

Syntheses, Structures, and Photoluminescent Properties of Ten Metal–Organic Frameworks Constructed by a Flexible Tetracarboxylate Ligand

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Table S1. Selected bond distances (Å) and angles (°) for compounds **1-10**

Compound 1					
O(1)-Zn(1)	2.135(3)	O(10)#3-Zn(1)-O(11)	99.63(13)	O(12)-Zn(1)-O(13)	99.16(16)
O(2)-Zn(2)	1.955(3)	O(10)#3-Zn(1)-O(1)	83.92(14)	O(12)-Zn(2)-O(12)#6	86.11(13)
O(3)-Zn(3)	2.135(4)	O(10)#3-Zn(1)-O(12)	92.33(16)	O(13)-Zn(1)-O(1)	82.25(15)
O(7)-Zn(2)#1	1.891(3)	O(10)#3-Zn(1)-O(13)	162.07(18)	O(2)-Zn(2)-O(12)	117.30(13)
O(9)-Zn(3)#2	1.996(3)	O(11)#5-Zn(3)-O(15)	178.20(14)	O(2)-Zn(2)-O(12)#6	106.02(13)
O(10)-Zn(1)#3	2.024(3)	O(11)#5-Zn(3)-O(3)	90.23(14)	O(3)-Zn(3)-O(15)	88.01(15)
O(13)-Zn(1)	2.072(4)	O(11)#8-Zn(3)-O(11)#5	85.66(12)	O(7)#10-Zn(2)-O(12)	106.54(15)
O(11)-Zn(3)#4	2.040(3)	O(11)#8-Zn(3)-O(15)	95.65(15)	O(7)#10-Zn(2)-O(12)#6	117.23(15)
O(11)-Zn(1)	2.045(3)	O(11)#8-Zn(3)-O(3)	149.59(13)	O(7)#10-Zn(2)-O(2)	119.30(15)
O(11)-Zn(3)#5	2.107(3)	O(11)-Zn(1)-O(1)	171.07(13)	O(9)#7-Zn(3)-O(11)#5	98.46(13)
O(12)-Zn(2)	1.997(3)	O(11)-Zn(1)-O(12)	97.41(12)	O(9)#7-Zn(3)-O(11)#8	102.41(15)
O(12)-Zn(2)#6	2.011(3)	O(11)-Zn(1)-O(13)	92.53(14)	O(9)#7-Zn(3)-O(15)	82.49(15)
O(12)-Zn(1)	2.054(3)	O(12)-Zn(1)-O(1)	90.60(13)	O(9)#7-Zn(3)-O(3)	107.99(16)
Compound 2					
Zn(1)-O(2)	1.942(6)	O(2)-Zn(1)-O(12)	130.4(2)	O(6)-Zn(1)-O(10)	88.3(4)
Zn(1)-O(12)	1.948(5)	O(2)-Zn(1)-O(6)	95.6(3)	O(2)-Zn(1)-O(11)	90.0(3)
Zn(1)-O(6)	1.964(6)	O(12)-Zn(1)-O(6)	134.1(3)	O(12)-Zn(1)-O(11)	90.1(3)
Zn(1)-O(10)	2.103(10)	O(2)-Zn(1)-O(10)	94.3(4)	O(6)-Zn(1)-O(11)	91.4(4)
Zn(1)-O(11)	2.123(9)	O(12)-Zn(1)-O(10)	87.0(3)	O(10)-Zn(1)-O(11)	175.7(3)
Compound 3					
O(1)-Zn(1)	2.023(3)	O(5)#2-Zn(1)-O(1)	107.51(11)	O(5)#2-Zn(1)-O(3)	84.30(12)
O(3)-Zn(1)	2.170(3)	O(1)-Zn(1)-O(3)	91.81(12)	O(5)#2-Zn(1)-O(4)	103.74(12)
O(4)-Zn(1)	2.063(3)	O(1)-Zn(1)-O(4)	148.35(12)	O(5)#2-Zn(1)-O(6)#4	92.26(12)
O(5)-Zn(1)#2	2.006(3)	O(1)-Zn(1)-O(6)#4	93.06(13)	O(6)#4-Zn(1)-O(3)	174.71(13)
O(6)-Zn(1)#3	2.044(3)	O(4)-Zn(1)-O(3)	86.38(12)	O(6)#4-Zn(1)-O(4)	90.55(13)
Compound 4'					
Co(1)-O(11)	2.026(3)	O(16)-Co(1)-O(16)#2	75.92(11)	O(1)-Co(1)-O(16)	135.08(11)
Co(1)-N(1)	2.062(4)	N(1)-Co(1)-O(16)#2	171.32(13)	O(11)-Co(1)-O(16)	129.01(12)
Co(1)-O(1)	2.045(3)	O(1)-Co(1)-O(16)#2	87.15(11)	O(1)-Co(1)-N(1)	98.42(14)

