Two pillared-layer metal-organic frameworks constructed with Co(II), 1,2,4,5-benzenetetracarboxylate, and 4,4'-bipydine: syntheses, crystal structures, and gas adsorption properties

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Supporting Information

Table S1. Selected Bond Lengths (Å) and angles (°) for compound **1**.

Co(1)-O(2)#1	2.0598(16)
Co(1)-O(7)#2	2.0696(15)
Co(1)-O(4)#1	2.1143(15)
Co(1)-O(1)	2.1177(15)
Co(1)-N(2)	2.143(2)
Co(1)-N(1)#3	2.2089(18)
Co(2)-O(6)#4	2.0732(17)
Co(2)-O(3)	2.0924(16)
Co(2)-O(8)#4	2.0965(15)
Co(2)-O(9)	2.1057(16)
Co(2)-N(3)#5	2.138(2)
Co(2)-N(4)	2.1709(19)
O(2)#1-Co(1)-O(7)#2	173.88(6)
O(2)#1-Co(1)-O(4)#1	85.54(6)
O(7)#2-Co(1)-O(4)#1	91.21(6)
O(2)#1-Co(1)-O(1)	89.49(6)
O(7)#2-Co(1)-O(1)	85.65(6)
O(4)#1-Co(1)-O(1)	95.47(6)
O(2)#1-Co(1)-N(2)	90.51(7)
O(7)#2-Co(1)-N(2)	92.52(7)
O(4)#1-Co(1)-N(2)	175.49(7)
O(1)-Co(1)-N(2)	82.30(7)
O(2)#1-Co(1)-N(1)#3	90.56(7)
O(7)#2-Co(1)-N(1)#3	94.96(7)
O(4)#1-Co(1)-N(1)#3	96.32(7)
O(1)-Co(1)-N(1)#3	168.18(7)
N(2)-Co(1)-N(1)#3	85.88(7)
O(6)#4-Co(2)-O(3)	175.11(6)
O(6)#4-Co(2)-O(8)#4	86.33(7)
O(3)-Co(2)-O(8)#4	91.27(6)
O(6)#4-Co(2)-O(9)	90.45(7)
O(3)-Co(2)-O(9)	94.04(7)
O(8)#4-Co(2)-O(9)	95.80(6)
O(6)#4-Co(2)-N(3)#5	91.08(8)
O(3)-Co(2)-N(3)#5	91.12(8)
O(8)#4-Co(2)-N(3)#5	176.34(8)
O(9)-Co(2)-N(3)#5	86.80(8)
O(6)#4-Co(2)-N(4)	88.28(7)
O(3)-Co(2)-N(4)	87.34(7)
O(8)#4-Co(2)-N(4)	87.07(7)
O(9)-Co(2)-N(4)	176.78(7)

N(3)#5-Co(2)-N(4)	90.27(8)

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y,-z+1 #2 -x+2,-y,-z+1 #3 x,y,z+1 #4 x-1,y,z #5 -x+1,-y+1,-z+1 #6 x+1,y,z #7 x,y,z-1

Table S2. Selected Bond Lengths (Å) and angles (°) for compound **2**.

Co(1)-O(5)	2.0510(19)
Co(1)-O(4)#1	2.0676(18)
Co(1)-N(1)	2.089(2)
Co(1)-O(1)	2.1242(19)
Co(1)-O(3)#1	2.2391(17)
Co(1)-O(2)	2.2492(19)
Co(1)-C(4)#1	2.474(2)
Co(1)-C(1)	2.503(3)
O(5)-Co(1)-O(4)#1	100.46(8)
O(5)-Co(1)-N(1)	94.80(8)
O(4)#1-Co(1)-N(1)	101.65(8)
O(5)-Co(1)-O(1)	93.18(8)
O(4)#1-Co(1)-O(1)	159.88(8)
N(1)-Co(1)-O(1)	91.78(8)
O(5)-Co(1)-O(3)#1	91.07(7)
O(4)#1-Co(1)-O(3)#1	60.69(7)
N(1)-Co(1)-O(3)#1	162.19(8)
O(1)-Co(1)-O(3)#1	104.69(7)
O(5)-Co(1)-O(2)	150.15(8)
O(4)#1-Co(1)-O(2)	103.33(8)
N(1)-Co(1)-O(2)	97.77(8)
O(1)-Co(1)-O(2)	59.57(7)
O(3)#1-Co(1)-O(2)	85.13(7)
O(5)-Co(1)-C(4)#1	96.77(8)
O(4)#1-Co(1)-C(4)#1	30.44(8)
N(1)-Co(1)-C(4)#1	132.05(9)
O(1)-Co(1)-C(4)#1	133.57(8)
O(3)#1-Co(1)-C(4)#1	30.25(8)
O(2)-Co(1)-C(4)#1	94.69(8)
O(5)-Co(1)-C(1)	121.65(9)
O(4)#1-Co(1)-C(1)	131.57(9)
N(1)-Co(1)-C(1)	97.77(8)
O(1)-Co(1)-C(1)	30.02(8)
O(3)#1-Co(1)-C(1)	93.39(7)
O(2)-Co(1)-C(1)	29.70(7)
C(4)#1-Co(1)-C(1)	114.59(9)

