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Syntheses, structures, luminescent sensor, and magnetism of a series of coordination polymers constructed by 3-carboxy-1-(4'-carboxy-benzyl)-2-oxidopyridinium

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Table S1a. Selected bond distances (Å) and angles (°) for **1**.

Co(1)-O(1)$^{\#1}$	2.063(3)	Co(1)-O(2W)	2.109(4)
Co(1)-O(4)	2.072(3)	Co(1)-O(1W)	2.116(3)
Co(1)-O(2)$^{\#1}$	2.080(3)	Co(1)-O(5)$^{\#2}$	2.123(3)
O(1)$^{\#1}$-Co(1)-O(4)	89.53(13)	O(1)$^{\#1}$-Co(1)-O(2)$^{\#1}$	85.52(11)
O(4)-Co(1)-O(2)$^{\#1}$	96.38(13)	O(1)$^{\#1}$-Co(1)-O(2W)	98.80(13)
O(4)-Co(1)-O(2W)	171.00(13)	O(2)$^{\#1}$-Co(1)-O(2W)	87.71(13)
O(1)$^{\#1}$-Co(1)-O(1W)	172.53(12)	O(4)-Co(1)-O(1W)	88.11(13)
O(2)$^{\#1}$-Co(1)-O(1W)	87.69(11)	O(2W)-Co(1)-O(1W)	84.04(13)
O(1)$^{\#1}$-Co(1)-O(5)$^{\#2}$	89.68(11)	O(4)-Co(1)-O(5)$^{\#2}$	94.51(12)
O(2)$^{\#1}$-Co(1)-O(5)$^{\#2}$	168.06(12)	O(2W)-Co(1)-O(5)$^{\#2}$	82.21(12)
O(1W)-Co(1)-O(5)$^{\#2}$	97.57(12)		

Table S1b. Hydrogen bonds for **1** (Å and °).

D-H···A	d (D-H)	d (H···A)	d (D···A)	< (DHA)
O(1W)-H(1A)···O(5)	0.899(10)	1.88(2)	2.728(5)	156(5)
O(1W)-H(1A)···O(2W)$^{\#3}$	0.899(10)	2.43(4)	3.003(4)	122(4)
O(1W)-H(1B)···O(3)$^{\#4}$	0.900(10)	1.982(18)	2.841(5)	159(4)
O(2W)-H(2A)···O(2)$^{\#5}$	0.898(10)	1.90(3)	2.717(4)	151(5)
O(2W)-H(2B)···O(3)$^{\#4}$	0.896(10)	1.92(3)	2.718(4)	148(5)

Symmetry transformations used to generate equivalent atoms: $^{\#1}$ -x,-y,-z; $^{\#2}$ x-1,y,z; $^{\#3}$ x+1,y,z; $^{\#4}$ x,y,z-1; $^{\#5}$ -x-1,-y,-z.

Table S2a. Selected bond distances (Å) and angles (°) for **2**.

Ni(1)-O(2)	1.998(4)	Ni(1)-O(2W)	2.058(4)
Ni(1)-O(1)	2.036(4)	Ni(1)-O(3W)	2.069(4)
Ni(1)-O(5)$^{\#1}$	2.050(4)	Ni(1)-O(1W)	2.102(4)
O(2)-Ni(1)-O(1)	88.18(16)	O(2)-Ni(1)-O(5)$^{\#1}$	176.24(17)
O(1)-Ni(1)-O(5)$^{\#1}$	88.09(16)	O(2)-Ni(1)-O(2W)	90.91(19)

O(1)-Ni(1)-O(2W)	92.29(17)	O(5)$^{\#1}$-Ni(1)-O(2W)	89.73(17)
O(2)-Ni(1)-O(3W)	91.68(16)	O(1)-Ni(1)-O(3W)	176.93(17)
O(5)$^{\#1}$-Ni(1)-O(3W)	92.02(16)	O(2W)-Ni(1)-O(3W)	90.77(17)
O(2)-Ni(1)-O(1W)	89.4(2)	O(1)-Ni(1)-O(1W)	88.92(17)
O(5)$^{\#1}$-Ni(1)-O(1W)	90.03(19)	O(2W)-Ni(1)-O(1W)	178.76(19)
O(3W)-Ni(1)-O(1W)	88.02(17)		

Table S2b. Hydrogen bonds for **2** (Å and °).