Co(1)-O(16)#2	2.314(3)	O(11)-Co(1)-O(16)#2	87.34(11)	O(11)-Co(1)-N(1)	99.21(14)
Co(1)-O(16)	2.103(3)	N(1)-Co(1)-O(16)	95.48(14)	O(11)-Co(1)-O(1)	90.45(12)
Compound 5					
N(1)-Zn(1)	2.094(4)	O(11)-Zn(1)-O(8)#3	100.50(13)	O(1)-Zn(1)-N(1)	87.61(14)
N(2)-Zn(1)	2.173(4)	O(11)-Zn(1)-O(1)	106.20(13)	O(11)-Zn(1)-N(2)	92.19(14)
O(1)-Zn(1)	2.089(3)	O(8)#3-Zn(1)-O(1)	92.66(14)	O(8)#3-Zn(1)-N(2)	95.87(15)
O(8)-Zn(1)#1	2.043(3)	O(11)-Zn(1)-N(1)	102.45(14)	O(1)-Zn(1)-N(2)	157.95(14)
O(11)-Zn(1)	1.985(3)	O(8)#3-Zn(1)-N(1)	156.00(14)	N(1)-Zn(1)-N(2)	76.42(16)
Compound 6					
Zn(1)-O(13)	1.972(4)	O(13)-Zn(1)-O(2)	100.88(16)	O(2)-Zn(1)-N(1)	95.20(15)
Zn(1)-O(2)	2.041(4)	N(2)-Zn(1)-N(1)	77.44(16)	O(2)-Zn(1)-N(2)	156.49(14)
Zn(1)-O(8)#1	2.087(4)	O(13)-Zn(1)-N(1)	91.35(15)	O(2)-Zn(1)-O(8)#1	93.06(15)
Zn(1)-N(2)	2.095(4)	O(13)-Zn(1)-N(2)	101.58(15)	O(8)#1-Zn(1)-N(1)	157.83(15)
Zn(1)-N(1)	2.181(4)	O(13)-Zn(1)-O(8)#1	107.24(14)	O(8)#1-Zn(1)-N(2)	86.86(15)
Compound 7					
Zn(1)-O(5)#1	1.936(2)	O(5)#1-Zn(1)-O(1)	103.85(10)	O(1)-Zn(1)-N(1)	97.43(10)
Zn(1)-O(1)	1.948(2)	O(5)#1-Zn(1)-N(2)#2	134.96(11)	N(2)#2-Zn(1)-N(1)	99.56(10)
Zn(1)-N(1)	2.087(2)	O(1)-Zn(1)-N(2)#2	109.56(10)		
Zn(1)-N(2)#2	2.029(2)	O(5)#1-Zn(1)-N(1)	105.21(11)		
Compound 8					
N(1)-Zn(1)	2.022(5)	O(1)-Zn(1)-O(3)#4	107.24(18)	O(3)#4-Zn(1)-N(2)#5	106.2(2)
N(2)-Zn(1)#2	2.066(5)	O(1)-Zn(1)-N(1)	111.64(19)	N(1)-Zn(1)-N(2)#5	99.4(2)
O(1)-Zn(1)	1.927(4)	O(3)#4-Zn(1)-N(1)	128.6(2)		
Zn(1)-O(3)#4	1.942(4)	O(1)-Zn(1)-N(2)#5	99.3(2)		
Compound 9					
N(1)-Zn(1)	2.048(5)	O(1)-Zn(1)-O(4)#4	104.29(18)	O(4)#4-Zn(1)-N(1)	108.6(2)
O(1)-Zn(1)	1.954(4)	O(1)-Zn(1)-N(4)#5	113.81(19)	N(4)#5-Zn(1)-N(1)	106.8(2)
O(4)-Zn(1)#3	1.974(5)	O(4)#4-Zn(1)-N(4)#5	121.6(2)		
Zn(1)-N(4)#5	2.025(5)	O(1)-Zn(1)-N(1)	99.50(19)		
Compound 10					
N(1)-Zn(1)	2.073(4)	Zn(1)-N(4)#5	2.022(4)	O(4)#4-Zn(1)-O(1)	110.66(14)
N(4)-Zn(1)#2	2.023(4)	O(4)#4-Zn(1)-N(1)	105.70(16)	O(4)#4-Zn(1)-N(4)#5	129.47(15)
O(1)-Zn(1)	1.952(3)	O(1)-Zn(1)-N(1)	97.13(14)	O(1)-Zn(1)-N(4)#5	107.62(14)
Zn(1)-O(4)#4	1.938(3)	N(4)#5-Zn(1)-N(1)	100.89(16)		

