Supplementary Material for CrystEngComm

Supporting Information

Syntheses, structures, photoluminescence and magnetic properties of five compounds with 1,3,5-benzenetricarboxylate acid and imidazole ligands

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Table S1 Selected Bond Distances (Å) and Angles (deg) for complexes

Complex **1**			
Zn1─N1	2.041(3)	Zn1─N4_a	1.993(3)
Zn1─O1	1.952(3)	Zn1─O4_a	1.989(3)
O1─ Zn1 ─O4_b	106.01(13)	O1─ Zn1 ─N4_b	113.73(14)
O4_b─ Zn1 ─N4_b	122.56(13)	O1─ Zn1 ─N1	95.47(13)
O4_b─ Zn1 ─N1	109.33(13)	N4_b─ Zn1 ─N1	106.33(15)
C23─ N4─ Zn1_a	131.3(3)	C9─ O1─ Zn1	116.9(3)
C7 ─O4─ Zn1_a	105.1(3)	C21─N4 ─Zn1_a	122.9(3)
Complex **2**			
Zn1─N1	2.009(5)	Zn2─N4_a	2.033(4)
Zn2─N6_b	2.026(5)	Zn1─O1_c	1.992(4)
Zn2─O3_d	1.958(4)	Zn1─O6	1.946(4)
Zn1─O7	1.932(4)	Zn2─O7	1.938(4)
O7─ Zn1 ─O6	106.01(17)	O7─ Zn1 ─O1_b	107.54(17)
O6─ Zn1 ─O1_b	107.94(17)	O7─ Zn1 ─N1	109.04(18)
O6─ Zn1 ─N1	122.53(19)	O1_b─ Zn1 ─N1	103.02(17)
O7 ─ Zn2 ─ O3_e	129.36(18)	O7 ─ Zn2 ─N6_c	114.79(18)
O3_e─ Zn2 ─N6_c	102.15(19)	O7 ─ Zn2 ─N4_a	104.87(18)
O3_e─ Zn2 ─N4_a	101.04(19)	N6_c─ Zn2 ─N4_a	100.21(18)
C9─ N1─ Zn1	124.1(4)	C11─N1─Zn1	126.4(4)
C18─ N4─ Zn2_a	122.1(4)	C19─ N4─ Zn2_a	131.1(4)
C23─ N6─ Zn2_b	126.5(4)	C22─ N6─ Zn2_b	125.3(4)
C7─ O1─ Zn1_c	119.1(3)	C24 ─O3 ─Zn2_d	109.6(4)
C8 ─O6 ─Zn1	117.0(4)	Zn1─ O7 ─Zn2	130.2(2)
Complex **3**			
Zn1─N1	2.042(5)	Zn2─N3	2.044(5)
Zn2─O1	2.167(4)	Zn1─O2	2.005(3)
Zn1─O3_a	2.315(4)	Zn1─O4_a	2.083(4)
Zn1─O6_b	2.063(4)	Zn2─O7	2.153(3)
Zn1─C27_a	2.526(6)		
O2─ Zn1─ N1	107.91(16)	O2─ Zn1─ O6_c	95.12(16)
N1─ Zn1 ─O6_c	93.27(18)	O2 ─ Zn1─ O4_d	108.21(16)
N1─Zn1─ O4_d	98.00(18)	O6_c─ Zn1─ O4_d	149.31(16)
O2─ Zn1─ O3_d	88.20(15)	N1─ Zn1─ O3_d	155.66(17)
O6_c─ Zn1 ─O3_d	103.57(15)	O4_d─Zn1─ O3_d	58.90(14)
O2─Zn1─C27_d	100.60(17)	N1─ Zn1─ C27_d	126.8(2)
O6_d─ Zn1─C27_c	128.14(19)	O4_c─Zn1─C27_c	29.46(17)
O3_c─ Zn1─C27_c	29.49(16)	N3_e─ Zn2─ N3	180.0

