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Supporting Information for

Syntheses, structures, luminescence, and magnetic properties of eleven coordination polymers constructed by a N,N'-sulfuryldiimidazole ligand

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

Zn(1)-N(4)$^{\#1}$	2.037(2)	Zn(1)-N(1)	2.041(2)
Zn(1)-O(7)	2.0734(19)	Zn(1)-O(3)	2.136(2)
Zn(1)-O(4)	2.156(2)	Zn(1)-O(9)	2.457(2)
N(4)$^{\#1}$-Zn(1)-N(1)	106.65(9)	N(4)$^{\#1}$-Zn(1)-O(7)	149.18(9)
N(1)-Zn(1)-O(7)	104.11(9)	N(4)$^{\#1}$-Zn(1)-O(3)	89.36(9)
N(1)-Zn(1)-O(3)	91.45(10)	O(7)-Zn(1)-O(3)	87.97(8)
N(4)$^{\#1}$-Zn(1)-O(4)	94.51(9)	N(1)-Zn(1)-O(4)	102.83(9)
O(7)-Zn(1)-O(4)	80.44(8)	O(3)-Zn(1)-O(4)	163.40(9)
N(4)$^{\#1}$-Zn(1)-O(9)	92.79(8)	N(1)-Zn(1)-O(9)	159.77(8)
O(7)-Zn(1)-O(9)	56.41(7)	O(3)-Zn(1)-O(9)	83.05(9)
O(4)-Zn(1)-O(9)	80.65(8)		

Symmetry transformations used to generate equivalent atoms:

$^{\#1}$ -x+1/2,-y+1/2,-z.

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

Zn(1)-N(1)	2.1237(13)	Zn(1)-N(1)$^{\#1}$	2.1237(13)
Zn(1)-N(4)$^{\#2}$	2.1477(15)	Zn(1)-N(4)$^{\#3}$	2.1477(15)
Zn(1)-O(3)	2.1604(12)	Zn(1)-O(3)$^{\#1}$	2.1604(12)
N(1)-Zn(1)-N(1)$^{\#1}$	180	N(1)-Zn(1)-N(4)$^{\#2}$	89.18(5)
N(1)$^{\#1}$-Zn(1)-N(4)$^{\#2}$	90.82(5)	N(1)-Zn(1)-N(4)$^{\#3}$	90.82(5)
N(1)$^{\#1}$-Zn(1)-N(4)$^{\#3}$	89.18(5)	N(4)$^{\#2}$-Zn(1)-N(4)$^{\#3}$	180
N(1)-Zn(1)-O(3)	85.98(5)	N(1)$^{\#1}$-Zn(1)-O(3)	94.02(5)
N(4)$^{\#2}$-Zn(1)-O(3)	92.53(5)	N(4)$^{\#3}$-Zn(1)-O(3)	87.47(5)
N(1)-Zn(1)-O(3)$^{\#1}$	94.02(5)	N(1)$^{\#1}$-Zn(1)-O(3)$^{\#1}$	85.98(5)
N(4)$^{\#2}$-Zn(1)-O(3)$^{\#1}$	87.47(5)	N(4)$^{\#3}$-Zn(1)-O(3)$^{\#1}$	92.53(5)
O(3)-Zn(1)-O(3)$^{\#1}$	180		

Symmetry transformations used to generate equivalent atoms:

$^{\#1}$ -x+1,-y,-z+1; $^{\#2}$ x,y-1,z; $^{\#3}$ -x+1,-y+1,-z+1.

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

Co(1)-O(3)	2.127(2)	Co(1)-O(3)$^{\#1}$	2.127(2)
Co(1)-N(1)$^{\#1}$	2.131(2)	Co(1)-N(1)	2.131(2)
Co(1)-N(4)$^{\#2}$	2.147(2)	Co(1)-N(4)$^{\#3}$	2.147(2)
O(3)-Co(1)-O(3)$^{\#1}$	180	O(3)-Co(1)-N(1)$^{\#1}$	86.17(8)
O(3)$^{\#1}$-Co(1)-N(1)$^{\#1}$	93.83(8)	O(3)-Co(1)-N(1)	93.83(8)
O(3)$^{\#1}$-Co(1)-N(1)	86.17(8)	N(1)$^{\#1}$-Co(1)-N(1)	180
O(3)-Co(1)-N(4)$^{\#2}$	87.34(9)	O(3)$^{\#1}$-Co(1)-N(4)$^{\#2}$	92.66(9)
N(1)$^{\#1}$-Co(1)-N(4)$^{\#2}$	90.98(9)	N(1)-Co(1)-N(4)$^{\#2}$	89.02(9)
O(3)-Co(1)-N(4)$^{\#3}$	92.66(9)	O(3)$^{\#1}$-Co(1)-N(4)$^{\#3}$	87.34(9)

N(1)$^{\#1}$-Co(1)-N(4)$^{\#3}$	89.02(9)	N(1)-Co(1)-N(4)$^{\#3}$	90.98(9)
N(4)$^{\#2}$-Co(1)-N(4)$^{\#3}$	180		

Symmetry transformations used to generate equivalent atoms:

$^{\#1}$ -x+1,-y,-z+1; $^{\#2}$ x,y-1,z; $^{\#3}$ -x+1,-y+1,-z+1.

