Electronic Supplementary Material for CrystEngComm

Supplementary Information

Microwave Synthesis and Single-Crystal-to-Single-Crystal Transformation of Magnesium Coordination Polymers Exhibiting Selective Gas Adsorption and Luminescence Properties

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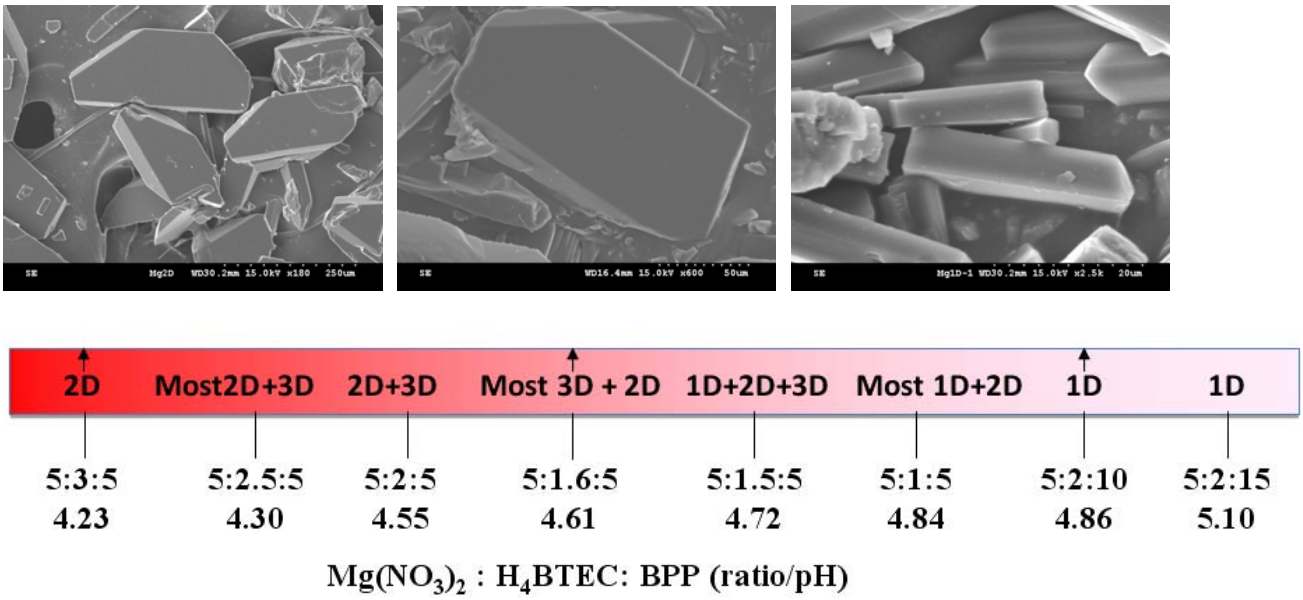


Fig. S1 The SEM photos of the crystals of **2**, **1**, and **3** from left to right were shown. The crystal sizes are ranged form about 0.01 to 0.5 mm. The ratio of the reaction materials and resulting phases are represented above. All these microwave reactions are done at 150^{o}C for 20 minutes.

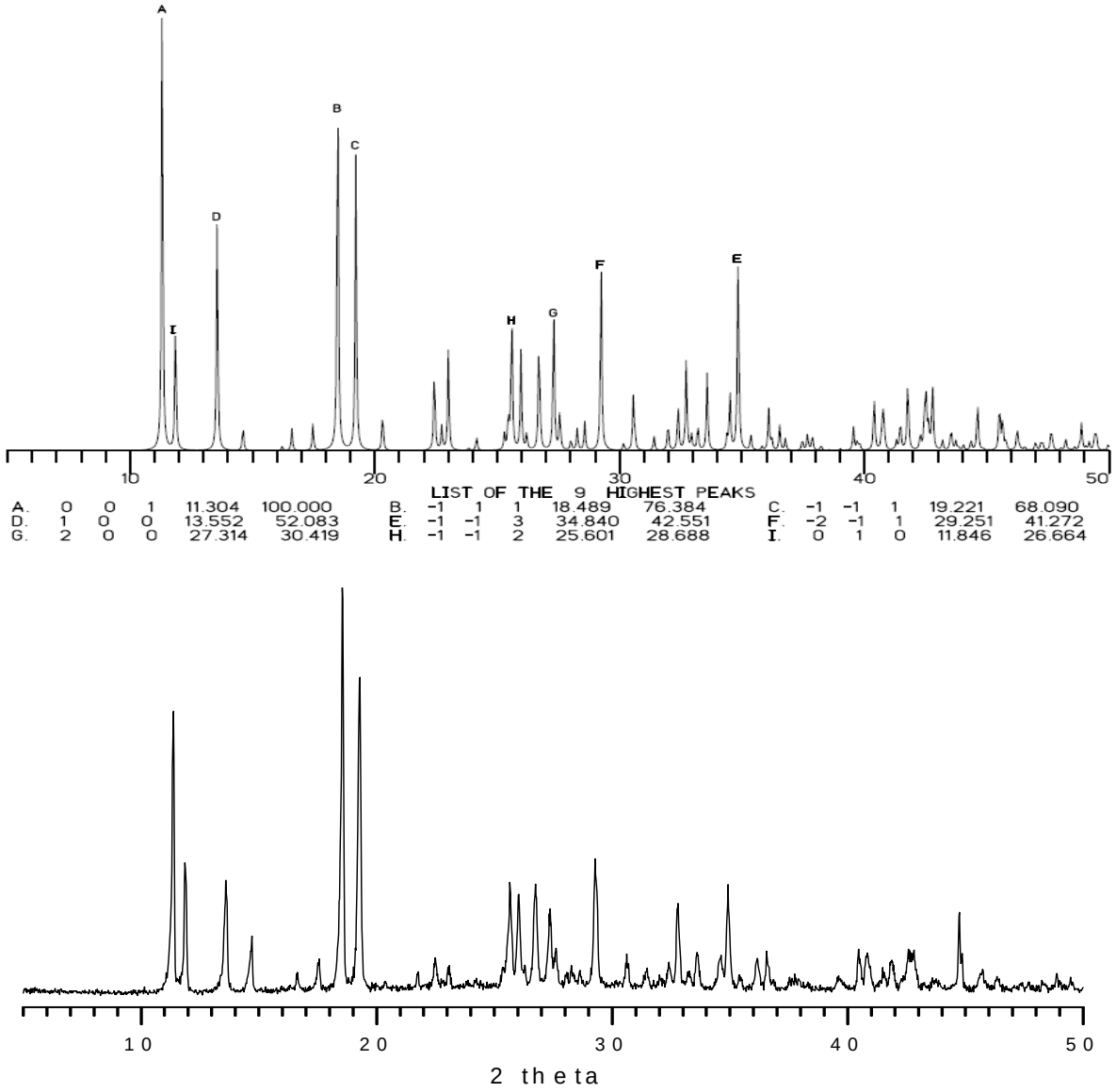


Fig. S2 Powder XRD patterns of **1** (calculated, top; measured, bottom).