Symmetry transformations used to generate equivalent atoms: #1 $x+1, y+1, z$, #2 $x+2, y, z-1$, #3 $-x+1, -y+1, -z$, #4 $x, y-1, z$, #5 $-x-1, -y+1, -z+1$, #6 $-x, -y, -z+1$, #7 $x-2, y, z+1$, #8 $x, y+1, z$, #9 $-x-1, -y+2, -z+1$, #10 $x-1, y-1, z$ for **1**; #1 $-x+1, -y+1, -z+1$, #2 $-x+1, -y+1, -z$, #3 $-x, -y, -z$ for **2**; #1 $-x+1, y, -z+5/2$, #2 $-x+1/2, -y+1/2, -z$, #3 $-x+1/2, y+1/2, -z+1/2$, #4 $-x+1/2, y-1/2, -z+1/2$ for **3**; #1 $-x+1, -y+1, -z-1$, #2 $-x+1, -y+1, -z$ for **4**; #1 $x, y, z-1$, #2 $x, y, z+1$, #3 $-x+3, -y+3, -z+1$ for **5**; #1 $x, y, z+1$, #2 $-x, -y-1, -z+1$, #3 $x, y, z-1$ for **6**. #1 $x+1/2, -y+3/2, z+1/2$, #2 $-x+5/2, y+1/2, -z+3/2$, #3 $-x+5/2, y-1/2, -z+3/2$, #4 $-x-1, -y+2, -z+1$, #5 $x-1/2, -y+3/2, z-1/2$ for **7**; #1 $-x-2, -y+1, -z+1$, #2 $-x+3/2, y+1/2, -z+3/2$, #3 $x-1/2, -y+1/2, z-1/2$, #4 $x+1/2, -y+1/2, z+1/2$, #5 $-x+3/2, y-1/2, -z+3/2$ for **8**; #1 $-x-2, -y+1, -z$, #2 $-x+3/2, y+1/2, -z+1/2$, #3 $x-1/2, -y+3/2, z-1/2$, #4 $x+1/2, -y+3/2, z+1/2$, #5 $-x+3/2, y-1/2, -z+1/2$ for **9**; #1 $-x+4, -y, -z$, #2 $-x+1, y+1/2, -z+1/2$, #3 $x, -y+1/2, z-1/2$, #4 $x, -y+1/2, z+1/2$, #5 $-x+1, y-1/2, -z+1/2$ for **10**.

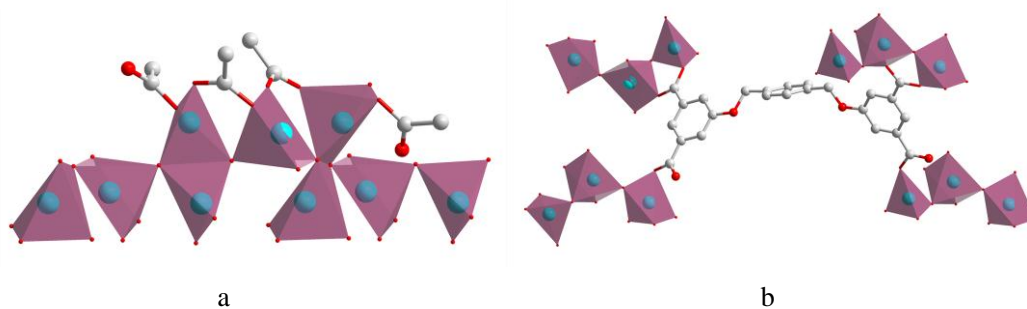


Fig. S1 a) Each Zn₃ cluster is linked by four L1 ligands and two Zn₃ clusters. b) Each L1 ligand links four Zn₃ clusters in compound **1**.

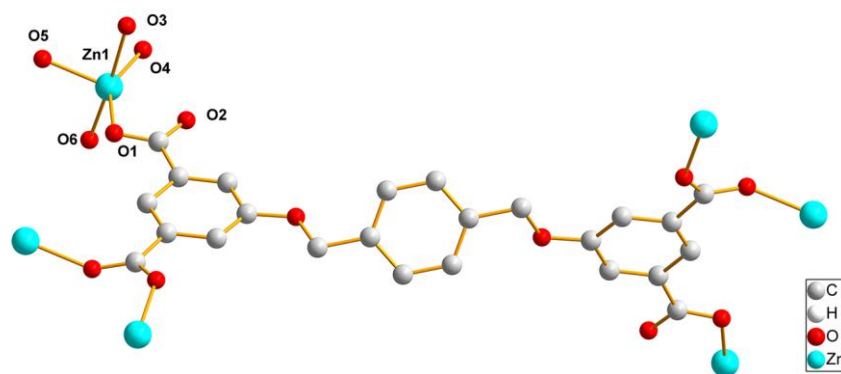


Fig. S2 The coordination geometries of Zn^{II} Center in compound **3**

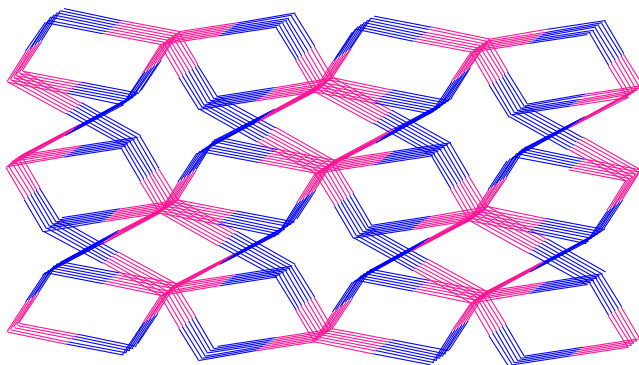


Fig. S3 (3.6)-connected 2-nodal net with a ant topology in **3**. (blue for 3-connected node and red for 6-connected node)

