Supporting Information

Syntheses, Structures, and Photochemical Properties of Six New Metal–Organic Frameworks Based on Aromatic Dicarboxylate Acid and V-shape Imidazole Ligand

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Table S1. Selected Bond Lengths (Å) and Angles (deg) for Complexes **1-6**.

		Complex **1**	
Co1-O4#1	1.989(4)	Co1-O1	2.033(3)
Co1-N1	2.036(4)	Co1-N3	2.057(4)
Co1-O2	2.387(4)	O4#1-Co1-O1	140.60(2)
O4#1-Co1-N1	101.57(18)	O1-Co1-N1	105.47(17)
O4#1-Co1-N3	106.60(17)	O1-Co1-N3	95.72(13)
N1-Co1-N3	101.18(18)	O4#1-Co1-O2	93.97(19)
O1-Co1-O2	58.15(12)	N1-Co1-O2	90.38(16)
N3-Co1-O2	153.62(19)		
		Complex **2**	
Cd1-N3	2.236(3)	Cd1-O2	2.256(3)
Cd1-N1	2.272(3)	Cd1-O3	2.305(3)
Cd1-O4	2.379(3)	Cd1-O1	2.390(3)
N3-Cd1-O2	95.77(13)	N3-Cd1-N1	98.78(14)
N1-Cd1-O2	108.24(13)	N3-Cd1-O3	93.07(11)
O2-Cd1-O3	144.89(13)	N1-Cd1-O3	144.8(6)
N3-Cd1-O4	95.46(13)	O2-Cd1-O4	98.62(12)
N1-Cd1-O4	144.97(11)	O3-Cd1-O4	55.11(10)
N3-Cd1-O1	149.40(13)	O2-Cd1-O1	54.51(12)
N1-Cd1-O1	85.85(12)	O3-Cd1-O1	101.41(10)
O4-Cd1-O1	96.21(11)		
		Complex **3**	
Zn1-O1	1.945(5)	Zn1-O4#1	1.984(4)
Zn1-N3	2.010(5)	Zn1-N1	2.047(6)
O1-Zn1-O4#1	130.0(2)	O1-Zn1-N3	105.8(2)

O4#1-Zn1-N3	108.9(2)	O1-Zn1-N1	106.9(2)
O4#1-Zn1-N1	99.2(2)	N3-Zn1-N1	102.9(2)
Complex **4**			
Cd1-O1	2.256(5)	Cd1-O4	2.265(5)
Cd1-N2	2.281(6)	Cd1-O33	2.635(5)
Cd1-O17	2.754(5)	Cd2-N3	2.280(5)
Cd2-O33	2.326(5)	Cd2-O2	2.348(4)
O3-Cd1-O1	127.06(19)	O3-Cd1-O4	122.6(2)
O1-Cd1-O4	107.76(19)	O3-Cd1-N2	106.0(2)
O1-Cd1-N2	88.08(19)	O4-Cd1-N2	90.0(2)
O3-Cd1-O33	98.35(19)	O1-Cd1-O33	100.61(17)
O4-Cd1-O33	51.55(16)	N2-Cd1-O33	141.50(18)
O3-Cd1-O17	51.15(16)	O1-Cd1-O17	164.84(18)
O4-Cd1-O17	80.38(17)	N2-Cd1-O17	78.99(18)
O33-Cd1-O17	94.45(16)	N3-Cd2-N3#1	180.0(3)
N3-Cd2-O33	88.26(18)	N3#1-Cd2-O33	91.74(18)
N3-Cd2-O33#1	91.74(18)	N3#1-Cd2-O33#1	88.26(18)
O33-Cd2-O33#1	180.000(1)	N3-Cd2-O2	91.68(17)
N3#1-Cd2-O2	88.32(17)	O33-Cd2-O2	97.36(17)
O33#1-Cd2-O2	82.64(17)	O33#1-Cd2-O2#1	82.64(17)
N3-Cd2-O2	88.32(17)	N3#1-Cd2-O2	91.68(17)
N3#1-Cd2-O2#1	91.68(17)	O33-Cd2-O2	82.64(17)
O33#1-Cd2-O2	97.36(17)	O33#1-Cd2-O2#1	97.36(17)
O2-Cd2-O2	180.0(2)	O2#1-Cd2-O2	180.0(2)
Complex **5**			
Ni1-N1	2.032(3)	Ni1-N3#3	2.039(3)
Ni1-O2	2.047(2)	Ni1-O5#2	2.077(2)