D-H···A	d (D-H)	d (H···A)	d (D···A)	< (DHA)
O(3W)-H(3B)···O(4)$^{\#1}$	0.903(10)	1.85(3)	2.699(6)	156(7)
O(3W)-H(3A)···O(3)$^{\#3}$	0.901(10)	1.79(2)	2.669(6)	165(7)

Symmetry transformations used to generate equivalent atoms: $^{\#1}$ x,-y+1/2,z+1/2; $^{\#2}$ x,-y+1/2,z-1/2; $^{\#3}$ -x+2,-y+1,-z+2.

Table S3. Selected bond distances (Å) and angles (°) for **3**.

Cu(1)-O(5)$^{\#1}$	1.904(4)	Cu(1)-O(2)	1.922(5)
Cu(1)-O(1)	1.943(4)	Cu(1)-O(3)$^{\#2}$	1.977(4)
Cu1-O2$^{\#2}$	2.656(4)		
O(5)$^{\#1}$-Cu(1)-O(2)	170.5(2)	O(5)$^{\#1}$-Cu(1)-O(1)	90.9(2)
O(2)-Cu(1)-O(1)	91.1(2)	O(5)$^{\#1}$-Cu(1)-O(3)$^{\#2}$	93.6(2)
O(2)-Cu(1)-O(3)$^{\#2}$	86.0(2)	O(1)-Cu(1)-O(3)$^{\#2}$	169.5(3)
O(2)$^{\#2}$-Cu(1)-O(3)$^{\#2}$	54.22(1)	O(2)$^{\#2}$-Cu(1)-O(1)	115.3(2)
O(2)$^{\#2}$-Cu(1)-O(2)	78.41(2)	O(2)$^{\#2}$-Cu(1)-O(5)$^{\#1}$	109.05(2)

Symmetry transformations used to generate equivalent atoms: $^{\#1}$ -x,y-1/2,-z+1; $^{\#2}$ -x,y-1/2,-z+2; $^{\#3}$ -x,y+1/2,-z+2; $^{\#4}$ -x,y+1/2,-z+1.

Table S4. Selected bond distances (Å) and angles (°) for **4**.

Cd(1)-O(4)$^{\#1}$	2.209(3)	Cd(1)-O(1)	2.263(3)
Cd(1)-O(2)	2.275(3)	Cd(1)-O(2)$^{\#2}$	2.279(3)

Cd(1)-O(5)$^{\#3}$	2.282(3)	Cd(1)-O(3)$^{\#4}$	2.311(3)
O(4)$^{\#1}$-Cd(1)-O(1)	94.17(13)	O(4)#1-Cd(1)-O(2)	171.99(12)
O(1)-Cd(1)-O(2)	78.44(10)	O(4)$^{\#1}$-Cd(1)-O(2)$^{\#2}$	90.78(13)
O(1)-Cd(1)-O(2)$^{\#2}$	175.01(11)	O(2)-Cd(1)-O(2)$^{\#2}$	96.58(14)
O(4)$^{\#1}$-Cd(1)-O(5)$^{\#3}$	91.67(13)	O(1)-Cd(1)-O(5)$^{\#3}$	89.53(13)
O(2)-Cd(1)-O(5)$^{\#3}$	91.36(12)	O(2)$^{\#2}$-Cd(1)-O(5)$^{\#3}$	90.97(12)
O(4)$^{\#1}$-Cd(1)-O(3)$^{\#4}$	87.51(15)	O(1)-Cd(1)-O(3)$^{\#4}$	81.17(12)
O(2)-Cd(1)-O(3)$^{\#4}$	88.30(13)	O(2)$^{\#2}$-Cd(1)-O(3)$^{\#4}$	98.43(11)
O(5)$^{\#3}$-Cd(1)-O(3)$^{\#4}$	170.57(13)		

Symmetry transformations used to generate equivalent atoms: $^{\#1}$ x-y+1/3,-y+2/3,-z+1/6; $^{\#2}$ y+1,-x+y+1,-z; $^{\#3}$ x-1/3,x-y-2/3,z-1/6; $^{\#4}$ -x+y+2,-x+1,z; $^{\#5}$ x-y,x-1,-z; $^{\#6}$ -y+1,x-y-1,z; $^{\#7}$ x+1/3,x-y-1/3,z+1/6.