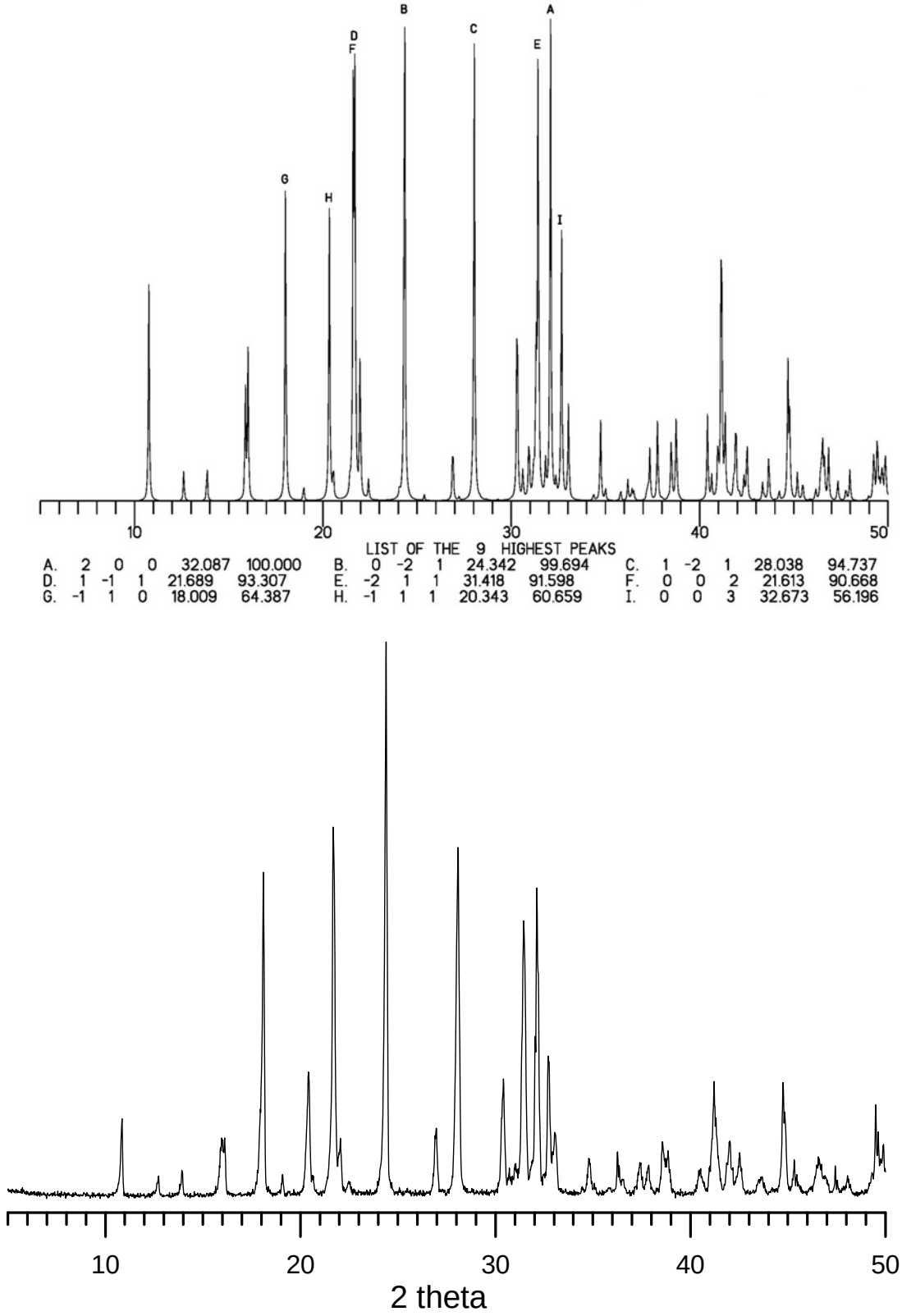


Fig. S3 Powder XRD patterns of **2** (calculated, top; measured, bottom).

