The Influence of 1-alkyl-3-methy Imidazolium Ionic Liquids on A Series of Cobalt-1,4-benzenedicarboxylate Metal-organic Frameworks

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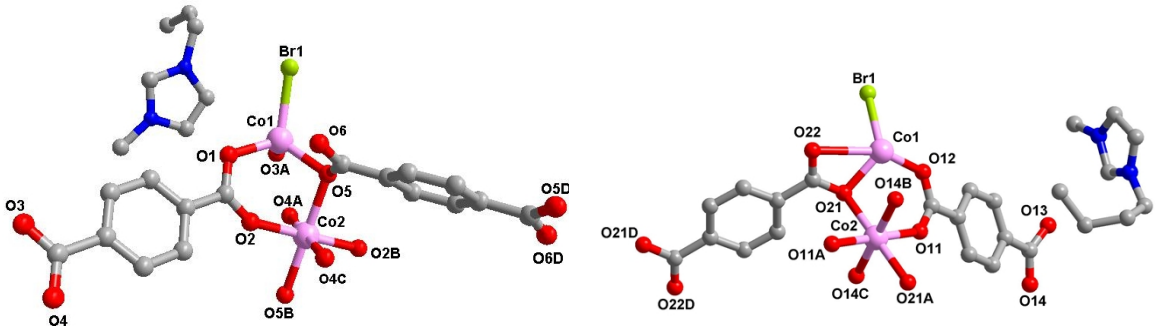
Table S1. Selected bond distances (Å) and bond angles (º) of compounds **1-4**.

1	**2**	**3**	**4**
Co1-O14A = 1.963(3)	Co1-O1=1.9584(18)	Co1-O13A = 1.9712(15)	Co1-O11 = 1.9664(18)
Co1-O12 = 1.964(3)	Co1-O3A=1.9648(19)	Co1-O12 = 1.9828(16)	Co1-O13A = 1.9871(18)
Co1-O21 = 1.982(4)	Co1-O5=1.9817(19)	Co1-O21 = 2.0010(16)	Co1-O32 = 2.0164(16)
Co1-Br1 = 2.3942(9)	Co1-Br1=2.3951(5)	Co1-Br1 = 2.4059(4)	Co1-O22 = 2.030(3)
Co2-O13A = 2.044(3)	Co2-O4A=2.0414(18)	Co2-O11 = 2.0283(15)	Co2-O12 = 2.0520(16)
Co2-O11 = 2.067(4)	Co2-O2=2.0521(19)	Co2-O14C = 2.0596(16)	Co2-O14#3 = 2.0578(17)
Co2-O21 = 2.163(3)	Co2-O5=2.1744(18)	Co2-O21 = 2.1910(16)	Co2-O32 = 2.1587(16)
O14A-Co1-O12 = 111.41(15)	O1-Co1-O3A=111.67(9)	O13A-Co1-O12 = 110.35(7)	O11-Co1-O13A = 112.42(8)
O14A-Co1-O21 = 102.08(15)	O1-Co1-O5=112.84(8)	O13A-Co1-O21 = 115.69(6)	O11-Co1-O32 = 108.47(7)
O12-Co1-O21 = 112.07(14)	O3A-Co1-O5=101.35(8)	O12-Co1-O21 = 101.08(7)	O13A-Co1-O32 = 97.94(7)
O14A-Co1-Br1 = 105.37(11)	O1-Co1-Br1=110.56(6)	O13A-Co1-Br1 = 107.10(5)	O11-Co1-O22 = 126.47(10)
O12-Co1-Br1 = 111.43(12)	O3A-Co1-Br1=103.68(6)	O12-Co1-Br1 = 102.51(5)	O13A-Co1-O22 = 103.52(10)
O21-Co1-Br1 = 113.90(10)	O5-Co1-Br1=115.97(5)	O21-Co1-Br1 = 118.94(5)	O32-Co1-O22 = 104.14(9)
O13A-Co2-O11 = 94.78(15)	O4B-Co2-O2=84.68(9)	O11-Co2-O14A = 94.90(7)	O12-Co2-O14A = 94.43(7)
O13B-Co2-O11 = 85.22(15)	O4A-Co2-O2=95.32(9)	O11-Co2-O14C = 85.10(7)	O12-Co2-O14#3 = 85.57(7)
O13A-Co2-O21 = 91.95(13)	O2-Co2-O5C=91.63(7)	O11B-Co2-O14C = 94.90(7)	O12-Co2-O32B = 89.32(6)
O13B-Co2-O21 = 88.05(13)	O4B-Co2-O5=88.25(7)	O11-Co2-O21B = 87.57(6)	O12B-Co2-O32 = 89.32(6)
O11C-Co2-O21 = 92.34(14)	O4A-Co2-O5=91.75(7)	O11-Co2-O21 = 92.43(6)	O12-Co2-O32 = 90.68(6)
O11-Co2-O21 = 87.66(14)	O2C-Co2-O5=91.63(7)	O11B-Co2-O21 = 87.57(6)	O14A-Co2-O32 = 90.38(6)
O11-Co2-O21C = 92.34(14)	O2-Co2-O5=88.37(7)	O14A-Co2-O21 = 89.38(6)	O14C-Co2-O32 = 89.62(6)