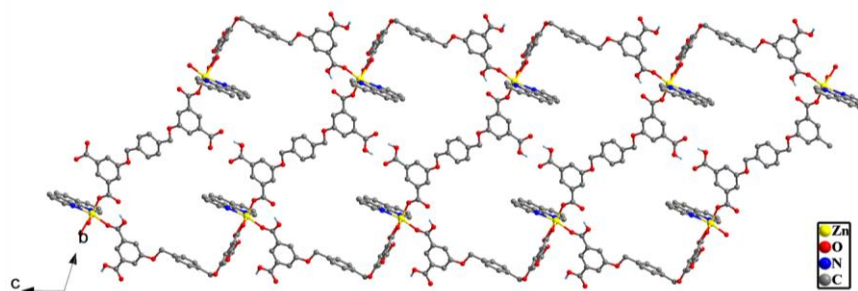


Fig. S4 1D ladder-like chain structure of **6** viewed down from a axis, the lattice water and hydrogen atoms are omitted for clarity.

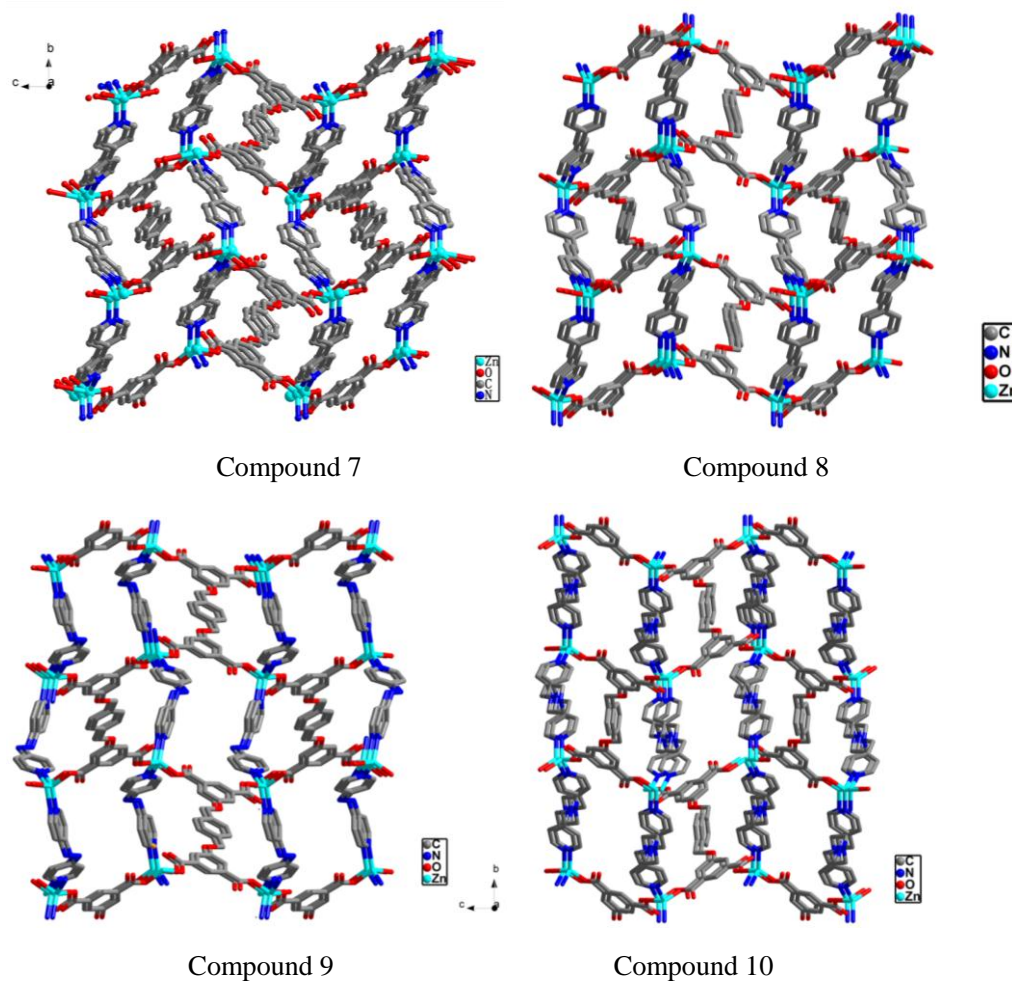
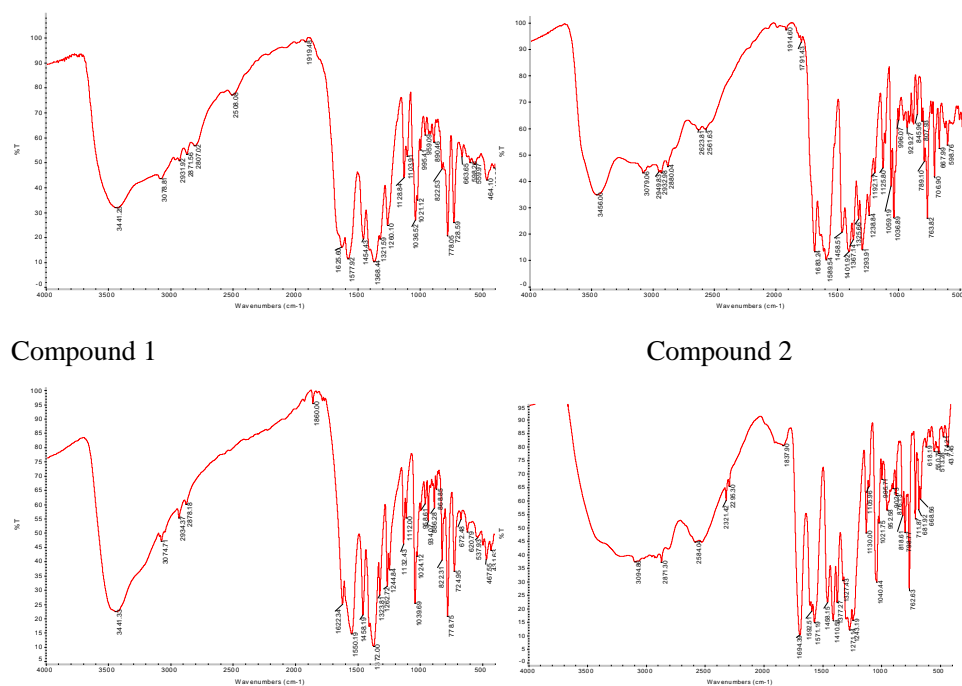
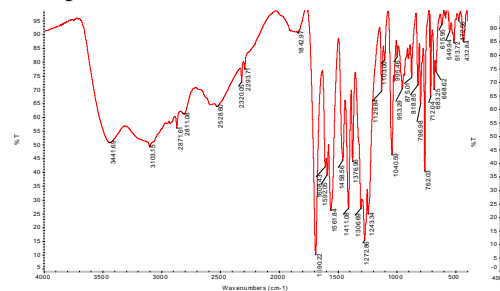