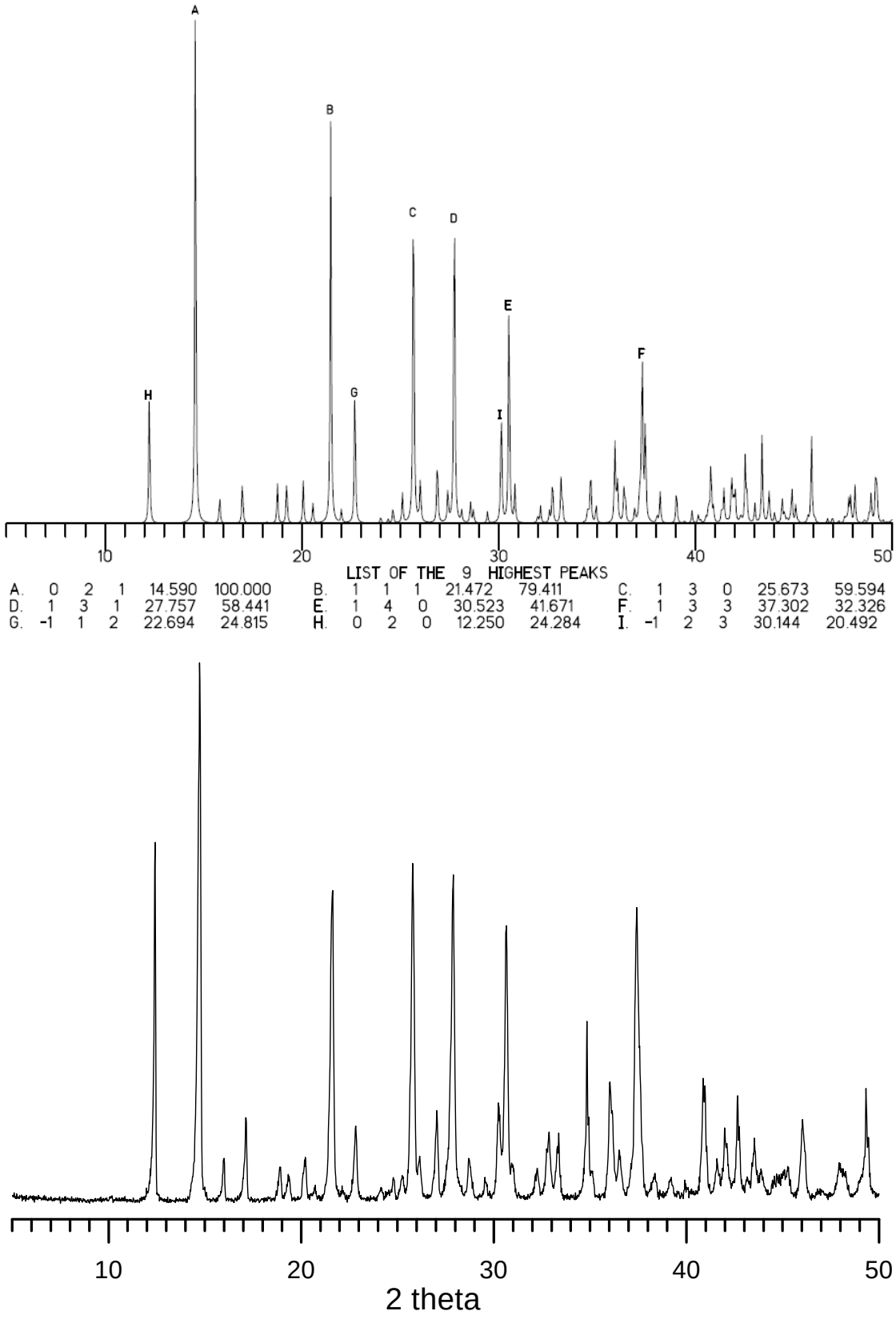
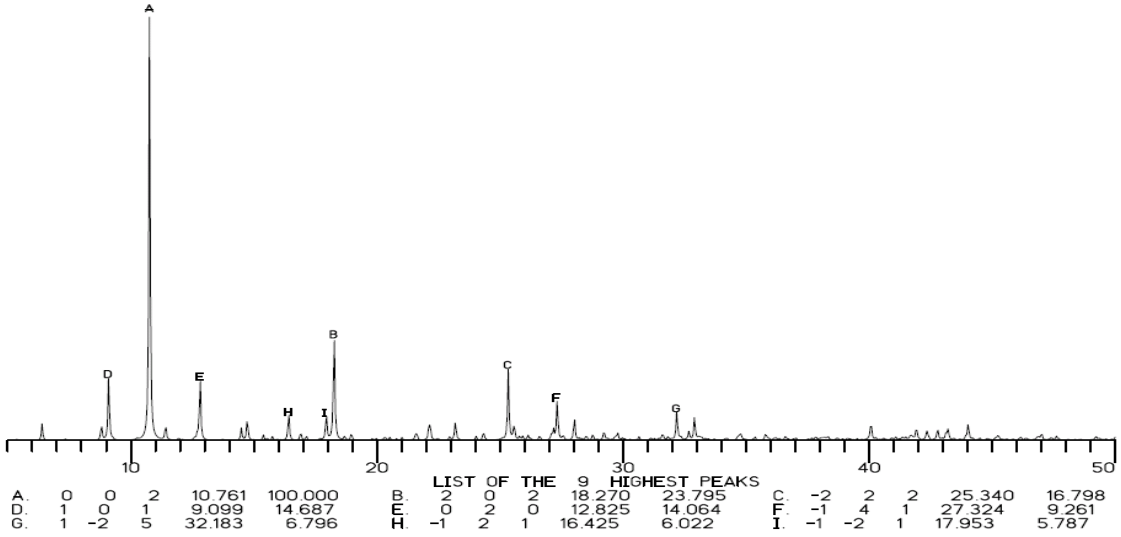
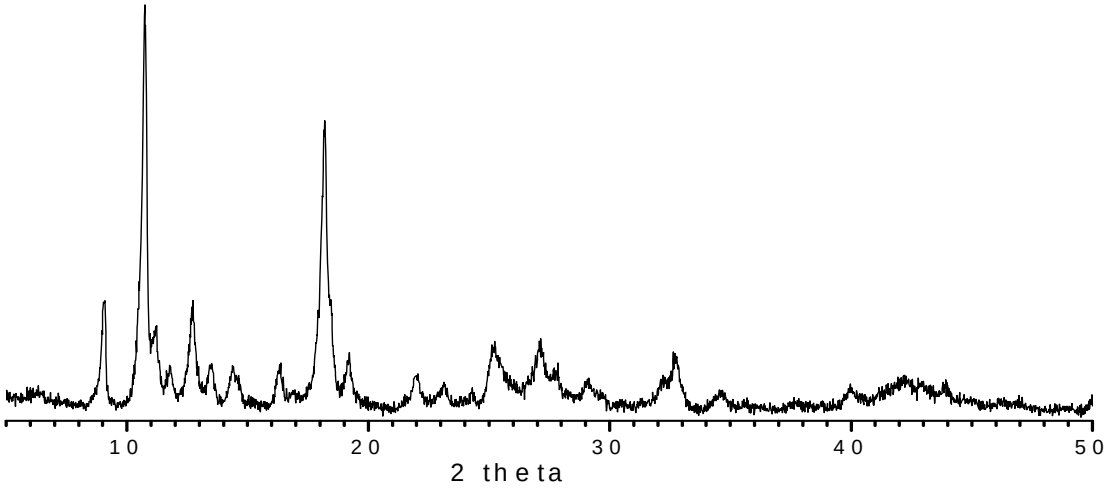


Fig. S4 Powder XRD patterns of **3** (calculated, top; measured, bottom).





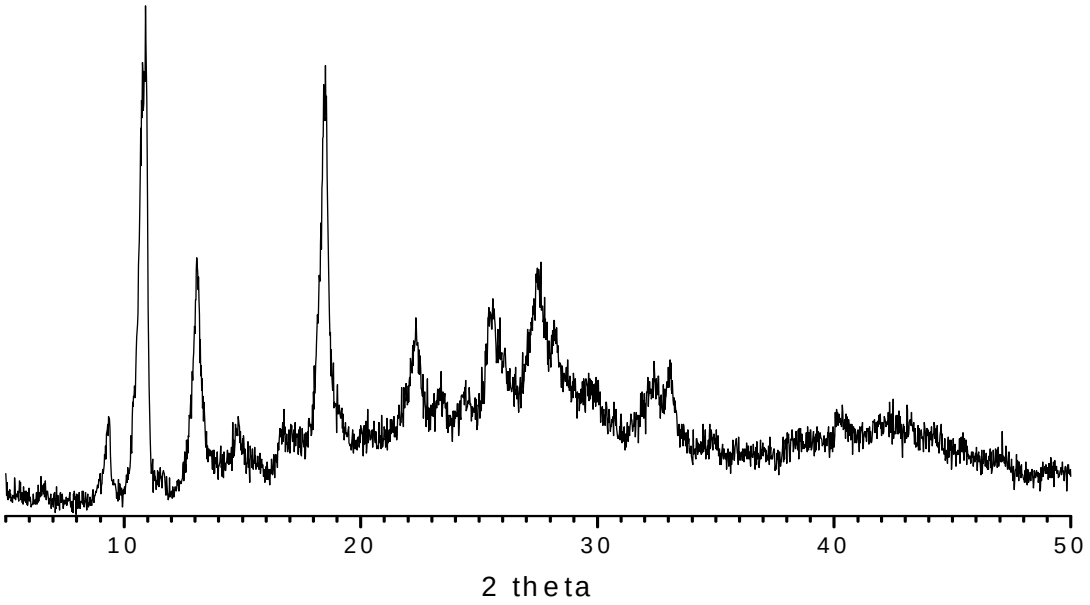


Fig. S5 Powder XRD patterns of **1a** (calculated, top; measured before gas sorption , middle, measured after gas sorption ,bottom).