Symmetry codes: 1) *A* = x-1/2, -y-1/2, z-1/2; *B* = -x+1/2, y+1/2, -z+1/2; *C* = -x, -y, -z. 2) *A* = x-1/2, -y-1/2, z-1/2; *B* = -x+5/2, y+1/2, -z+1/2; *C* = -x+2, -y, -z; 3) *A* = x+1/2, -y+1/2, z+1/2; *B* = -x+1, -y, -z+2; *C* = -x+1/2, y-1/2, -z+3/2; 4) *A* = x, -y, z+1/2; *B* = -x+1/2, -y+1/2, -z+1; *C* = -x+1/2, y+1/2, -z+1/2.

Table S2. The main IR characteristic absorption peaks for compounds **1**-**4**.

compounds	υ_{as}(COO–)/cm^{-1}	υs(COO–)/cm^{-1}	δ(C-H)(MI)/cm^{-1}	δ(C-N)(MI)/cm^{-1}	δ(C-H)/cm^{-1}
1	1627, 1596	1504, 1380	3145, 3105	1165	2991, 2934
2	1614, 1581	1504. 1380	3145, 3088	1161	2960, 2925
3	1625, 1584	1508, 1387	3141, 3080	1161	2978, 2938
4	1635,1508	1455, 1380	3162, 3106	1097	2978, 2934



(a) (b)

Figure S1. Coordination spheres of Co(II) centers in compounds **2** (a) and **3** (b).

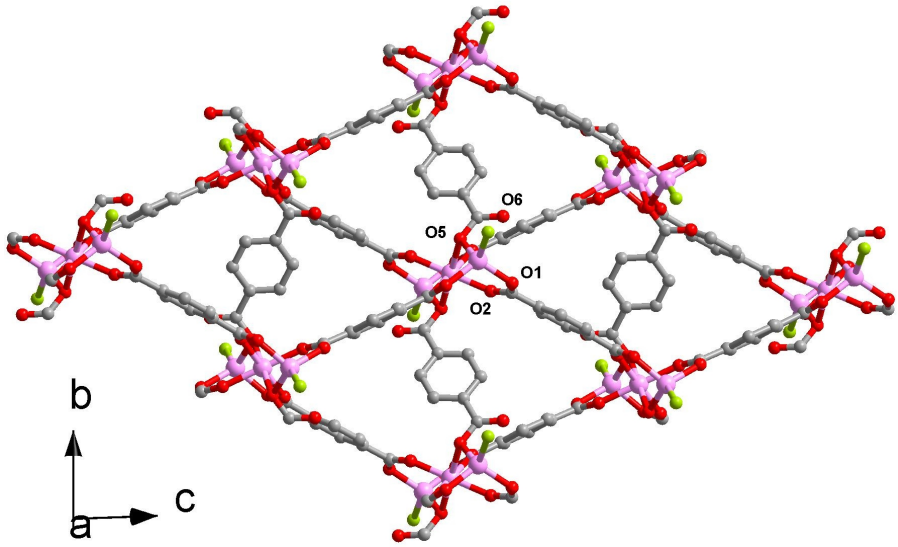


Figure S2. The 2D layers along the *bc*-plane in compound **2**.

