

Electronic supporting information (ESI)

Two Coordination Polymers of Benzene-1,2,4,5-tetracarboxylic Acid (H₄BTC): In Situ Ligand Syntheses, Structures, and Luminescent Property

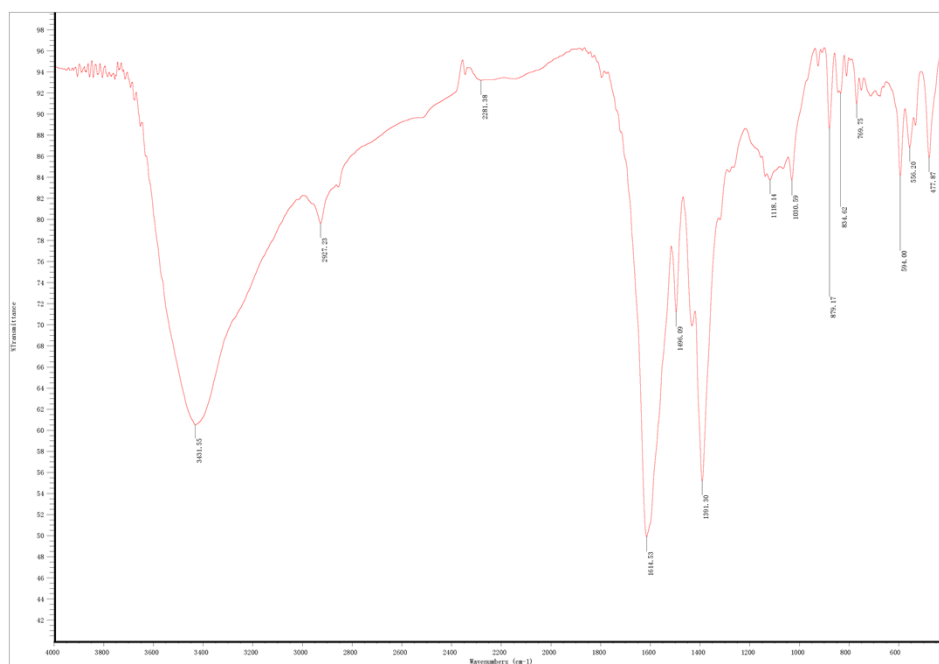
Di-Chang Zhong,^{*} Hua-Bin Guo, Ji-Hua Deng, Qing Chen,^{*} and Xu-Zhong Luo

