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A series of coordination polymers based on flexible 5-carboxy-1-(4'-carboxybenzyl)-2-oxidopyridinium and structurally related N-donor ligands: syntheses, structures and photoluminescent properties

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Table S1. Selected bond distances (Å) and angles (°) for **1**.

Zn(1)-O(5)	1.976(3)	Zn(1)-O(1)$^{\#1}$	1.978(3)
Zn(1)-N(2)	2.009(3)	Zn(1)-N(5)$^{\#2}$	2.020(3)
O(5)-Zn(1)-O(1)$^{\#1}$	104.35(13)	O(5)-Zn(1)-N(2)	109.67(14)
O(1)$^{\#1}$-Zn(1)-N(2)	101.70(13)	O(5)-Zn(1)-N(5)$^{\#2}$	124.62(14)
O(1)$^{\#1}$-Zn(1)-N(5)$^{\#2}$	108.25(14)	N(2)-Zn(1)-N(5)$^{\#2}$	105.96(15)

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

Table S2. Selected bond distances (Å) and angles (°) for **2**.

Co(1)-O(5)	2.008(2)	Co(1)-N(2)	2.030(16)
Co(1)-O(1)$^{\#1}$	2.0314(19)	Co(1)-O(2)$^{\#2}$	2.0595(19)
Co(1)-O(4)$^{\#3}$	2.076(2)		
O(5)-Co(1)-N(2)	102.9(5)	O(5)-Co(1)-O(1)$^{\#1}$	91.64(9)
N(2)-Co(1)-O(1)$^{\#1}$	103.5(7)	O(1)$^{\#1}$-Co(1)-O(4)$^{\#3}$	87.74(8)
O(5)-Co(1)-O(2)$^{\#2}$	87.78(9)	N(2)-Co(1)-O(2)$^{\#2}$	94.5(7)
O(1)$^{\#1}$-Co(1)-O(2)$^{\#2}$	161.63(8)	O(2)$^{\#2}$-Co(1)-O(4)$^{\#3}$	87.29(8)
O(5)-Co(1)-O(4)$^{\#3}$	162.29(8)	N(2)-Co(1)-O(4)$^{\#3}$	94.4(5)

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

Table S3a. Selected bond distances (Å) and angles (°) for **3**.

Zn(1)-O(4)	1.965(5)	Zn(1)-O(1)$^{\#1}$	2.004(5)
Zn(1)-N(3)	2.073(5)	Zn(1)-N(4)	2.158(6)
Zn(1)-N(2)	2.178(6)		
O(4)-Zn(1)-O(1)$^{\#1}$	92.9(3)	O(4)-Zn(1)-N(3)	124.7(2)
O(1)$^{\#1}$-Zn(1)-N(3)	142.4(2)	O(4)-Zn(1)-N(4)	103.0(2)
O(1)$^{\#1}$-Zn(1)-N(4)	98.0(2)	N(3)-Zn(1)-N(4)	75.2(2)
O(4)-Zn(1)-N(2)	96.4(2)	O(1)$^{\#1}$-Zn(1)-N(2)	103.0(2)

N(3)-Zn(1)-N(2)	75.6(2)	N(4)-Zn(1)-N(2)	150.5(2)

Table S3b. Hydrogen bonds for **3** (Å and °).

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(1W)-H(1B)···O(5)	0.92	1.74	2.640(9)	166(3)
O(1W)-H(1A)···O(3)[#3]	0.97	1.85	2.793(10)	165(4)