Table S5. Selected bond distances (Å) and angles (°) for **5**.

Mn(1)-O(4)$^{\#1}$	2.118(5)	Mn(1)-O(1)$^{\#2}$	2.158(5)
Mn(1)-O(5)	2.177(5)	Mn(1)-O(2)$^{\#2}$	2.182(5)
Mn(1)-O(2)$^{\#3}$	2.189(4)	Mn(1)-O(3)$^{\#4}$	2.203(5)
O(4)$^{\#1}$-Mn(1)-O(1)$^{\#2}$	93.3(2)	O(4)$^{\#1}$-Mn(1)-O(5)	91.3(2)
O(1)$^{\#2}$-Mn(1)-O(5)	90.1(2)	O(4)$^{\#1}$-Mn(1)-O(2)$^{\#2}$	173.92(19)
O(1)$^{\#2}$-Mn(1)-O(2)$^{\#2}$	81.27(18)	O(5)-Mn(1)-O(2)$^{\#2}$	91.53(19)
O(4)$^{\#1}$-Mn(1)-O(2)$^{\#3}$	89.9(2)	O(1)$^{\#2}$-Mn(1)-O(2)$^{\#3}$	176.0(2)
O(5)-Mn(1)-O(2)$^{\#3}$	92.25(18)	O(2)$^{\#2}$-Mn(1)-O(2)$^{\#3}$	95.4(2)
O(4)$^{\#1}$-Mn(1)-O(3)$^{\#4}$	87.8(2)	O(1)$^{\#2}$-Mn(1)-O(3)$^{\#4}$	82.12(19)
O(5)-Mn(1)-O(3)$^{\#4}$	172.12(19)	O(2)$^{\#2}$-Mn(1)-O(3)$^{\#4}$	88.7(2)
O(2)$^{\#3}$-Mn(1)-O(3)$^{\#4}$	95.58(18)		

Symmetry transformations used to generate equivalent atoms: $^{\#1}$ y+1,-x+y+1,-z; $^{\#2}$ x+1/3,x-y-1/3,z+1/6; $^{\#3}$ x-y+2/3,-y+1/3,-z-1/6; $^{\#4}$ -y+4/3,-x+2/3,z+1/6; $^{\#5}$ x-1/3,x-y-2/3,z-1/6; $^{\#6}$ x-y-1/3,-y+1/3,-z-1/6; $^{\#7}$ -y+2/3,-x+4/3,z-1/6; $^{\#8}$ x-y,x-1,-z.

Table S6. Selected bond distances (Å) and angles (°) for **6**.

Cu(1)-O(1)	1.9449(15)	Cu(1)-O(2)	1.9624(15)
Cu(1)-O(5)$^{\#1}$	1.9854(15)	Cu(1)-N(2)	1.9992(17)
Cu(1)-O(1W)	2.348(2)	Cu(1)-O(4)$^{\#1}$	2.4952(19)
O(1)-Cu(1)-O(2)	90.68(6)	O(1)-Cu(1)-O(5)$^{\#1}$	90.56(7)
O(2)-Cu(1)-O(5)$^{\#1}$	158.41(7)	O(1)-Cu(1)-N(2)	170.07(7)
O(2)-Cu(1)-N(2)	92.46(7)	O(5)$^{\#1}$-Cu(1)-N(2)	89.98(7)
O(1)-Cu(1)-O(1W)	86.11(7)	O(2)-Cu(1)-O(1W)	98.77(7)
O(5)$^{\#1}$-Cu(1)-O(1W)	102.82(7)	N(2)-Cu(1)-O(1W)	84.11(7)
O(1)-Cu(1)-O(4)$^{\#1}$	95.67(8)	O(2)-Cu(1)-O(4)$^{\#1}$	100.67(7)
O(5)$^{\#1}$-Cu(1)-O(4)$^{\#1}$	57.77(7)	O(4)$^{\#1}$-Cu(1)-O(1W)	160.44(7)
N(2)-Cu(1)-O(4)$^{\#1}$	93.00(8)		

Symmetry transformations used to generate equivalent atoms: $^{\#1}$ -x+1,-y,-z+1; $^{\#2}$ -x+2,-y+1,-z+1.