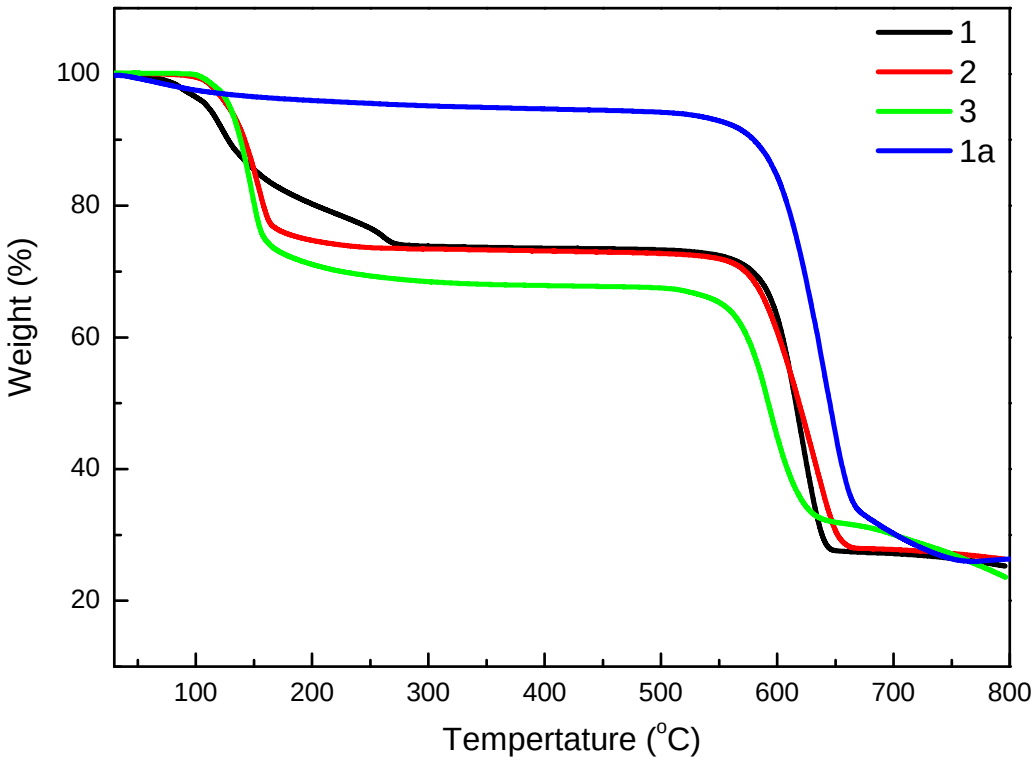


Fig. S6 TGA curves of compound **1**, **2**, **3**, and **1a**.

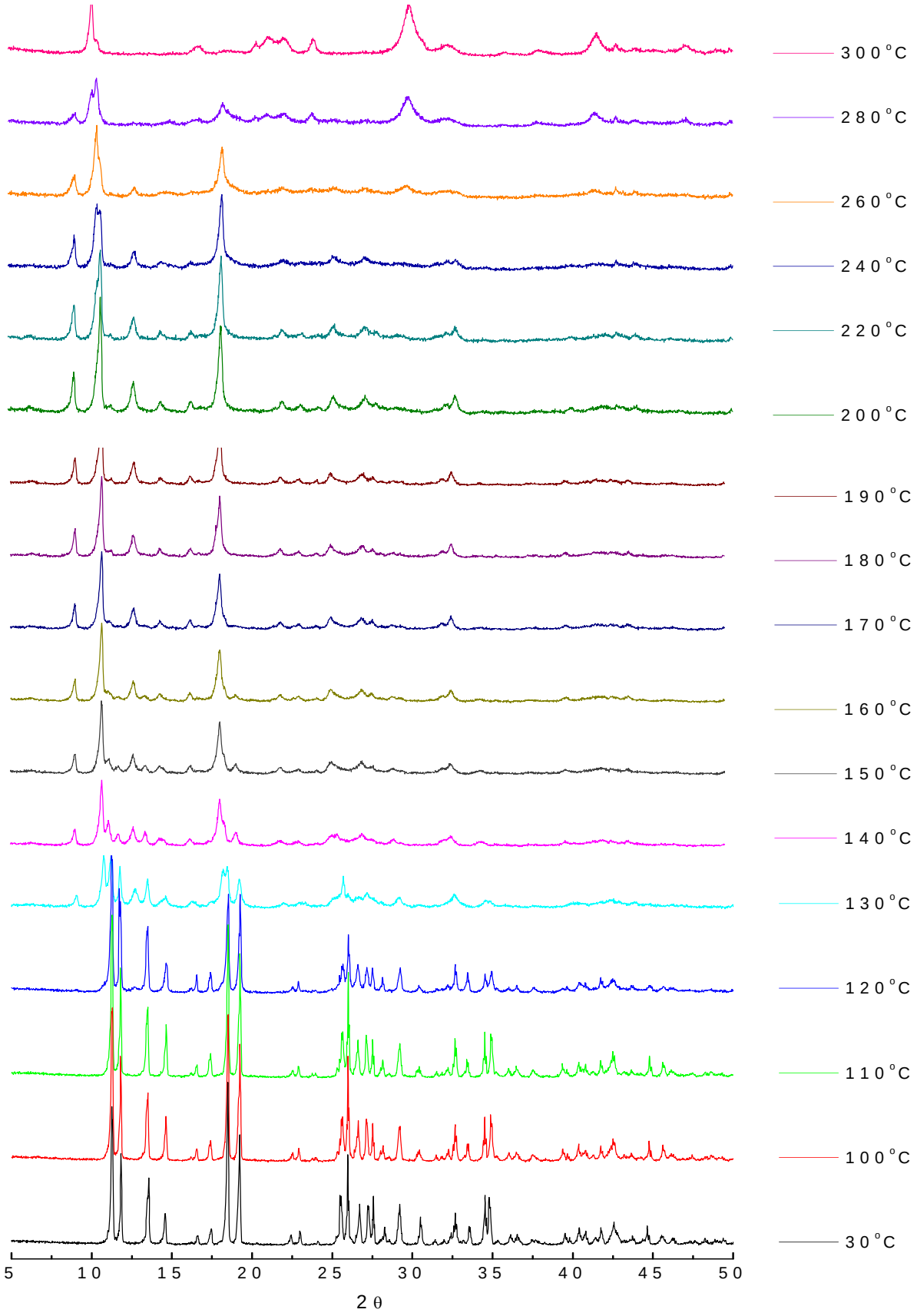


Fig. S7 Powder XRD patterns of compound **1** under various temperatures.

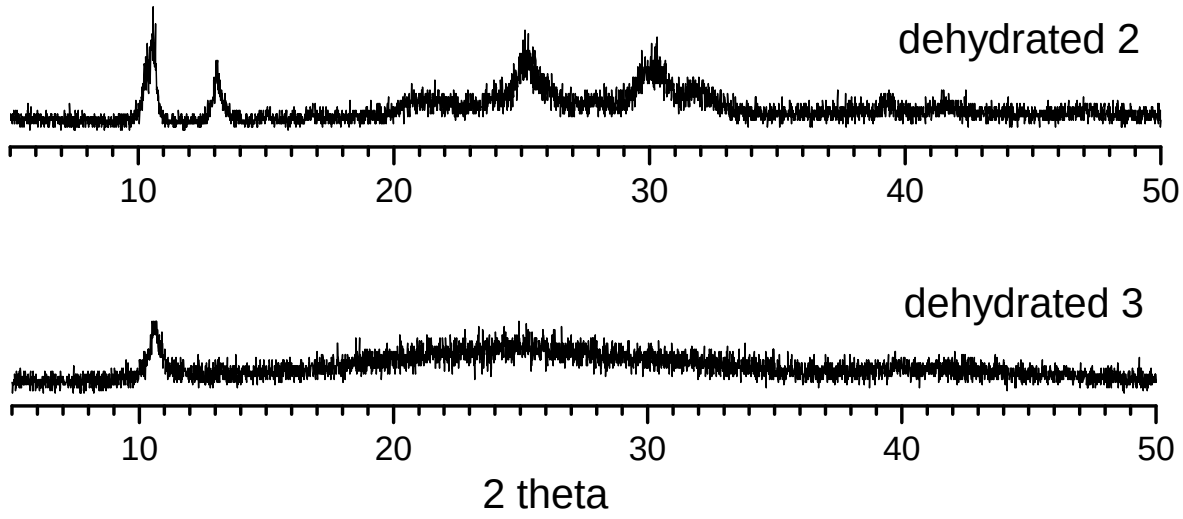


Fig. S8 Powder XRD patterns of dehydrated **2** and **3** heated at the temperature of 250 ^{o}C.