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

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

Co(1)-O(1)[#1]	2.002(3)	Co(1)-N(3)	2.074(3)
Co(1)-O(5)	2.098(3)	Co(1)-N(2)	2.148(4)
Co(1)-N(4)	2.153(3)	Co(1)-O(4)	2.252(3)
O(1)[#1]-Co(1)-N(3)	98.62(13)	O(1)[#1]-Co(1)-O(5)	92.87(13)
N(3)-Co(1)-O(5)	167.54(14)	O(1)[#1]-Co(1)-N(2)	105.93(14)
N(3)-Co(1)-N(2)	75.29(14)	O(5)-Co(1)-N(2)	96.98(11)
O(1)[#1]-Co(1)-N(4)	89.82(13)	N(3)-Co(1)-N(4)	74.62(13)
O(5)-Co(1)-N(4)	110.40(13)	N(2)-Co(1)-N(4)	147.76(14)
O(1)[#1]-Co(1)-O(4)	149.17(11)	N(3)-Co(1)-O(4)	110.12(13)
O(5)-Co(1)-O(4)	59.78(12)	N(2)-Co(1)-O(4)	92.30(14)
N(4)-Co(1)-O(4)	87.33(13)		

Symmetry transformation used to generate equivalent atoms: [#1] x-1/2, -y+3/2, z+1/2.

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

Cd(1)-O(5)	2.2439(19)	Cd(1)-O(2)[#1]	2.295(2)
Cd(1)-N(2)	2.308(3)	Cd(1)-N(3)	2.335(2)
Cd(1)-O(1W)	2.344(2)	Cd(1)-O(1)[#1]	2.415(2)
O(5)-Cd(1)-O(2)[#1]	97.30(8)	O(5)-Cd(1)-N(2)	99.02(8)
O(2)[#1]-Cd(1)-N(2)	163.37(9)	O(5)-Cd(1)-N(3)	171.49(9)

O(2)$^{\#1}$-Cd(1)-N(3)	91.21(9)	N(2)-Cd(1)-N(3)	72.48(9)
O(5)-Cd(1)-O(1W)	90.64(8)	O(2)$^{\#1}$-Cd(1)-O(1W)	89.59(8)
N(2)-Cd(1)-O(1W)	93.41(8)	N(3)-Cd(1)-O(1W)	89.56(8)
O(5)-Cd(1)-O(1)$^{\#1}$	96.36(8)	O(2)$^{\#1}$-Cd(1)-O(1)$^{\#1}$	55.57(8)
N(2)-Cd(1)-O(1)$^{\#1}$	119.01(9)	N(3)-Cd(1)-O(1)$^{\#1}$	88.31(8)
O(1W)-Cd(1)-O(1)$^{\#1}$	145.02(8)		

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

Table S6a. Selected bond distances (Å) and angles (°) for **6.**

Cd(1)-O(6)	2.247(4)	Cd(1)-O(6)$^{\#1}$	2.247(4)
Cd(1)-O(1)	2.313(5)	Cd(1)-O(1)$^{\#1}$	2.313(5)
Cd(1)-O(5)$^{\#2}$	2.323(6)	Cd(1)-O(5)$^{\#3}$	2.323(6)
Cd(2)-O(4)$^{\#2}$	2.253(6)	Cd(2)-O(6)	2.292(5)
Cd(2)-O(6)$^{\#4}$	2.297(5)	Cd(2)-N(2)	2.334(6)
Cd(2)-O(2)	2.342(5)	Cd(2)-O(1W)	2.382(6)
O(6)-Cd(1)-O(1)	98.30(17)	O(6)$^{\#1}$-Cd(1)-O(1)	81.70(17)
O(6)-Cd(1)-O(1)$^{\#1}$	81.70(17)	O(6)$^{\#1}$-Cd(1)-O(1)$^{\#1}$	98.30(17)
O(6)-Cd(1)-O(5)$^{\#2}$	91.06(19)	O(6)$^{\#1}$-Cd(1)-O(5)$^{\#2}$	88.94(19)
O(1)-Cd(1)-O(5)$^{\#2}$	89.9(2)	O(1)$^{\#1}$-Cd(1)-O(5)$^{\#2}$	90.1(2)
O(6)-Cd(1)-O(5)$^{\#3}$	88.94(19)	O(6)$^{\#1}$-Cd(1)-O(5)$^{\#3}$	91.06(19)
O(1)-Cd(1)-O(5)$^{\#3}$	90.1(2)	O(1)$^{\#1}$-Cd(1)-O(5)$^{\#3}$	89.9(2)
O(4)$^{\#2}$-Cd(2)-O(6)	102.17(18)	O(4)$^{\#2}$-Cd(2)-O(6)$^{\#4}$	171.6(2)
O(6)-Cd(2)-O(6)$^{\#4}$	84.05(16)	O(4)$^{\#2}$-Cd(2)-N(2)	82.2(2)
O(6)-Cd(2)-N(2)	171.7(2)	O(6)$^{\#4}$-Cd(2)-N(2)	92.3(2)
O(4)$^{\#2}$-Cd(2)-O(2)	102.2(2)	O(6)-Cd(2)-O(2)	85.16(19)
O(6)$^{\#4}$-Cd(2)-O(2)	83.82(19)	N(2)-Cd(2)-O(2)	87.0(2)
O(4)$^{\#2}$-Cd(2)-O(1W)	87.6(2)	O(6)-Cd(2)-O(1W)	81.40(19)
O(6)$^{\#4}$-Cd(2)-O(1W)	87.73(19)	N(2)-Cd(2)-O(1W)	106.0(2)