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

Cu(1)-N(1)	2.012(2)	Cu(1)-N(1)$^{\#1}$	2.012(2)
Cu(1)-N(4)$^{\#2}$	2.035(2)	Cu(1)-N(4)$^{\#3}$	2.035(2)
Cu(1)-O(3)$^{\#1}$	2.3616(19)	Cu(1)-O(3)	2.3616(19)
N(1)-Cu(1)-N(1)$^{\#1}$	180	N(1)-Cu(1)-N(4)$^{\#2}$	88.39(8)
N(1)$^{\#1}$-Cu(1)-N(4)$^{\#2}$	91.61(8)	N(1)-Cu(1)-N(4)$^{\#3}$	91.61(8)
N(1)$^{\#1}$-Cu(1)-N(4)$^{\#3}$	88.39(8)	N(4)$^{\#2}$-Cu(1)-N(4)$^{\#3}$	180
N(1)-Cu(1)-O(3)$^{\#1}$	90.76(8)	N(1)$^{\#1}$-Cu(1)-O(3)$^{\#1}$	89.24(8)
N(4)$^{\#2}$-Cu(1)-O(3)$^{\#1}$	82.14(8)	N(4)$^{\#3}$-Cu(1)-O(3)$^{\#1}$	97.86(8)
N(1)-Cu(1)-O(3)	89.24(8)	N(1)$^{\#1}$-Cu(1)-O(3)	90.76(8)
N(4)$^{\#2}$-Cu(1)-O(3)	97.86(8)	N(4)$^{\#3}$-Cu(1)-O(3)	82.14(8)
O(3)$^{\#1}$-Cu(1)-O(3)	180		

Symmetry transformations used to generate equivalent atoms:

$^{\#1}$ -x+1/2,-y+1/2,-z+1; $^{\#2}$ x+1/2,-y+1/2,z+1/2; $^{\#3}$ -x,y,-z+1/2.

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

Mn(1)-O(3)	2.196(3)	Mn(1)-O(3)$^{\#1}$	2.196(3)
Mn(1)-N(1)	2.246(3)	Mn(1)-N(1)$^{\#1}$	2.246(3)
Mn(1)-N(4)$^{\#2}$	2.262(3)	Mn(1)-N(4)$^{\#3}$	2.262(3)
O(3)-Mn(1)-O(3)$^{\#1}$	87.71(19)	O(3)-Mn(1)-N(1)	92.19(12)
O(3)$^{\#1}$-Mn(1)-N(1)	83.61(12)	O(3)-Mn(1)-N(1)$^{\#1}$	83.61(12)
O(3)$^{\#1}$-Mn(1)-N(1)$^{\#1}$	92.19(13)	N(1)-Mn(1)-N(1)$^{\#1}$	174.20(15)
O(3)-Mn(1)-N(4)$^{\#2}$	173.63(13)	O(3)$^{\#1}$-Mn(1)-N(4)$^{\#2}$	89.48(13)
N(1)-Mn(1)-N(4)$^{\#2}$	93.18(10)	N(1)$^{\#1}$-Mn(1)-N(4)$^{\#2}$	90.78(10)
O(3)-Mn(1)-N(4)$^{\#3}$	89.48(13)	O(3)$^{\#1}$-Mn(1)-N(4)$^{\#3}$	173.63(13)
N(1)-Mn(1)-N(4)$^{\#3}$	90.78(10)	N(1)$^{\#1}$-Mn(1)-N(4)$^{\#3}$	93.18(10)
N(4)$^{\#2}$-Mn(1)-N(4)$^{\#3}$	93.87(17)		

Symmetry transformations used to generate equivalent atoms:

$^{\#1}$ -x+2,y,-z+1/2; $^{\#2}$ -x+3/2,-y+1/2,-z; $^{\#3}$ x+1/2,-y+1/2,z+1/2.

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

Co(1)-N(1)	2.142(3)	Co(1)-N(1)$^{\#1}$	2.142(3)
Co(1)-N(4)$^{\#2}$	2.144(3)	Co(1)-N(4)$^{\#3}$	2.144(3)
Co(1)-O(7)$^{\#1}$	2.150(3)	Co(1)-O(7)	2.150(3)
N(1)-Co(1)-N(1)$^{\#1}$	95.26(17)	N(1)-Co(1)-N(4)$^{\#2}$	92.96(11)

N(1)$^{\#1}$-Co(1)-N(4)$^{\#2}$	92.49(11)	N(1)-Co(1)-N(4)$^{\#3}$	92.49(11)
N(1)$^{\#1}$-Co(1)-N(4)$^{\#3}$	92.96(11)	N(4)$^{\#2}$-Co(1)-N(4)$^{\#3}$	171.92(17)
N(1)-Co(1)-O(7)$^{\#1}$	173.55(12)	N(1)$^{\#1}$-Co(1)-O(7)$^{\#1}$	90.74(12)
N(4)$^{\#2}$-Co(1)-O(7)$^{\#1}$	84.38(12)	N(4)$^{\#3}$-Co(1)-O(7)$^{\#1}$	89.58(12)
N(1)-Co(1)-O(7)	90.74(12)	N(1)$^{\#1}$-Co(1)-O(7)	173.55(12)
N(4)$^{\#2}$-Co(1)-O(7)	89.58(12)	N(4)$^{\#3}$-Co(1)-O(7)	84.38(12)
O(7)$^{\#1}$-Co(1)-O(7)	83.37(18)		

Symmetry transformations used to generate equivalent atoms:

$^{\#1}$ -x+1,y,-z+1/2; $^{\#2}$ x+1/2,-y+1/2,z+1/2; $^{\#3}$ -x+1/2,-y+1/2,-z.

Table S7a. Selected bond distances (Å) and angles (°) for **7**.