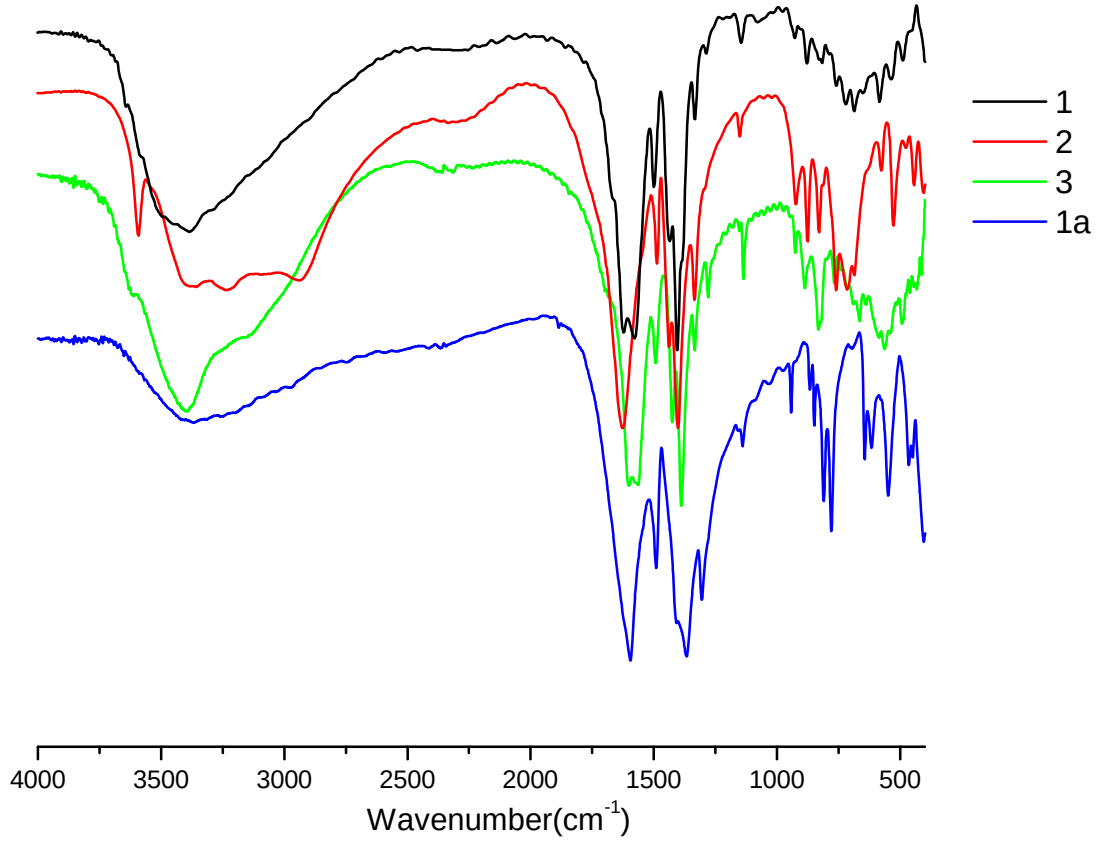


Fig. S9. FT-IR spectra of **1**, **2**, **3**, and **1a**.

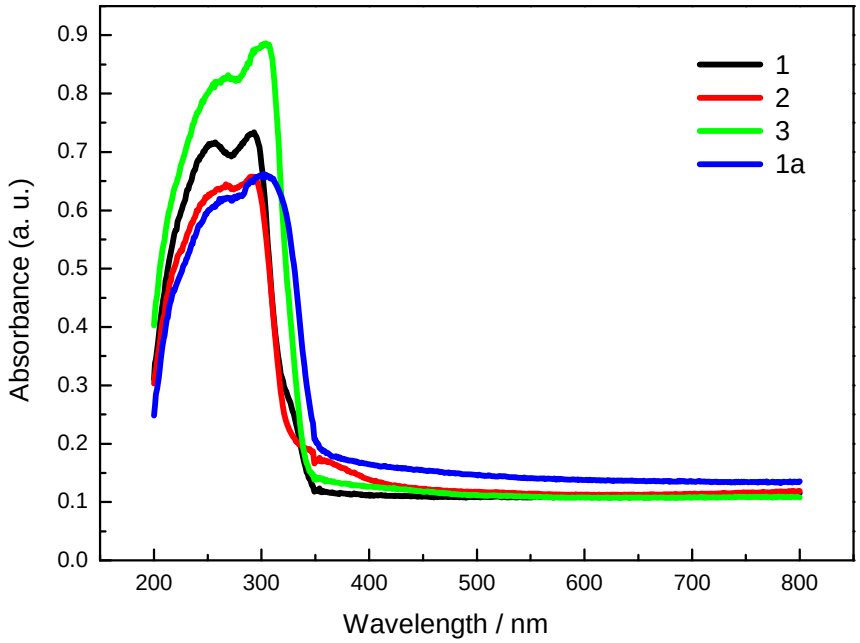


Fig. S10 UV-vis absorption spectra of compound **1**, **2**, **3**, and **1a**.