O(2)-Cd(2)-O(1W)	164.8(2)

Table S6b. Hydrogen bonds for **6** (Å and °).

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(1W)-H(1A)···O(2)$^{\#4}$	0.84(9)	1.97(10)	2.807(8)	172(10)
O(1W)-H(1B)···O(3)$^{\#5}$	0.897(10)	1.81(2)	2.690(8)	167(8)

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

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

Pb(1)-O(4)	2.350(6)	Pb(1)-O(1)$^{\#1}$	2.352(6)
Pb(1)-O(2)$^{\#2}$	2.422(6)	Pb(1)-O(1W)	2.52(2)
Pb(1)-O(3)$^{\#3}$	2.748(7)		
O(4)-Pb(1)-O(1)$^{\#1}$	77.9(2)	O(4)-Pb(1)-O(2)$^{\#2}$	76.1(2)
O(1)$^{\#1}$-Pb(1)-O(2)#2	95.6(2)	O(4)-Pb(1)-O(1W)	78.5(4)
O(1)$^{\#1}$-Pb(1)-O(1W)	92.2(4)	O(2)$^{\#2}$-Pb(1)-O(1W)	151.1(4)
O(4)-Pb(1)-O(3)$^{\#3}$	145.3(2)	O(1)$^{\#1}$-Pb(1)-O(3)$^{\#3}$	84.6(2)
O(2)$^{\#2}$-Pb(1)-O(3)$^{\#3}$	76.1(2)	O(1W)-Pb(1)-O(3)$^{\#3}$	132.4(4)

