

Electronic Supplementary Information

Four MOFs with 2,2'-Dimethoxy-4,4'-biphenyldicarboxylic Acid: Syntheses, Structures, Topologies, and Properties

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

1			
Mn1-O1 ⁱ	2.123(3)	Mn1-O4	2.252(4)
Mn1-O2	2.133(3)	Mn1-O4 ^{iv}	2.258(4)
O1 ⁱ -Mn1-O1 ⁱⁱ	95.98(12)	O2-Mn1-O2 ⁱⁱⁱ	92.16(19)
O1 ⁱ -Mn1-O2	178.05(15)	O2-Mn1-O4 ^{iv}	93.01(12)
O1 ⁱ -Mn1-O2 ⁱⁱⁱ	85.92(11)	O4-Mn1-O4 ^{iv}	175.79(14)
O1 ⁱ -Mn1-O4 ^{iv}	87.46(11)	Mn1-O4-Mn1 ⁱ	112.57(13)
2			
Ni1-O4 ⁱ	2.044(2)	Ni2-O1	2.002(2)
Ni1-O7	2.092(2)	Ni2-O2W	2.088(2)
Ni1-O1W	2.110(2)	Ni2-O1W	2.109(2)

O4 ⁱ -Ni1-O7 ⁱⁱⁱ	90.48(16)	O1-Ni2-O1W	89.14(16)
O4 ⁱ -Ni1-O1W	87.93(16)	O1-Ni2-O2W	91.83(17)
O4 ⁱⁱ -Ni1-O1W	92.07(16)	O1-Ni2-O2W ^{iv}	88.16(17)
O7-Ni1-O1W	91.03(16)	O2W-Ni2-O1W ^{iv}	91.00(17)

3

Cu1-O1	1.959(2)	Cu1-O1W	2.120(4)
Cu1-O2 ⁱⁱⁱ	1.966(2)	Cu1...Cu1 ⁱⁱⁱ	2.5910(11)
O1-Cu1-O1 ⁱ	89.33(17)	O1-Cu1-O1W	95.63(14)
O1-Cu1-O2 ⁱⁱ	89.80(12)	O2 ⁱⁱ -Cu1-O2 ⁱⁱⁱ	88.95(15)
O1-Cu1-O2 ⁱⁱⁱ	168.98(11)	O2 ⁱⁱ -Cu1-O1W	95.39(14)

4

Cd1-O1	2.370(4)	Cd2-O4 ⁱⁱ	2.302(4)
Cd1-O2	2.404(4)	Cd2-O8	2.302(4)
Cd1-O3 ⁱⁱ	2.361(4)	Cd2-O10 ⁱ	2.211(3)
Cd1-O4 ⁱⁱ	2.537(4)	Cd3-O13	2.302(6)
Cd1-O7	2.382(4)	Cd3-O14	2.501(7)
Cd1-O8	2.431(4)	Na1-O1	2.301(5)
Cd1-O9 ⁱ	2.181(4)	Na1-O7	2.369(5)
Cd1...Cd2	3.601(4)	Cd1...Na1	3.6602(5)
O1-Cd1-O2	55.00(15)	O4 ⁱⁱ -Cd2-O4 ^{iv}	95.88(19)
O1-Cd1-O3 ⁱⁱ	110.60(15)	O4 ⁱⁱ -Cd2-O8	81.38(13)
O1-Cd1-O4 ⁱⁱ	163.09(14)	O4 ⁱⁱ -Cd2-O8 ^v	175.06(14)
O1-Cd1-O7	77.20(16)	O4 ⁱⁱ -Cd2-O10 ⁱ	85.24(14)
O1-Cd1-O8	118.71(14)	O4 ⁱⁱ -Cd2-O10 ⁱⁱⁱ	92.62(14)
O1-Cd1-O9 ⁱ	103.96(15)	O8-Cd2-O8 ^v	101.6(2)
O2-Cd1-O3 ⁱⁱ	86.80(16)	O8-Cd2-O10 ⁱ	91.25(14)
O2-Cd1-O4 ⁱⁱ	114.71(13)	O10 ⁱ -Cd2-O10 ⁱⁱⁱ	176.8(2)
O2-Cd1-O7	128.91(16)	O13-Cd3-O13 ^{vi}	121.3(3)
O2-Cd1-O8	166.16(14)	O13-Cd3-O13 ^{vii}	103.88(14)

O2-Cd1-O9 ⁱ	85.03(15)	O13-Cd3-O14	52.3(2)
O3 ⁱⁱ -Cd1-O4 ⁱⁱ	53.05(13)	O13-Cd3-O14 ^{vi}	83.0(2)
O3 ⁱⁱ -Cd1-O7	95.04(18)	O13-Cd3-O14 ^{vi}	152.9(2)
O3 ⁱⁱ -Cd1-O8	106.99(15)	O13-Cd3-O14 ^{viii}	81.1(2)
O3 ⁱⁱ -Cd1-O9 ⁱ	130.49(17)	O14-Cd3-O14 ^{vi}	82.9(4)
O4 ⁱⁱ -Cd1-O7	106.38(15)	O14-Cd3-O14 ^{vii}	124.2(2)
O4 ⁱⁱ -Cd1-O8	74.30(12)	O1-Na1-O1 ^{ix}	106.9(3)
O7-Cd1-O8	52.68(15)	O1-Na1-O7	78.81(14)
O7-Cd1-O9 ⁱ	127.04(19)	O1-Na1-O7 ^{ix}	155.13(17)
O8-Cd1-O9 ⁱ	84.97(15)	O7-Na1-O7 ^{ix}	106.5(3)

Symmetry codes: for **1**: i) 1.5-x, 2.5-y, 0.5+z; ii) x, 2.5-y, 0.5+z; iii) 1.5-x, y, z; iv) 1.5-x, 2.5-y, z-0.5. for **2**: i) x, y-1, z-1; ii) 1-x, 2-y, 3-z; iii) 1-x, 1-y, 2-z; iv) -x, 1-y, 2-z. for **3**: i) x-0.5, 0.5+y, z; ii) 0.5-x, 0.5-y, -z; iii) 1-x, -y, -z. for **4**: i) -x, -0.5-y, z-0.25; ii) -0.5-x, -1-y, 0.25+z; iii) x-0.5, -0.5-y, -1.5-z; iv) x, -1-y, -2-z; v) x, -0.5-y, -1.75-z; vi) -x, -y, z; vii) -x, y, -1-z; viii) x, -y, -1-z; ix) -x, -1-y, z.