Zn(1)-O(3)$^{\#1}$	1.9724(19)	Zn(1)-O(3)	1.9724(19)
Zn(1)-N(4)$^{\#1}$	2.034(3)	Zn(1)-N(4)	2.034(3)
Zn(2)-N(1)	2.121(3)	Zn(2)-N(1)$^{\#1}$	2.121(3)
Zn(2)-O(6)$^{\#1}$	2.122(2)	Zn(2)-O(6)	2.122(2)
Zn(2)-O(5)$^{\#1}$	2.144(2)	Zn(2)-O(5)	2.144(2)
O(3)$^{\#1}$-Zn(1)-O(3)	120.02(12)	O(3)$^{\#1}$-Zn(1)-N(4)$^{\#1}$	110.67(9)
O(3)-Zn(1)-N(4)$^{\#1}$	106.78(9)	O(3)$^{\#1}$-Zn(1)-N(4)	106.78(9)
O(3)-Zn(1)-N(4)	110.67(9)	N(4)$^{\#1}$-Zn(1)-N(4)	100.15(14)
N(1)-Zn(2)-N(1)$^{\#1}$	92.68(14)	N(1)-Zn(2)-O(6)$^{\#1}$	178.07(9)
N(1)$^{\#1}$-Zn(2)-O(6)$^{\#1}$	89.23(9)	N(1)-Zn(2)-O(6)	89.23(9)
N(1)$^{\#1}$-Zn(2)-O(6)	178.07(10)	O(6)$^{\#1}$-Zn(2)-O(6)	88.86(13)
N(1)-Zn(2)-O(5)$^{\#1}$	90.56(10)	N(1)$^{\#1}$-Zn(2)-O(5)$^{\#1}$	93.04(10)
O(6)$^{\#1}$-Zn(2)-O(5)$^{\#1}$	89.02(10)	O(6)-Zn(2)-O(5)$^{\#1}$	87.26(10)
N(1)-Zn(2)-O(5)	93.04(10)	N(1)$^{\#1}$-Zn(2)-O(5)	90.56(10)
O(6)$^{\#1}$-Zn(2)-O(5)	87.26(10)	O(6)-Zn(2)-O(5)	89.02(10)
O(5)$^{\#1}$-Zn(2)-O(5)	174.79(14)		

Symmetry transformations used to generate equivalent atoms:

$^{\#1}$ -x-1,y,-z+1/2.

Table S7b. Hydrogen bonds for **7** (Å and °).

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(6)-H(6A)···O3#1	0.82	2.41	2.810(3)	111.2

Symmetry transformations used to generate equivalent atoms:

$^{\#1}$ -x-1,y,-z+1/2.

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

Cd(1)-N(8)	2.308(2)	Cd(1)-N(5)$^{\#1}$	2.338(3)
Cd(1)-N(5)	2.346(3)	Cd(1)-N(1)	2.356(2)
Cd(1)-N(4)$^{\#2}$	2.366(3)	Cd(1)-N(8)$^{\#3}$	2.436(3)

N(8)-Cd(1)-N(5)$^{\#1}$	106.78(10)	N(8)-Cd(1)-N(5)	94.83(10)
N(5)$^{\#1}$-Cd(1)-N(5)	76.62(11)	N(8)-Cd(1)-N(1)	158.39(9)
N(5)$^{\#1}$-Cd(1)-N(1)	94.82(10)	N(5)-Cd(1)-N(1)	89.71(10)
N(8)-Cd(1)-N(4)$^{\#2}$	90.13(10)	N(5)$^{\#1}$-Cd(1)-N(4)$^{\#2}$	92.96(9)
N(5)-Cd(1)-N(4)$^{\#2}$	169.38(9)	N(1)-Cd(1)-N(4)$^{\#2}$	89.09(9)
N(8)-Cd(1)-N(8)$^{\#3}$	76.69(10)	N(5)$^{\#1}$-Cd(1)-N(8)$^{\#3}$	171.70(9)
N(5)-Cd(1)-N(8)$^{\#3}$	95.70(9)	N(1)-Cd(1)-N(8)$^{\#3}$	81.85(8)
N(4)$^{\#2}$-Cd(1)-N(8)$^{\#3}$	94.57(9)		

Symmetry transformations used to generate equivalent atoms:

$^{\#1}$ -x+1,-y+1,-z+1; $^{\#2}$ -x+2,-y+1,-z; $^{\#3}$ -x+2,-y+1,-z+1.

Table S9. Selected bond distances (Å) and angles (°) for **9**.

Mn(1)-N(4)$^{\#1}$	2.2081(13)	Mn(1)-N(4)	2.2081(13)
Mn(1)-N(3)$^{\#2}$	2.2235(13)	Mn(1)-N(3)$^{\#3}$	2.2235(13)
Mn(1)-N(1)	2.2515(13)	Mn(1)-N(1)$^{\#1}$	2.2515(13)
N(4)$^{\#1}$-Mn(1)-N(4)	180	N(4)$^{\#1}$-Mn(1)-N(3)$^{\#2}$	89.34(5)
N(4)-Mn(1)-N(3)$^{\#2}$	90.66(5)	N(4)$^{\#1}$-Mn(1)-N(3)$^{\#3}$	90.66(5)
N(4)-Mn(1)-N(3)$^{\#3}$	89.34(5)	N(3)$^{\#2}$-Mn(1)-N(3)$^{\#3}$	180
N(4)$^{\#1}$-Mn(1)-N(1)	93.55(5)	N(4)-Mn(1)-N(1)	86.45(5)
N(3)$^{\#2}$-Mn(1)-N(1)	89.43(5)	N(3)$^{\#3}$-Mn(1)-N(1)	90.57(5)
N(4)$^{\#1}$-Mn(1)-N(1)$^{\#1}$	86.45(5)	N(4)-Mn(1)-N(1)$^{\#1}$	93.55(5)
N(3)$^{\#2}$-Mn(1)-N(1)$^{\#1}$	90.57(5)	N(3)$^{\#3}$-Mn(1)-N(1)$^{\#1}$	89.43(5)
N(1)-Mn(1)-N(1)$^{\#1}$	180		

Symmetry transformations used to generate equivalent atoms:

$^{\#1}$ -x+1,-y+1,-z+1; $^{\#2}$ x-1/2,y,-z+3/2; $^{\#3}$ -x+3/2,-y+1,z-1/2.