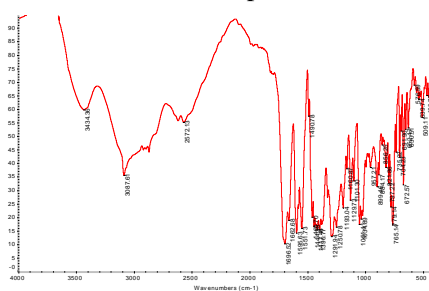
Fig. S5 3D structure of compounds 7~10.



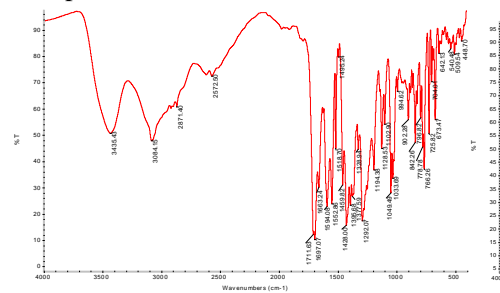
Compound 3



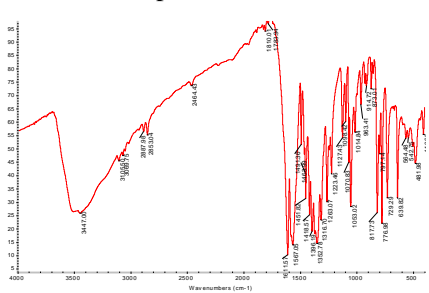
Compound 4



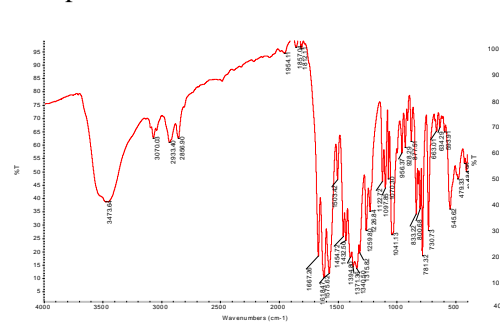
Compound 4'



