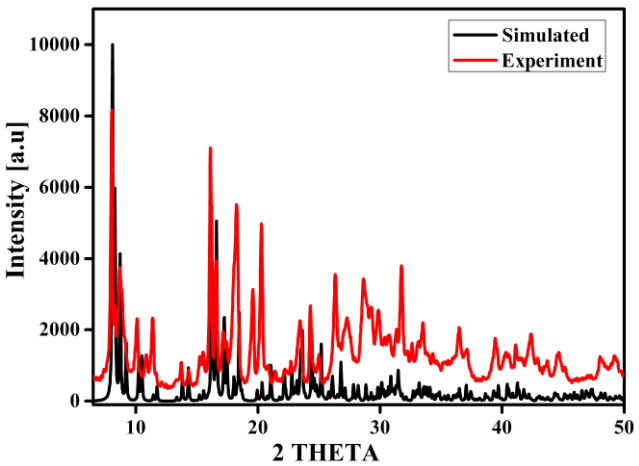

Fig. S2 Comparison of the experimental PXRD pattern of as-synthesized **1** with the one simulated from its single crystal structure.

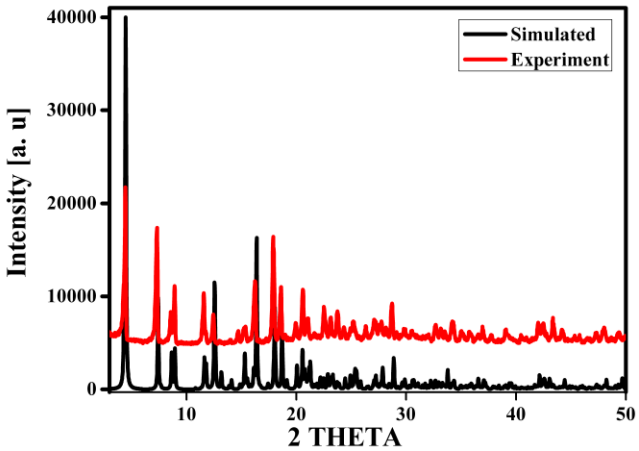

Fig. S3 Comparison of the experimental PXRD pattern of as-synthesized **2** with the one simulated from its single crystal structure

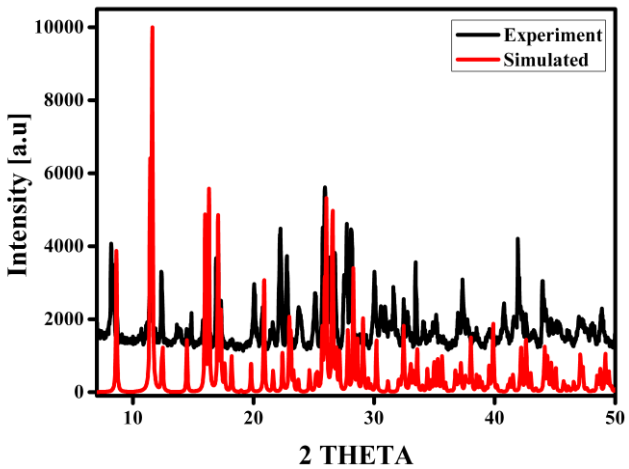

Fig. S4 Comparison of the experimental PXRD pattern of as-synthesized **3** with the one simulated from its single crystal structure