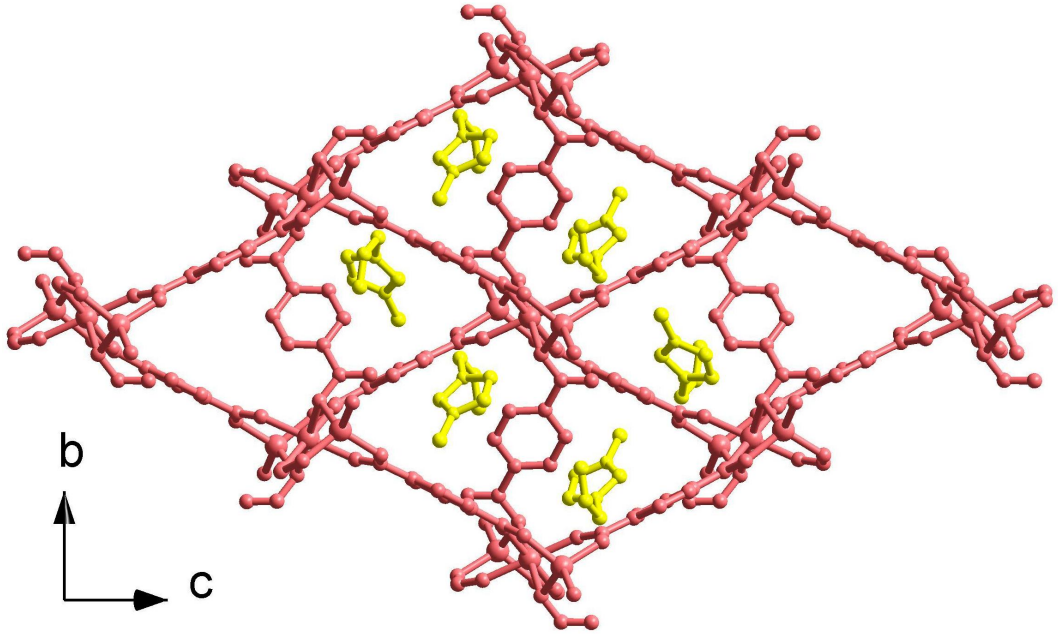


Figure S3. The 2D layers with $[EMI]^+$ templates in compound **2**.