Table S10. Selected bond distances (Å) and angles (°) for **10**.

Ni(1)-O(3)$^{\#1}$	2.0586(19)	Ni(1)-O(3)	2.0586(19)
Ni(1)-N(4)$^{\#2}$	2.100(2)	Ni(1)-N(4)$^{\#3}$	2.100(2)
Ni(1)-N(1)	2.119(2)	Ni(1)-N(1)$^{\#1}$	2.119(2)
O(3)$^{\#1}$-Ni(1)-O(3)	180	O(3)$^{\#1}$-Ni(1)-N(4)$^{\#2}$	91.79(9)
O(3)-Ni(1)-N(4)$^{\#2}$	88.21(9)	O(3)$^{\#1}$-Ni(1)-N(4)$^{\#3}$	88.21(9)
O(3)-Ni(1)-N(4)$^{\#3}$	91.79(9)	N(4)$^{\#2}$-Ni(1)-N(4)$^{\#3}$	180
O(3)$^{\#1}$-Ni(1)-N(1)	94.29(9)	O(3)-Ni(1)-N(1)	85.71(9)
N(4)$^{\#2}$-Ni(1)-N(1)	93.60(9)	N(4)$^{\#3}$-Ni(1)-N(1)	86.40(9)
O(3)$^{\#1}$-Ni(1)-N(1)$^{\#1}$	85.71(9)	O(3)-Ni(1)-N(1)$^{\#1}$	94.29(9)
N(4)$^{\#2}$-Ni(1)-N(1)$^{\#1}$	86.40(9)	N(4)$^{\#3}$-Ni(1)-N(1)$^{\#1}$	93.60(9)
N(1)-Ni(1)-N(1)$^{\#1}$	180		

Symmetry transformations used to generate equivalent atoms:

$^{\#1}$ -x+1,-y,-z+2; $^{\#2}$ x+1/2,-y-1/2,z+1/2; $^{\#3}$ -x+1/2,y+1/2,-z+3/2.

Table S11. Selected bond distances (Å) and angles (°) for **11**.

Cd(1)-O(3)	2.240(3)	Cd(1)-N(1)	2.257(3)
Cd(1)-O(2)	2.316(3)	Cd(1)-O(5)$^{\#1}$	2.363(3)
Cd(1)-O(6)$^{\#1}$	2.388(3)	Cd(1)-O(3)$^{\#2}$	2.458(3)
O(3)-Cd(1)-N(1)	124.79(11)	O(3)-Cd(1)-O(2)	95.50(11)
N(1)-Cd(1)-O(2)	90.91(12)	O(3)-Cd(1)-O(5)$^{\#1}$	142.08(9)
N(1)-Cd(1)-O(5)$^{\#1}$	91.32(11)	O(2)-Cd(1)-O(5)$^{\#1}$	94.99(11)
O(3)-Cd(1)-O(6)$^{\#1}$	87.61(9)	N(1)-Cd(1)-O(6)$^{\#1}$	146.28(10)
O(2)-Cd(1)-O(6)$^{\#1}$	95.32(10)	O(5)$^{\#1}$-Cd(1)-O(6)$^{\#1}$	55.17(9)
O(3)-Cd(1)-O(3)$^{\#2}$	81.66(9)	N(1)-Cd(1)-O(3)$^{\#2}$	89.32(10)
O(2)-Cd(1)-O(3)$^{\#2}$	176.68(9)	O(5)$^{\#1}$-Cd(1)-O(3)$^{\#2}$	88.32(9)
O(6)$^{\#1}$-Cd(1)-O(3)$^{\#2}$	86.31(9)		

Symmetry transformations used to generate equivalent atoms:

$^{\#1}$ x-1/2,y-1/2,z; $^{\#2}$ -x,-y-1,-z+1.