Table S7. Selected bond distances (Å) and angles (°) for **7**.

Cd(1)-O(4)	2.230(4)	Cd(1)-O(1W)	2.270(3)
Cd(1)-O(2)$^{\#1}$	2.292(3)	Cd(1)-O(2)$^{\#2}$	2.317(2)
Cd(1)-O(1)$^{\#2}$	2.334(3)	Cd(1)-N(2)	2.363(3)
O(4)-Cd(1)-O(1W)	174.45(12)	O(4)-Cd(1)-O(2)$^{\#1}$	95.25(12)
O(1W)-Cd(1)-O(2)$^{\#1}$	89.85(11)	O(4)-Cd(1)-O(2)$^{\#2}$	96.19(11)
O(1W)-Cd(1)-O(2)$^{\#2}$	87.45(10)	O(2)$^{\#1}$-Cd(1)-O(2)$^{\#2}$	72.17(10)
O(4)-Cd(1)-O(1)$^{\#2}$	87.69(12)	O(1W)-Cd(1)-O(1)$^{\#2}$	89.34(11)
O(2)$^{\#1}$-Cd(1)-O(1)$^{\#2}$	145.68(9)	O(2)$^{\#2}$-Cd(1)-O(1)$^{\#2}$	73.52(9)
O(4)-Cd(1)-N(2)	80.32(13)	O(1W)-Cd(1)-N(2)	94.87(12)
O(2)$^{\#1}$-Cd(1)-N(2)	126.88(11)	O(2)$^{\#2}$-Cd(1)-N(2)	160.73(11)
O(1)$^{\#2}$-Cd(1)-N(2)	87.36(11)		

Symmetry transformations used to generate equivalent atoms: $^{\#1}$ x,y,z+1; $^{\#2}$ -x+1,-y,-z+1; $^{\#3}$ -x+2,-y,-z+1; $^{\#4}$ x,y,z-1.

Table S8. Selected bond distances (Å) and angles (°) for **8**.

Mn(1)-O(5)$^{\#1}$	2.0824(17)	Mn(1)-O(2)	2.1373(16)
Mn(1)-O(1)	2.1843(14)	Mn(1)-O(1W)	2.2024(17)
Mn(1)-N(2)	2.2825(19)	Mn(1)-N(3)	2.296(2)
O(5)$^{\#1}$-Mn(1)-O(1)	94.52(6)	O(2)-Mn(1)-O(1)	81.16(6)
O(5)$^{\#1}$-Mn(1)-O(1W)	84.61(7)	O(2)-Mn(1)-O(1W)	102.16(7)
O(1)-Mn(1)-O(1W)	176.67(6)	O(5)$^{\#1}$-Mn(1)-N(2)	98.00(7)
O(2)-Mn(1)-N(2)	153.08(7)	O(1)-Mn(1)-N(2)	78.92(6)
O(1W)-Mn(1)-N(2)	98.00(7)	O(5)$^{\#1}$-Mn(1)-N(3)	168.28(7)
O(2)-Mn(1)-N(3)	90.25(7)	O(1)-Mn(1)-N(3)	87.69(6)
O(1W)-Mn(1)-N(3)	92.52(7)	N(2)-Mn(1)-N(3)	71.10(7)

Table S8b. Hydrogen bonds for **8** (Å and °).

