Supplementary Information

Four new MOFs based on imidazole-containing ligand and multicarboxylates: syntheses, structures and sorption properties

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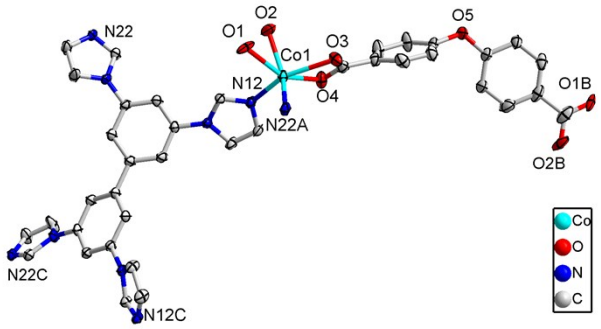
Table S1. Selected bond lengths (Å) and angles (°) for complexes **1 - 4**

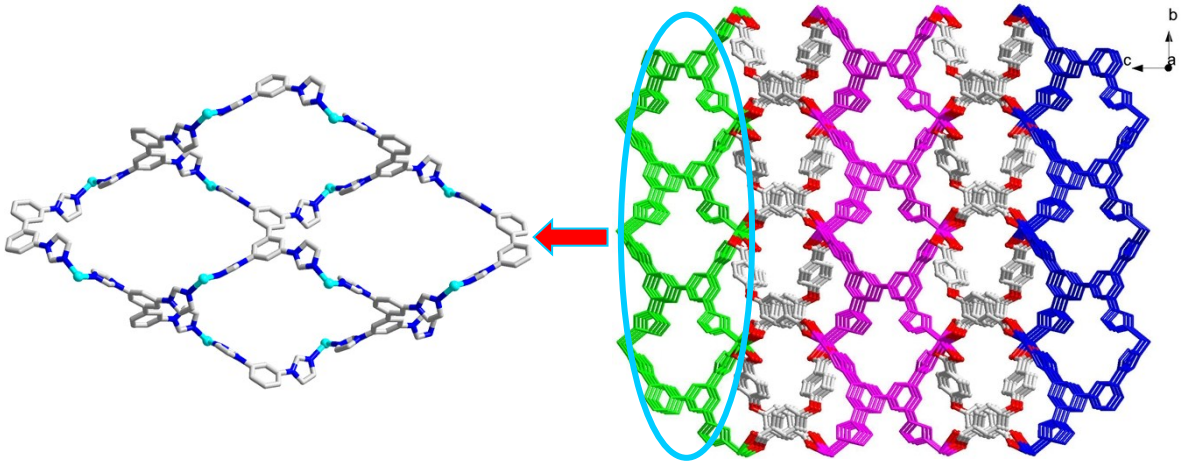
1			
Zn(1)-O(1)	1.993(3)	Zn(1)-O(3)	2.031(4)
Zn(1)-N(12)	2.029(4)	Zn(1)-N(22)#1	2.044(4)
O(1)-Zn(1)-N(12)	110.20(17)	O(1)-Zn(1)-O(3)	102.19(17)
N(12)-Zn(1)-O(3)	130.77(17)	O(1)-Zn(1)-N(22)#1	99.16(16)
N(12)-Zn(1)-N(22)#1	99.37(15)	O(3)-Zn(1)-N(22)#1	111.12(17)
2			
Zn(1)-O(5)	1.932(3)	Zn(1)-O(9)#1	1.936(3)
Zn(1)-N(32)#2	2.007(3)	Zn(1)-N(42)#3	2.011(3)
Zn(2)-O(2)	1.904(3)	Zn(2)-O(7)	1.958(3)
Zn(2)-N(22)#4	2.009(3)	Zn(2)-N(12)	2.043(3)
O(5)-Zn(1)-O(9)#1	106.16(14)	O(5)-Zn(1)-N(32)#2	107.87(14)
O(9)#1-Zn(1)-N(32)#2	111.36(14)	O(5)-Zn(1)-N(42)#3	129.99(14)

