Three luminescent metal-organic frameworks constructed from trinuclear zinc(II) clusters and furan-2,5-dicarboxylate

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Supporting information

1. X-ray crystallography

The selected crystal parameters, data collection and refinements are summarized in Table S1. The selected bond lengths and angles are listed in Table S2. CCDC reference numbers for **1**-**3** are 1036655, 1036654 and 1023610, respectively.

Table S1 Crystal data and structure refinement details for **1-3**

	1	**2**	**3**
formula	$C_{34}H_{38}N_4Zn_3O_{22}$	$C_{34}H_{38}N_4O_{22}Zn_3$	$C_{14}H_{17.068}NZn_3O_{14.034}$
fw	1050.85	1050.85	620.12
temp (K)	120	120	120
cryst system	Monoclinic	Triclinic	Monoclinic
space group	$P2_1/c$	P-1	$C2/c$
a (Å)	9.3468(12)	12.6947(8)	17.0962(9)
b (Å)	15.2267(8)	12.8242(6)	13.7039(7)
c (Å)	17.6517(8)	14.7971(7)	10.0192(5)
α (deg)	90	85.110(4)	90
β (deg)	95.599(8)	65.988(5)	105.432(6)
γ(deg)	90	89.663(4)	90
V (Å^3)	2500.2(4)	2191.4(2)	2262.7(2)
Z	2	2	4
D_c (g·cm^{-3})	1.396	1.593	1.814
μ (mm^{-1})	1.503	1.715	3.222
R_{int}	0.0364	0.0350	0.0388
GOF	1.077	1.062	1.129
R_1 [$I > 2\sigma(I)$]	0.0832	0.0499	0.0709
wR_2 [$I > 2\sigma(I)$]	0.2254	0.1282	0.1553
R_1 (all data)	0.1040	0.0640	0.0862
wR_2 (all data)	0.2447	0.1408	0.1642
$\triangle\rho_{max}$ (e Å^{-3})	0.89	1.47	0.87
$\triangle\rho_{min}$ (e Å^{-3})	-2.33	-0.91	-1.20

Table S2 Selected bond lengths [Å] and angles [°] for the complexes.