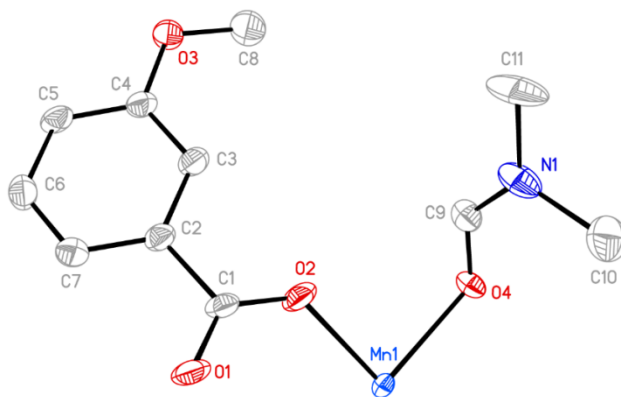


Fig. S1 The asymmetric unit of **1** (Hydrogen atoms are omitted for clarity).

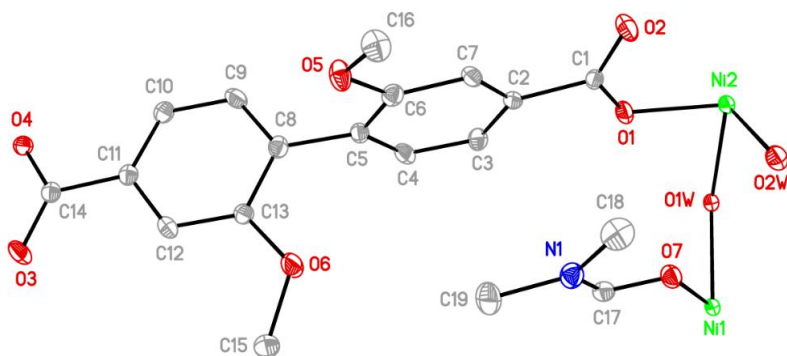


Fig. S2 The asymmetric unit of **2** (Hydrogen atoms are omitted for clarity).

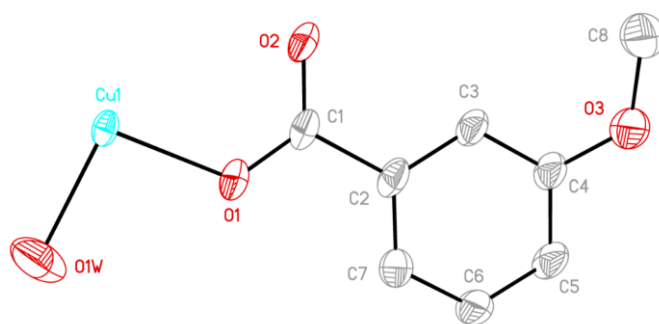


Fig. S3 The asymmetric unit of **3** (Hydrogen atoms are omitted for clarity).

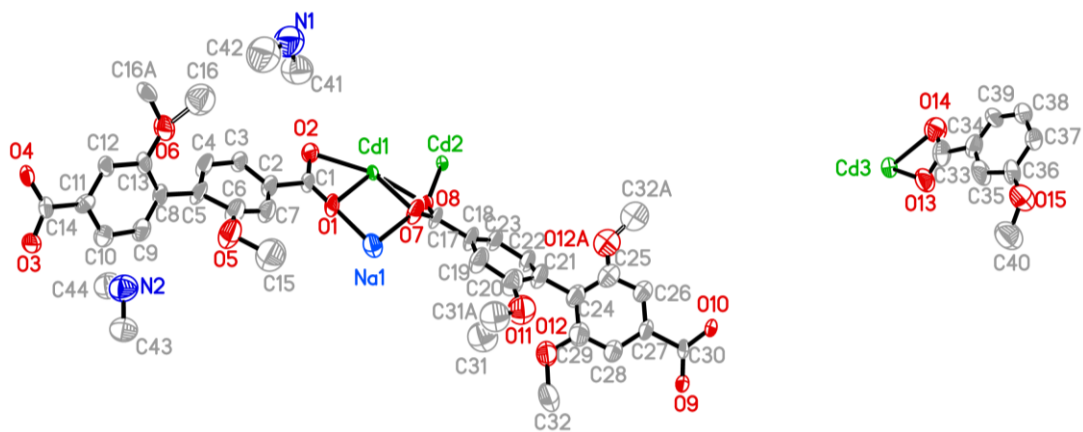


Fig. S4 The asymmetric unit of **4** (Hydrogen atoms are omitted for clarity).

