Electronic Supplementary Information

Crystal structures from 1D to 3D: triggered by the different coordination morphologies of ligands in different reaction systems

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Contents

Table S1. Selected bond lengths [Å] and angles [º] for seven complexes.

Complex **1**

Zn(1)-O(1)	1.966(6)	O(1)-Zn(1)-O(4)#1	110.0(2)
Zn(1)-O(6)	1.980(7)	O(6)-Zn(1)-O(4)#1	111.4(3)
Zn(1)-O(4)#1	2.008(5)	O(1)-Zn(1)-O(5)	105.1(4)
Zn(1)-O(5)	2.040(7)	O(6)-Zn(1)-O(5)	111.0(3)
O(1)-Zn(1)-O(6)	118.9(3)	O(4)#1-Zn(1)-O(5)	98.3(3)

Symmetry codes: #1: x+1, y+1, z; #2: x-1, y-1, z.

Complex **2**

Zn(1)-O(5)	1.988(4)	O(5)-Zn(1)-O(3)#2	96.22(15)
Zn(1)-O(4)#1	2.012(4)	O(4)#1-Zn(1)-O(3)#2	158.28(17)
Zn(1)-O(1)	2.015(4)	O(1)-Zn(1)-O(3)#2	93.78(16)
Zn(1)-O(3)#2	2.057(3)	O(5)-Zn(1)-O(2)#3	92.59(17)
Zn(1)-O(2)#3	2.077(4)	O(4)#1-Zn(1)-O(2)#3	86.86(18)
O(5)-Zn(1)-O(4)#1	103.84(16)	O(1)-Zn(1)-O(2)#3	158.59(17)
O(5)-Zn(1)-O(1)	108.81(17)	O(3)#2-Zn(1)-O(2)#3	83.99(16)
O(4)#1-Zn(1)-O(1)	87.62(18)		

Symmetry codes: #1: x+1, y, z; #2: -x, -y+2, -z; #3: -x+1, -y+2, -z.

Complex **3**

Zn(1)-O(7)#1	2.063(4)	O(4)#3-Zn(1)-O(1)#1	88.2(2)
Zn(1)-O(7)	2.063(4)	O(7)#1-Zn(1)-O(1)	85.06(16)
Zn(1)-O(4)#2	2.094(5)	O(7)-Zn(1)-O(1)	94.94(16)
Zn(1)-O(4)#3	2.094(5)	O(4)#2-Zn(1)-O(1)	88.2(2)
Zn(1)-O(1)#1	2.096(5)	O(4)#3-Zn(1)-O(1)	91.8(2)
Zn(1)-O(1)	2.096(5)	O(1)#1-Zn(1)-O(1)	180.0(3)
Zn(2)-O(7)	2.059(4)	O(7)-Zn(2)-O(7)#4	81.85(17)
Zn(2)-O(7)#4	2.070(4)	O(7)-Zn(2)-O(3)#5	95.17(17)
Zn(2)-O(3)#5	2.091(4)	O(7)#4-Zn(2)-O(3)#5	97.78(16)
Zn(2)-O(5)	2.133(4)	O(7)-Zn(2)-O(5)	95.74(18)
Zn(2)-O(6)	2.172(4)	O(7)#4-Zn(2)-O(5)	176.74(16)
Zn(2)-O(2)	2.218(4)	O(3)#5-Zn(2)-O(5)	84.59(17)
O(7)#1-Zn(1)-O(7)	180.0(2)	O(7)-Zn(2)-O(6)	173.11(16)
O(7)#1-Zn(1)-O(4)#2	95.43(18)	O(7)#4-Zn(2)-O(6)	93.73(17)
O(7)-Zn(1)-O(4)#2	84.57(18)	O(3)#5-Zn(2)-O(6)	90.66(18)
O(7)#1-Zn(1)-O(4)#3	84.57(18)	O(5)-Zn(2)-O(6)	88.46(18)
O(7)-Zn(1)-O(4)#3	95.43(18)	O(7)-Zn(2)-O(2)	94.62(16)
O(4)#2-Zn(1)-O(4)#3	180.00(18)	O(7)#4-Zn(2)-O(2)	91.48(16)
O(7)#1-Zn(1)-O(1)#1	94.94(16)	O(3)#5-Zn(2)-O(2)	167.38(17)
O(7)-Zn(1)-O(1)#1	85.06(16)	O(5)-Zn(2)-O(2)	86.52(17)
O(4)#2-Zn(1)-O(1)#1	91.8(2)	O(6)-Zn(2)-O(2)	80.15(17)

Symmetry codes: #1: -x+1, -y+1, -z; #2: -x+1, y-1/2, -z+1/2; #3: x, -y+3/2, z-1/2; #4: -

x+1, -y+2, -z; #5: -x+1, y+1/2, -z+1/2.