Symmetry transformation used to generate equivalent atoms: $^{\#1}$ -x+3/2, y+1/2, -z+1/2; $^{\#2}$ -x+1/2, y+1/2, -z+1/2; $^{\#3}$ x+1, y+1, z.
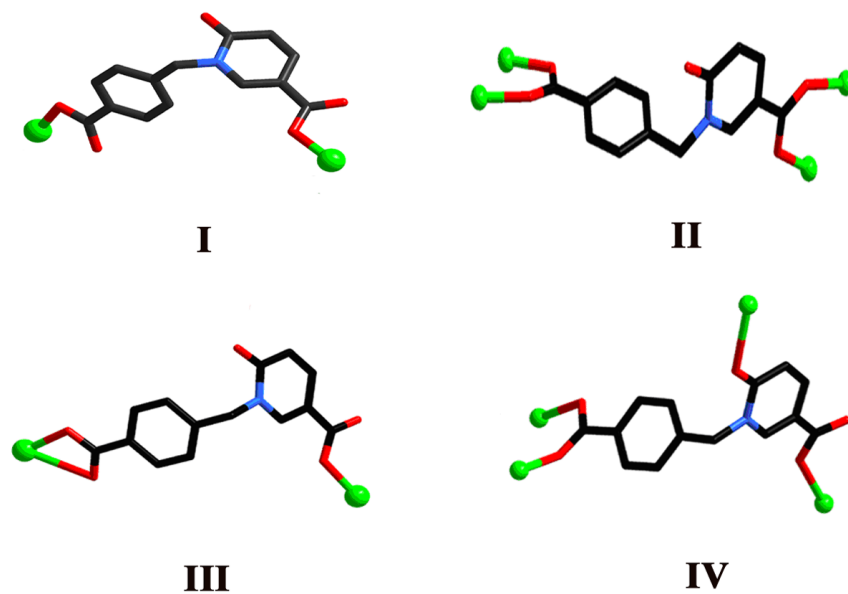
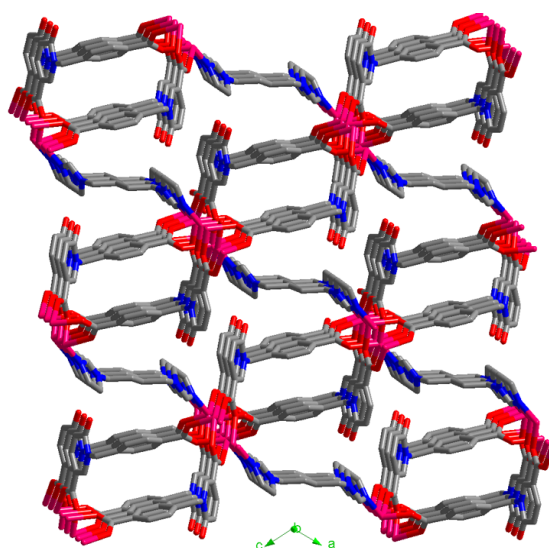**Scheme S1** Coordination modes of the H$_2$L ligand.