N3_e─ Zn2─ O7_e	88.72(16)	O7_e─ Zn2─ O7_e	180.0
N3_e─ Zn2─ O1	93.21(16)	O7_e─ Zn2─ O1	86.24(14)
O1─ Zn2─O1_e	180.00(16)	O4─ C27─ Zn1_a	55.2(3)
O3─C27─Zn1_a	65.8(3)	C24─ C27─ Zn1_a	173.1(5)
C1─ N1─ Zn1	122.4(4)	C2─ N1─ Zn1	132.8(4)
C10─ N3─ Zn2	128.4(4)	C11─ N3─ Zn2	127.5(4)
C19─ O1─ Zn2	134.1(4)	C19─ O2─ Zn1	128.6(4)
C27─ O3─ Zn1_a	84.7(4)	C27─ O4─ Zn1_a	95.3(4)
C26─ O6─ Zn1_b	99.6(4)	Zn2 ─O7 ─H7B	109.1
Zn2 ─O7 ─H7C	109.1		

Complex **4**

N1─Ni2	2.016(4)	Ni2─O5_c	2.082(3)
N3─Ni1	2.052(4)	Ni2─O3_b	2.193(3)
Ni1─O7_a	2.075(3)	Ni2─O6_c	2.208(3)
Ni1─O1	2.088(3)	Ni2─C5_a	2.448(5)
Ni2─O2	2.037(3)	Ni2─C8_c	2.459(5)
Ni2─O4_b	2.054(3)		
N3─ Ni1─ N3_a	180.000	O7─ Ni1─ O1	86.86(13)
O1─ Ni1─ O1_a	180.000(14)	O3_b─ Ni2─ O6_c	87.28(12)
N3─ Ni1─ O7	92.07(14)	N1─ Ni2─ O2	101.41(15)
O7_a─ Ni1─ O7	180.00(13)	N1─ Ni2─ O4_b	97.99(15)
N3─ Ni1─ O1	86.73(13)	O2─ Ni2─ O4_b	102.57(13)
N1─ Ni2─ O5_c	90.84(14)	O5_c─ Ni2─ O3_a	106.98(12)
O2─ Ni2─ O5_c	92.64(12)	N1─ Ni2─ O6_c	91.78(14)
O4_b─ Ni2─ O5_c	160.19(13)	O2─ Ni2─ O6_c	151.00(12)
N1─ Ni2─ O3_b	158.92(13)	O4_b─ Ni2─ O6_c	100.87(12)
O2─ Ni2─ O3_b	89.06(12)	O5_c─ Ni2─ O6_c	61.10(11)
O4_b─ Ni2─ O3_b	61.55(12)	N1─ Ni2─ C5_b	128.27(16)
O4─ C5─ Ni2_d	57.0(2)	O2─ Ni2─ C5_b	98.57(14)
O3─ C5─ Ni2_d	63.3(3)	O5_c─ Ni2─ C5_b	135.11(15)
C4─ C5─ Ni2_d	173.5(3)	O6_c─ Ni2─ C5_b	92.88(14)
O6─ C8─ Ni2_e	63.6(2)	N1─ Ni2─ C8_c	88.86(15)
O5─ C8─ Ni2_e	57.8(2)	O2─ Ni2─ C8_c	123.23(14)
C7─ C8─ Ni2_e	169.0(3)	O4_b─ Ni2─ C8_c	131.10(15)
C10─ N1─ Ni2	125.6(3)	C21─ N3─ Ni1	127.6(3)
C11─ N1─ Ni2	129.0(3)	C19─ N3─ Ni1	126.4(3)
O3_b─ Ni2─ C8_c	100.60(14)	C5─ O3─ Ni2_d	85.9(3)
O6_c─ Ni2─ C8_c	30.48(13)	C5─ O4─ Ni2_d	92.3(3)
C5_b─ Ni2─ C8_c	117.82(16)	C1─ O2─ Ni2	128.3(3)
C1─ O1─ Ni1	136.5(3)	Ni1─ O7─ H7A	119.8
Ni1─ O7─ H7	109.5		