O(9)#1-Zn(1)-N(42)#3	93.14(13)	N(32)#2-Zn(1)-N(42)#3	106.90(13)
O(2)-Zn(2)-O(7)	121.43(16)	O(2)-Zn(2)-N(22)#4	125.57(15)
O(7)-Zn(2)-N(22)#4	104.22(14)	O(2)-Zn(2)-N(12)	101.20(15)
O(7)-Zn(2)-N(12)	94.49(14)	N(22)#4-Zn(2)-N(12)	103.22(14)
3			
Co(1)-O(4)#1	2.042(4)	Co(1)-N(12)	2.062(4)
Co(1)-N(22)#2	2.066(4)	Co(1)-O(1)	2.191(4)
O(4)#1-Co(1)-N(12)	98.27(16)	O(4)#1-Co(1)-N(22)#2	112.78(16)
N(12)-Co(1)-N(22)#2	96.45(15)	O(4)#1-Co(1)-O(1)	150.8(2)
N(12)-Co(1)-O(1)	94.26(16)	N(22)#2-Co(1)-O(1)	91.71(18)
4			
Zn(1)-O(1)	1.958(3)	Zn(1)-O(3)#1	2.004(3)
Zn(1)-N(32)#2	2.025(4)	Zn(1)-N(12)	2.043(4)
Zn(2)-O(7)#3	1.938(5)	Zn(2)-O(5)	1.970(7)
Zn(2)-N(22)#4	1.984(4)	Zn(2)-N(42)	2.012(4)
O(1)-Zn(1)-O(3)#1	105.84(14)	O(1)-Zn(1)-N(32)#2	110.13(15)
O(3)#1-Zn(1)-N(32)#2	121.70(15)	O(1)-Zn(1)-N(12)	115.61(15)
O(3)#1-Zn(1)-N(12)	101.10(14)	N(32)#2-Zn(1)-N(12)	102.65(15)
O(7)#3-Zn(2)-O(5)	104.6(2)	O(7)#3-Zn(2)-N(22)#4	132.17(18)
O(5)-Zn(2)-N(22)#4	97.2(2)	O(7)#3-Zn(2)-N(42)	100.7(2)
O(5)-Zn(2)-N(42)	112.48(19)	N(22)#4-Zn(2)-N(42)	109.41(17)

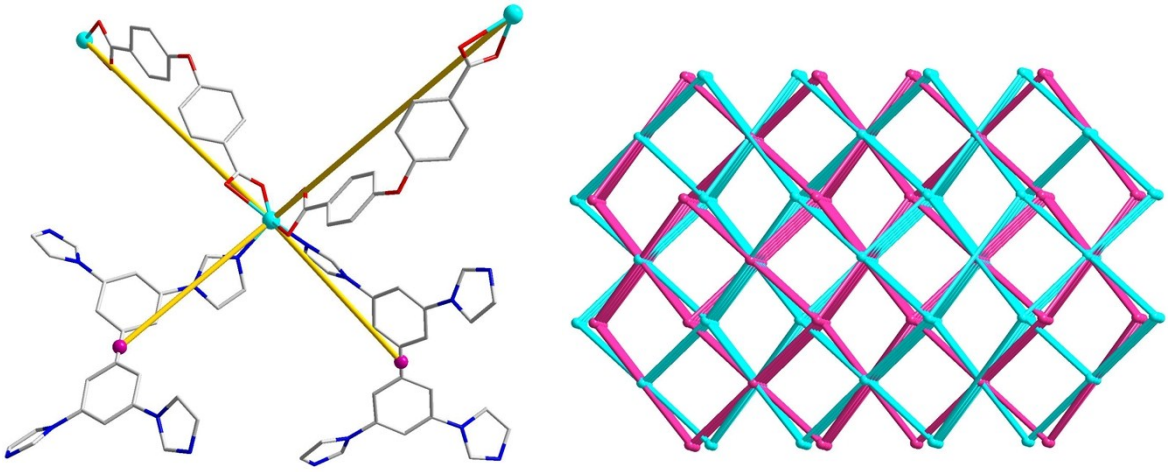
Symmetry transformations used to generate equivalent atoms: #1 *x*-1/2,-*y*+3/2,*z*+1/2 for **1**; #1 *x*,*y*-1,*z*-1; #2 *x*+1,*y*-1,*z*; #3 *x*+1,-*y*+1/2,*z*-1/2; #4 *x*,-*y*+1/2,*z*+1/2 for **2**; #1 *x*-1/2,*y*+1/2,-*z*+1/2; #2 -*x*+1/2,*y*+1/2,*z* for **3**; #1 -*x*,*y*,-*z*+1/2; #2 *x*+1/2,*y*+1/2,*z*;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



(a)

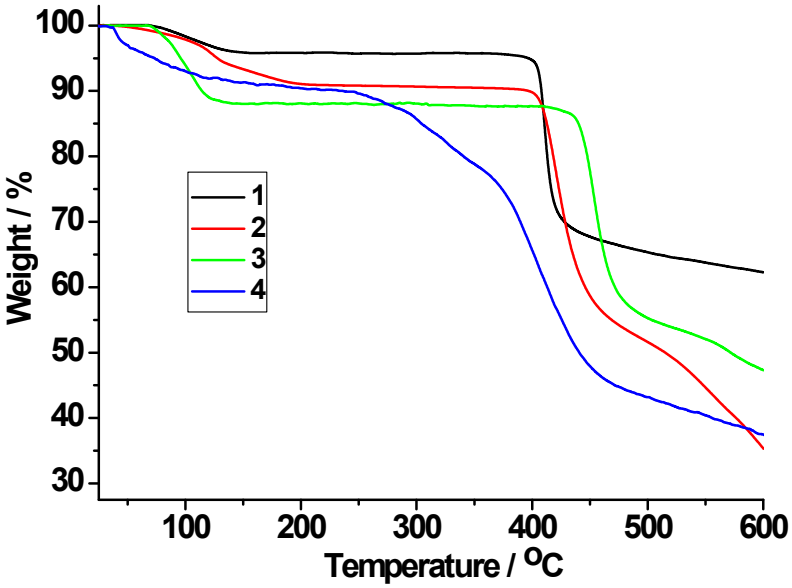


(b) (c)