Fig. S1 View of the 3D framework constructed by the L anions and biim-4 ligands.
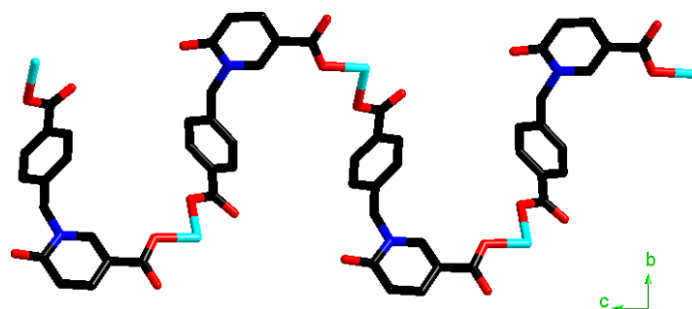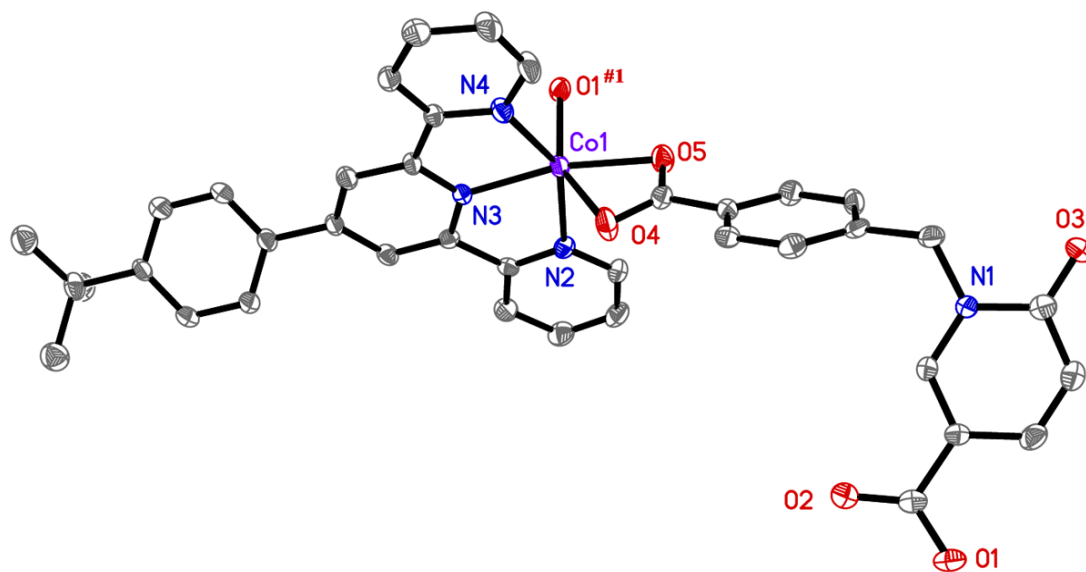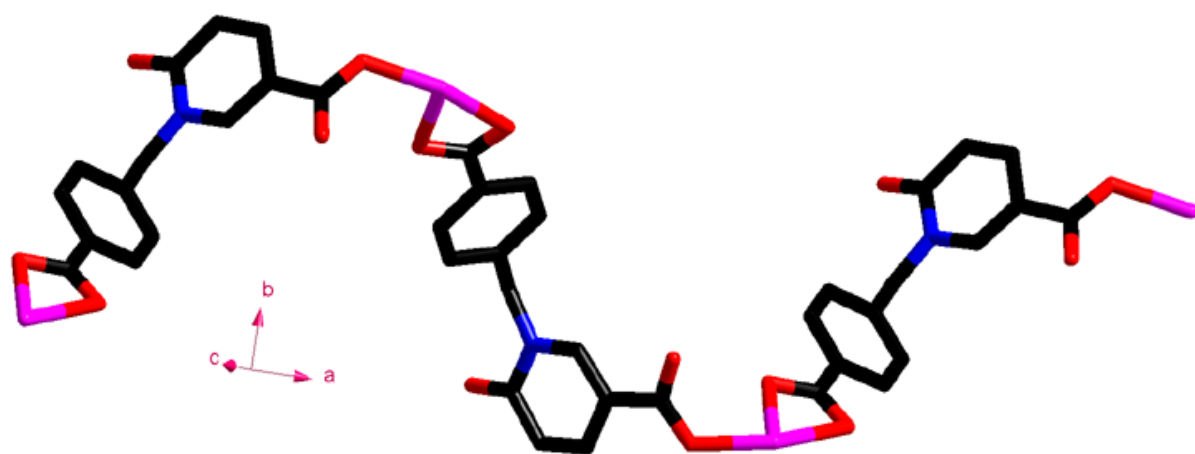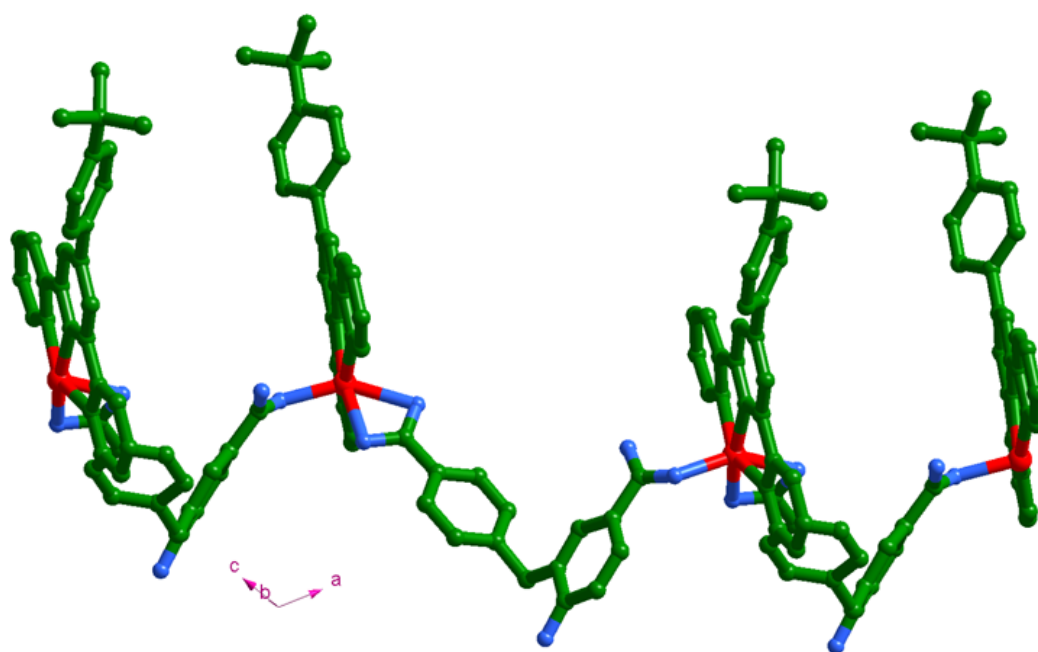