D-H···A	d (D-H)	d (H···A)	d (D···A)	< (DHA)
O(1W)-H(1B)···O(3)$^{\#3}$	0.890(10)	1.967(14)	2.820(2)	160(3)
O(1W)-H(1B)···O(2)$^{\#3}$	0.890(10)	2.50(2)	3.232(2)	140(2)
O(1W)-H(1A)···O(3)$^{\#4}$	0.891(10)	1.989(12)	2.863(2)	167(3)

Symmetry transformations used to generate equivalent atoms: $^{\#1}$ x,y+1,z; $^{\#2}$ x,y-1,z; $^{\#3}$ -x,-y+1,-z; $^{\#4}$ x+1,y,z.

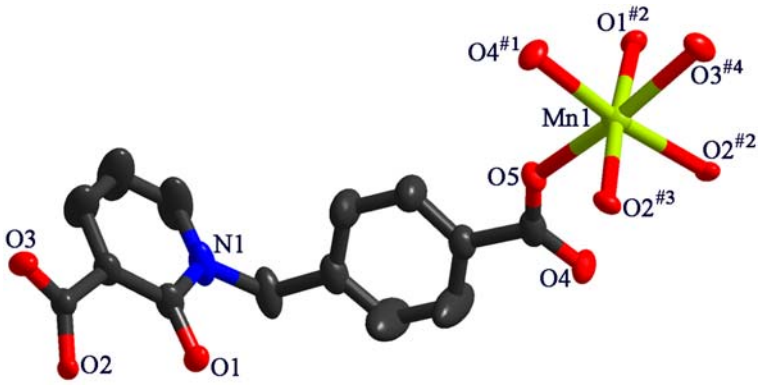

Fig. S1. Coordination environment of the Mn(II) cation in **5**. Symmetry codes: $^{\#1}$ y+1, -x+y+1, -z; $^{\#2}$ x+1/3, x-y-1/3, z+1/6; $^{\#3}$ x-y+2/3, -y+1/3, -z-1/6; $^{\#4}$ -y+4/3, -x+2/3,

z+1/6.

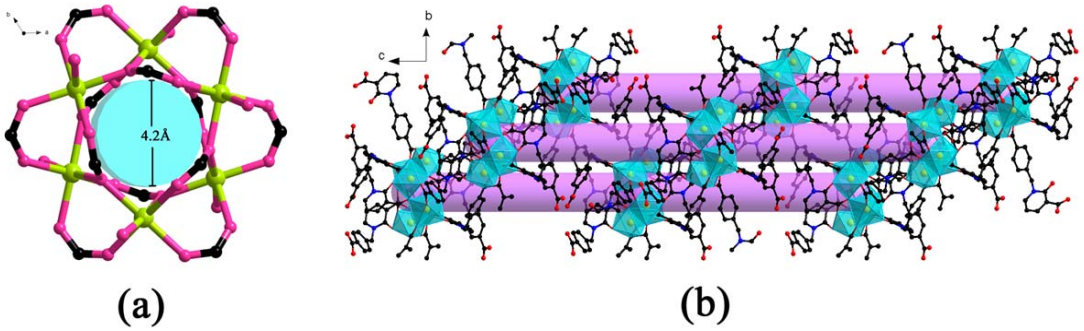

Fig. S2. (a) The diameter of the channel is about 4.2Å. (b) View of the 1D cylindrical channel running along the *c* axis shown.