Ni1-O4	2.121(2)	Ni1-O3	2.122(2)
N1-Ni1-N3#2	178.81(12)	N1-Ni1-O2	88.07(11)
N3#2-Ni1-O2	91.04(11)	N1-Ni1-O5#1	92.65(11)
N3#2-Ni1-O5#2	88.27(11)	O2-Ni1-O5#1	178.12(10)
N1-Ni1-O4	87.79(11)	N3#2-Ni1-O4	91.49(11)
O2-Ni1-O4	94.24(9)	O5#1-Ni1-O4	87.53(9)
N1-Ni1-O3	90.88(11)	N3#2-Ni1-O3	89.88(11)
O2-Ni1-O3	87.73(9)	O5#1-Ni1-O3	90.51(9)
O4-Ni1-O3	177.58(9)		
Complex **6**			
Mn1-O7#3	2.118(3)	Mn1-O11	2.190(3)
Mn1-N3	2.230(4)	Mn1-O9	2.247(3)
Mn1-N4#2	2.253(4)	Mn1-O10	2.341(3)
Mn2-O1	2.088(3)	Mn2-O6	2.154(3)
Mn2-O3#1	2.212(3)	Mn2-N2	2.238(4)
Mn2-N1#2	2.258(4)	Mn2-O4#1	2.335(3)
O7#3-Mn1-O11	111.39(12)	O7#3-Mn1-N3	86.16(13)
O11-Mn1-N3	88.10(13)	O7#3-Mn1-O9	163.01(12)
O11-Mn1-O9	83.62(11)	N3-Mn1-O9	86.47(13)
O7#3-Mn1-N4#2	83.83(12)	O11-Mn1-N4#2	86.50(12)
N3-Mn1-N4#2	166.02(14)	O9-Mn1-N4#2	105.70(13)
O7#3-Mn1-O10	110.09(12)	O11-Mn1-O10	137.71(12)
N3-Mn1-O10	102.55(13)	O9-Mn1-O10	56.89(11)
N4#2-Mn1-O10	90.07(12)	O1-Mn2-O6	106.04(13)
O1-Mn2-O3#1	162.71(12)	O6-Mn2-O3#1	89.55(12)
O1-Mn2-N2	90.23(14)	O6-Mn2-N2	89.48(14)
O3#1-Mn2-N2	97.49(14)	O1-Mn2-N1#2	86.31(13)

O6-Mn2-N1#2	92.60(13)	O3#1-Mn2-N1#2	85.53(13)
N2-Mn2-N1#2	176.35(15)	O1-Mn2-O4#1	106.99(12)
O6-Mn2-O4#1	146.96(12)	O3#1-Mn2-O4#1	57.63(10)
N2-Mn2-O4#1	91.17(13) 4	N1#2-Mn2-O4#1	88.73(12)

Symmetry codes: Compound **1:** #1 = 0.5+*x*, 1-*y*, *z*; **3:** #1=0.5+*x*, 1-*y*, *z*; **4:** #1 = 2-*x*, -*y*, 1-*z*; **5:** #1 = 0.5+*x*, 0.5-*y*, 0.5+*z*; #2 = -1.5+ *x*, 0.5-*y*, 0.5+*z*; **6:** #1 = *x*, 0.5-*y*, -0.5+*z*; #2 = 1+*x*, 0.5-*y*, 0.5+*z*; #3 = *x*, 0.5-*y*, 0.5+*z*.