Fig. S2 The 1D infinite chain constructed by L anions and Zn(II) ions.
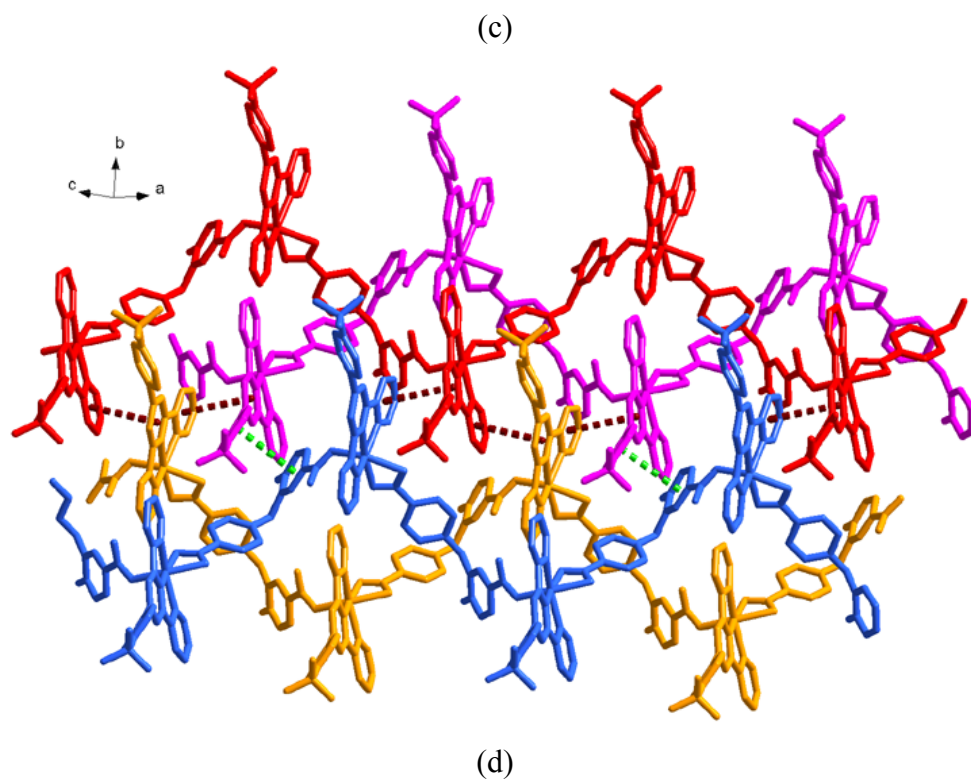
(a)

(b)

(c)

(d)

Fig. S3 (a) Coordination environment of the Co(II) ion in **4** (30% probability displacement ellipsoids). Symmetry code:[#1] x-1/2, -y+3/2, z+1/2. (b) The 1D infinite chain constructed by L anions and Co(II) ions. (c) View of the 1D chain of compound **4**. (d) View of the 2D supramolecular layer formed by π-π interactions in **4**.