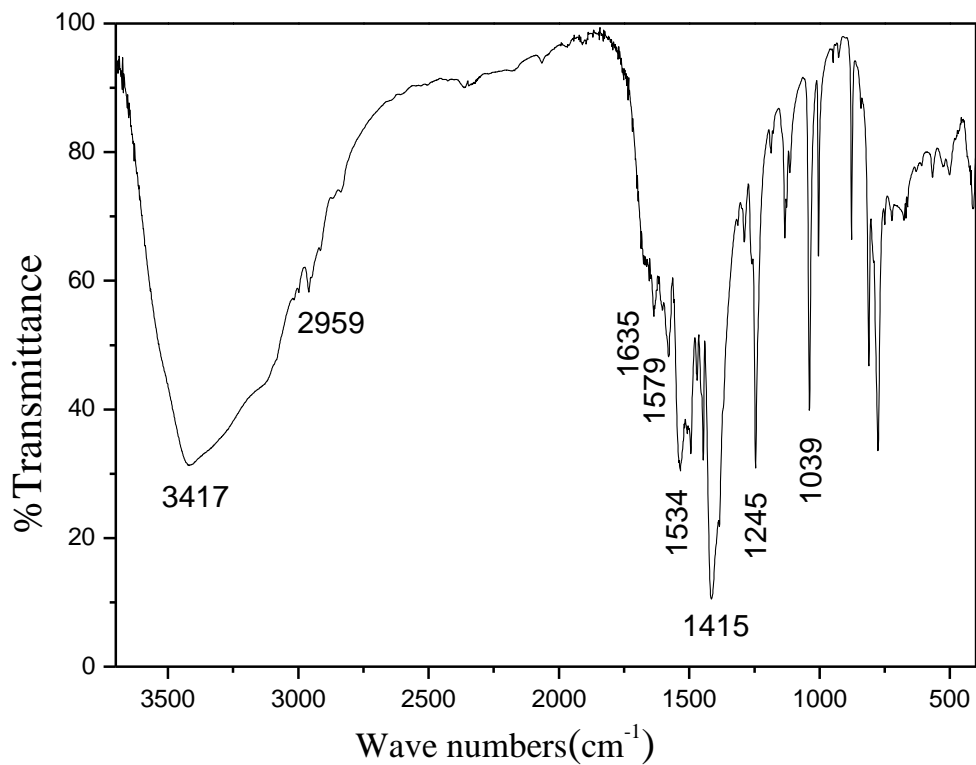


Fig. S5 The IR spectra of **1**.

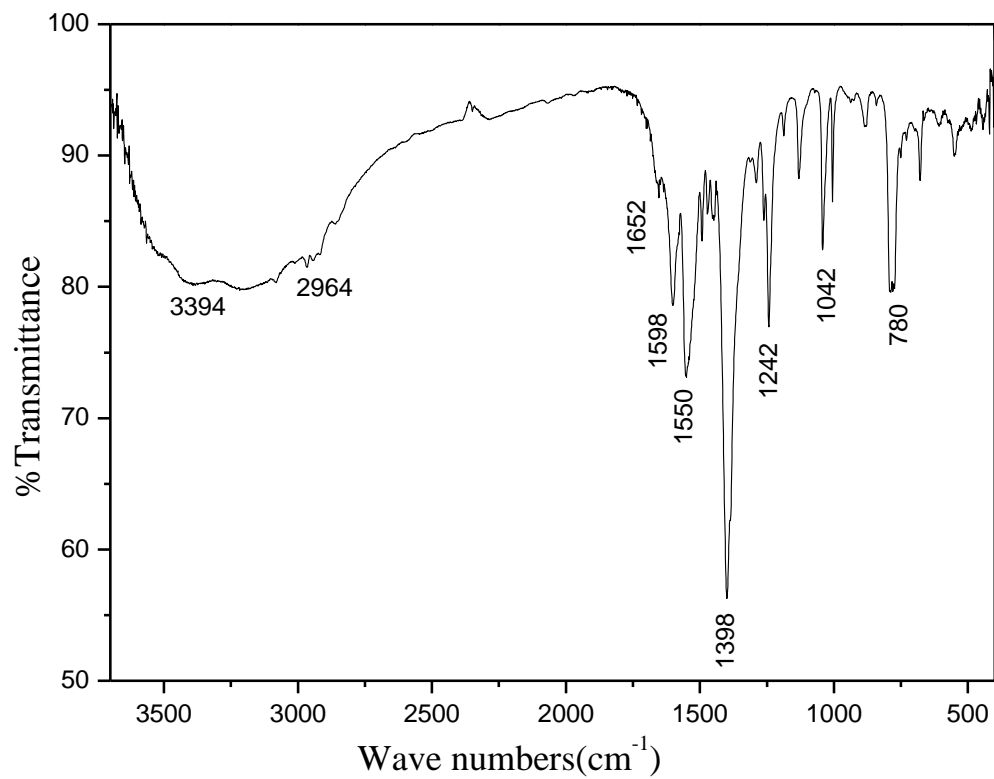


Fig. S6 The IR spectra of **2**.

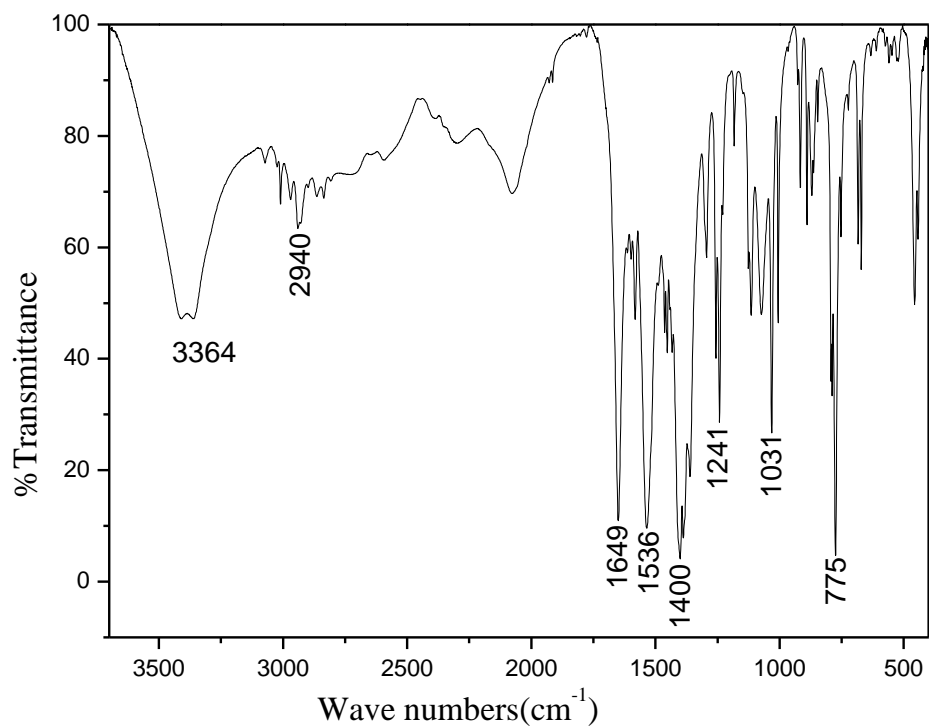


Fig. S7 The IR spectra of **3**.