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

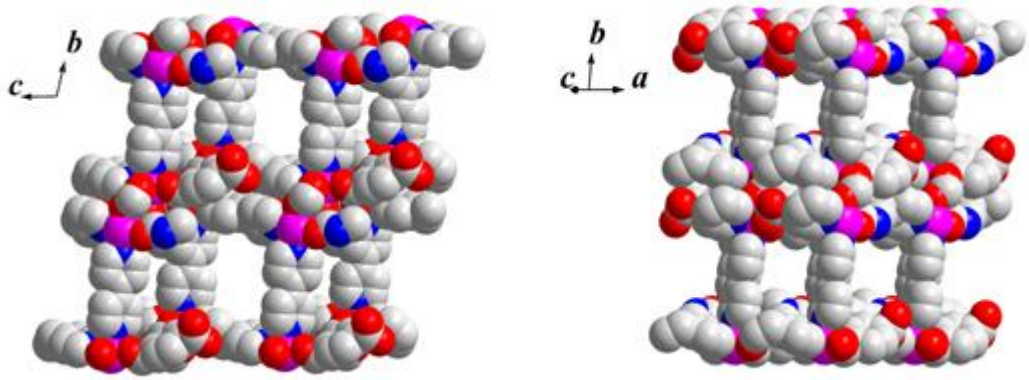

Fig. S1 Packing diagram of compound **1** along the a) [100] and b) [101] directions.

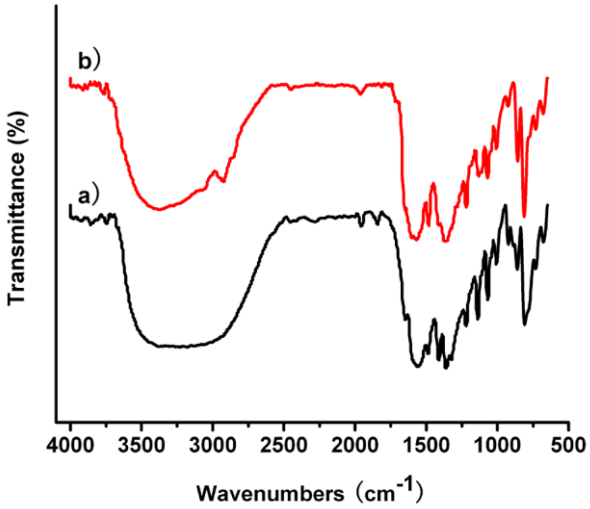

Fig. S2. IR spectra of compound **1**: a) as-synthesized; b) evacuated at 120°C for 2 h.

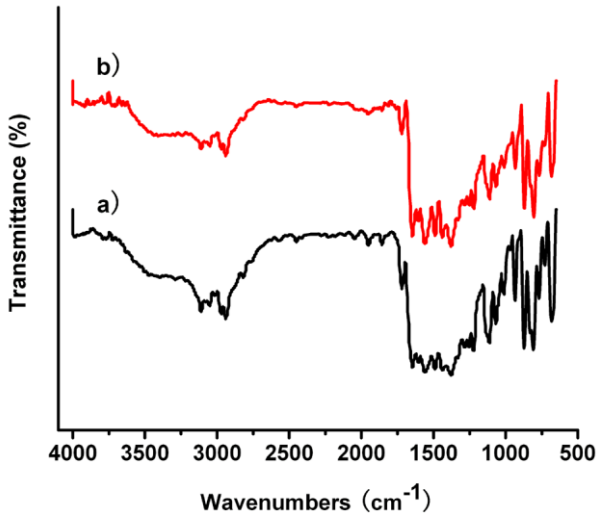

Fig. S3. IR spectra of compound **2**: a) as synthesized; b) evacuated at 120°C for 2 h.