1			
Zn(1)-O(1)#1	1.985(5)	O(2)#1-Zn(2)-O(5)#4	93.8(2)
Zn(1)-O(5)	2.013(5)	O(2)#3-Zn(2)-O(5)#4	86.2(2)
Zn(1)-O(6)	1.979(5)	O(2)#3-Zn(2)-O(5)	93.8(2)
Zn(1)-O(10)#2	1.971(5)	O(2)#1-Zn(2)-O(5)	86.2(2)
Zn(2)-O(2)#3	2.097(6)	O(2)#3-Zn(2)-O(7)#4	96.1(2)
Zn(2)-O(2)#1	2.097(6)	O(2)#1-Zn(2)-O(7)#4	83.9(2)
Zn(2)-O(5)	2.265(5)	O(2)#1-Zn(2)-O(7)	96.1(2)
Zn(2)-O(5)#4	2.265(5)	O(2)#3-Zn(2)-O(7)	83.9(2)
Zn(2)-O(7)#4	2.252(5)	O(5)-Zn(2)-O(5)#4	180.0
Zn(2)-O(7)	2.252(5)	O(7)#4-Zn(2)-O(5)#4	89.87(16)
O(1)#1-Zn(1)-O(5)	109.1(2)	O(7)-Zn(2)-O(5)#4	90.13(16)
O(6)-Zn(1)-O(1)#1	100.0(2)	O(7)-Zn(2)-O(5)	89.87(16)
O(6)-Zn(1)-O(5)	108.9(2)	O(7)#4-Zn(2)-O(5)	90.13(16)
O(10)#2-Zn(1)-O(1)#1	107.1(2)	O(7)#4-Zn(2)-O(7)	180.0
O(10)#2-Zn(1)-O(5)	127.1(2)	O(2)#3-Zn(2)-O(2)#1	180.0
O(10)#2-Zn(1)-O(6)	101.3(2)		
2			
Zn(1)-O(5)	2.004(3)	Zn(2)-O(15)#4	2.072(3)
Zn(1)-O(7)#1	1.986(3)	Zn(3)-O(2)	1.958(3)
Zn(1)-O(14)#2	1.972(3)	Zn(3)-O(10)#5	1.957(3)
Zn(1)-O(19)#3	2.137(3)	Zn(3)-O(11)	1.963(3)
Zn(1)-O(20)#3	2.113(13)	Zn(3)-O(17)#6	1.942(3)
Zn(1)-O(20)'#3	2.326(11)	Zn(4)-O(16)	2.145(3)
Zn(2)-O(5)	2.136(3)	Zn(4)-O(1)	2.144(3)
Zn(2)-O(5)#1	2.136(3)	Zn(4)-O(9)#5	2.07 1(3)
Zn(2)-O(6)#1	2.062(3)	Zn(4)-O(9)#7	2.071(3)
Zn(2)-O(6)	2.062(3)	Zn(4)-O(16)	2.107(3)
Zn(2)-O(15)#2	2.072(3)	Zn(4)-O(16)#6	2.107(3)
O(5)-Zn(1)-Zn(2)	39.89(8)	O(6)#2-Zn(2)-O(15)#4	86.63(12)
O(5)-Zn(1)-O(19)#1	95.37(14)	O(6)-Zn(2)-O(15)#4	93.37(12)
O(5)-Zn(1)-O(20)#1	150.8(4)	O(6)-Zn(2)-O(15)#3	86.63(12)
O(5)-Zn(1)-O(20)'#1	154.4(3)	O(6)#2-Zn(2)-O(15)#3	93.37(12)
O(7)#2-Zn(1)-Zn(2)	82.57(9)	O(15)#4-Zn(2)-Zn(1)	109.23(8)
O(7)#2-Zn(1)-O(5)	96.36(12)	O(15)#3-Zn(2)-Zn(1)	70.77(8)
O(7)#2-Zn(1)-O(19)#1	106.34(13)	O(15)#4-Zn(2)-Zn(1)#2	70.77(8)
O(7)#2-Zn(1)-O(20)#1	100.5(3)	O(15)#3-Zn(2)-Zn(1)#2	109.23(8)
O(7)#2-Zn(1)-O(20)'#1	84.5(3)	O(15)#4-Zn(2)-O(5)#2	92.04(11)