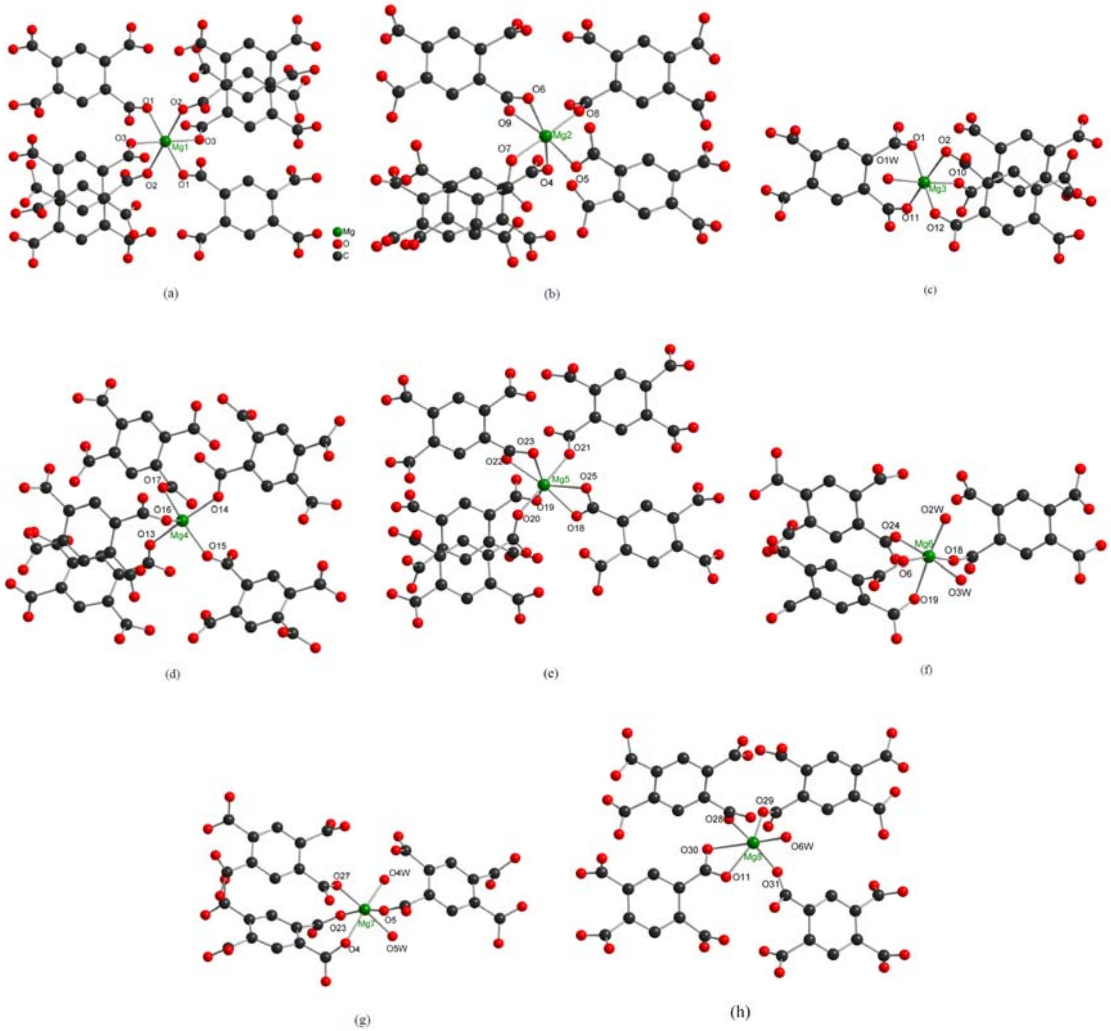


Fig. S11 Views of the coordination environments of magnesium sites: (a) Mg(1); (b) Mg(2); (c) Mg(3); (d) Mg(4); (e) Mg(5); (f) Mg(6); (g) Mg(7); (h) Mg(8).

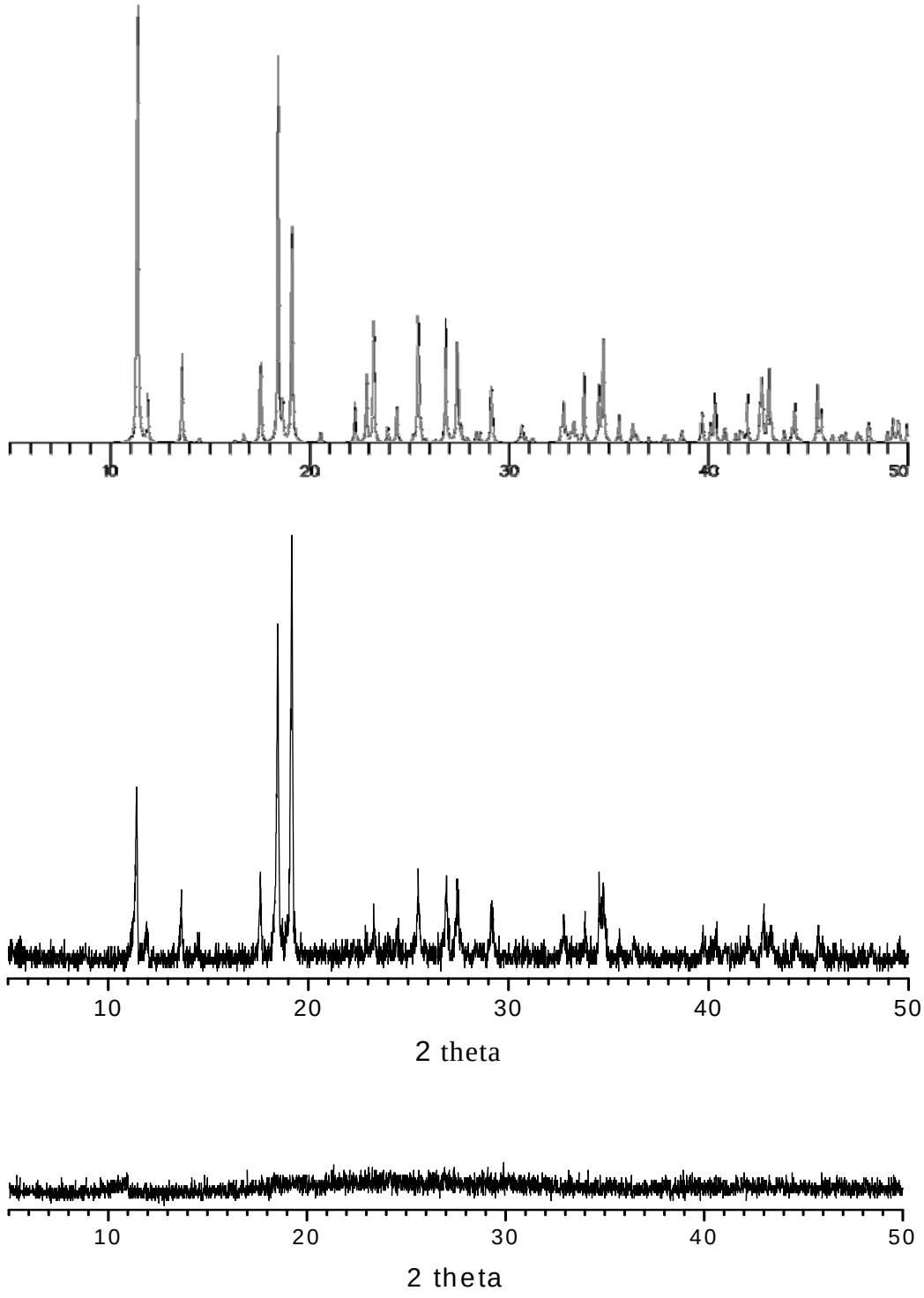


Fig. S12 Powder XRD patterns of $[Co_2(BTEC)(H_2O)_4]\cdot 2H_2O$ (calculated, top; measured, middle; heated by 150^{o}C, bottom).