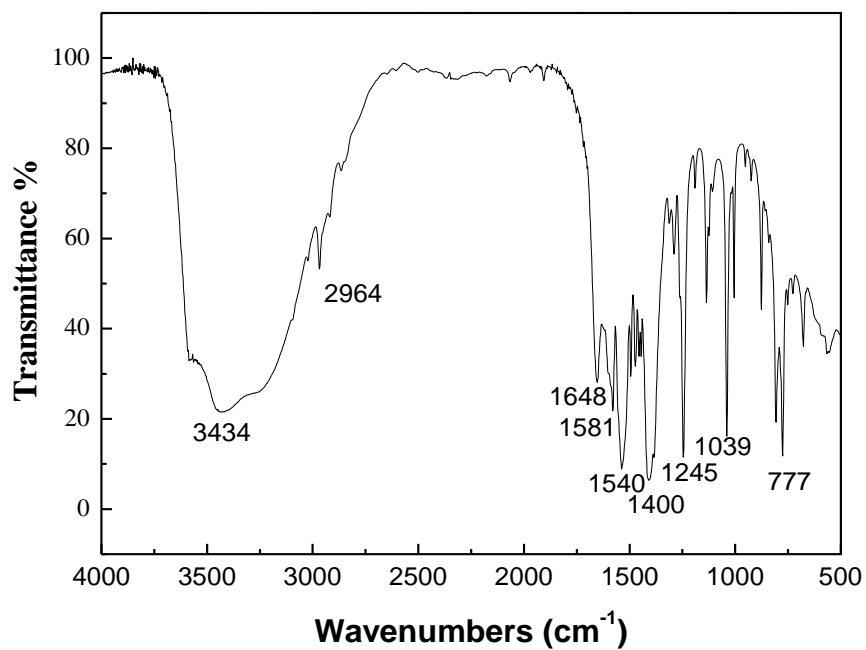


Fig. S8 The IR spectra of **4**.

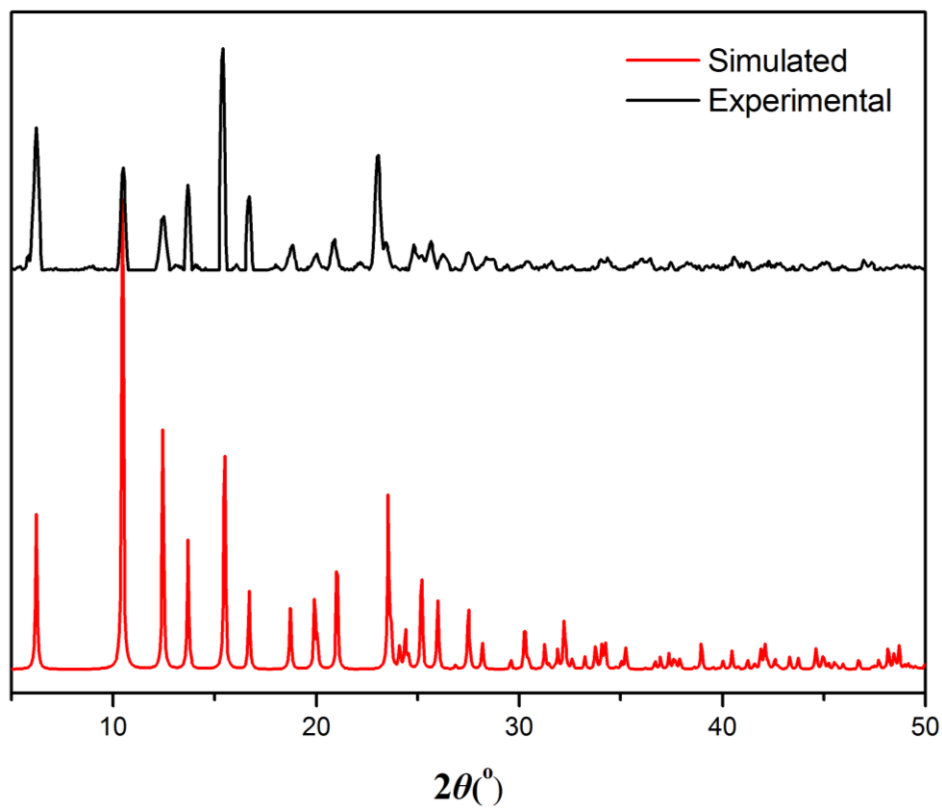


Fig. S9 The P-XRD patterns of **1**.

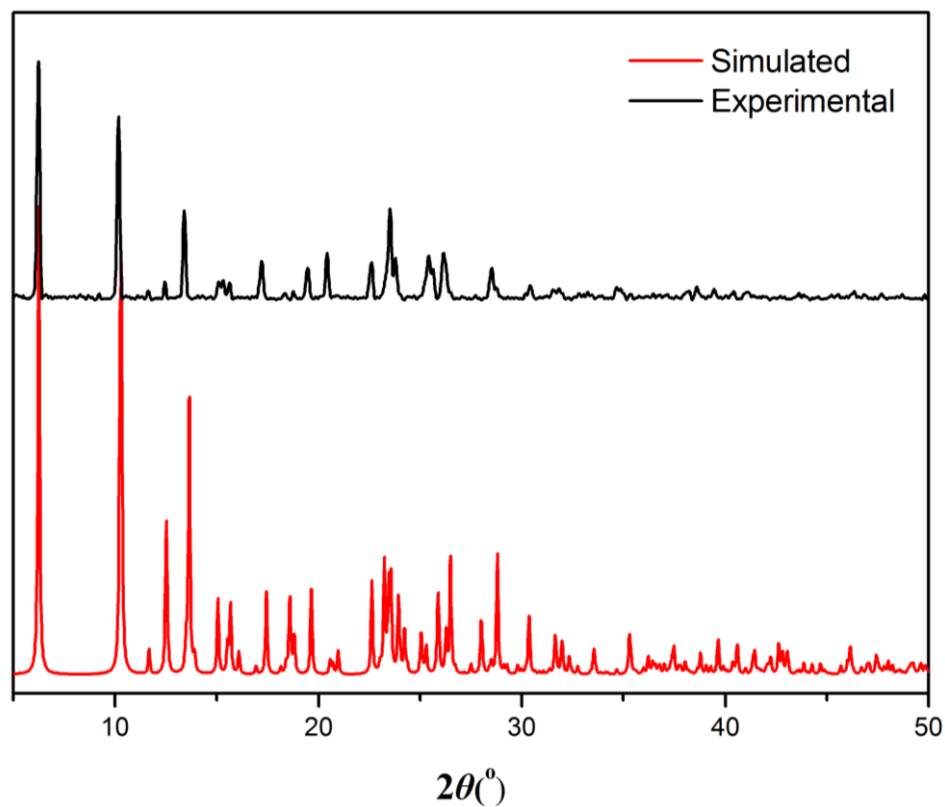


Fig. S10 The P-XRD patterns of **2**.