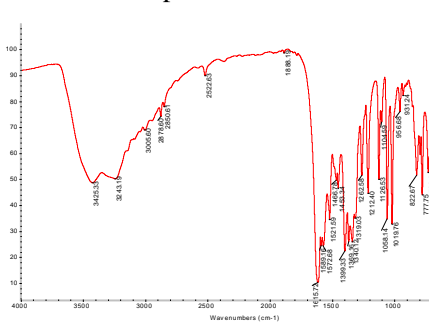
Compound 5



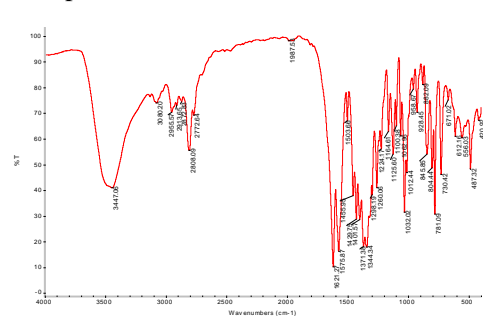
Compound 6



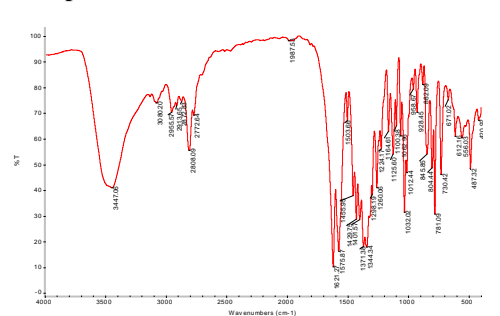
Compound 7



Compound 8

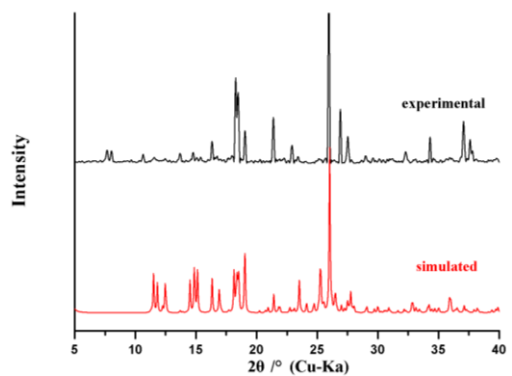


Compound 9

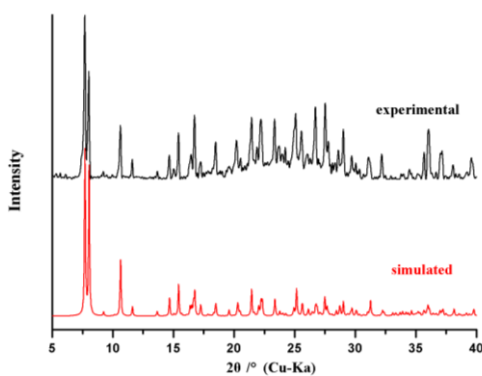


Compound 10

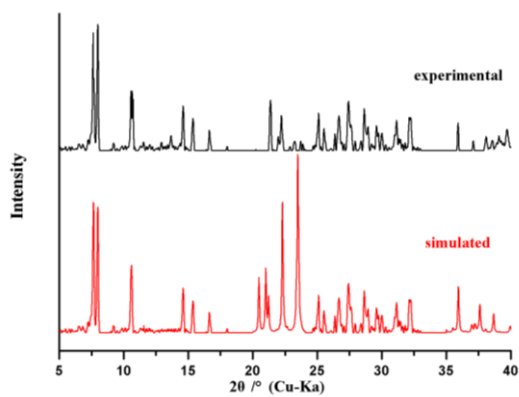
Fig. S6 IR Spectra of compounds 1~10.