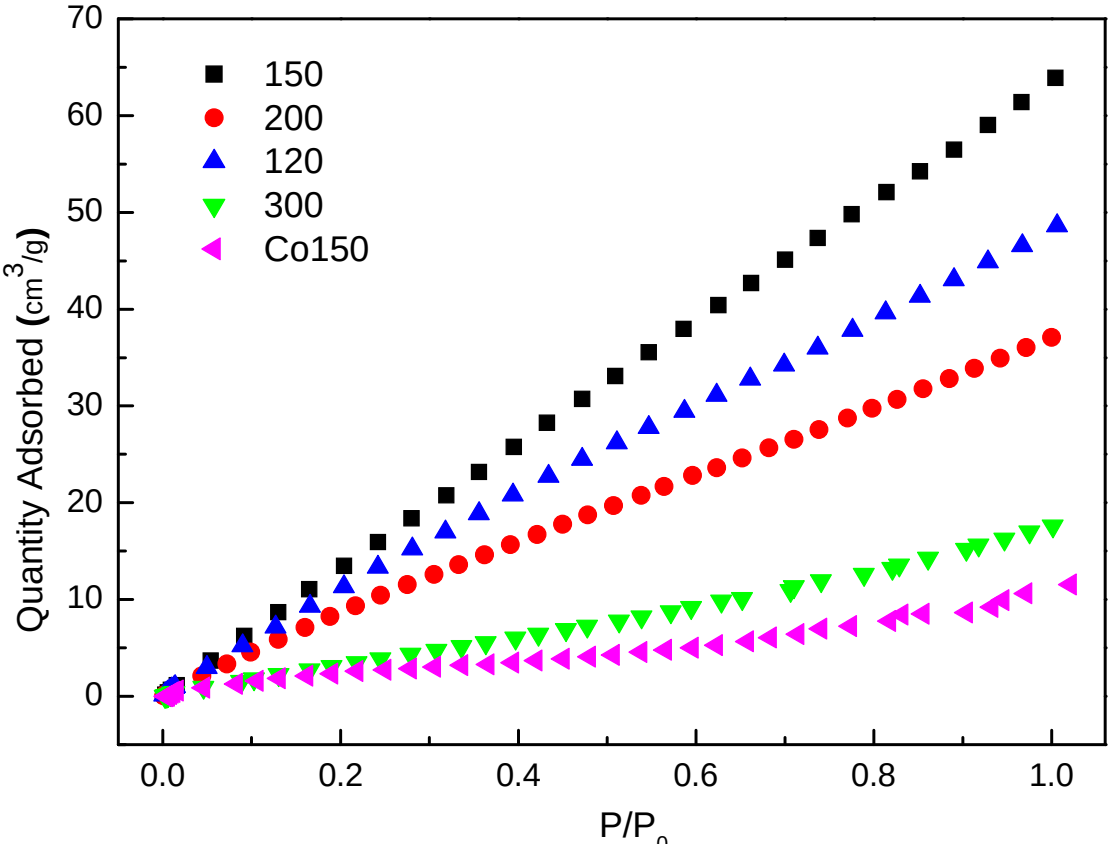


Fig. S13 The hydrogen gas sorption isotherms for the samples of **1** (blue, heated at 120 ^{o}C), **1a** (black, heated at 150 ^{o}C), **1a** (red, heated at 200 ^{o}C), and amorphous phases heated from **1** (green, heated at 300 ^{o}C) and $[Co_2(BTEC)(H_2O)_4]\cdot 2H_2O$ (magenta, heated at 150 ^{o}C) at 77 K.

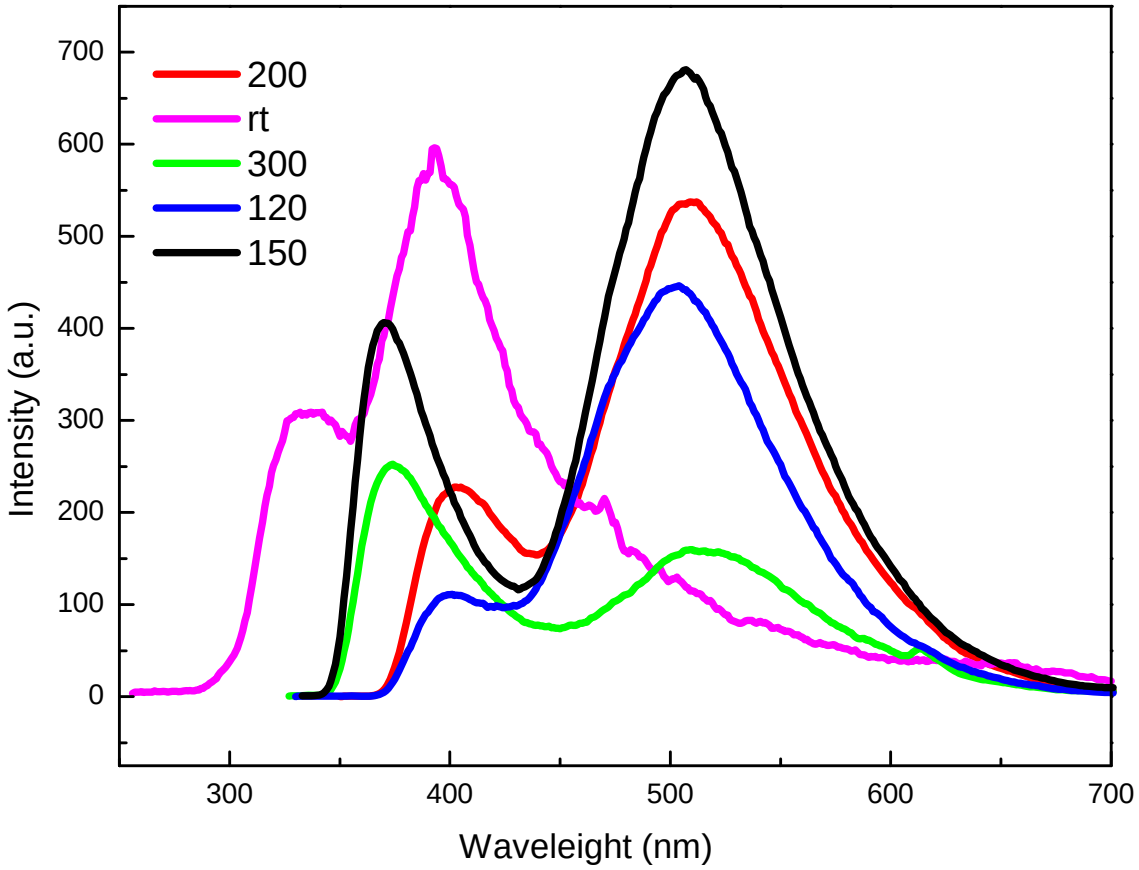


Fig. S14 Emission spectra of samples heated under various temperatures from **1** (excitation at 246 for room temperature and 317 nm for others).

Table S1 Hydrogen bonding distance (Å) and angle (^{o}) data for **1**, **2**, **3**, and **1a**.