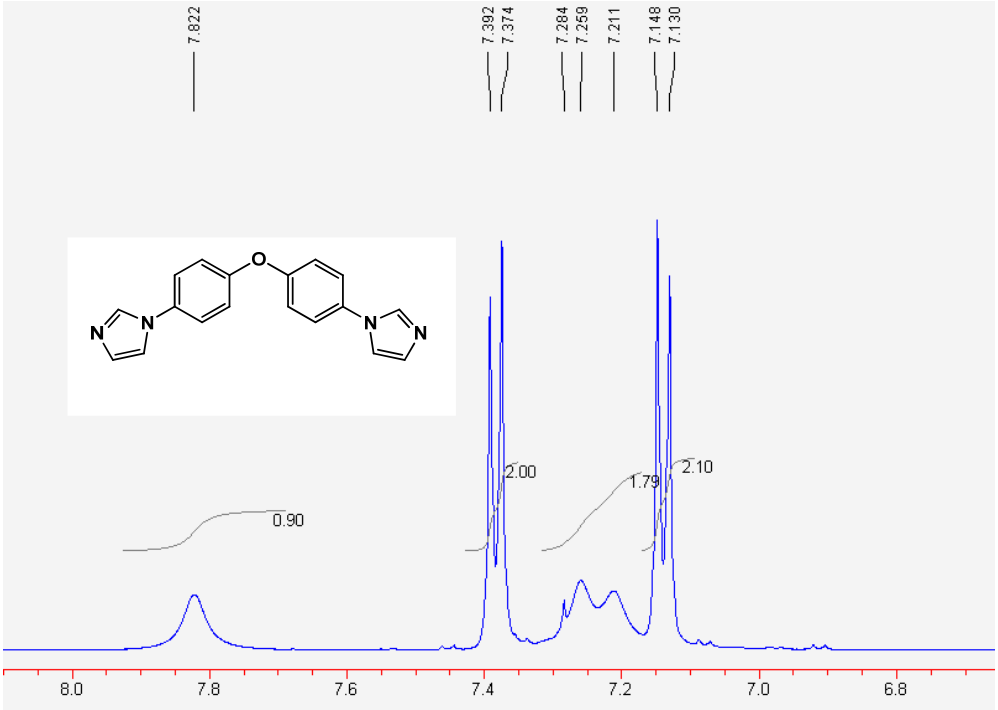

Figure S1. The ^{1}HNMR spectra of BIDPE

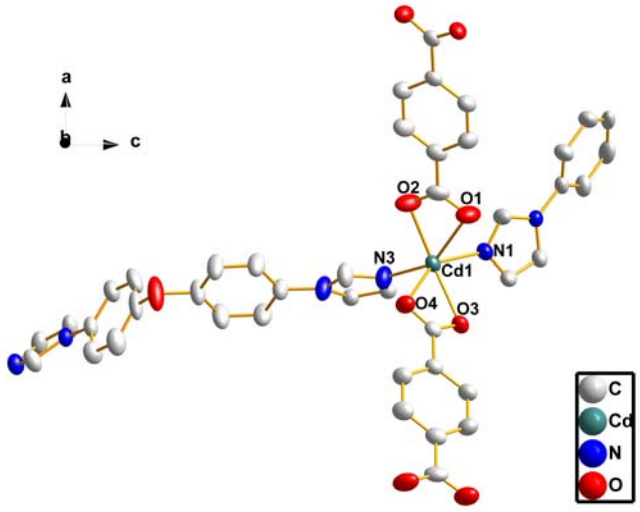

Figure S2. An ORTEP drawing of **2** showing 30% ellipsoid probability (hydrogen atoms are omitted for clarity).

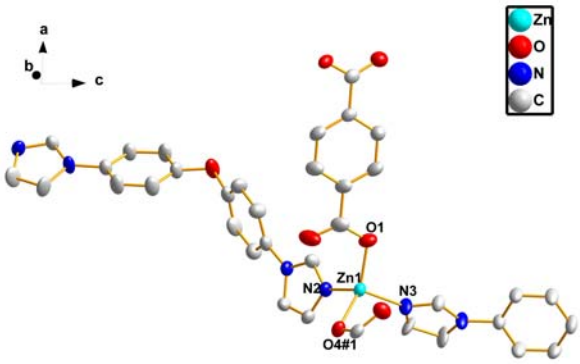

Figure S3. An ORTEP drawing of **3** showing 30% ellipsoid probability (hydrogen atoms are omitted for clarity). Symmetry codes: #1 = 0.5+*x*, 1-*y*, *z*.