Complex **5**

Cu1─ N1	1.953(3)	Cu1─ O5	1.972(2)
Cu2─ N3	1.951(3)	Cu2 ─O2_a	1.963(3)
Cu2─ O3_b	2.024(3)	Cu2─ O4_b	2.063(2)
Cu2─ O6	2.208(2)	Cu2─ C26_b	2.357(4)
N1─Cu1─N1_c	180.000(1)	N1─Cu1─O5	86.97(11)
O5─Cu1─O5_c	180.0	N1─Cu1─O7	92.02(15)
O5─Cu─O7	104.89(13	N3─Cu2─O2_b	92.04(12)
N3─Cu2─O3_d	96.25(12)	O2_b─Cu2─O3_d	154.90(10)
N3─ Cu2─ O4_d	159.72(13)	O2_a─ Cu2─ O4_d	103.67(10)
O3_d─ Cu2─ O4_d	64.24(10)	N3─ Cu2─ O6	104.72(11)
O2_a─ Cu2─ O6	94.08(10)	O3_d─ Cu2─ O6	106.55(10)
O4_d─ Cu2─ O6	87.12(10)	N3─ Cu2─ C26_d	128.17(14)
O2_a─ Cu2─ C26_d	131.11(11)	O3_d─ Cu2─ C26_d	32.45(10)
O4_d─ Cu2─ C26_d	31.89(11)	O6─ Cu2─ C26_d	99.73(11)
C24─ C26─ Cu2_b	171.9(3)	C3─ N1─ C1	105.6(3)
C3─ N1─ Cu1	125.2(3)	C1─ N1─ Cu1	128.7(3)
C12─ N3─ Cu2	125.0(3)	C10─ N3─ Cu2	130.2(3)
C19 ─O2─ Cu2_e	106.5(2)	C27─ O5─ Cu1	124.2(2)
C27─ O6─ Cu2	134.3(2)		

Symmetry transformations used to generate equivalent atoms:

a = *x* - 1/2, -*y* + 3/2 , *z* – 1/2; b= *x*+ 1/2, -*y* + 3/2 , *z* + 1/2. (compond **1**)

a = -*x* + 2, -*y* + 1, -*z* + 1; b= -*x* + 2, -*y* + 1/2 , -*z* + 3/2; c= -*x* + 2, -*y* - 1/2 , -*z* + 3/2; d=-*x* + 3, -*y* - 1/2 , -*z* + 3/2; e=-*x* + 3, -*y* + 1/2 , -*z* + 3/2. (compond **2**)

a = *x* + 1, *y*, *z*; b= *x* + 1/2, -*y* + 1/2 , *z* + 1/2; c= *x* -1/2, -*y* + 1/2 , *z* - 1/2; d= *x* - 1, *y*, *z*; e = -*x*,- *y*, -*z*+1 (compond **3**)

a = -*x,* -*y* + 1, -*z*; b= *x* - 2, *y* , *z*; c= *x* - 1/2, -*y* + 1/2 , *z* -*1*/2; d=*x* + 2, *y* , *z*; e=*x* + 1/2, -*y* + 1/2 , *z* + 1/2. (compond **4**)

a = *x* - 1/2, -*y* + 1/2 , *z* – 1/2; b= *x* + 1, *y*, *z*; c= -*x* + 1,- *y*+ 1, -*z*; d= *x* -1, -*y* + 1/2 , *z* + 1/2; e = *x*- 1/2, -*y* +1/2 , *z* + 1/2.(compond **5**)