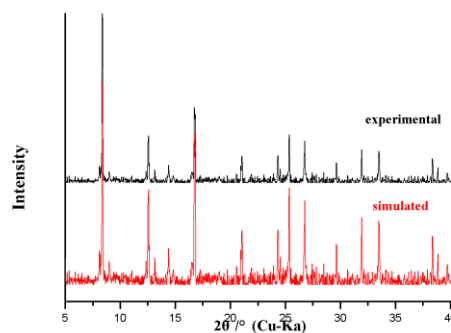
Compound 1



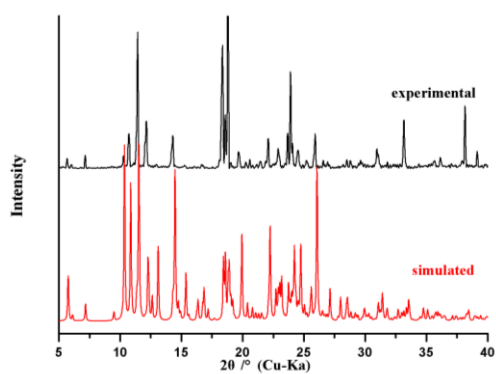
Compound 2



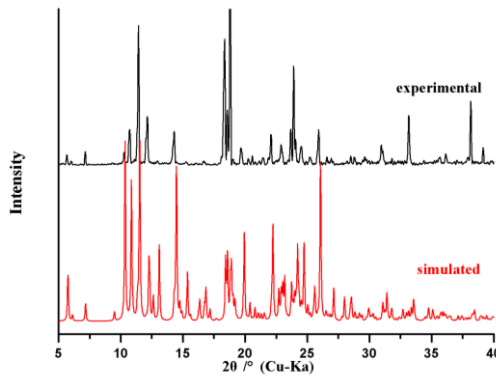
Compound 3



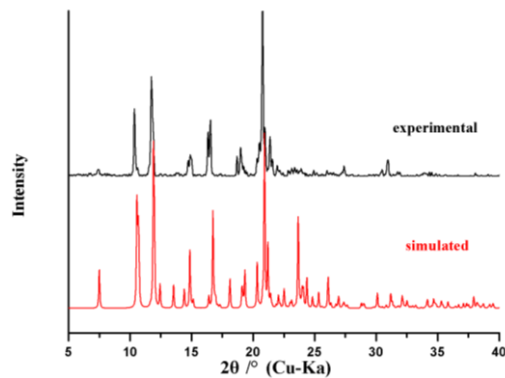
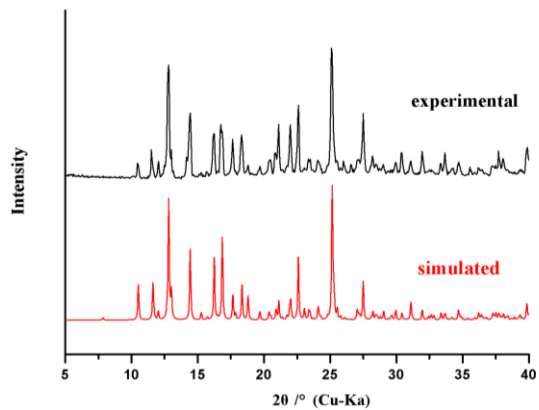
Compound 4



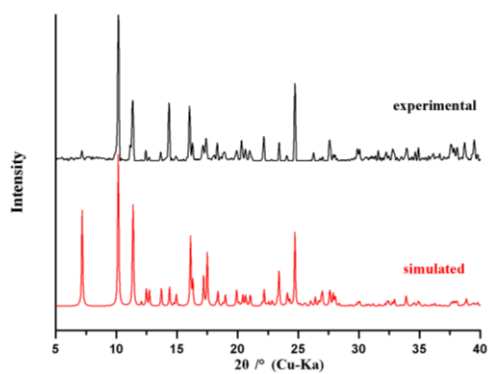
Compound 5



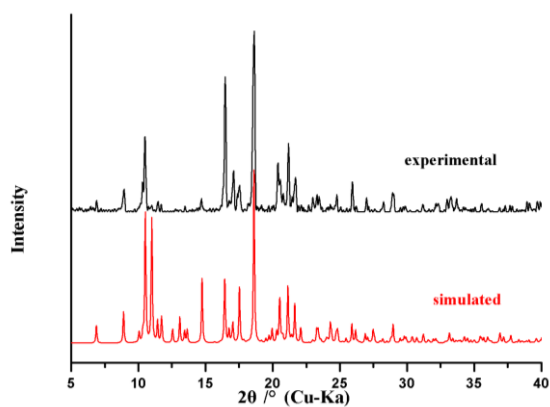
Compound 6



Compound 7



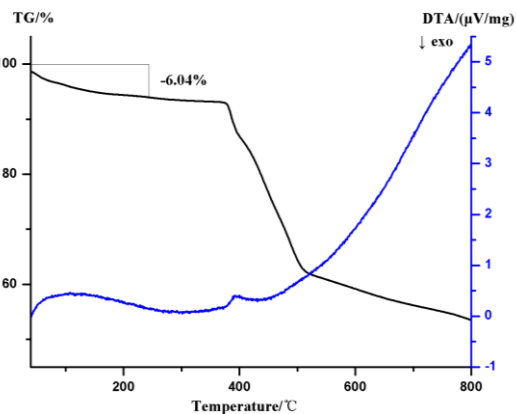
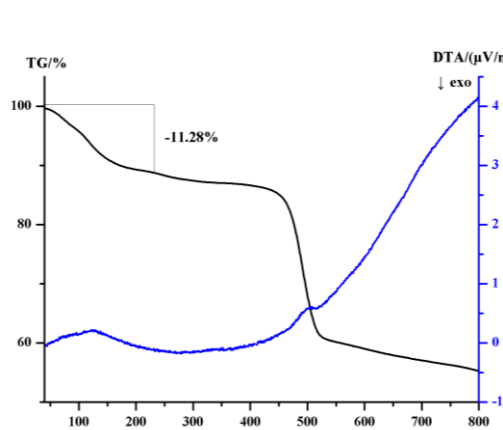
Compound 8