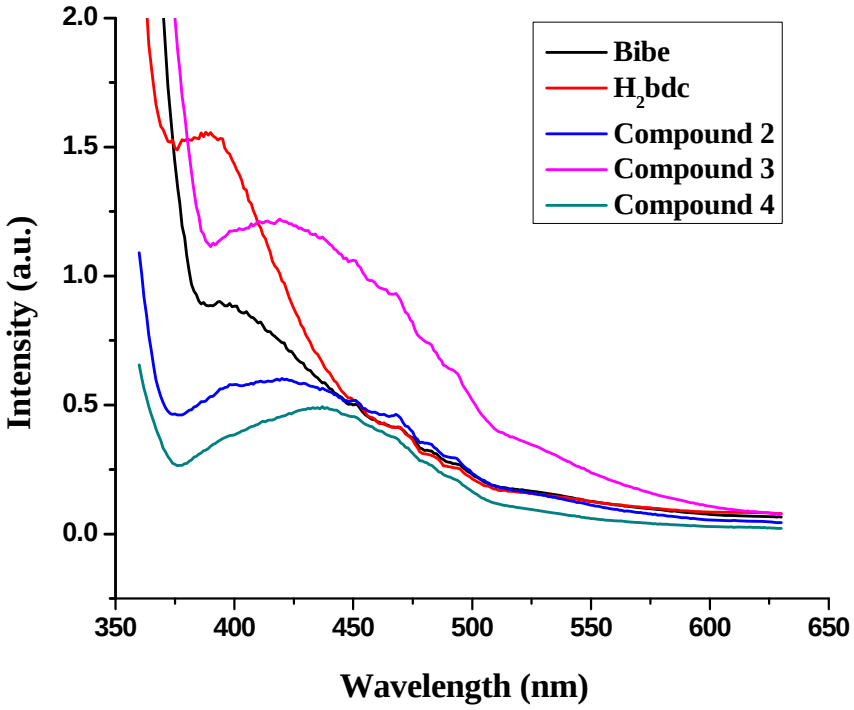

Figure S4. Solid-state photoluminescent spectra of **2**, **3**, **4**, BIDPE, and H_2bdc at room temperature.

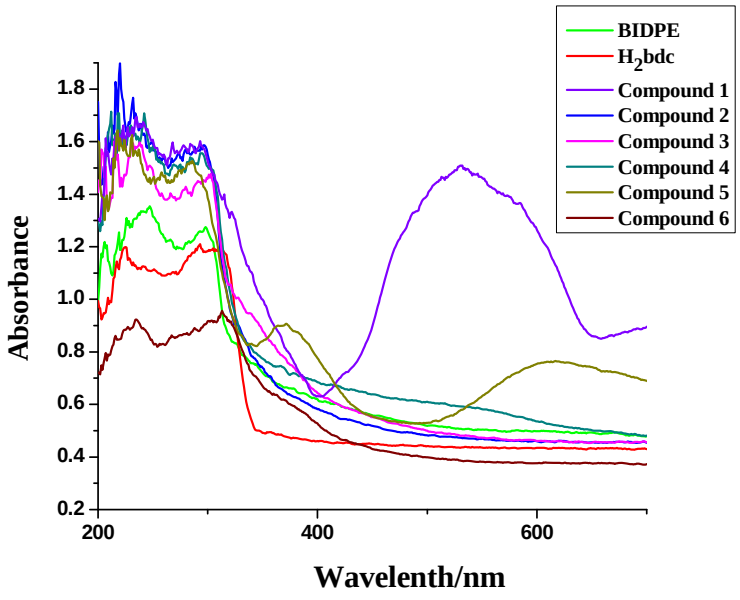

Figure S5. UV–vis of compounds **1–6** and ligands

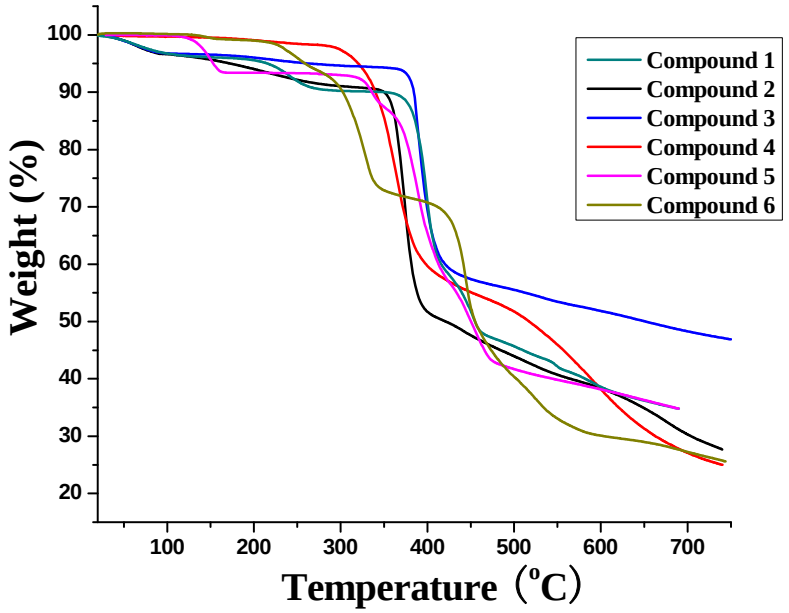

Figure S6. TG plots of polymers **1**–**6**.