O(14)#3-Zn(1)- Zn(2)	81.17(9)	O(15)#3-Zn(2)-O(5)#2	87.96(11)
O(14)#3-Zn(1)-O(5)	104.91(12)	O(15)#3-Zn(2)-O(5)	92.04(11)
O(14)#3-Zn(1)-O(7)#2	122.29(13)	O(15)#4-Zn(2)-O(5)	87.96(11)
O(14)#3-Zn(1)-O(19)#1	123.69(14)	O(15)#3-Zn(2)-O(15)#4	180.00(16)
O(14)#3-Zn(1)-O(20) #1	85.9(3)	O(2)-Zn(3)-O(11)	103.77(13)
O(14)#3-Zn(1)-O(20)'#1	96.0(3)	O(10)#5-Zn(3)-O(2)	106.84(14)
O(19)#1-Zn(1)-Zn(2)	135.21(11)	O(10)#5-Zn(3)-O(11)	101.90(13)
O(19)#1-Zn(1)-O(20)'#1	60.2(3)	O(17)#6-Zn(3)-O(2)	125.95(13)
O(20)#1-Zn(1)-Zn(2)	166.3(3)	O(17)#6-Zn(3)-O(10)#5	109.30(13)
O(20)#1-Zn(1)-O(19)#1	57.0(4)	O(17)#6-Zn(3)-O(11)	106.44(13)
O(20)#1-Zn(1)-O(20)'#1	16.1(3)	O(1)-Zn(4)-O(16)	180.0
O(20)#1-Zn(1)-Zn(2)	162.6(2)	O(9)#7-Zn(4)-O(16)	94.28(12)
O(5)#2-Zn(2)-Zn(1)#2	36.98(8)	O(9)#5-Zn(4)-O(1)	94.28(12)
O(5)#2-Zn(2)-Zn(1)	143.02(8)	O(9)#7-Zn(4)-O(1)	85.72(12)
O(5)-Zn(2)-Zn(1)	36.98(8)	O(9)#5-Zn(4)-O(16)	85.72(12)
O(5)-Zn(2)-Zn(1)#2	143.02(8)	O(9)#5-Zn(4)-O(9)#7	180.0
O(5)-Zn(2)-O(5)#2	180.0	O(9)#5-Zn(4)-O(16)#6	94.52(11)
O(6)#2-Zn(2)-Zn(1)#2	116.03(8)	O(9)#5-Zn(4)-O(16)	85.48(11)
O(6)-Zn(2)-Zn(1)#2	63.97(8)	O(9)#7-Zn(4)-O(16)#6	85.48(11)
O(6)#2-Zn(2)-Zn(1)	63.97(8)	O(9)#7-Zn(4)-O(16)	94.52(11)
O(6)-Zn(2)-Zn(1)	116.03(8)	O(16)#6-Zn(4)-O(16)	81.37(11)
O(6)-Zn(2)-O(5)	88.42(11)	O(16)#6-Zn(4)-O(1)	98.63(11)
O(6)#2-Zn(2)-O(5)#2	88.42(11)	O(16)-Zn(4)-O(16)	98.63(11)
O(6)-Zn(2)-O(5)#2	91.58(11)	O(16)-Zn(4)-O(1)	81.37(11)
O(6)#2-Zn(2)-O(5)	91.58(11)	O(16)#6-Zn(4)-O(16)	180.0
O(6)-Zn(2)-O(6)#2	180.0		
3			
Zn(1)-O(1)#1	2.168(5)	Zn(2)-O(2)	2.029(6)
Zn(1)-O(4)	2.031(5)	Zn(2)-O(6)	1.865(5)
Zn(1)-O(5)#2	2.129(5)	Zn(2)-O(6)#5	1.981(6)
Zn(1)-O(6)#3	1.960(5)	Zn(2)-O(7)	1.880(7)
Zn(1)-O(7)#4	1.946(12)	Zn(2)-O(7)#5	1.966(7)
Zn(1)-O(7)#1	2.094(12)	Zn(2)#5-Zn(2)-O(2)	167.5(5)
O(4)-Zn(1)-O(1)#1	98.9(3)	Zn(2)#5-Zn(2)-O(6)#5	70.1(4)
O(4)- Zn(1)-O(5)#2	94.9(2)	Zn(2)#5-Zn(2)-O(6)	87.7(4)
O(4)-Zn(1)-O(7)#1	94.3(3)	Zn(2)#5-n(2)-O(7)#5	72.4(3)
O(5)#2-Zn(1)-O(1)#1	164.8(2)	Zn(2)#5-Zn(2)-O(7)	85.3(3)
O(6)#3-Zn(1)-O(1)#1	85.4(2)	O(6)-Zn(2)-O(2)	104.8(2)
O(6)#3-Zn(1)-O(4)	97.6(2)	O(6)#5-Zn(2)-O(2)	102.2(2)
O(6)#3-Zn(1)-O(5)#2	86.5(2)	O(6)-Zn(2)-O(6)#5	118.0(3)

O(6)#3-Zn(1)-O(7)#1	167.7(3)	O(6)-Zn(2)-O(7)#5	122.5(4)
O(7)#1-Zn(1)-O(1)#1	89.7(3)	O(6)-Zn(2)-O(7)	113.5(4)
O(7)#4-Zn(1)-O(1)#1	93.6(3)	O(7)-Zn(2)-O(2)	90.7(4)
O(7)#4-Zn(1)-O(4)	108.8(3)	O(7)#5-Zn(2)-O(2)	101.1(4)
O(7)#4-Zn(1)-O(5)#2	87.9(3)	O(7)-Zn(2)-O(6)#5	120.9(4)
O(7)#1-Zn(1)-O(5)#2	95.7(3)	O(7)#5-Zn(2)-O(6)#5	105.0(3)
O(7)#4-Zn(1)-O(6)#3	153.4(3)	O(7)-Zn(2)-O(7)#5	17.0(5)
O(7)#4-Zn(1)-O(7)#1	15.9(5)		