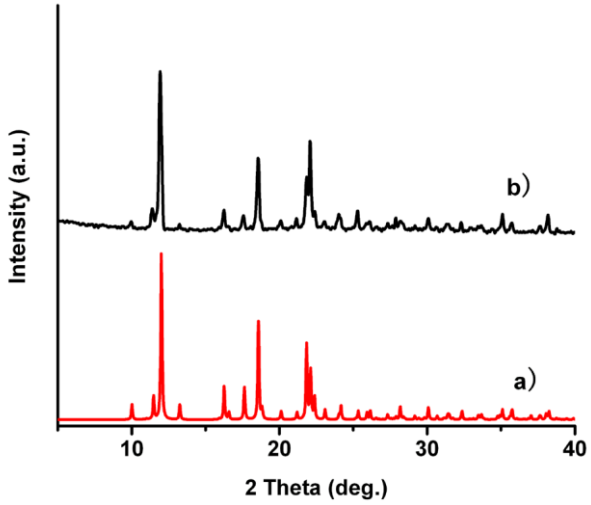

Fig. S4. PXRD patterns of a) the simulation, b) the as-synthesized sample of compound **2**.

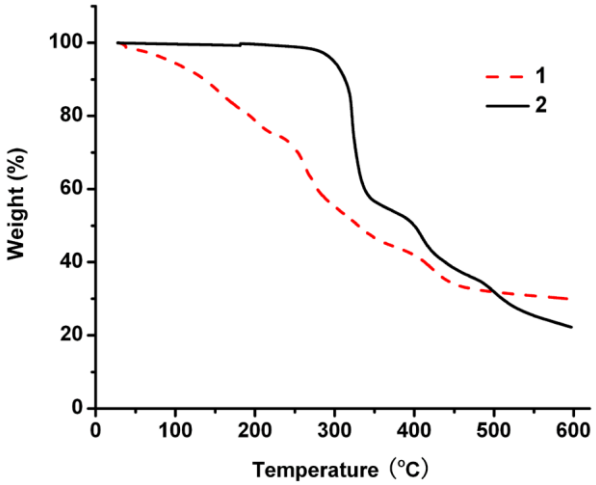

Fig. S5. TGA curves of **1** (dash), **2** (solid)

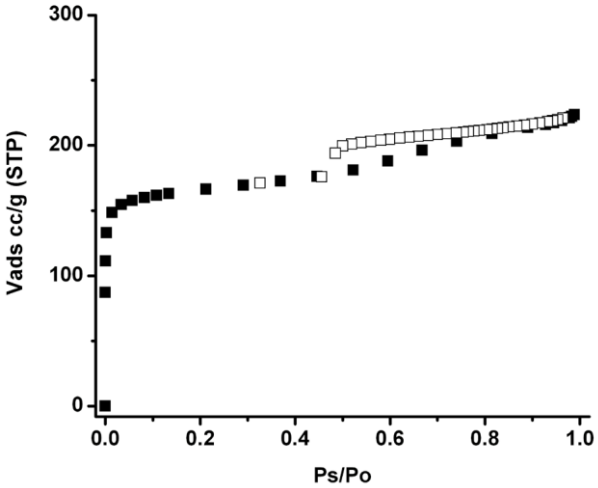

Fig. S6. N_2 isotherms for compound **1** at 77 K. The shaded symbols and open symbols represent adsorption and desorption, respectively.

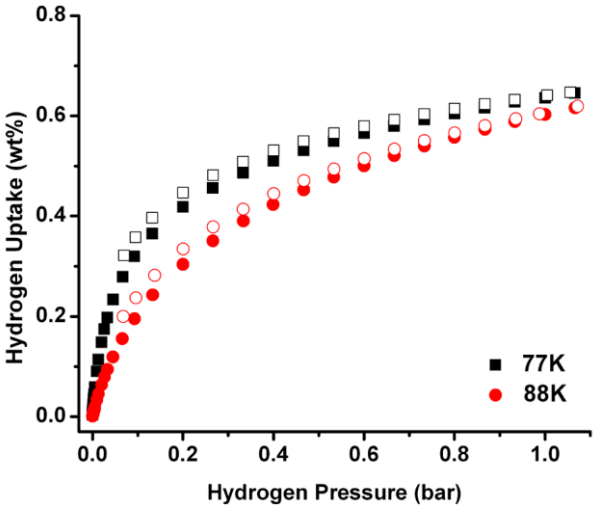

Fig. S7. The H_2 isotherms of **1** at 77 K and 88 K under 0-1 bar.