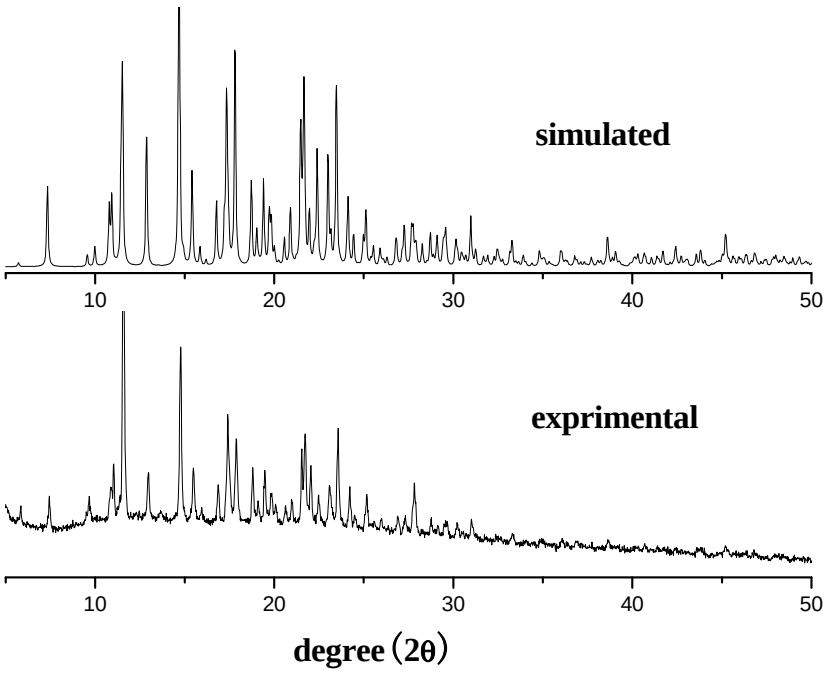

Figure S7. Powder X-ray diffraction patterns of complex **1**

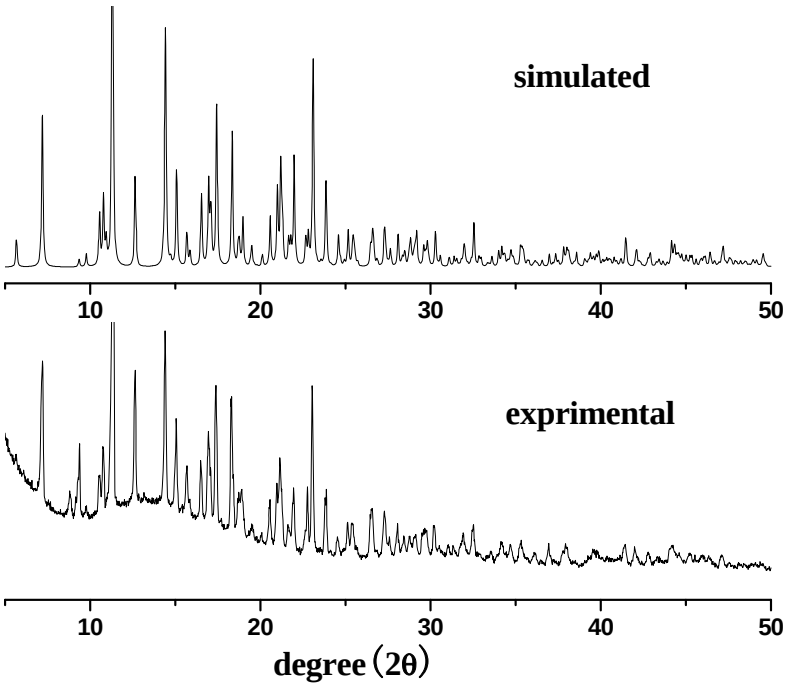

Figure S8. Powder X-ray diffraction patterns of complex **2**

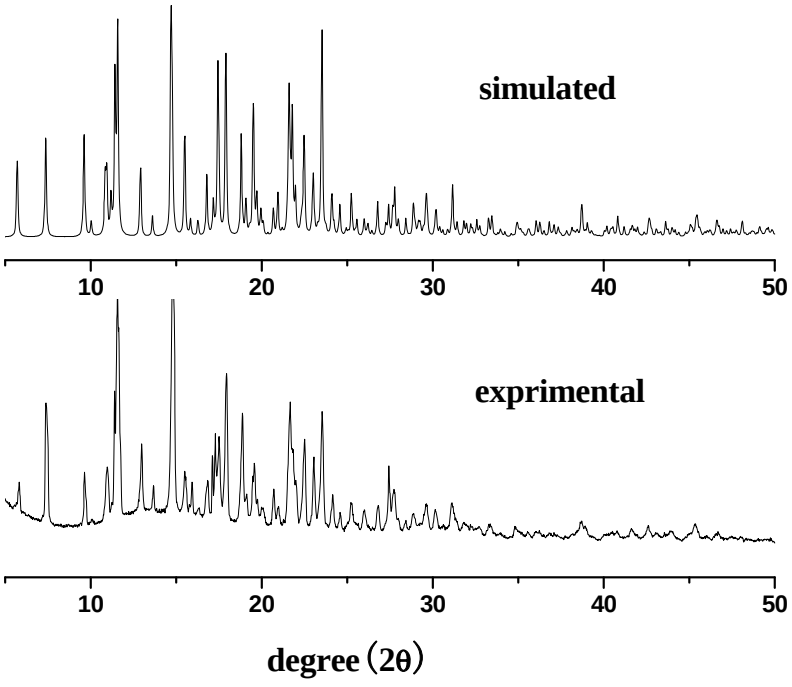

Figure S9. Powder X-ray diffraction patterns of complex **3**