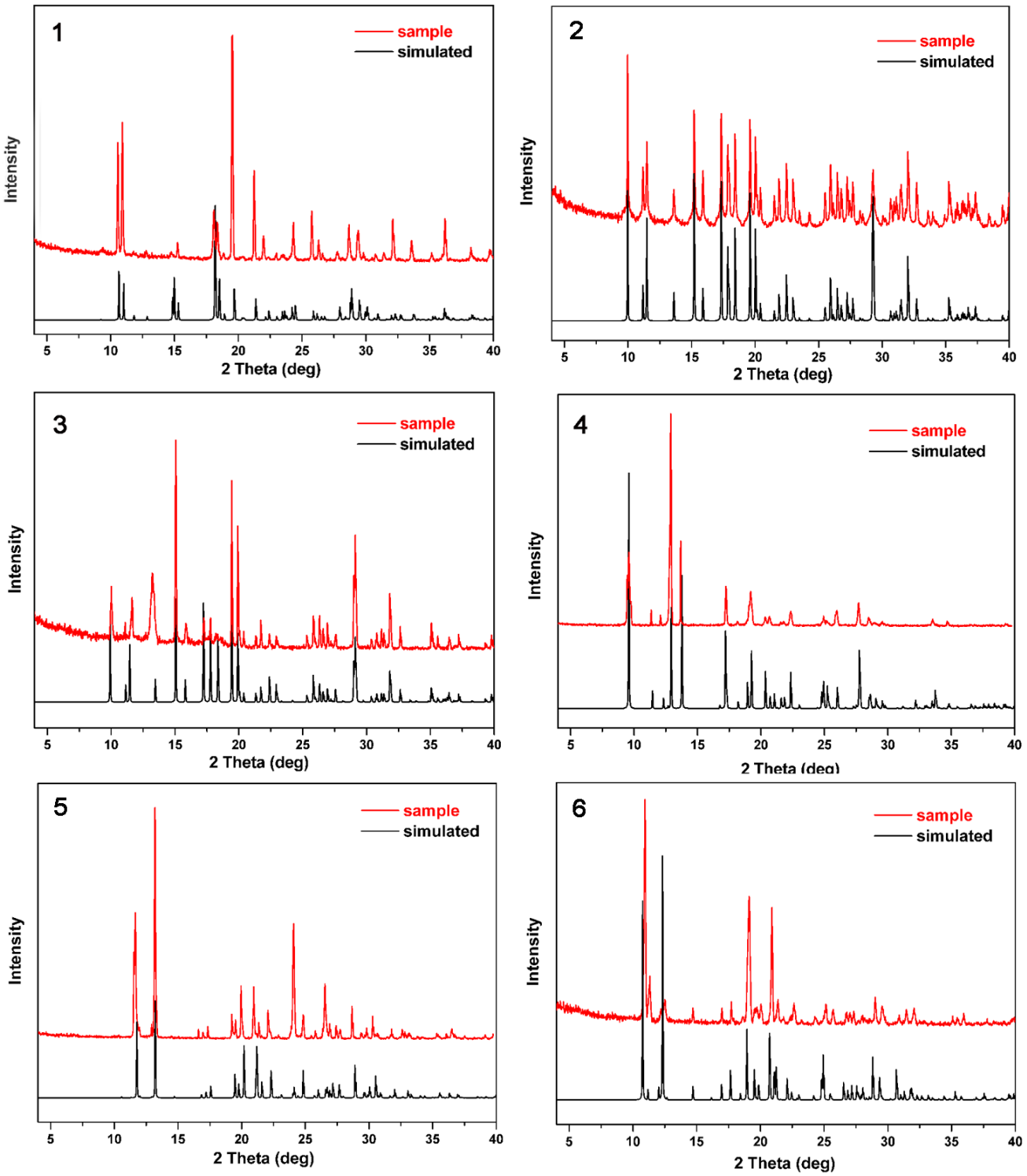

Fig. S1 Simulated (black) and experimental (red) PXRD patterns of compounds **1**-**6**.