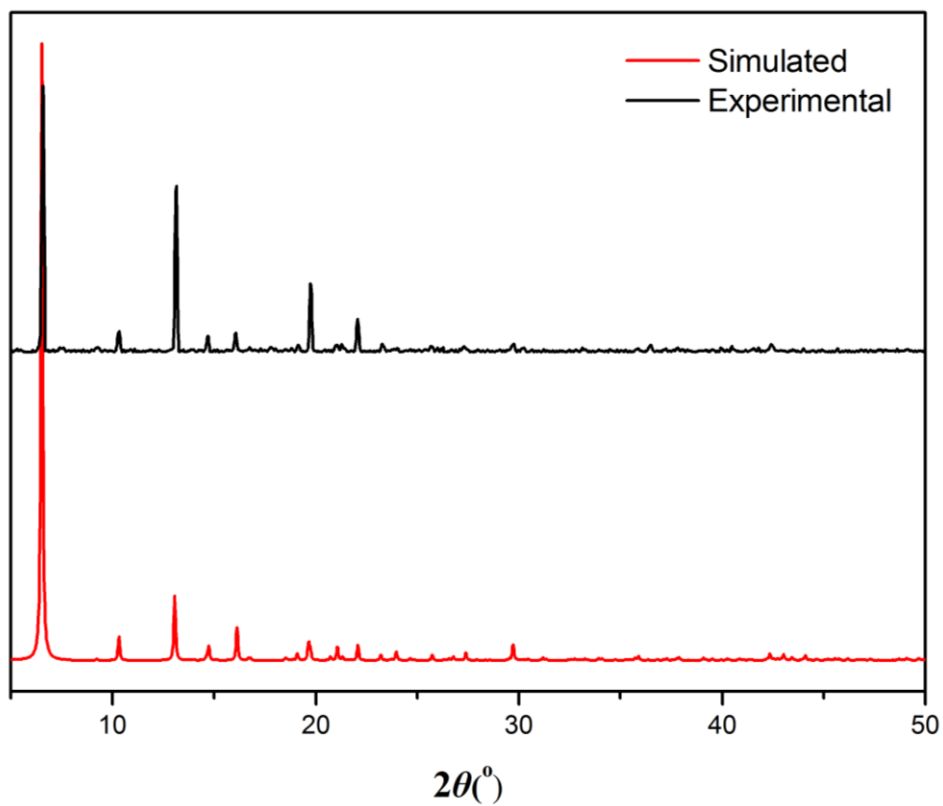


Fig. S11 The P-XRD patterns of **3**.

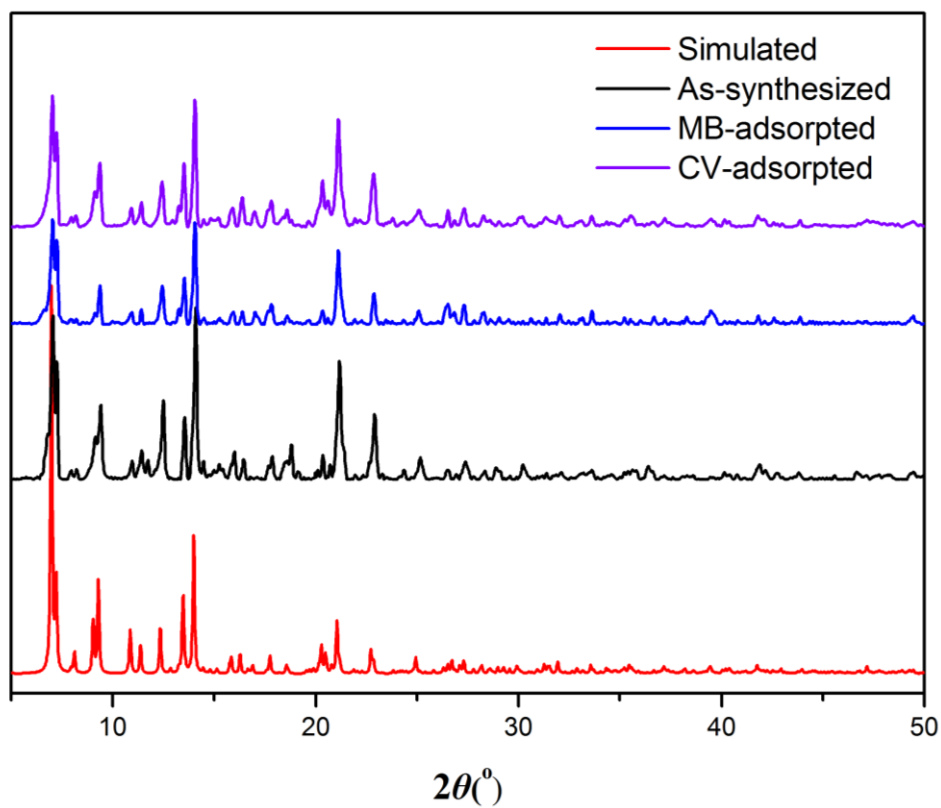


Fig. S12 The P-XRD patterns of **4**.