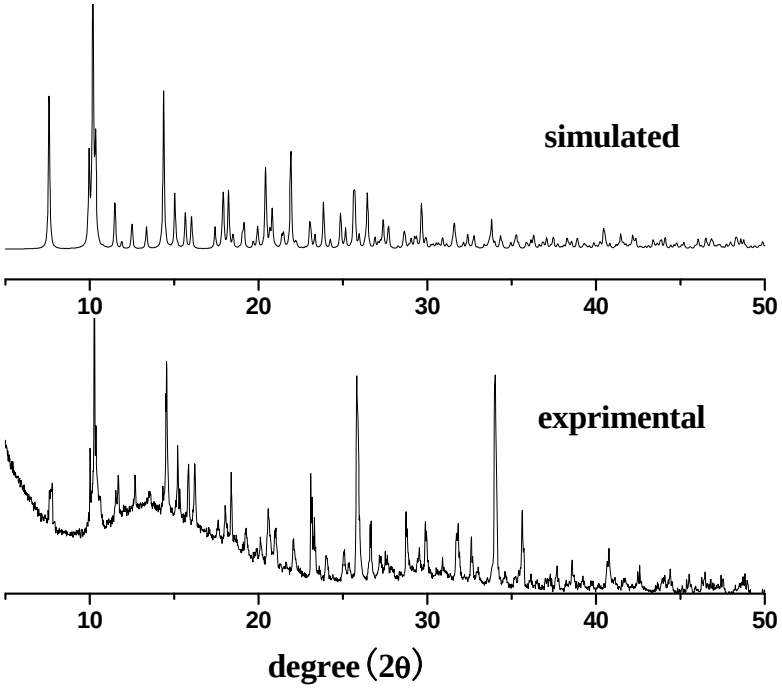

Figure S10. Powder X-ray diffraction patterns of complex **4**

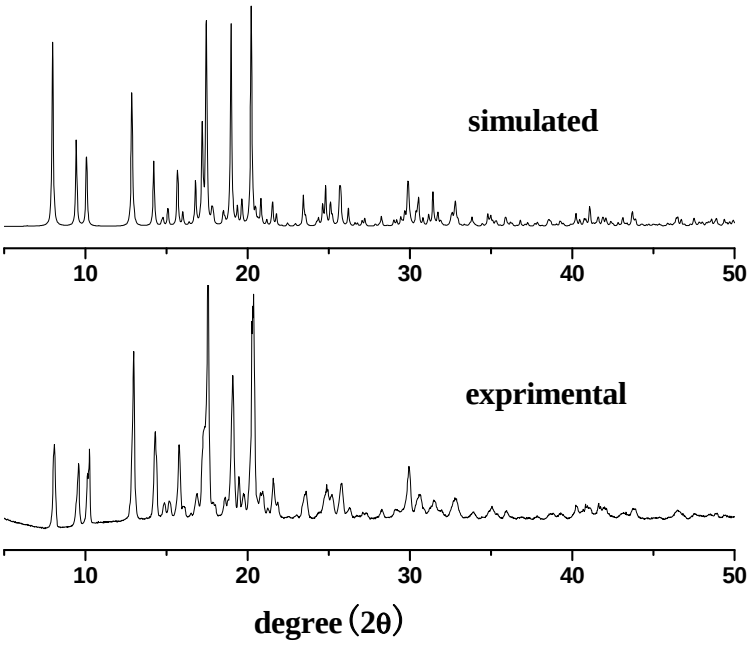

Figure S11. Powder X-ray diffraction patterns of complex **5**

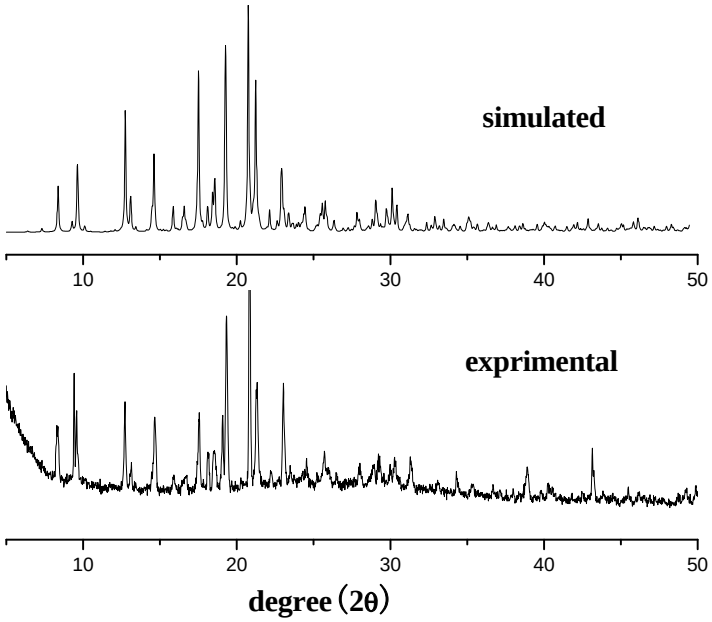