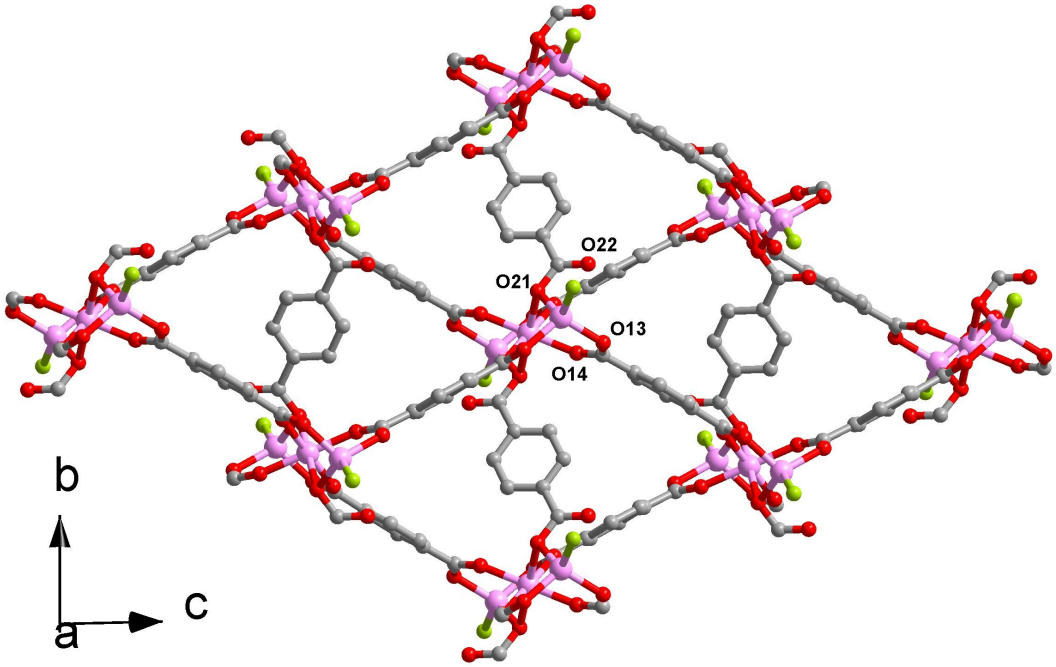


Figure S4. The 2D layers along the *bc*-plane in compound **3**.

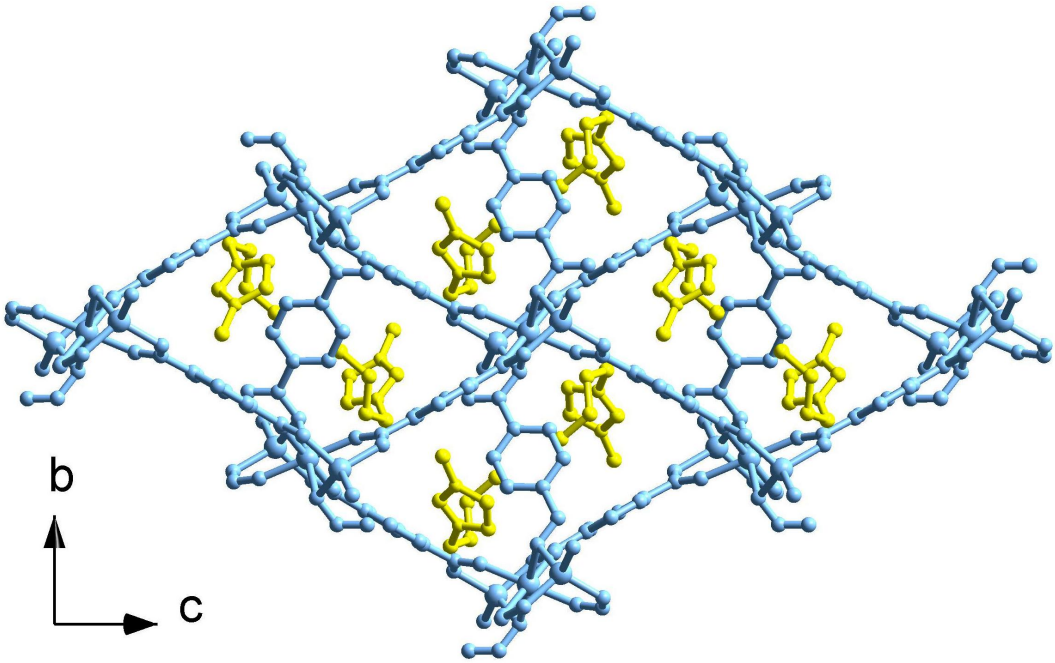


Figure S5. The 2D layers with $[EMI]^+$ templates in compound **3**.