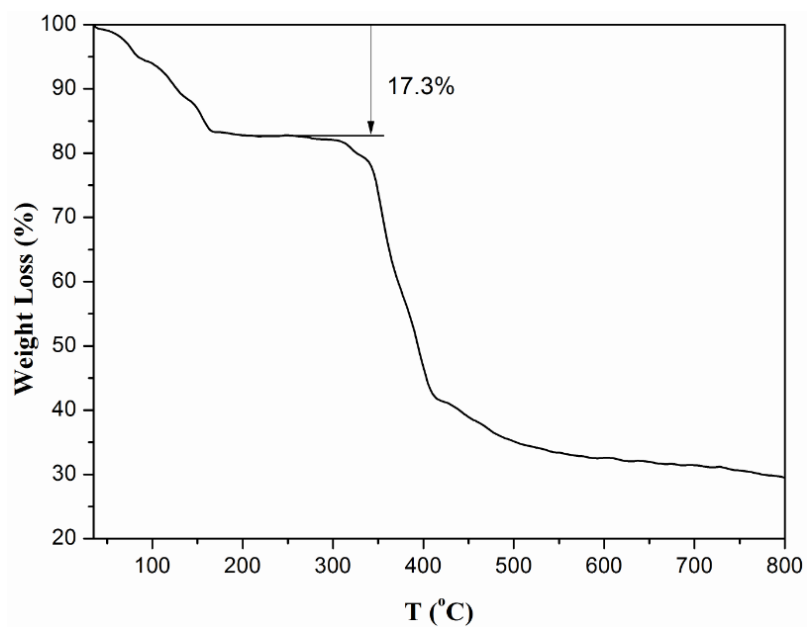


Fig. S13 The TGA curve for **1**.

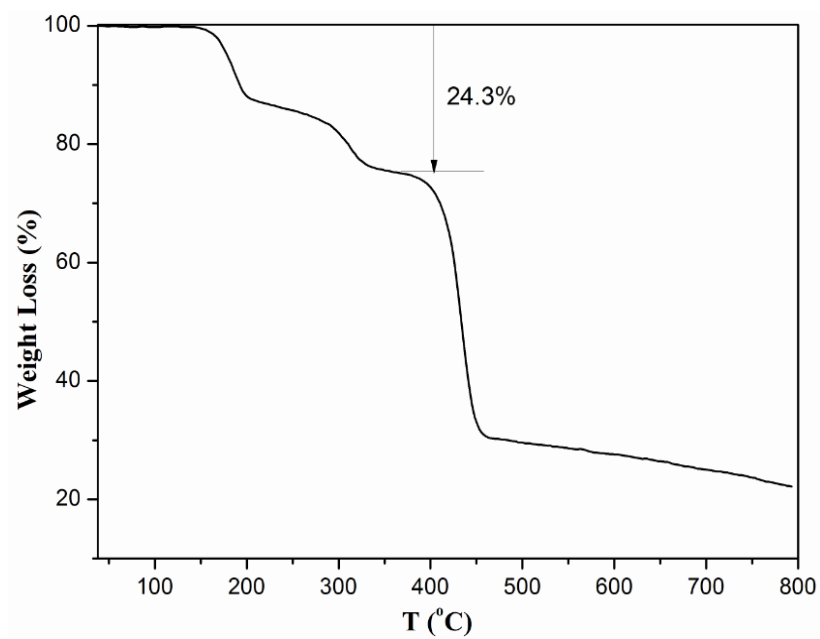


Fig. S14 The TGA curve for **2**.

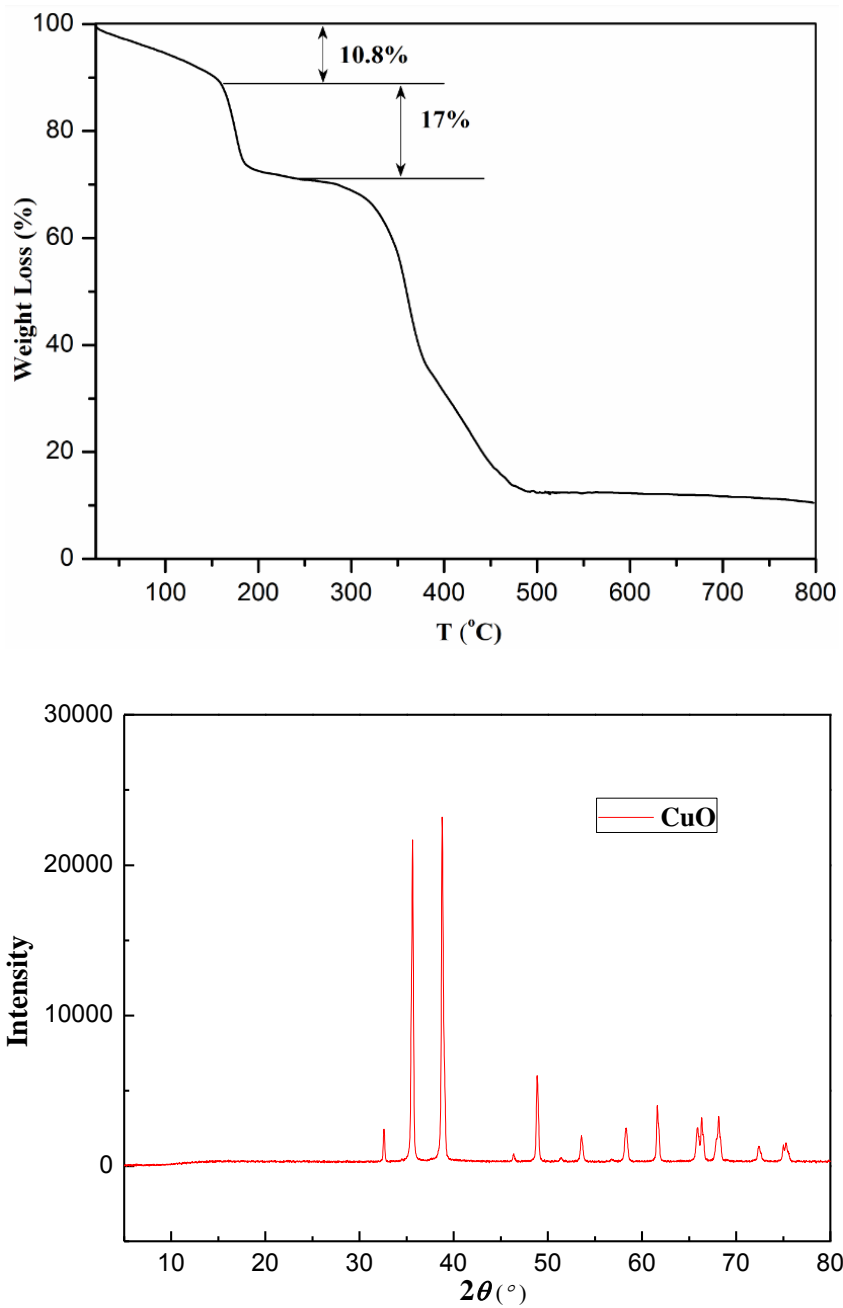


Fig. S15 The TGA curve for **3** (top). The P-XRD patterns of the final residues (bottom).