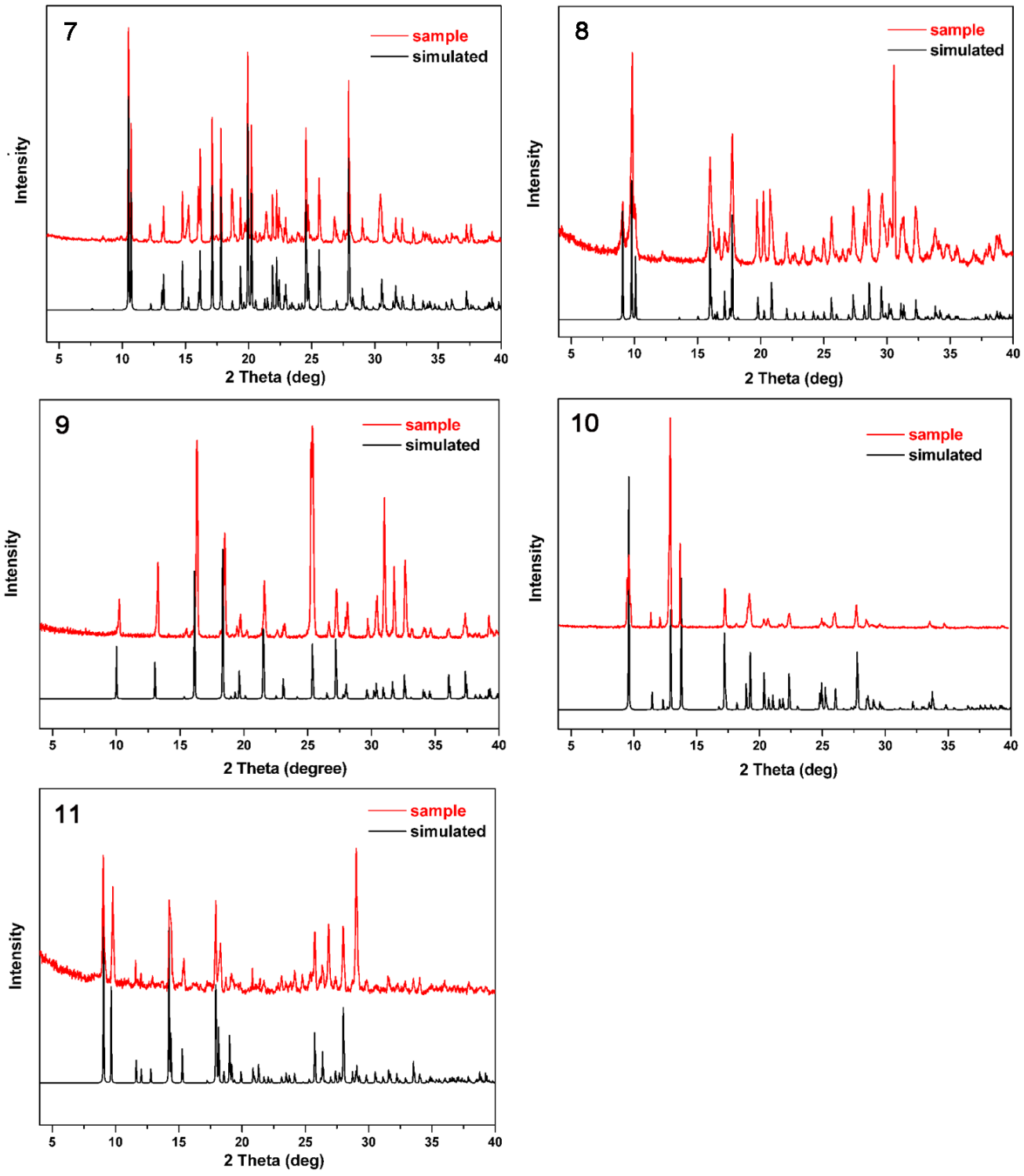

Fig. S2 Simulated (black) and experimental (red) PXRD patterns of compounds **7**-**11**.

Thermogravimetric (TGA) experiments were carried out to study the thermal stability of **1**-**11** (Fig. S3 and Fig. S4). The TG curves of **1**, **5** and **6** exhibited two steps of weight losses of 4.53% (30-130°C) and 50.22% (170-500°C) (**1**), or 5.19% (30-185°C) and 60.15% (200-500°C) (**5**), or 4.59% (30-115°C) and 63.01% (170-500°C) (**6**), which corresponded to the loss of the coordinated water molecules and the sdi ligands, respectively. The remaining weight corresponds to the formation of ZnO for **1** (obsd 21.27%, calcd 20.06%), MnO for **5** (obsd 11.88%, calcd 11.60%) and Co_2O_3 for **6** (obsd 14.14%, calcd 12.01%). Thermal analysis of **2** showed that the weight is almost unchanged in the temperature range of 30-130 °C. Above 130 °C, the residue begins to decompose. The residue corresponds to the formation of ZnO (obsd 14.16%, calcd 13.89%). Compound **3** has similar thermodynamic properties to those of **2**, and compound **3** is stable up to 155 °C. The remaining residue corresponding to the formation of Co_2O_3 is 14.90% (calcd 14.31%). The TG curve of **4** showed two steps of weight losses of 6.41% (30-190°C) and 56.87% (200-350 °C), which could be assigned to the loss of the free acetone molecules and the sdi ligands, respectively. The remaining residue corresponds to the formation of CuO (obsd 11.66%, calcd 11.36%). Compounds **8**, **9** and **10** had similar weight loss stages to that of **2**. Compound **8** released the sdi ligands in the range of 200-500°C with a weight loss of 52.44%, leading to the formation of CdO as the residue (obsd 32.73%, calcd 32.53%). Compound **9** released the sdi ligands in the range of 220-570°C with a weight loss of 61.28%. The departure of the structure leads to the formation of MnO as the residue (obsd 21.68%, calcd 21.04%). Compound **10** released the sdi ligands in the range of 290-520°C with a weight loss of 72.56%. The remaining residue is assigned to the formation of NiO (obsd 13.98%, calcd 13.55%). The TG curves of **7** and **11** displayed three stages of weight losses of 9.82% (30-150°C), 38.62% (180-380°C) and 16.85% (400-600°C) (**7**), or 6.29% (30-180°C), 22.03% (190-310°C) and 46.07% (350-700°C) (**11**), which could be assigned to the loss of the coordinated methanol molecules and water molecules, the sdi ligands, and bdc ligand(**7**) (btc ligand(**11**)), respectively. The remaining weight corresponds to the formation of ZnO for **7** (obsd 16.46%, calcd 15.95%) and CdO for **11** (obsd 28.98%, calcd 28.56%).