D-H	d(D-H)	d(H..A)	<DHA	d(D..A)	A	Symmetry Code
1						
O1W-H1	0.868	2.049	151.17	2.841	O3	[x-1, y, z]
O1W-H2	0.775	2.315	129.99	2.875	O4	[-x+1, -y+1, -z+2]
O1W-H2	0.775	2.422	151.98	3.127	O3	[-x+1, -y+1, -z+2]
O2W-H3	0.820	2.048	172.35	2.863	O1	[x+1, y, z]
O2W-H4	0.865	2.076	160.42	2.906	O3W	[x, y, z-1]
O2W-H4	0.865	2.648	133.46	3.304	O4W	[x, y, z-1]
O3W-H5	0.698	2.568	126.00	3.032	O2W	[-x+2, -y, -z+2]
O3W-H5	0.698	2.586	110.62	2.906	O2W	[x, y, z+1]
O3W-H6	0.874	2.230	172.31	3.098	O2	
O4W-H8	0.850	2.216	165.64	3.047	O2	
2						
O1W-H1	0.870	1.981	161.52	2.820	O3W	[-x, -y+2, -z+2]
O1W-H2	0.831	2.297	144.58	3.013	O1W	[-x+1, -y+2, -z+2]
O2W-H3	0.820	1.850	172.28	2.666	O4	[-x, -y+1, -z+1]
O2W-H4	0.840	1.973	169.00	2.803	O2	[-x, -y+1, -z+1]
O3W-H5	0.860	1.842	166.19	2.686	O4	[x, y+1, z]
O3W-H6	0.804	2.123	177.97	2.926	O2W	[x-1, y, z]
3						
O1W-H1	0.810	2.113	143.44	2.805	O1	[-x, -y, -z]
O1W-H1	0.810	2.637	133.71	3.249	O3	[-x, -y, -z]
O1W-H2	0.880	1.946	164.52	2.804	O1	[x-1, y, z]
O1W-H2	0.880	2.599	139.45	3.318	O3	[x-1, y, z]
O2W-H3	0.879	1.909	167.73	2.774	O4	[x-1/2, -y+1/2, z-1/2]
O2W-H4	0.859	1.824	169.30	2.673	O3	[-x+1/2, y+1/2, -z+1/2]
O3W-H5	0.798	2.513	132.91	3.112	O4	
O3W-H6	0.850	2.129	150.11	2.897	O2W	[x+1, y, z]
O4W-H7	0.905	1.766	176.25	2.670	O4	[x+1/2, -y+1/2, z-1/2]
O4W-H8	0.959	2.005	154.02	2.897	O3	[-x+1, -y, -z]
1a						
O32-H32A	0.820	1.364	141.42	2.069	O7W	[x-1, y, z]
O32-H32A	0.820	2.285	139.76	2.959	O31	[x-1, y, z]
O1W-H1WA	0.850	2.647	133.03	3.286	O3	
O1W-H1WB	0.858	2.132	177.97	2.990	O14	[-x+1, -y, -z]
O2W-H2WB	0.850	2.229	128.38	2.836	O7	[-x, -y+1, -z-1]
O2W-H2WA	0.850	2.454	141.39	3.163	O2W	[-x, -y+1, -z-1]
O3W-H3WA	0.850	2.287	125.23	2.863	O26	

O3W-H3WA	0.850	2.455	112.90	2.894	O2W	
O3W-H3WB	0.850	2.320	173.86	3.166	O8	
O4W-H4WA	0.850	2.075	122.87	2.635	O25	[x, y+1, z]
O4W-H4WB	0.850	1.912	152.76	2.696	O20	[-x, -y+1, -z-1]
O5W-H5WA	0.850	2.561	114.97	3.020	O5	
O5W-H5WB	0.852	2.086	166.37	2.921	O22	[-x-1, -y+1, -z-1]
O6W-H6WB	0.848	2.008	153.34	2.792	O16	
O7W-H7WA	0.851	1.909	117.47	2.423	O31	
O7W-H7WB	0.860	1.759	111.49	2.223	O32	[-x, -y+1, -z]
O7W-H7WB	0.860	2.225	139.19	2.931	O29	[-x, -y+1, -z]
O8W-H8WA	0.842	2.546	168.58	3.376	O16	
O8W-H8WB	0.826	1.635	112.09	2.091	O7W	
O8W-H8WB	0.826	2.532	178.06	3.358	O31	

Table 2 Selected bond lengths (Å) for **1**-**3** and **1a**

Complex **1**[a]					
Mg(1)-O(2)#1	2.0725(6)	Mg(1)-O(1)#1	2.0792(5)	Mg(2)-O(3)	2.0373(6)
Mg(1)-O(2)	2.0725(6)	Mg(1)-O(1)	2.0792(5)	Mg(2)-O(3)#2	2.0373(6)
Mg(1)-O(1W)#1	2.0774(7)	Mg(2)-O(4)#2	2.0177(6)	Mg(2)-O(2W)#2	2.1366(7)
Mg(1)-O(1W)	2.0774(7)	Mg(2)-O(4)	2.0177(6)	Mg(2)-O(2W)	2.1366(7)
Complex **2**					
Mg(1)-O(1)	2.0053(9)	Mg(1)-O(2)	2.0805(8)	Mg(1)-O(3W)	2.1105(9)
Mg(1)-O(3)	2.0069(9)	Mg(1)-O(2W)	2.0880(9)	Mg(1)-O(1W)	2.1569(10)
Complex **3**					
Mg(1)-O(2)	2.017(2)	Mg(1)-O(3W)	2.065(2)	Mg(1)-O(4W)	2.085(2)
Mg(1)-O(1W)	2.037(2)	Mg(1)-O(1)	2.078(2)	Mg(1)-O(2W)	2.128(2)
Complex **1a**[b]					
Mg(1)-O(1)#1	2.067(6)	Mg(3)-O(1W)	2.090(9)	Mg(6)-O(18)	2.086(9)
Mg(1)-O(1)	2.067(6)	Mg(3)-O(2)#1	2.148(8)	Mg(6)-O(3W)	2.103(9)
Mg(1)-O(3)#1	2.071(7)	Mg(4)-O(16)	1.967(8)	Mg(6)-O(6)	2.104(8)
Mg(1)-O(3)	2.071(7)	Mg(4)-O(15)	1.994(8)	Mg(6)-O(19)	2.174(7)
Mg(1)-O(2)	2.192(8)	Mg(4)-O(17)	2.042(8)	Mg(7)-O(27)	1.994(8)
Mg(1)-O(2)#1	2.192(8)	Mg(4)-O(14)	2.064(7)	Mg(7)-O(4W)	2.003(9)
Mg(2)-O(8)	2.029(8)	Mg(4)-O(13)	2.072(8)	Mg(7)-O(23)#2	2.086(9)
Mg(2)-O(7)	2.056(8)	Mg(5)-O(21)	2.009(8)	Mg(7)-O(5)	2.087(8)
Mg(2)-O(5)	2.060(8)	Mg(5)-O(20)	2.038(7)	Mg(7)-O(5W)	2.080(10)
Mg(2)-O(9)	2.102(8)	Mg(5)-O(19)	2.128(7)	Mg(7)-O(4)	2.142(8)
Mg(2)-O(4)	2.156(8)	Mg(5)-O(22)	2.138(8)	Mg(8)-O(29)	1.940(10)
Mg(2)-O(6)	2.280(8)	Mg(5)-O(18)	2.141(8)	Mg(8)-O(6W)	1.973(16)
Mg(3)-O(12)	2.016(9)	Mg(5)-O(25)	2.391(10)	Mg(8)-O(28)	2.020(9)
Mg(3)-O(10)	2.017(8)	Mg(5)-O(23)	2.508(9)	Mg(8)-O(11)#3	2.095(8)
Mg(3)-O(11)	2.021(8)	Mg(6)-O(2W)	2.009(9)	Mg(8)-O(31)#3	2.202(13)
Mg(3)-O(1)	2.051(7)	Mg(6)-O(24)	2.046(8)	Mg(8)-O(30)#3	2.422(11)

[a]Symmetry transformations used to generate equivalent atoms for **1**: #1 -x+1,-y+1,-z+2; #2 -x+2,-y,-z+2.

[b]Symmetry transformations used to generate equivalent atoms for **1a**: #1 -x+1,-y,-z; ; #2 x,y+1,z; #3 x-1,y,z.