Compound 9

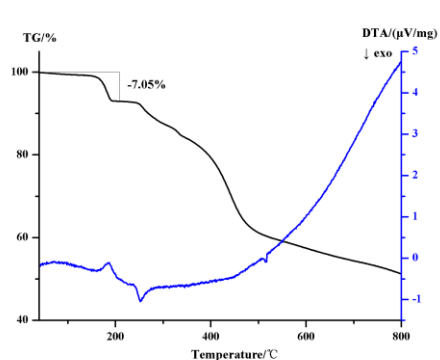
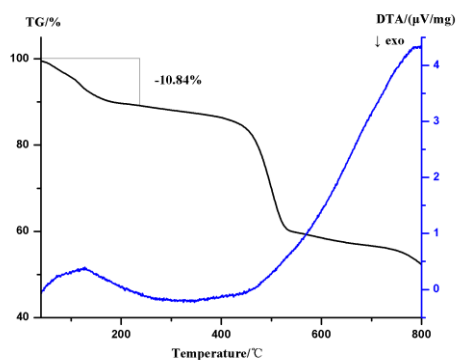
Compound 10

Fig S7 Powder X-ray diffractions (PXRD) for complexes **1-10**.



Compound 1

Compound 2



Compound 3

Compound 4

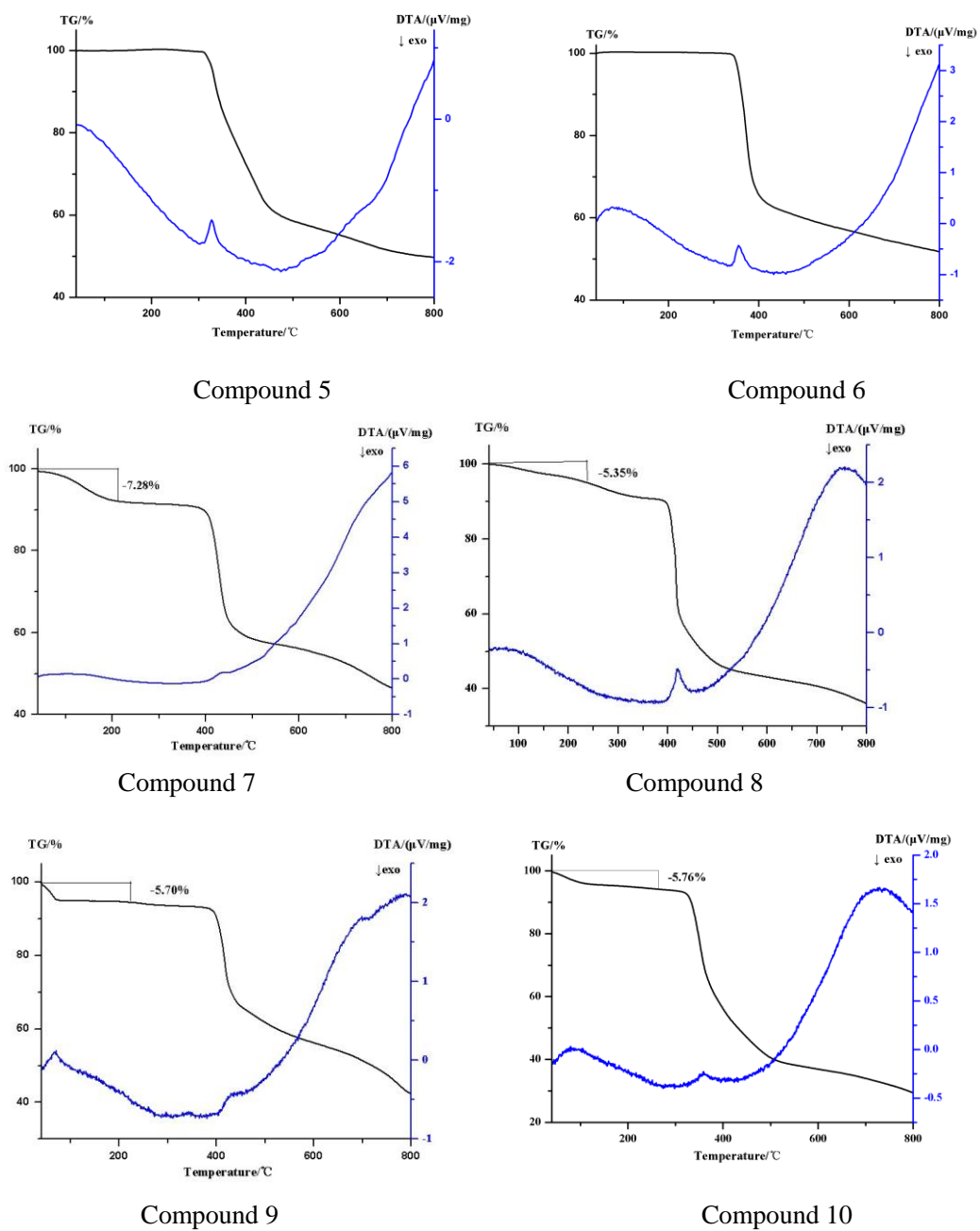


Fig S8 TGA curve for compounds 1-10.