1, #1 -1+X, +Y, +Z; #2 +X, 3/2-Y, -1/2+Z; #3 1-X, 1-Y, 1-Z; #4 -X, 1-Y, 1-Z; #5 1+X, +Y, +Z; #6 +X, 3/2-Y, 1/2+Z

2, #1 1-X, -Y, 1-Z; #2 1-X, -Y, -Z; #3 -1+X, +Y, +Z; #4 +X, +Y, 1+Z; #5 2-X, -Y, -Z; #6 2-X, 1-Y, -Z; #7 +X, 1+Y, +Z; #8 +X, -1+Y, +Z; #9 +X, +Y, -1+Z; #10 1+X, +Y, +Z

3, #1 1/2-X, 1/2+Y, 1/2-Z; #2 1-X, +Y, 1/2-Z; #3 1/2-X, 1/2-Y, 1-Z; #4 1/2+X, 1/2+Y, +Z; #5 -X, +Y, 1/2-Z; #6 1/2-X, -1/2+Y, 1/2-Z; #7 -1/2+X, -1/2+Y, +Z

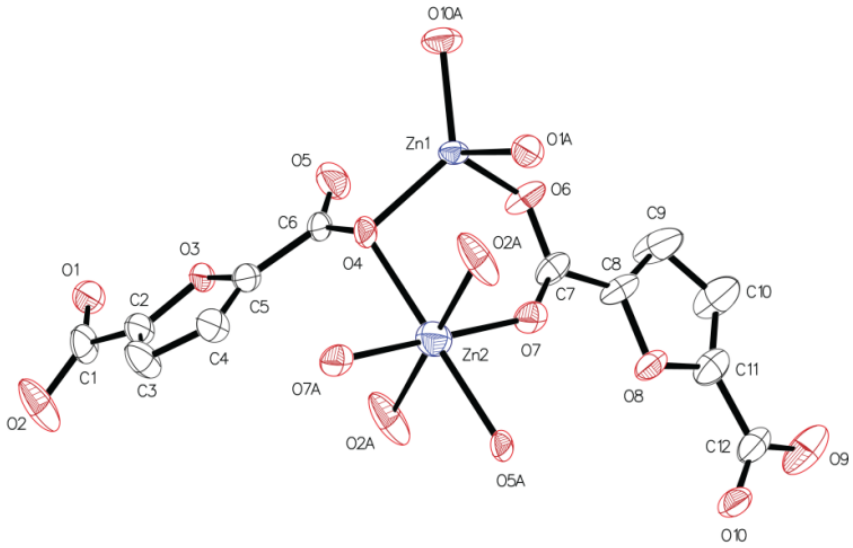


Fig. S1. ORTEP drawing of the structural unit of **1** (thermal ellipsoids are drawn at the 30% probability level; H atoms were omitted for clarity).

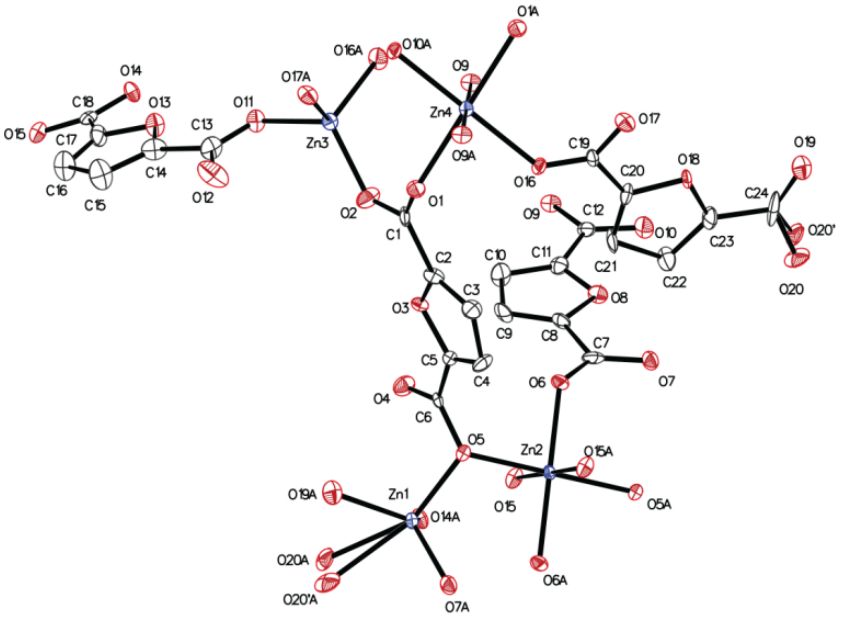


Fig. S2. ORTEP drawing of the structural unit of **2** (thermal ellipsoids are drawn at the 30% probability level; H atoms were omitted for clarity).