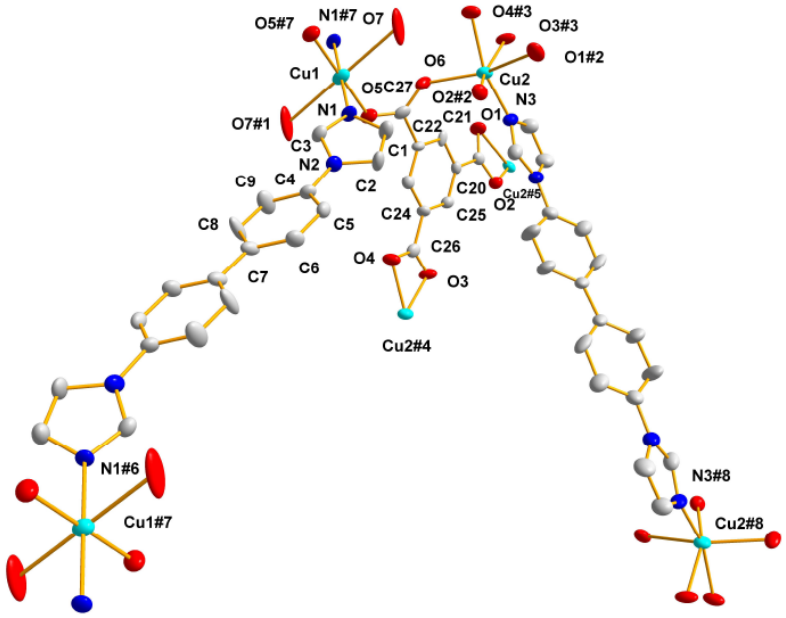

Figure S1. An ORTEP drawing of **5** showing 30% ellipsoid probability (hydrogen atoms are omitted for clarity). Symmetry codes: #1 = 1 - *x*, 1 - *y*, - *z*; #2 = -0.5 + *x*, 0.5 - *y*, -0.5 + *z*; #3 = -1 + *x*, *y*, *z*; #4 = 1 + *x*, *y*, *z*; #5 = 0.5 + *x*, 0.5 - *y*, 0.5 + *z*; #6 = 2- *x*, 1 - *y*, - 1-*z*; #7 = 1 + *x*, *y*, -1 + *z*; #8 = 2 - *x*, -*y*, -*z*.

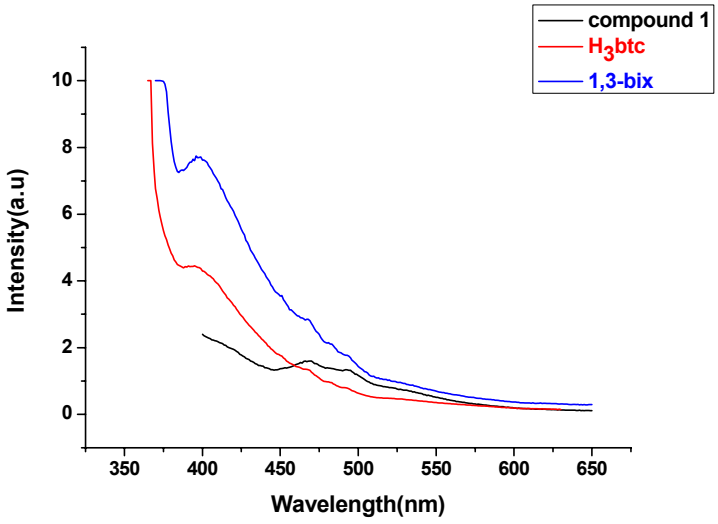

Figure S2. Emission spectra of free H_3btc,1,3-bix and compound **1** in the solid state at room temperature.