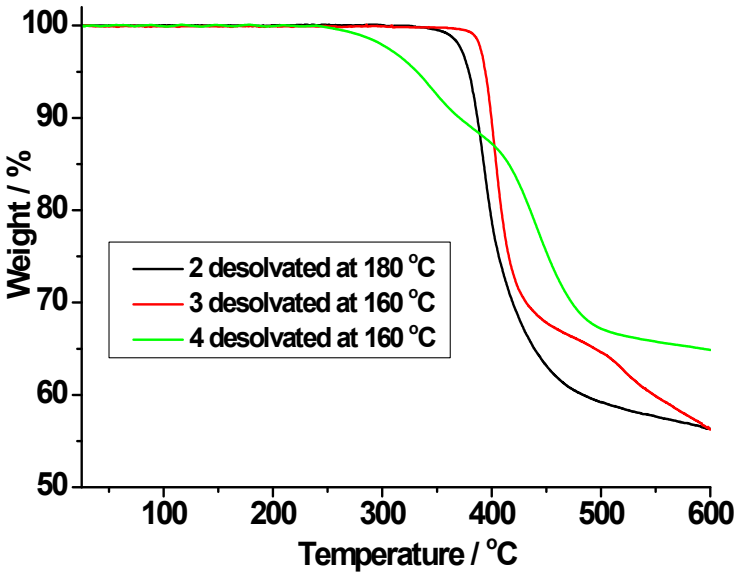


(d) (e)

Fig. S1. (a) Coordination environment of Co(II) atom in **3** with the ellipsoid drawn at the 30% probability level. Hydrogen atoms and free water molecules are omitted for charity. Symmetry codes: A 1.5-*x*, 0.5+*y*, *z*; B -0.5+*x*, 0.5+*y*, 0.5-*z*; C 1-*x*, *y*, -0.5-*z*. (b) The structure of Co(II)-L layer. (c) 3D framework of **3** with different 2D layers displayed by distinct colors. (d) The 4-connected node of Co(II). (e) Schematic representation of the (4,4)-connected binodal 2-fold interpenetrating 3D framework of **3** with point (Schläfli) symbol of $(6^2.8^4)$.

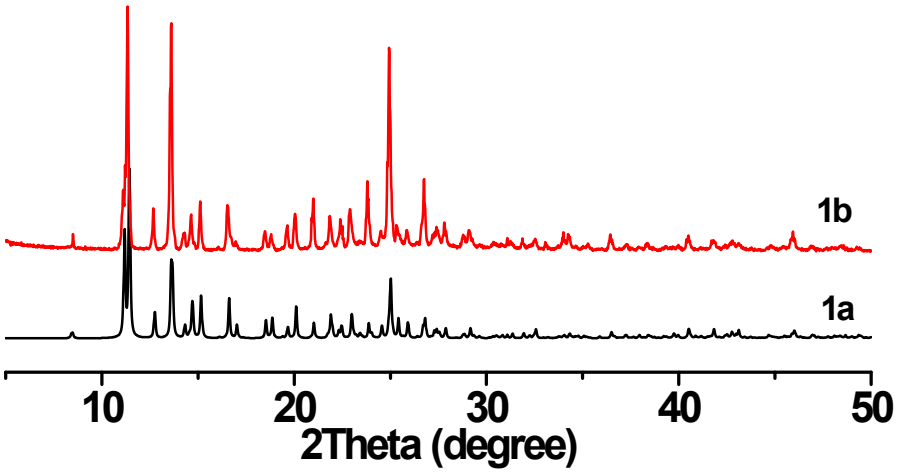


(a)