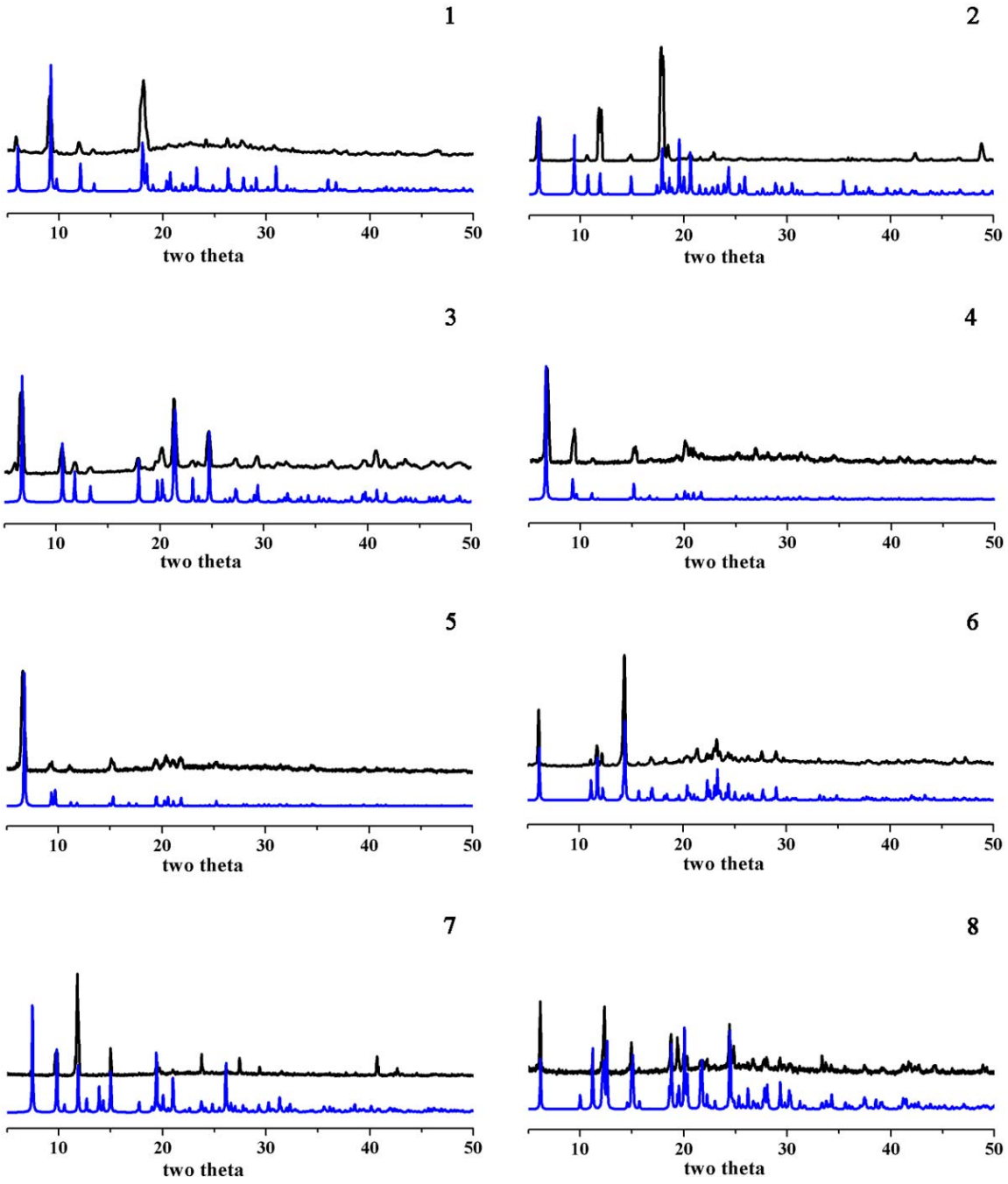

Fig. S3. Simulated (blue) and experimental (black) PXRD patterns of **1**–**8**.

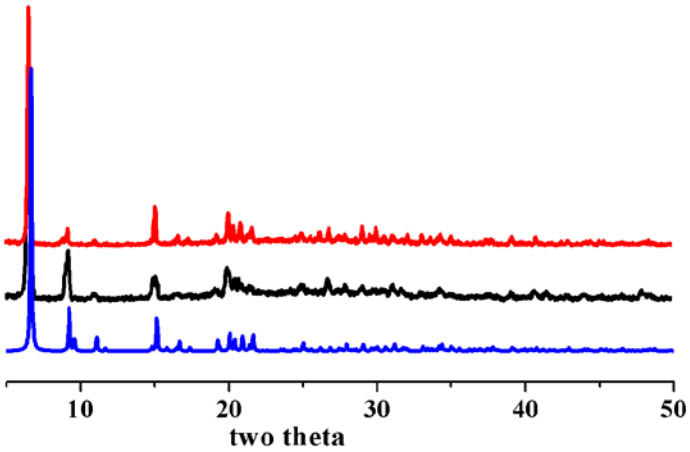

Fig. S4. Simulated (blue), experimental (black) and anhydrous compound **4** (red) PXRD patterns.