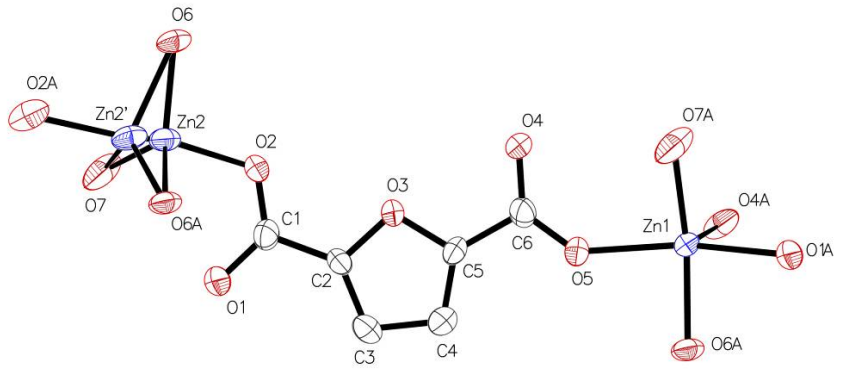


Fig. S3. ORTEP drawing of structural unit of **3** (thermal ellipsoids are drawn at the 30% probability level; H atoms were omitted for clarity.)

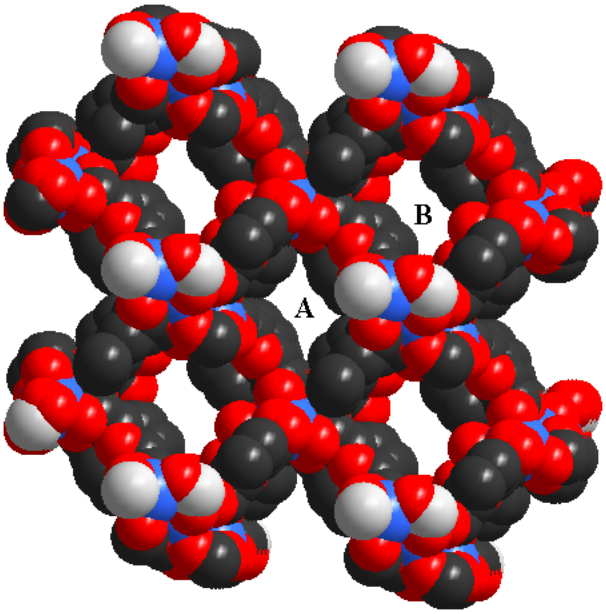


Fig. S4. Space filling view of the 3D framework along the [1,0,0] direction of **2**. Zn is in blue, O in red, and C in gray.