Fig. S4 The TGA curves of compounds **1–7.**
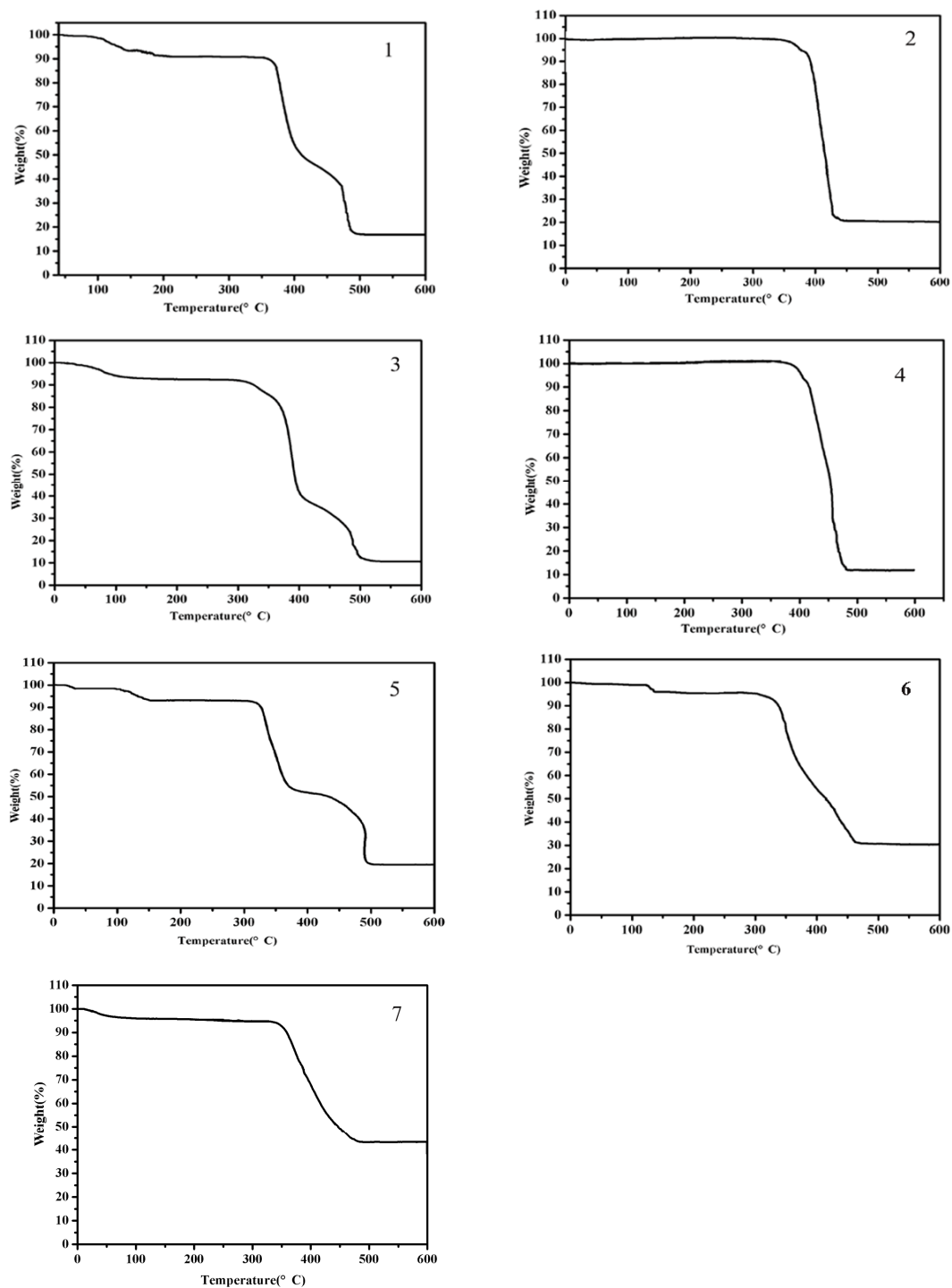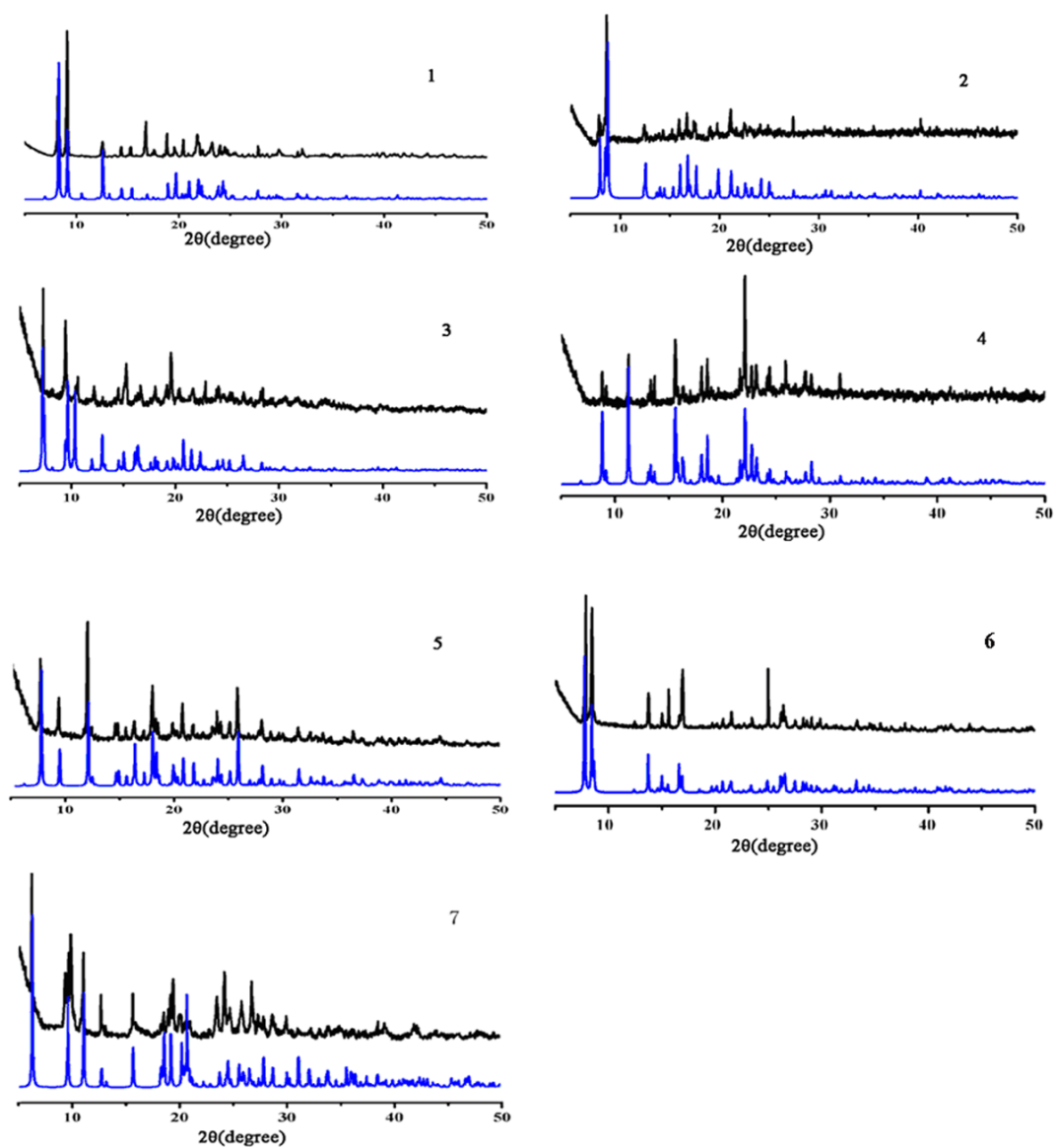
Fig. S5 The simulated (blue) and experimental (black) PXRD patterns for compounds **1**-**7**.