Figure S12. Powder X-ray diffraction patterns of complex **6**

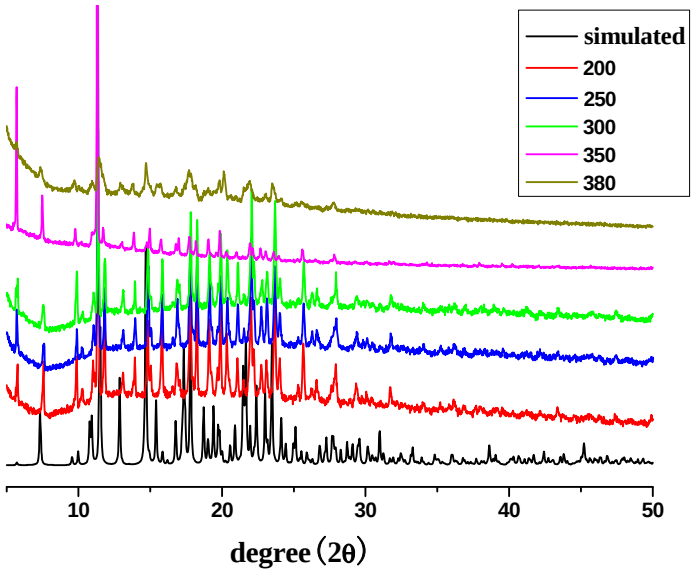

Figure S13. Powder X-ray diffraction patterns of complex **1** in different temperatures.

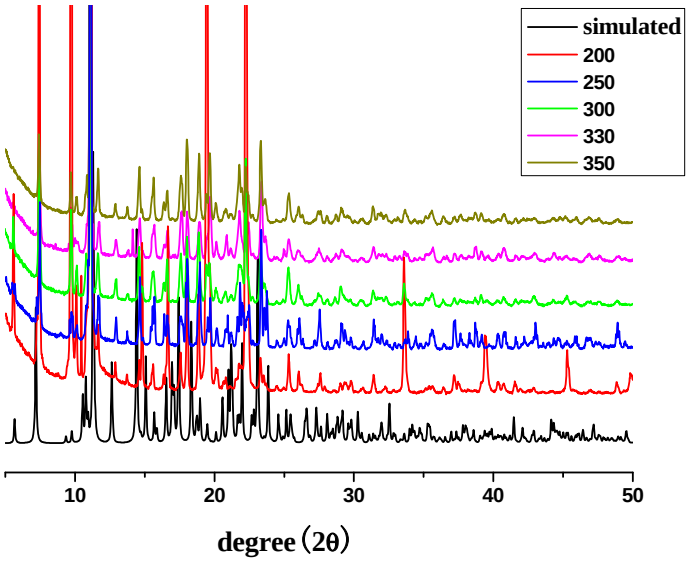

Figure S14. Powder X-ray diffraction patterns of complex **2** in different temperatures.