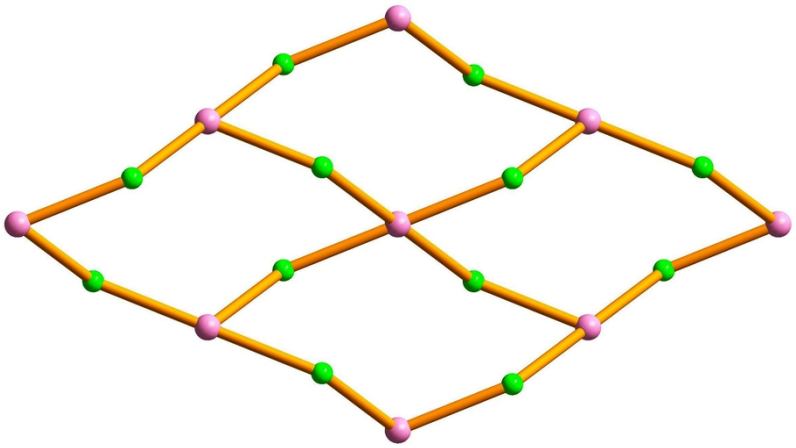


Figure S6. The (4,4) topological network constructed by $[Co_3(COO)_6Br_2]$ nodes (purple) and the rest benzene moieties from BDC^{2-} ligands (green) in compound **1**.

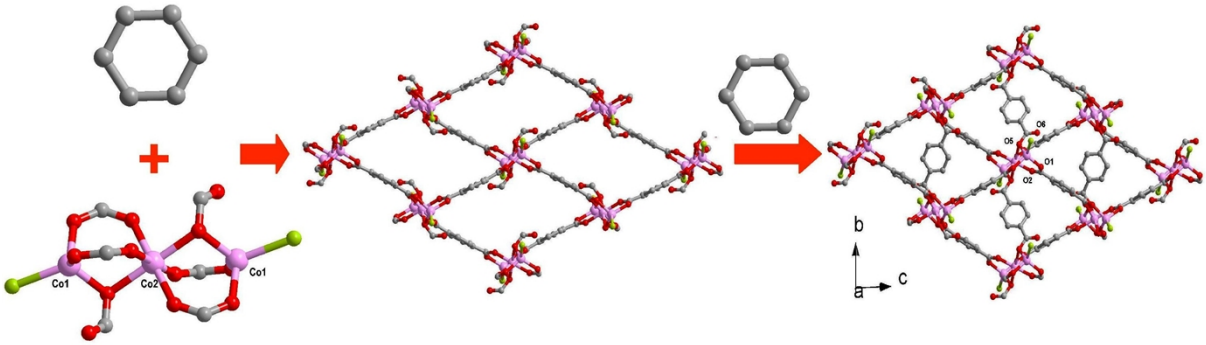


Figure S7. The final 2D (3,6) layer constructed by the $[Co_3(COO)_6Br_2]$ SBUs and the benzene moieties in compound **1**-**3**.