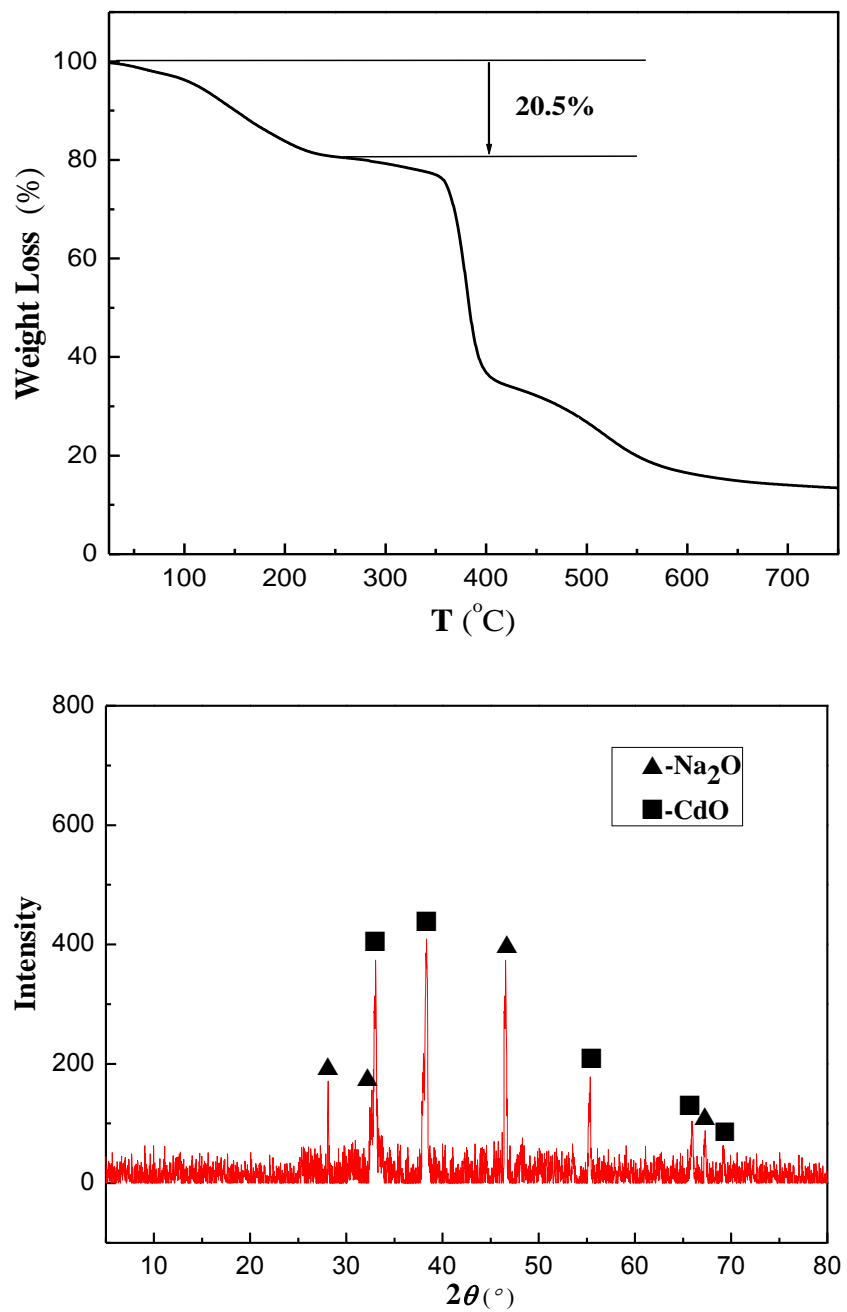


Fig. S16 The TGA curve for **4** (top). The P-XRD patterns of the final residues (bottom).