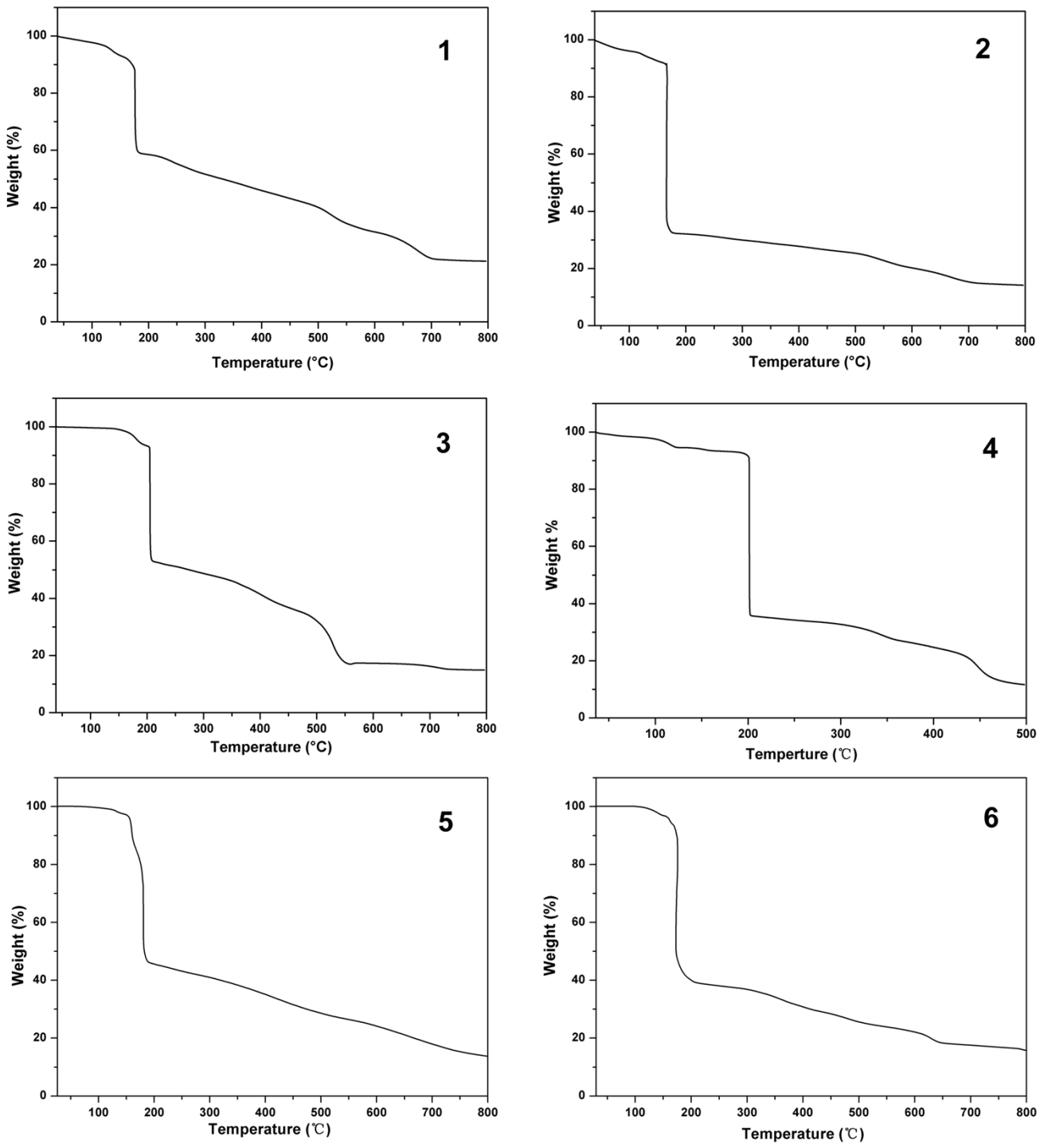

Fig. S3 TGA plot of compounds **1**-**6**.