Table S1 Selected bond length (Å) and angle (°) for **1** and **2**

Compound 1					
Co(1)-O(1)	2.228(3)	Co(1)-O(2)	2.159(3)	Co(1)-O(10)	2.276(7)
Co(1)-O(8)#1	2.000(4)	Co(1)-O(5)#2	2.001(3)	Co(1)-O(4)#3	2.012(3)
Co(2)-O(2)	2.042(3)	Co(2)-O(3)	2.063(3)	Co(2)-O(6)#4	2.057(3)
Co(2)-O(7)#4	2.108(3)	Co(2)-O(9)	2.030(5)	Co(2)-O(7)#1	2.223(3)
O(8)#1-Co(1)-O(5)#2	164.40(16)	O(8)#1-Co(1)-O(4)#3	92.28(15)	O(5)#2-Co(1)-O(4)#3	98.46(15)
O(8)#1-Co(1)-O(2)	87.33(14)	O(5)#2-Co(1)-O(2)	85.24(14)	O(4)#3-Co(1)-O(2)	164.77(14)
O(8)#1-Co(1)-O(1)	96.87(16)	O(5)#2-Co(1)-O(1)	91.18(13)	O(4)#3-Co(1)-O(1)	105.36(14)
O(2)-Co(1)-O(1)	59.64(12)	O(8)#1-Co(1)-O(10)	75.9(3)	O(5)#2-Co(1)-O(10)	91.1(2)
O(4)#3-Co(1)-O(10)	99.6(3)	O(2)-Co(1)-O(10)	95.1(2)	O(1)-Co(1)-O(10)	154.3(2)
O(9)-Co(2)-O(2)	97.61(17)	O(9)-Co(2)-O(6)#4	98.93(18)	O(2)-Co(2)-O(6)#4	89.82(14)
O(9)-Co(2)-O(3)	90.64(18)	O(2)-Co(2)-O(3)	87.44(14)	O(6)#4-Co(2)-O(3)	170.32(14)
O(9)-Co(2)-O(7)#4	92.92(17)	O(2)-Co(2)-O(7)#4	168.71(13)	O(6)#4-Co(2)-O(7)#4	84.49(13)
O(3)-Co(2)-O(7)#4	96.55(14)	O(9)-Co(2)-O(7)#1	171.51(18)	O(2)-Co(2)-O(7)#1	89.11(12)
O(6)#4-Co(2)-O(7)#1	86.22(13)	O(3)-Co(2)-O(7)#1	84.45(13)	O(7)#4-Co(2)-O(7)#1	80.80(13)
Compound 2					
Zn(1)-O(8)	1.936(14)	Zn(1)-O(9)	1.969(17)	Zn(1)-O(3)#1	1.990(14)
Zn(1)-O(1)#2	2.054(12)	Zn(2)-O(5)#3	1.943(14)	Zn(2)-O(10)	1.992(19)
Zn(2)-O(6)	2.077(11)	Zn(2)-O(11)	2.24(5)	Zn(2)-O(5)	2.381(14)
O(8)-Zn(1)-O(9)	109.1(7)	O(8)-Zn(1)-O(3)#1	106.5(5)	O(9)-Zn(1)-O(3)#1	107.8(6)
O(8)-Zn(1)-O(1)#2	103.6(6)	O(9)-Zn(1)-O(1)#2	118.8(7)	O(3)#1-Zn(1)-O(1)#2	110.2(6)
O(5)#3-Zn(2)-O(10)	96.9(8)	O(5)#3-Zn(2)-O(6)	102.3(6)	O(10)-Zn(2)-O(6)	93.0(8)
O(5)#3-Zn(2)-O(11)	104.8(7)	O(10)-Zn(2)-O(11)	122.4(12)	O(6)-Zn(2)-O(11)	131.3(10)
O(5)#3-Zn(2)-O(5)	158.0(5)	O(10)-Zn(2)-O(5)	93.7(6)	O(6)-Zn(2)-O(5)	57.8(5)
O(11)-Zn(2)-O(5)	85.2(8)				

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

(a)



(b)