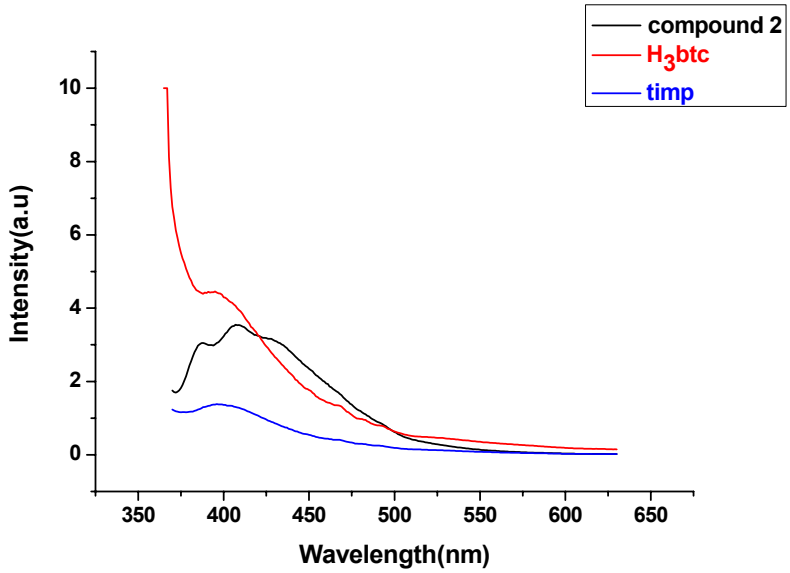

Figure S3. Emission spectra of free H_3btc,timp and compound **2** in the solid state at room temperature.

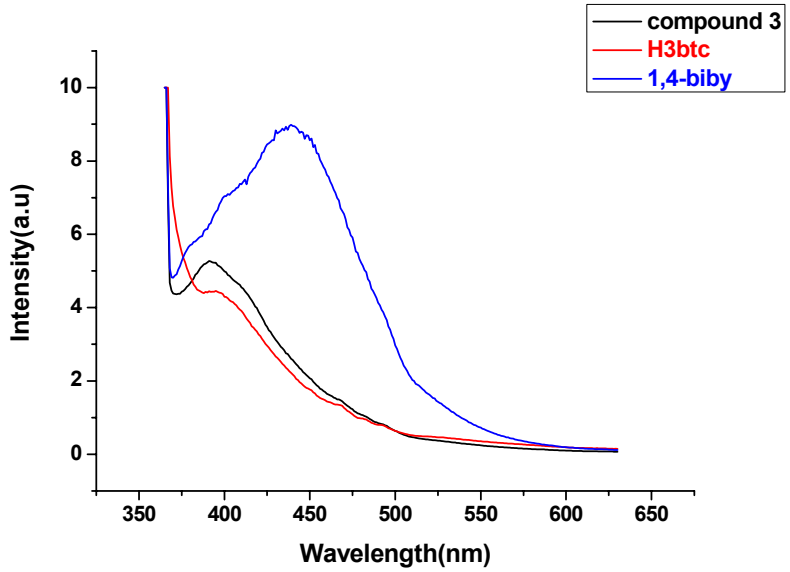

Figure S4. Emission spectra of free H_3btc, 1,4-biby and compound **3** in the solid state at room temperature.