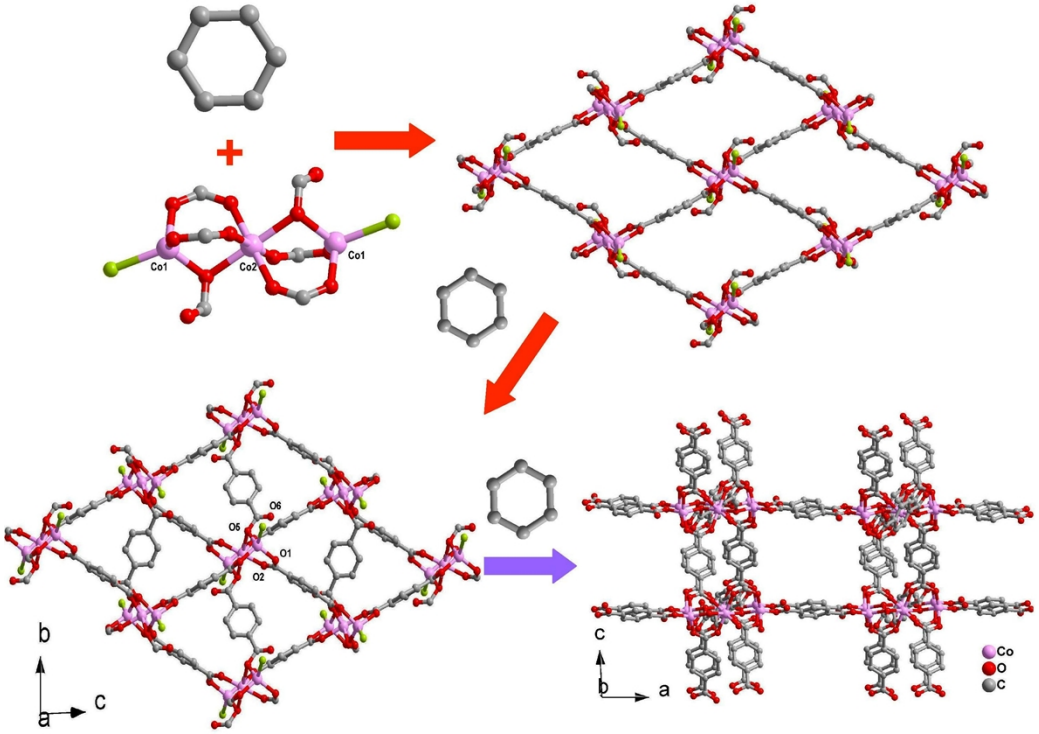
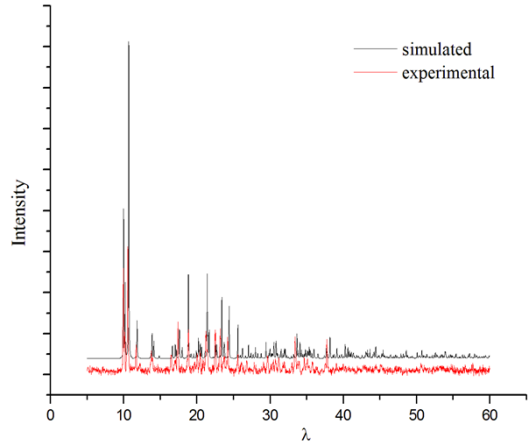
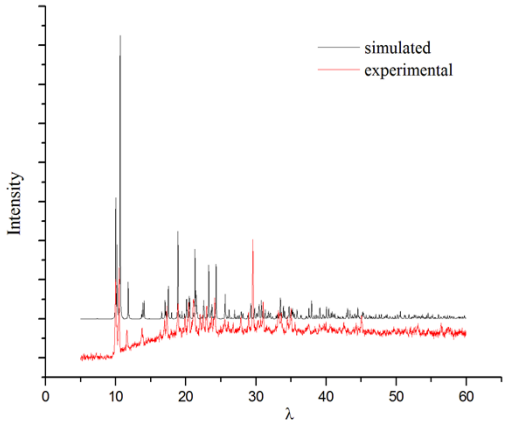


Figure S8. The structure construction of the 3D architecture in compound **4**.

(**1**)



(**2**)



(**3**)

(**4**)