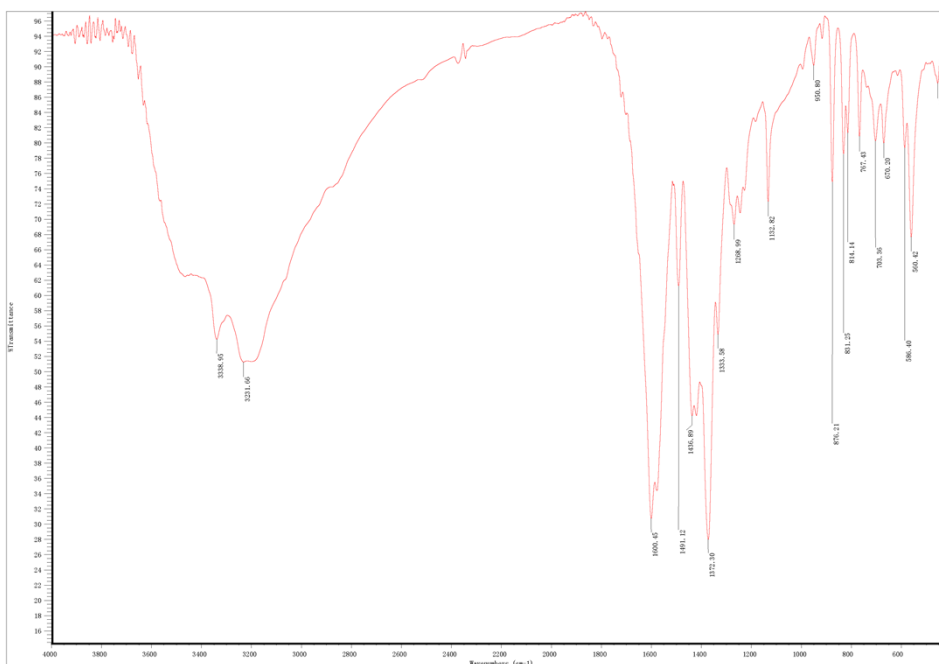


Fig. S1. IR spectra of (a) 1 and (b) 2.

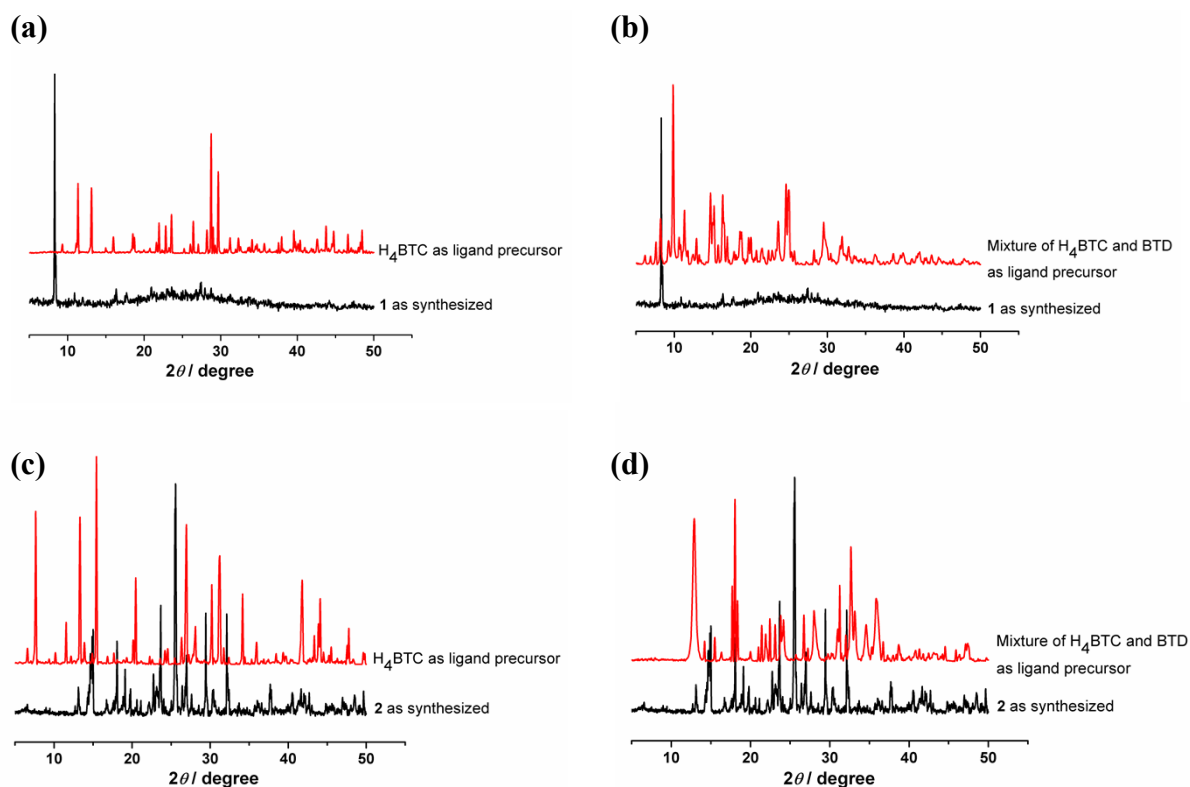


Fig. S2. Powder XRD patterns of crystalline products resulted from reactions as in situ ligand reactions except using H₄BTC or mixture of H₄BTC and BTD instead of ligand precursor BTD, (a) and (b) for **1**, (c) and (d) for **2**.