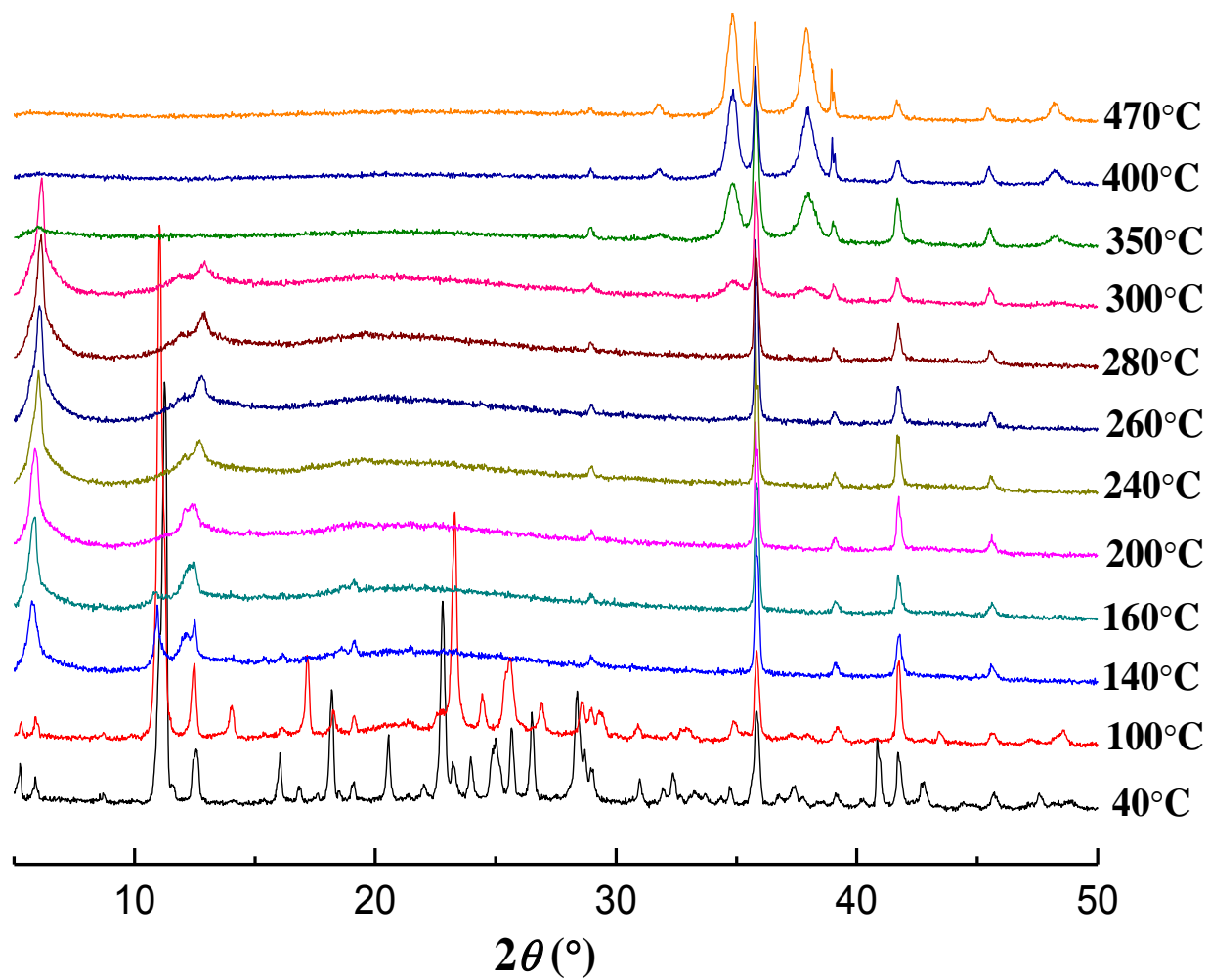


Fig. S17 The variable temperature PXRD patterns of **3**.

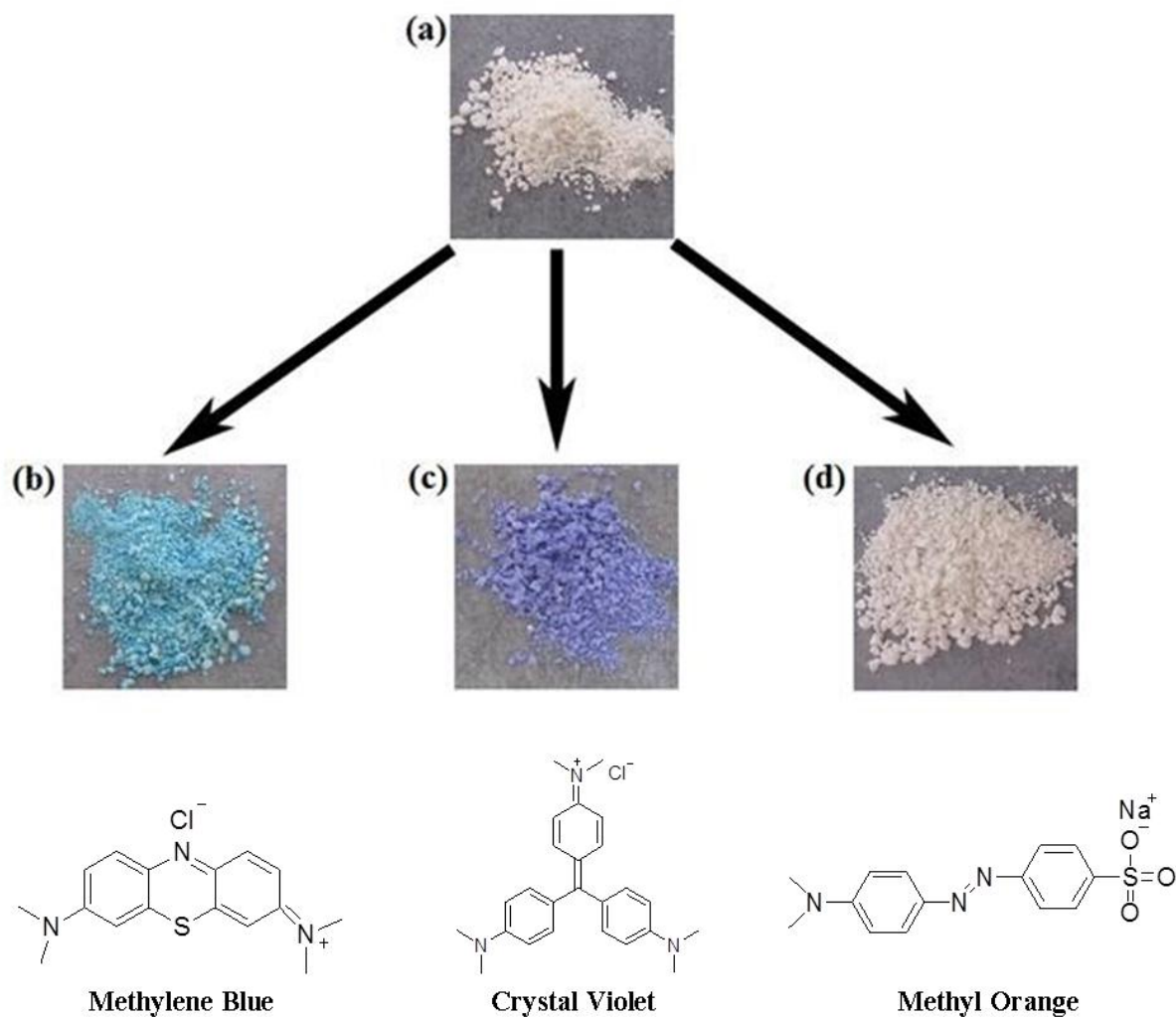


Fig. S18 (a) As-synthesized **4**. (b)-(d) Photos of **4** after soaked in DMF solutions of three kinds of dyes.