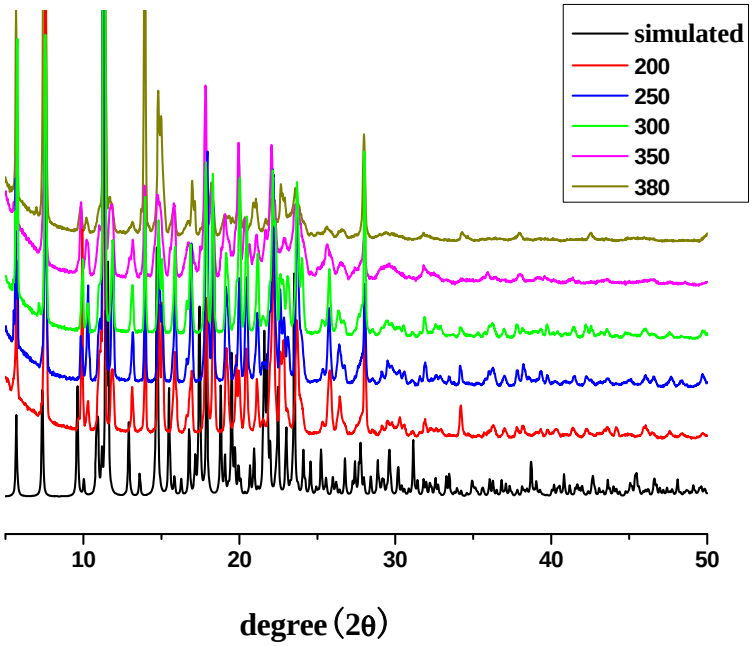

Figure S15. Powder X-ray diffraction patterns of complex **3** in different temperatures.

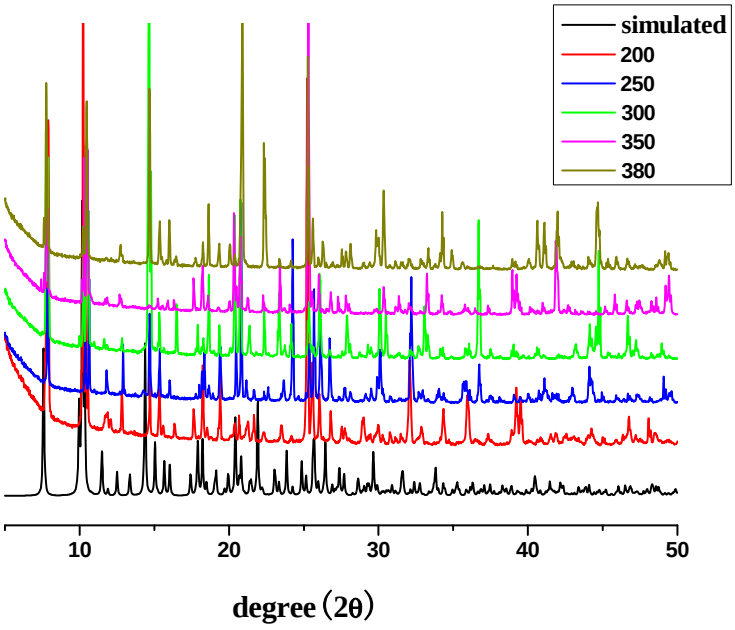

Figure S16. Powder X-ray diffraction patterns of complex **4** in different temperatures.

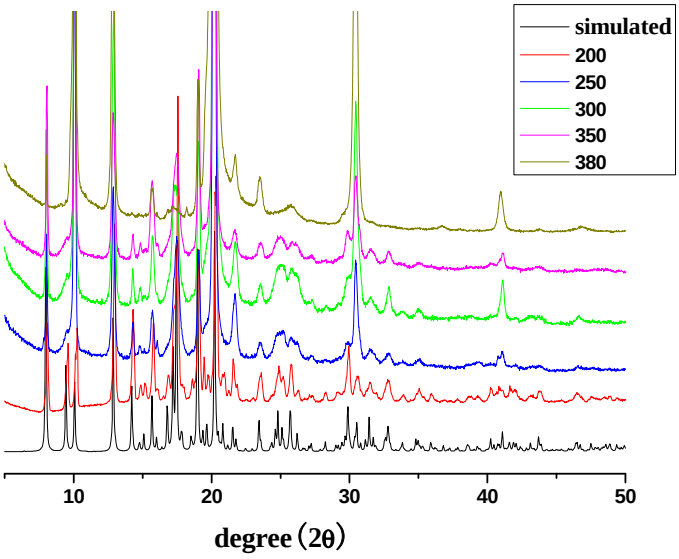

Figure S17. Powder X-ray diffraction patterns of complex **5** in different temperatures.

Table S2. Specified hydrogen bonds of compound **6**

D─H─A	d(D···H)(Å)	d(H···A)(Å)	d(D···A)(Å)	(DHA)(deg)
O6–H6B─O8[a]	0.85	2.05	2.616(4)	123.5
O6–H6C─O10[b]	0.85	2.03	2.770(4)	145.7
O11–H11C─O4[c]	0.85	2.04	2.790(3)	146.7
O11–H11A─O2[d]	0.85	1.87	2.633(6)	148.5

Symmetry codes: a = -1+*x*, -*y*+1/2, -1/2+*z*, b = -1+*x*, y, -1+*z*, c =*x*, 1/2-*y*, 1/2+*z*, d = *x*, *y*, 1+ *z*.