3. Infrared spectra

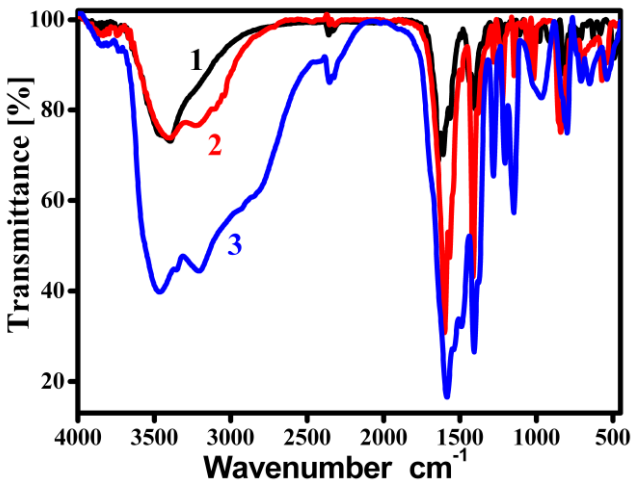

Fig. S5 IR spectra of **1-3**

4. Crystal Structures

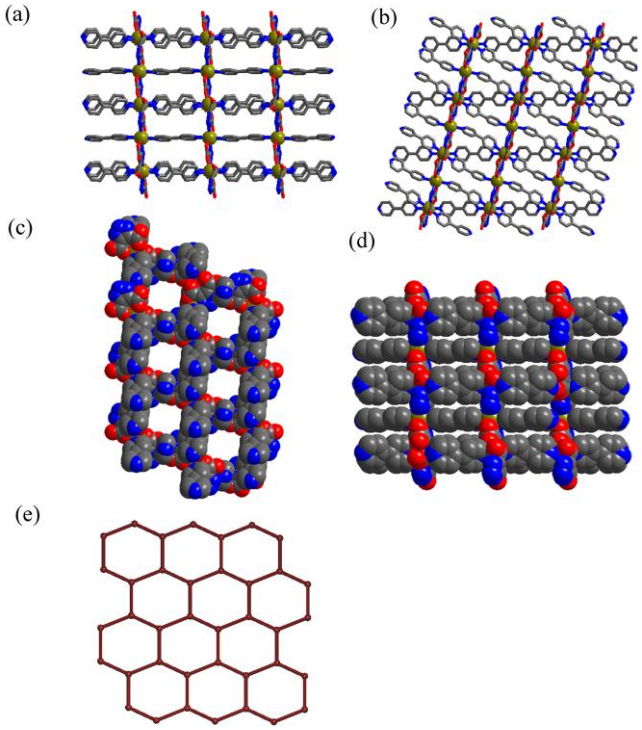

Fig. S6 View of the 3D structure of **1** along (a) the [0, 1, 0] direction, (b) the [0, 0 ,1] direction, (c) the space filling of **1** viewed along the [1, 0, 0] direction and (d) the [0, 1, 0] direction, (e) the **hcb** layers.

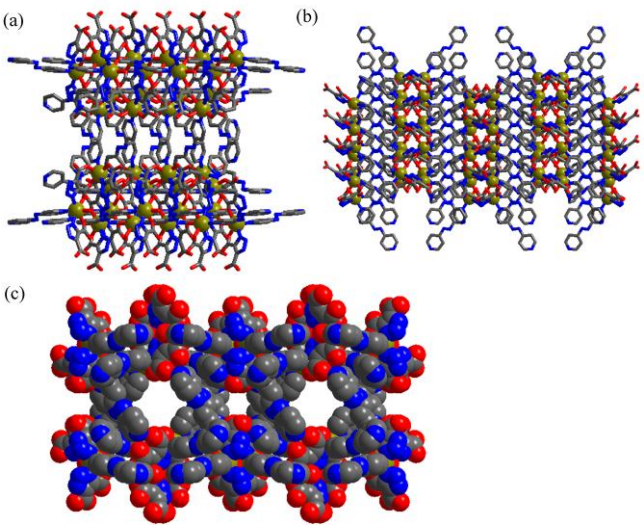

Fig. S7 View of the 3D structure of **2** along (a) the [1, 0, 0] direction, (b) the [0,1 ,0] direction, (c) the space filling of **2** viewed along the[0, 0 ,1] direction.

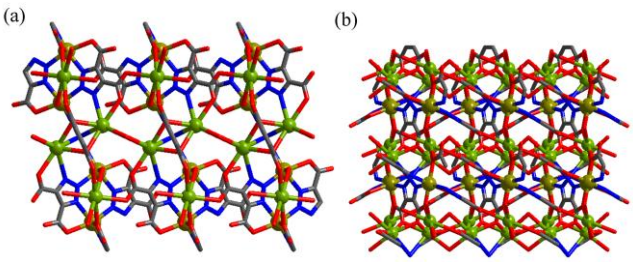

Fig. S8 View of the 3D structure of **3** along (a) the [0, 1, 0] direction, (b) the [0,0 ,1] direction.