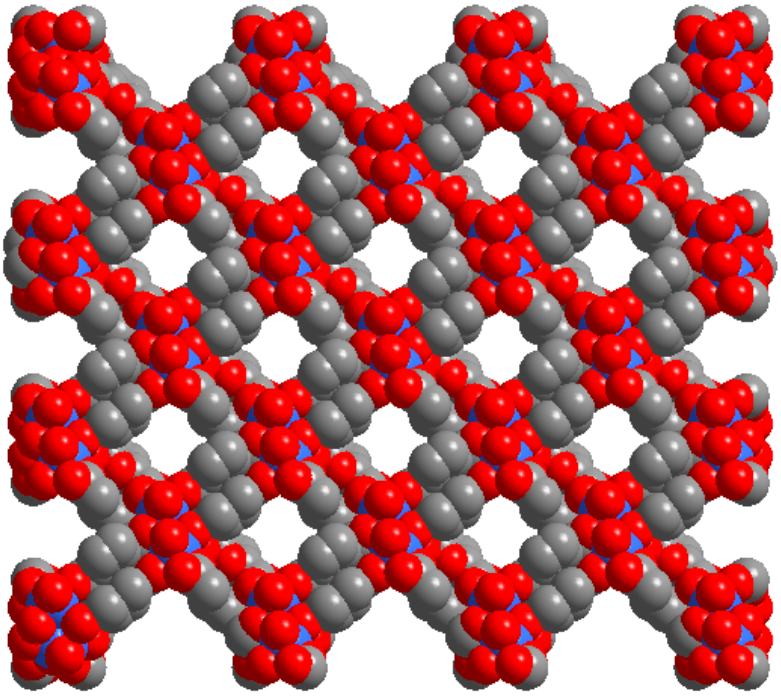
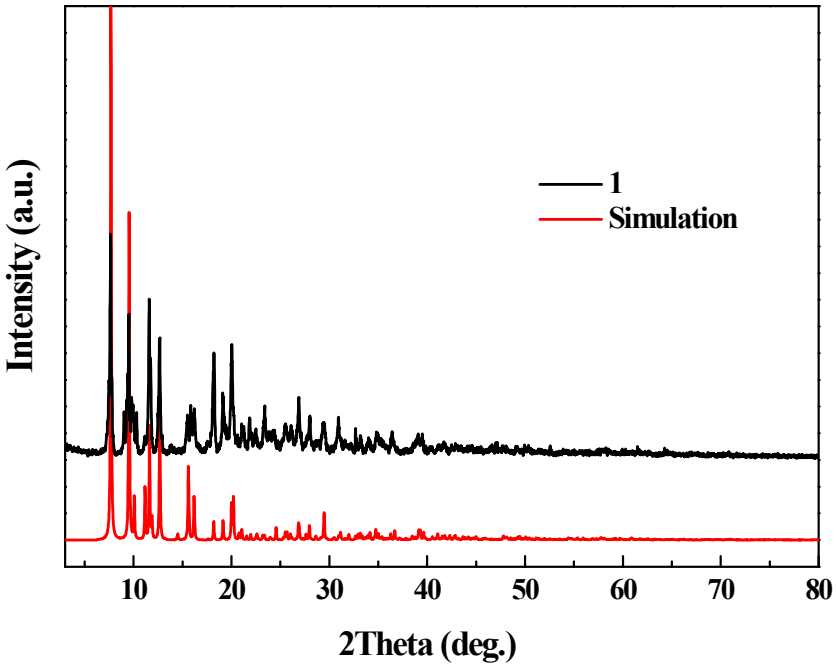
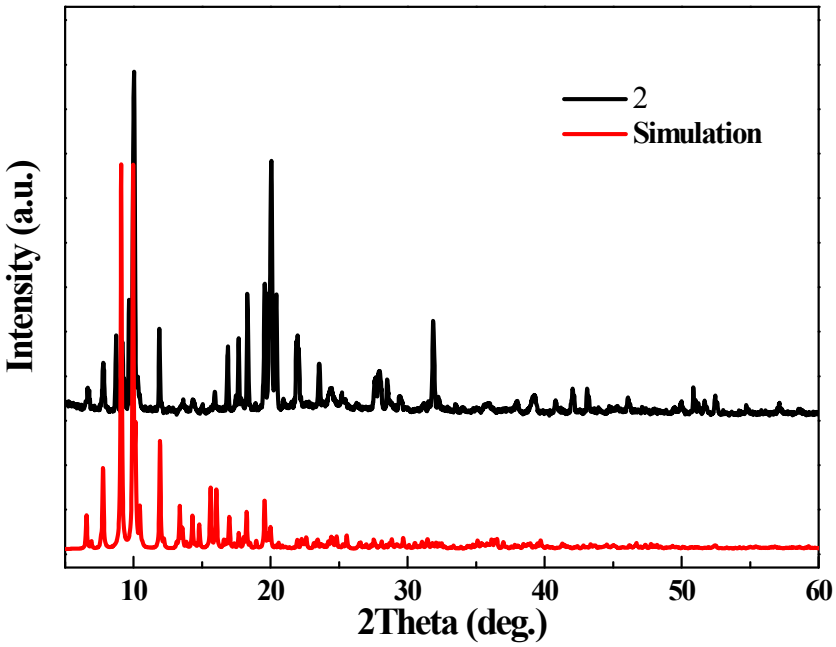


Fig. S5. Space filling view of the 3D framework along the [0,0,1] direction of **3**. Zn in blue, O in red, C in gray.