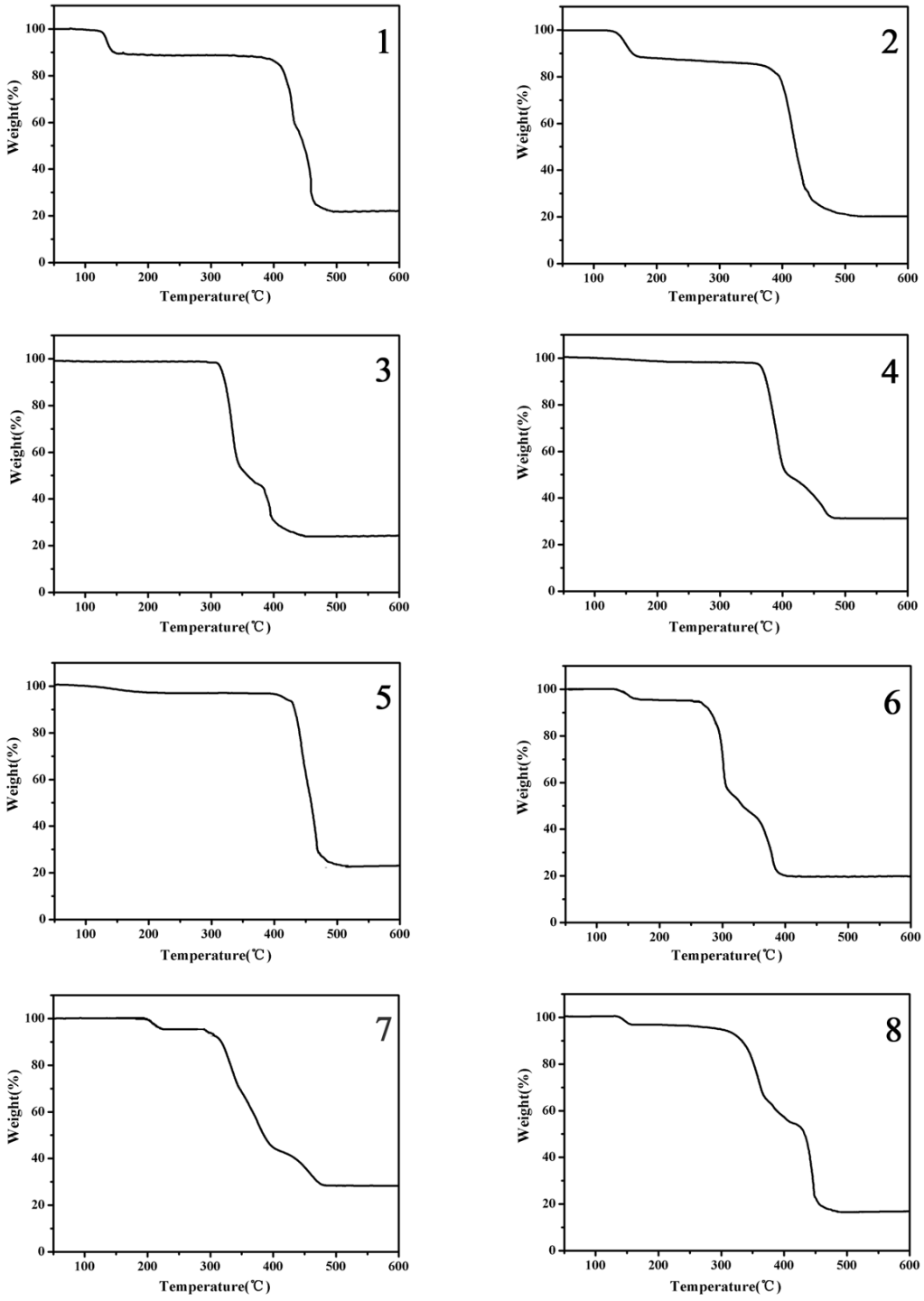

Fig. S5. The TGA curves of compounds **1-8.**