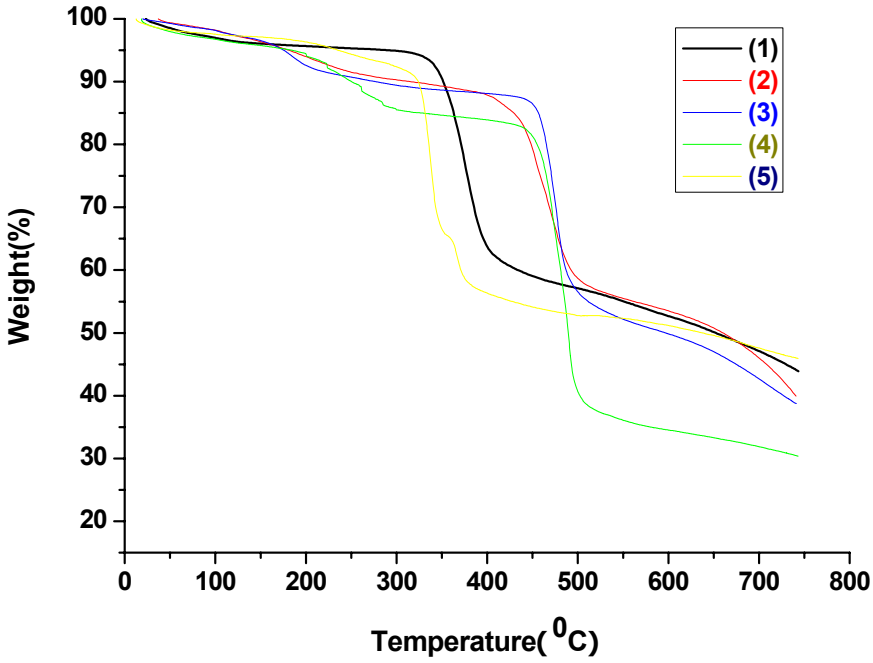

Figure S5. TGA plot of compounds **1 – 5.**

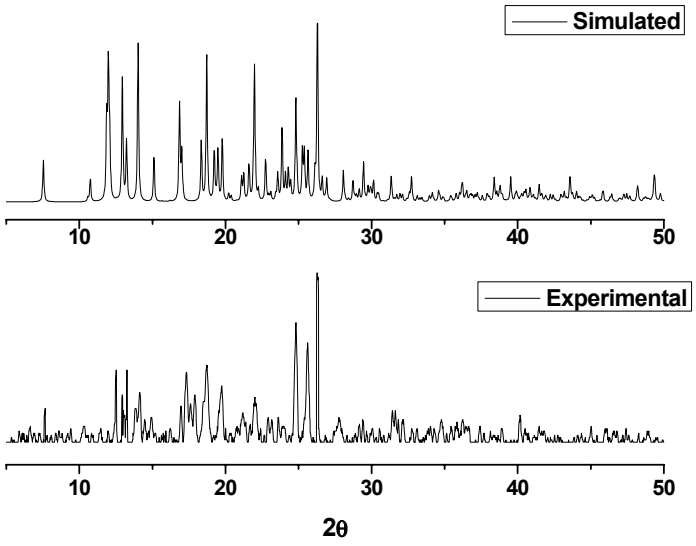

Figure S6. Experimental (bottom) and simulated (top) powder X-ray diffraction patterns of compound **1** at 293K.

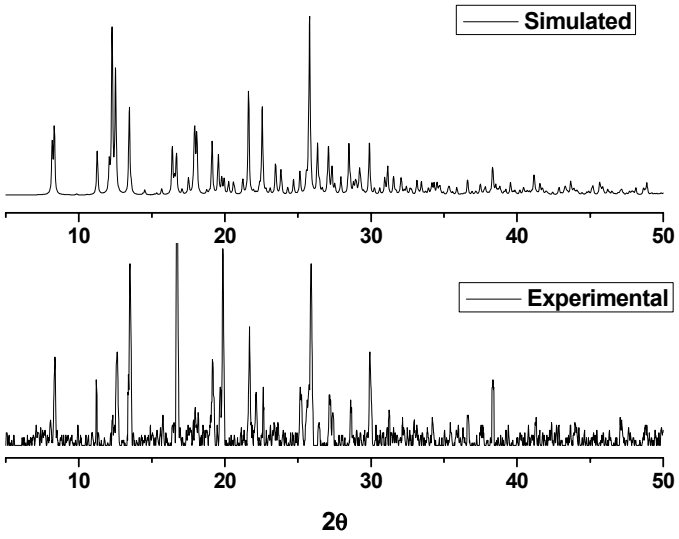

Figure S7. Experimental (bottom) and simulated (top) powder X-ray diffraction patterns of compound **2** at 293K.