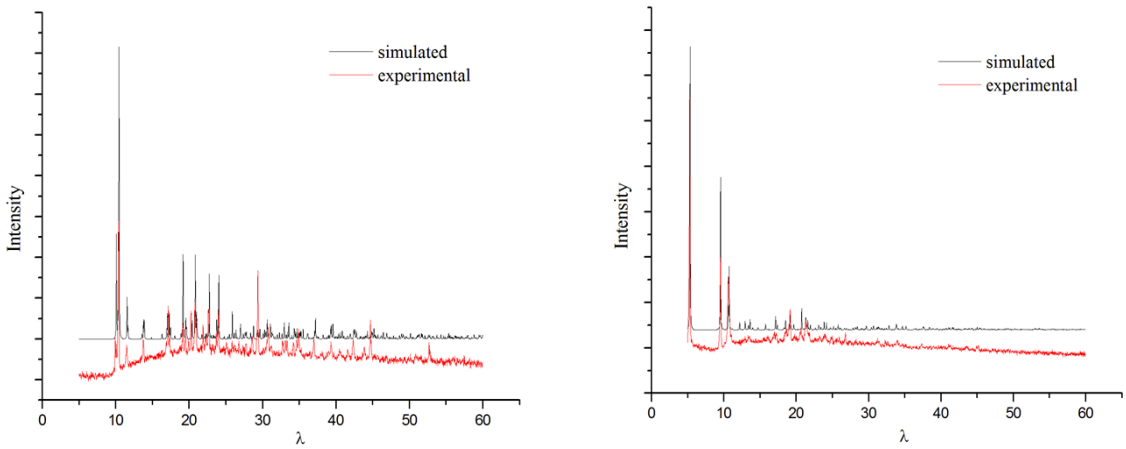
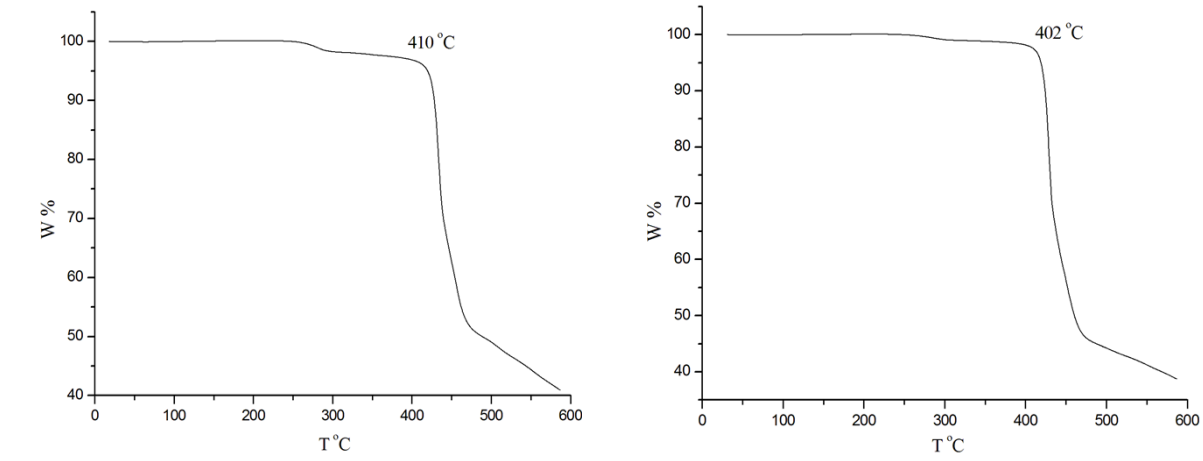


Fig. S9. Comparison of X-ray powder diffraction patterns of compounds **1**-**4** to those simulated from single crystal structure data.

(1) **(2)**



(3) **(4)**

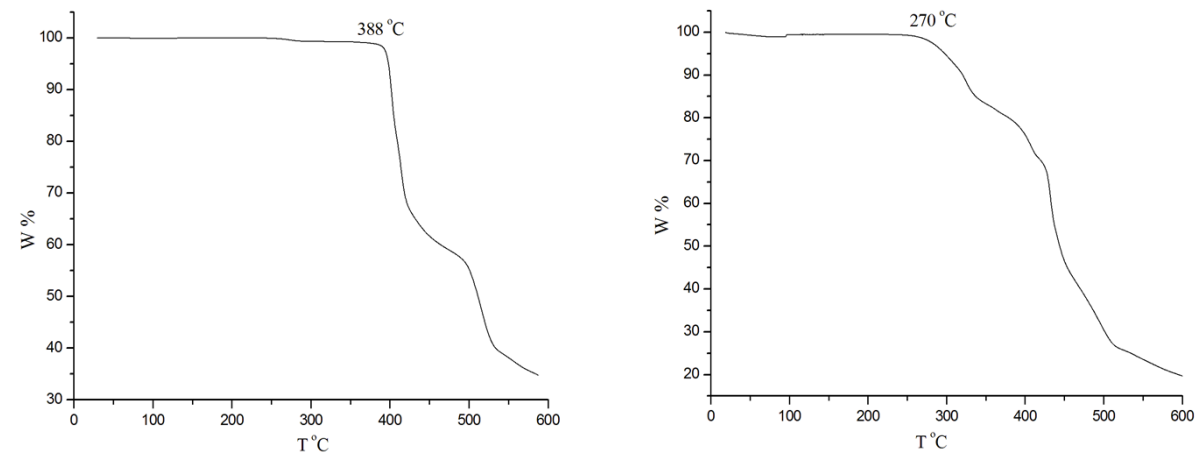


Figure. S10. TG curves of compounds **1**-**4**.