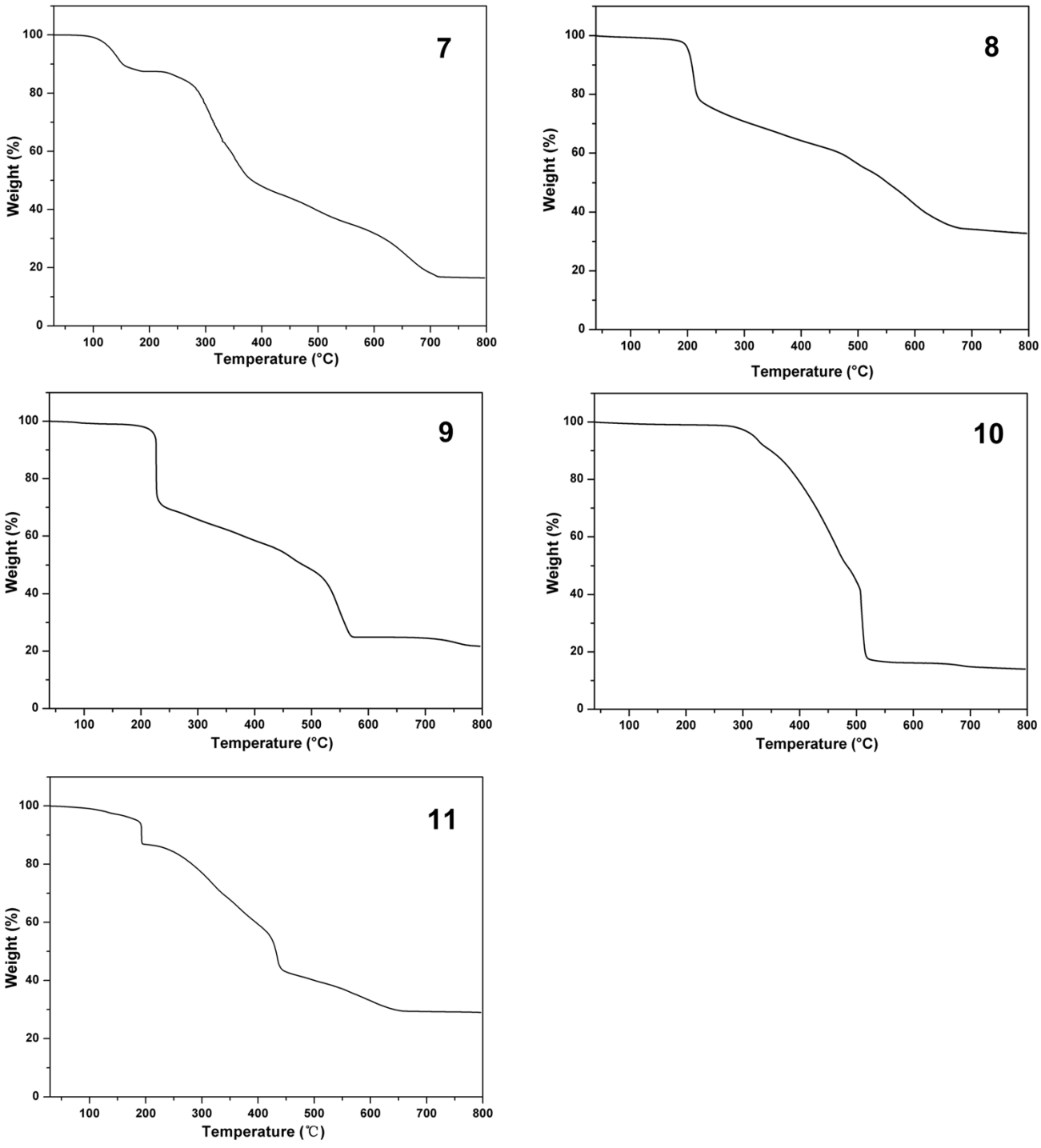

Fig. S4 TGA plot of compounds **7-11**.

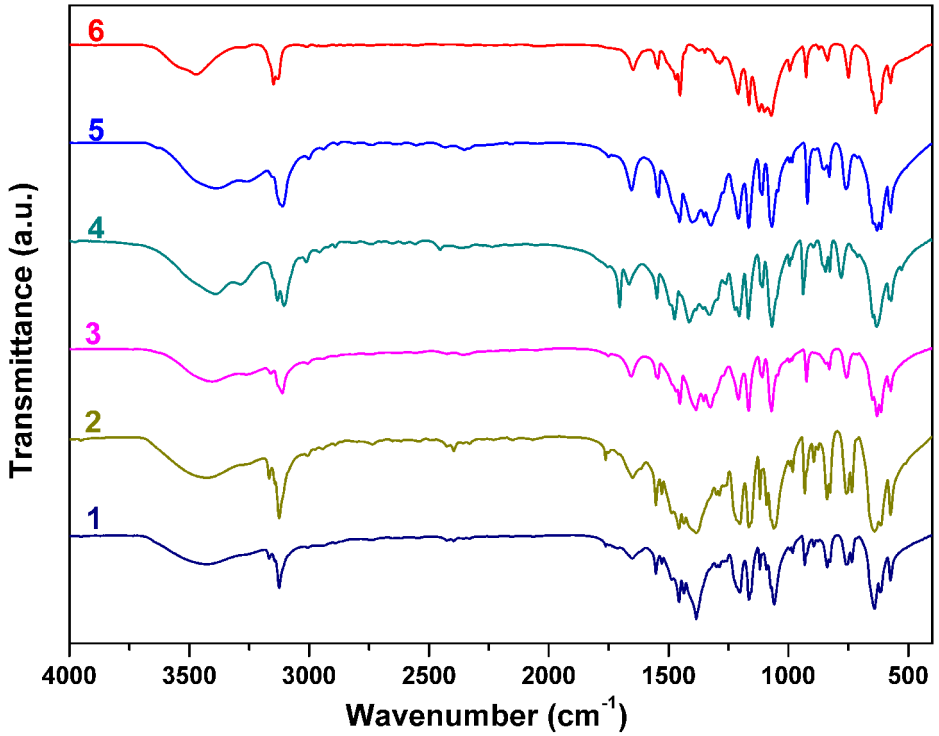

Fig. S5 IR spectra of compounds **1-6**.

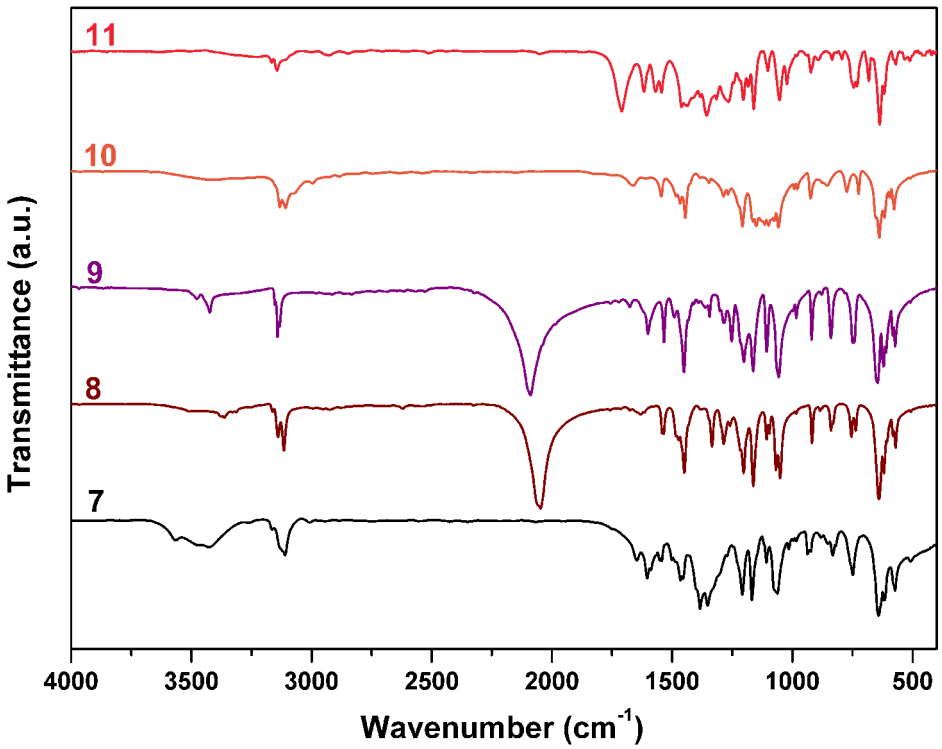

Fig. S6 IR spectra of compounds **7-11**.