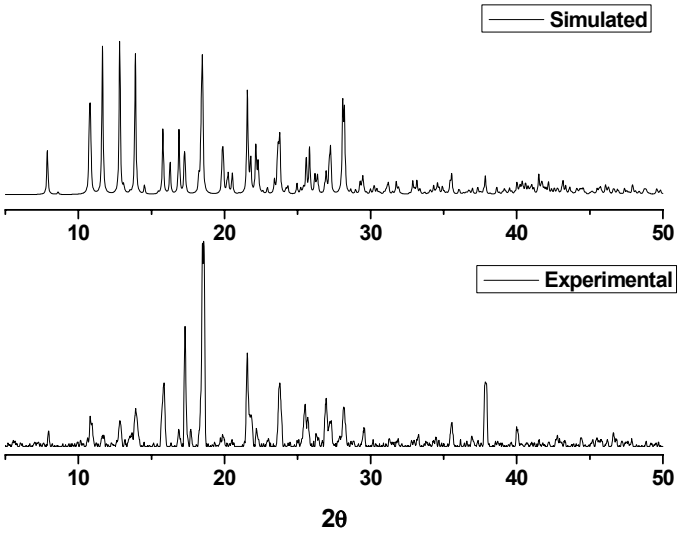

Figure S8. Experimental (bottom) and simulated (top) powder X-ray diffraction patterns of compound **3** at 293K.

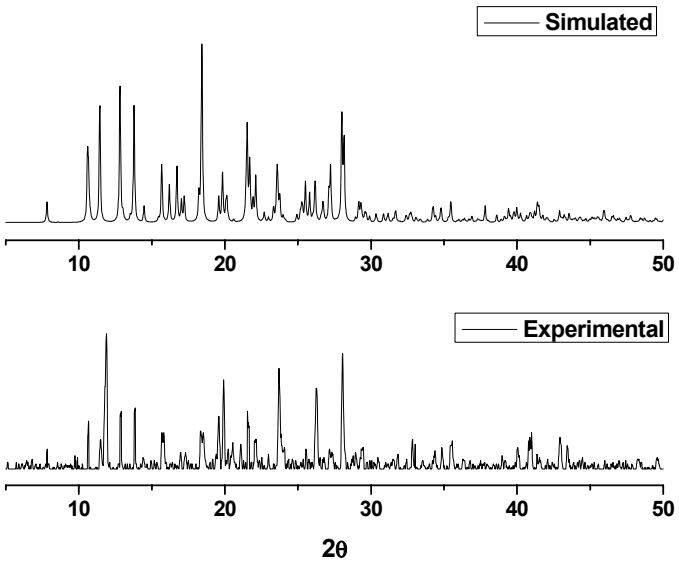

Figure S9. Experimental (bottom) and simulated (top) powder X-ray diffraction patterns of compound **4** at 293K.

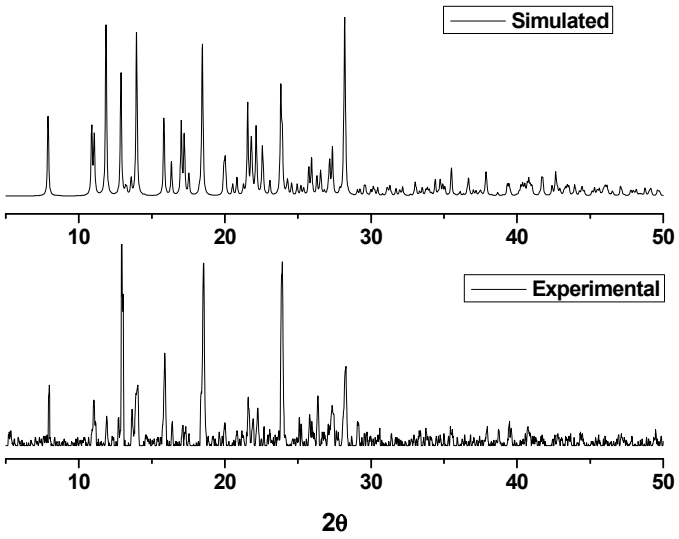

Figure S10. Experimental (bottom) and simulated (top) powder X-ray diffraction patterns of compound **5** at 293K.