Table S1 Selected bonds length and angles for MOFs **1-3**

1

Zn(1)-O(1)	2.113(3)	N(6)-Zn(1)-N(6)$^{\#1}$	180.0
Zn(1)-O(1)$^{\#1}$	2.113(3)	N(1)$^{\#2}$-Zn(2)-N(1)	180.0
Zn(1)-O(3)	2.091(3)	N(1)$^{\#2}$-Zn(2)-O(2)	101.61(13)
Zn(1)-O(3)$^{\#1}$	2.091(3)	N(1)-Zn(2)-O(2)	78.39(13)
Zn(1)-N(6)	2.149(4)	N(1)$^{\#2}$-Zn(2)-O(2)$^{\#2}$	78.39(13)
Zn(1)-N(6)$^{\#1}$	2.149(4)	N(1)-Zn(2)-O(2)$^{\#2}$	101.61(13)
Zn(2)-O(2)	2.132(3)	O(2)-Zn(2)-O(2)$^{\#2}$	180.0
Zn(2)-O(2)$^{\#2}$	2.132(3)	N(1)$^{\#2}$-Zn(2)-N(4)$^{\#2}$	90.12(14)
Zn(2)-N(1)	2.057(4)	N(1)-Zn(2)-N(4)$^{\#2}$	89.88(14)
Zn(2)-N(1)$^{\#2}$	2.057(4)	O(2)-Zn(2)-N(4)$^{\#2}$	94.11(14)
Zn(2)-N(4)	2.219(4)	O(2)$^{\#2}$-Zn(2)-N(4)$^{\#2}$	85.90(14)
Zn(2)-N(4)$^{\#2}$	2.219(4)	N(1)$^{\#2}$-Zn(2)-N(4)	89.88(14)
Zn(3)-O(4)	2.129(3)	N(1)-Zn(2)-N(4)	90.12(14)
Zn(3)-O(4)$^{\#3}$	2.129(3)	O(2)-Zn(2)-N(4)	85.89(14)
Zn(3)-N(3)	2.080(4)	O(2)$^{\#2}$-Zn(2)-N(4)	94.10(14)
Zn(3)-N(3)$^{\#3}$	2.080(4)	N(4)$^{\#2}$-Zn(2)-N(4)	180.0(2)
Zn(3)-N(5)	2.176(4)	N(3)-Zn(3)-N(3)$^{\#3}$	180.0
Zn(3)-N(5)$^{\#3}$	2.176(4)	N(3)-Zn(3)-O(4)$^{\#3}$	101.56(14)
O(3)$^{\#1}$-Zn(1)-O(3)	180.00(19)	N(3)$^{\#3}$-Zn(3)-O(4)$^{\#3}$	78.44(14)
O(3)$^{\#1}$-Zn(1)-O(1)	87.19(13)	N(3)-Zn(3)-O(4)	78.44(14)
O(3)-Zn(1)-O(1)	92.81(13)	N(3)$^{\#3}$-Zn(3)-O(4)	101.55(14)
O(3)$^{\#1}$-Zn(1)-O(1)$^{\#1}$	92.81(13)	O(4)$^{\#3}$-Zn(3)-O(4)	180.0
O(3)-Zn(1)-O(1)$^{\#1}$	87.19(13)	N(3)-Zn(3)-N(5)	90.72(15)
O(1)-Zn(1)-O(1)$^{\#1}$	180.0	N(3)$^{\#3}$-Zn(3)-N(5)	89.28(15)
O(3)$^{\#1}$-Zn(1)-N(6)	86.87(14)	O(4)$^{\#3}$-Zn(3)-N(5)	91.77(15)
O(3)-Zn(1)-N(6)	93.13(14)	O(4)-Zn(3)-N(5)	88.23(15)
O(1)-Zn(1)-N(6)	90.37(13)	N(3)-Zn(3)-N(5)$^{\#3}$	89.28(15)
O(1)$^{\#1}$-Zn(1)-N(6)	89.63(13)	N(3)$^{\#3}$-Zn(3)-N(5)$^{\#3}$	90.72(15)
O(3)$^{\#1}$-Zn(1)-N(6)$^{\#1}$	93.13(14)	O(4)$^{\#3}$-Zn(3)-N(5)$^{\#3}$	88.23(15)
O(3)-Zn(1)-N(6)$^{\#1}$	86.87(14)	O(4)-Zn(3)-N(5)$^{\#3}$	91.77(15)
O(1)-Zn(1)-N(6)$^{\#1}$	89.63(13)	N(5)-Zn(3)-N(5)$^{\#3}$	180.0
O(1)$^{\#1}$-Zn(1)-N(6)$^{\#1}$	90.37(13)		