2. PXRD and TGA patterns





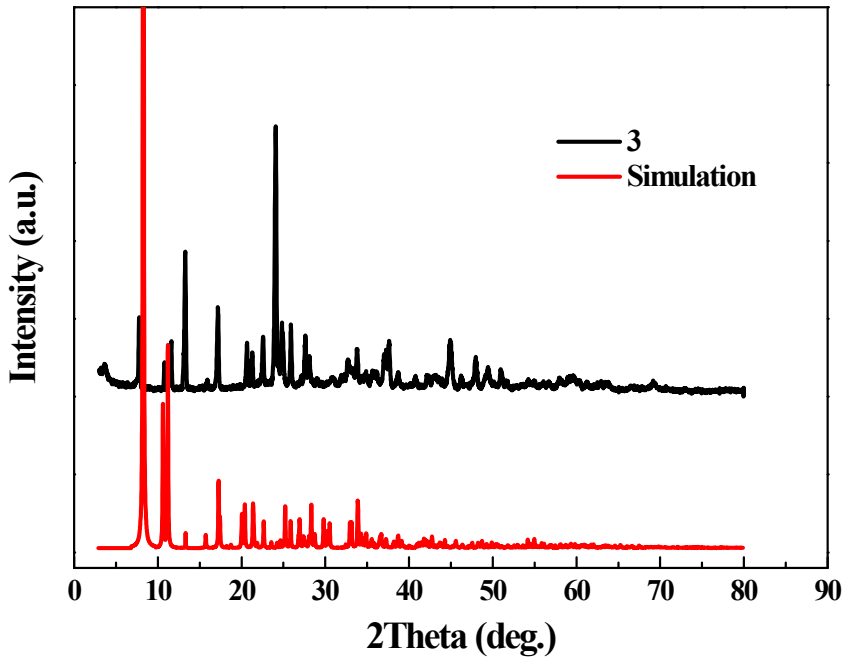


Fig. S6. The simulated X-ray powder diffraction patterns (lower) and the measured one (upper) of compound **1-3**.

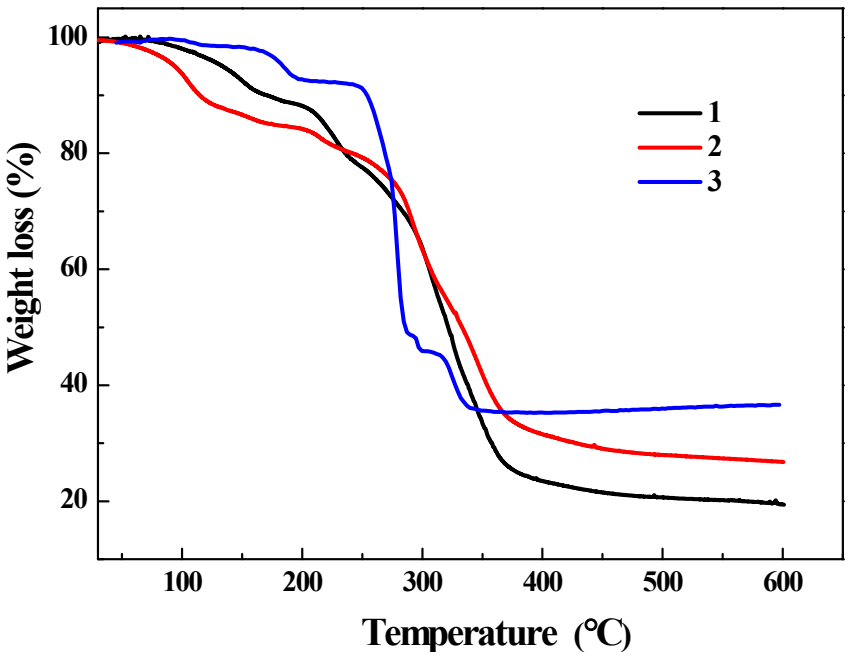


Fig. S7. TGA plots of **1-3.**