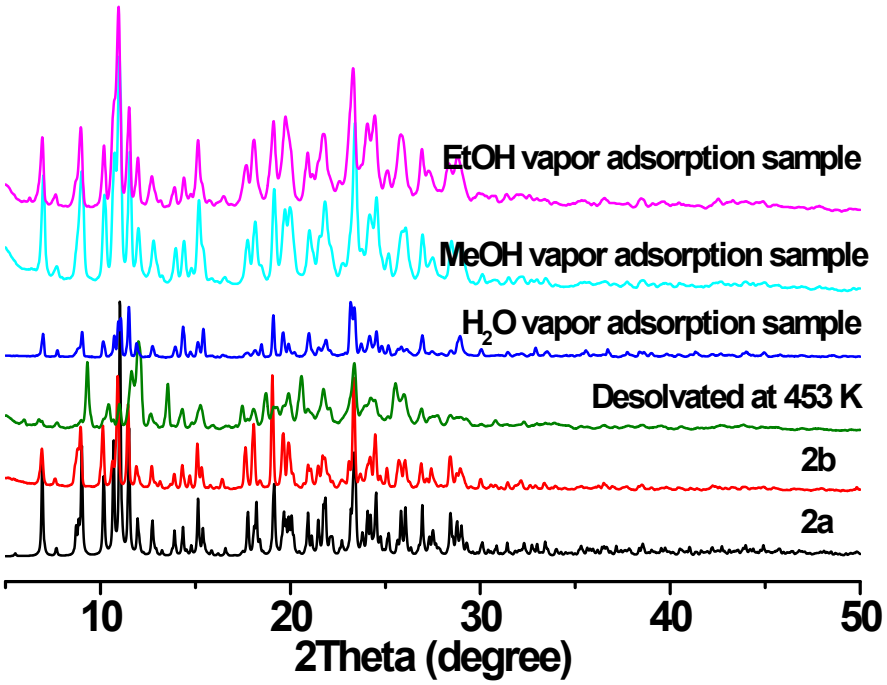


(b)

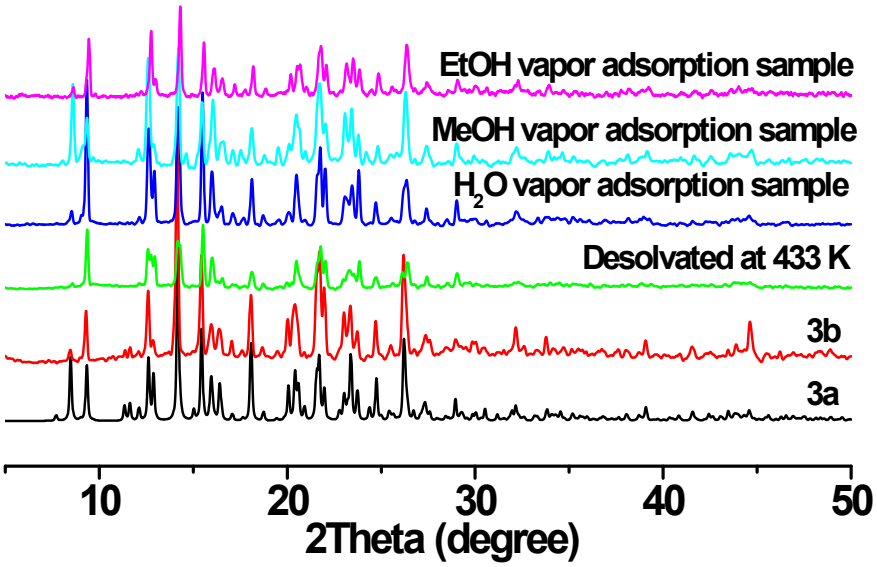
Fig. S2. TGA curves for complexes **1** - **4** (a) and desolvated samples **2** - **3** (b).



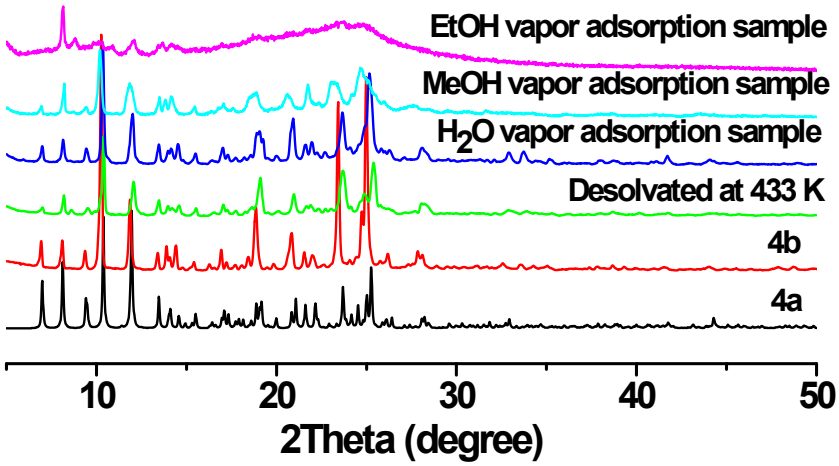
(a)



(b)



(c)



(d)

Fig. S3. (a) The PXRD pattern of complex **1**: a-simulated; b- as-synthesized. (b) - (d) The PXRD patterns of complexes **2** - **4** under different conditions: a-simulated; b- as-synthesized.