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

2

Zn(1)-O(4)	2.123(5)	O(5)-Zn(1)-N(3)	166.5(2)
Zn(1)-O(5)	2.130(5)	O(3)#1-Zn(2)-O(2)#1	92.9(2)
Zn(1)-O(9)	2.108(5)	O(3)#1-Zn(2)-O(1)	174.54(19)
Zn(1)-N(3)	2.169(6)	O(2)#1-Zn(2)-O(1)	88.3(2)
Zn(1)-N(4)	2.119(6)	O(3)#1-Zn(2)-N(1)	97.6(2)
Zn(1)-N(7)	2.110(6)	O(2)#1-Zn(2)-N(1)	95.4(2)
Zn(2)-O(1)	2.125(5)	O(1)-Zn(2)-N(1)	76.9(2)
Zn(2)-O(2)#1	2.109(5)	O(3)#1-Zn(2)-N(16)#2	93.7(2)
Zn(2)-O(3)#1	2.054(5)	O(2)#1-Zn(2)-N(16)#2	82.9(2)
Zn(2)-N(1)	2.138(6)	O(1)-Zn(2)-N(16)#2	91.7(2)
Zn(2)-N(12)#3	2.211(6)	N(1)-Zn(2)-N(16)#2	168.6(2)
Zn(2)-N(16)#2	2.147(6)	O(3)#1-Zn(2)-N(12)#3	89.4(2)
Zn(3)-O(6)#1	2.048(5)	O(2)#1-Zn(2)-N(12)#3	170.7(2)
Zn(3)-O(7)#1	2.091(5)	O(1)-Zn(2)-N(12)#3	90.3(2)
Zn(3)-O(8)	2.110(5)	N(1)-Zn(2)-N(12)#3	93.2(2)
Zn(3)-N(6)	2.161(6)	N(16)#2-Zn(2)-N(12)#3	87.9(2)
Zn(3)-N(9)	2.213(6)	O(6)#1-Zn(3)-O(7)#1	94.23(19)
Zn(3)-N(13)	2.155(6)	O(6)#1-Zn(3)-O(8)	171.57(19)
O(9)-Zn(1)-N(7)	175.6(2)	O(7)#1-Zn(3)-O(8)	87.5(2)
O(9)-Zn(1)-N(4)	85.1(2)	O(6)#1-Zn(3)-N(13)	94.1(2)
N(7)-Zn(1)-N(4)	95.8(2)	O(7)#1-Zn(3)-N(13)	82.6(2)
O(9)-Zn(1)-O(4)	87.1(2)	O(8)-Zn(3)-N(13)	94.3(2)
N(7)-Zn(1)-O(4)	92.7(2)	O(6)#1-Zn(3)-N(6)	95.1(2)
N(4)-Zn(1)-O(4)	167.7(2)	O(7)#1-Zn(3)-N(6)	99.3(2)
O(9)-Zn(1)-O(5)	88.1(2)	O(8)-Zn(3)-N(6)	76.5(2)
N(7)-Zn(1)-O(5)	96.4(2)	N(13)-Zn(3)-N(6)	170.4(2)
N(4)-Zn(1)-O(5)	77.2(2)	O(6)#1-Zn(3)-N(9)	93.0(2)
O(4)-Zn(1)-O(5)	92.95(18)	O(7)#1-Zn(3)-N(9)	167.9(2)
O(9)-Zn(1)-N(3)	83.1(2)	O(8)-Zn(3)-N(9)	86.7(2)
N(7)-Zn(1)-N(3)	92.6(2)	N(13)-Zn(3)-N(9)	87.2(2)
N(4)-Zn(1)-N(3)	112.0(2)	N(6)-Zn(3)-N(9)	89.7(2)
O(4)-Zn(1)-N(3)	76.5(2)		

Symmetry transformations used to generate equivalent atoms:

#1 x,-y+3/2,z-1/2 #2 x-1/2,-y+2,-z+1/2 #3 -x,-y+2,-z+2

3

Cd(1)-O(1)	2.498(4)	O(9)-K(1)-O(4)$^{\#6}$	84.60(9)
Cd(1)-O(5)	2.301(4)	O(6)-K(1)-O(6)$^{\#3}$	60.93(15)
Cd(1)-O(7)	2.243(5)	O(9)-K(1)-O(6)$^{\#3}$	107.85(9)
Cd(1)-N(1)	2.314(4)	O(4)$^{\#6}$-K(1)-O(6)$^{\#3}$	154.21(13)
Cd(1)-N(2)$^{\#1}$	2.285(5)	O(6)-K(1)-O(8)	114.76(13)
Cd(1)-N(4)	2.260(4)	O(9)-K(1)-O(8)	76.63(14)
K(1)-O(4)$^{\#6}$	2.807(4)	O(4)$^{\#6}$-K(1)-O(8)	80.49(9)
K(1)-O(6)$^{\#3}$	2.861(5)	O(6)$^{\#3}$-K(1)-O(8)	80.64(10)
K(1)-O(8)	2.970(4)	O(6)-K(1)-N(5)$^{\#8}$	75.22(11)
K(1)-O(9) $^{\#7}$	2.805(4)	O(9)-K(1)-N(5)$^{\#8}$	86.11(11)
K(1)-O(6)	2.754(5)	O(4)$^{\#6}$-K(1)-N(5)$^{\#8}$	130.72(11)
K(1)-N(3)$^{\#6}$	3.106(5)	O(6)$^{\#3}$-K(1)-N(5)$^{\#8}$	73.78(11)
K(1)-N(5)$^{\#8}$	3.102(5)	O(8)-K(1)-N(5)$^{\#8}$	142.95(7)
K(2)-O(3)$^{\#9}$	2.908(4)	O(6)-K(1)-N(3)$^{\#6}$	80.67(13)
K(2)-O(3)$^{\#10}$	2.908(4)	O(9)-K(1)-N(3)$^{\#6}$	102.63(12)
K(2)-O(5)$^{\#6}$	2.818(4)	O(4)$^{\#6}$-K(1)-N(3)$^{\#6}$	55.93(12)
K(2)-O(5)	2.818(4)	O(6)$^{\#3}$-K(1)-N(3)$^{\#6}$	137.40(13)
O(7)-Cd(1)-N(4)	99.16(17)	O(8)-K(1)-N(3)$^{\#6}$	135.99(10)
O(7)-Cd(1)-N(2)$^{\#1}$	83.4(2)	N(5)$^{\#8}$-K(1)-N(3)$^{\#6}$	79.44(10)
N(4)-Cd(1)-N(2)$^{\#1}$	100.01(16)	O(5)-K(2)-O(5)$^{\#6}$	180.0
O(7)-Cd(1)-O(5)	170.13(18)	O(5)-K(2)-O(3)$^{\#9}$	70.11(11)
N(4)-Cd(1)-O(5)	72.74(14)	O(5)$^{\#6}$-K(2)-O(3)$^{\#9}$	109.88(11)
N(2)$^{\#1}$-Cd(1)-O(5)	103.32(15)	O(5)-K(2)-O(3)$^{\#10}$	109.89(11)
O(7)-Cd(1)-N(1)	98.20(16)	O(5)$^{\#6}$-K(2)-O(3)$^{\#10}$	70.11(11)
N(4)-Cd(1)-N(1)	157.48(17)	O(3)$^{\#9}$-K(2)-O(3)$^{\#10}$	180.0
N(2)$^{\#1}$-Cd(1)-N(1)	96.13(15)	O(5)-K(2)-O(7)$^{\#8}$	68.68(12)
O(5)-Cd(1)-N(1)	88.37(14)	O(5)$^{\#6}$-K(2)-O(7)$^{\#8}$	111.33(12)
O(7)-Cd(1)-O(1)	96.79(18)	O(3)$^{\#9}$-K(2)-O(7)$^{\#8}$	109.27(11)
N(4)-Cd(1)-O(1)	94.61(14)	O(3)$^{\#10}$-K(2)-O(7)$^{\#8}$	70.73(12)
N(2)$^{\#1}$-Cd(1)-O(1)	165.17(13)	O(5)-K(2)-O(7)$^{\#1}$	111.32(12)
O(5)-Cd(1)-O(1)	78.61(14)	O(5)$^{\#6}$-K(2)-O(7)$^{\#1}$	68.68(12)
N(1)-Cd(1)-O(1)	69.13(14)	O(3)$^{\#9}$-K(2)-O(7)$^{\#1}$	70.73(12)
O(6)-K(1)-O(9)	160.19(12)	O(3)$^{\#10}$-K(2)-O(7)$^{\#1}$	109.27(11)
O(6)-K(1)-O(4)$^{\#6}$	112.53(13)	O(7)$^{\#8}$-K(2)-O(7)$^{\#1}$	180.00(15)

Symmetry transformations used to generate equivalent atoms:

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