Complex **4**

O(3)-Zn(2)	1.991(4)	O(5)#2-Zn(1)-O(7)#3	97.86(17)
Zn(1)-O(5)#2	1.872(4)	O(4)#1-Zn(1)-O(7)#3	103.25(17)
Zn(1)-O(4)#1	1.900(4)	O(1)-Zn(1)-O(7)#3	110.96(18)
Zn(1)-O(1)	1.907(3)	O(2)-Zn(2)-O(10)	113.81(17)
Zn(1)-O(7)#3	1.936(4)	O(2)-Zn(2)-O(8)#3	129.73(19)
Zn(2)-O(2)	1.879(4)	O(10)-Zn(2)-O(8)#3	109.55(17)
Zn(2)-O(10)	1.889(4)	O(2)-Zn(2)-O(3)	105.41(18)
Zn(2)-O(8)#3	1.891(4)	O(10)-Zn(2)-O(3)	91.75(18)
Zn(2)-O(9)	2.347(8)	O(8)#3-Zn(2)-O(3)	97.30(16)
C(14)#1-O(3)-Zn(2)	138.6(3)	O(2)-Zn(2)-O(9)	79.2(3)
O(5)#2-Zn(1)-O(4)#1	117.42(19)	O(10)-Zn(2)-O(9)	85.2(3)
O(5)#2-Zn(1)-O(1)	112.11(19)	O(8)#3-Zn(2)-O(9)	80.4(2)
O(4)#1-Zn(1)-O(1)	113.53(17)	O(3)-Zn(2)-O(9)	175.2(3)

Symmetry codes: #1: -x+2, -y+1, -z+2; #2: x+1, -y+1/2, z+1/2; #3: x+1, y, z+1.

Complex **5**

Cd(1)-O(1)	2.343(4)	O(1)-Cd(1)-O(4)#3	109.87(12)
Cd(1)-O(1)#1	2.343(4)	O(1)#1-Cd(1)-O(4)#3	127.64(14)
Cd(1)-O(3)#2	2.346(4)	O(3)#2-Cd(1)-O(4)#3	138.83(17)
Cd(1)-O(3)#3	2.346(4)	O(3)#3-Cd(1)-O(4)#3	53.11(15)
Cd(1)-O(4)#2	2.519(5)	O(4)#2-Cd(1)-O(4)#3	87.39(18)
Cd(1)-O(4)#3	2.519(5)	O(1)-Cd(1)-O(2)#1	151.07(13)
Cd(1)-O(2)#1	2.522(4)	O(1)#1-Cd(1)-O(2)#1	53.29(13)
Cd(1)-O(2)	2.522(4)	O(3)#2-Cd(1)-O(2)#1	87.43(16)
O(1)-Cd(1)-O(1)#1	97.81(18)	O(3)#3-Cd(1)-O(2)#1	95.13(16)
O(1)-Cd(1)-O(3)#2	89.84(15)	O(4)#2-Cd(1)-O(2)#1	71.62(14)
O(1)#1-Cd(1)-O(3)#2	82.19(17)	O(4)#3-Cd(1)-O(2)#1	90.58(13)
O(1)-Cd(1)-O(3)#3	82.19(17)	O(1)-Cd(1)-O(2)	53.29(13)
O(1)#1-Cd(1)-O(3)#3	89.84(15)	O(1)#1-Cd(1)-O(2)	151.07(13)
O(3)#2-Cd(1)-O(3)#3	167.9(3)	O(3)#2-Cd(1)-O(2)	95.13(16)
O(1)-Cd(1)-O(4)#2	127.64(14)	O(3)#3-Cd(1)-O(2)	87.43(16)
O(1)#1-Cd(1)-O(4)#2	109.87(13)	O(4)#2-Cd(1)-O(2)	90.58(13)
O(3)#2-Cd(1)-O(4)#2	53.11(15)	O(4)#3-Cd(1)-O(2)	71.62(14)
O(3)#3-Cd(1)-O(4)#2	138.83(16)	O(2)#1-Cd(1)-O(2)	155.64(19)

Symmetry codes: #1: -x, y, -z+1/2; #2: -x+1, y, -z+1/2; #3: x-1, y, z.

Complex **6**

Cd(1)-O(2)	2.214(9)	O(8)#2-Cd(1)-O(6)#3	90.3(3)
Cd(1)-O(3)#1	2.247(8)	O(9)-Cd(1)-O(6)#3	91.7(3)
Cd(1)-O(8)#2	2.266(10)	O(5)#3-Cd(1)-O(6)#3	54.4(2)
Cd(1)-O(9)	2.308(9)	O(7)#4-Cd(2)-O(1)	92.6(4)

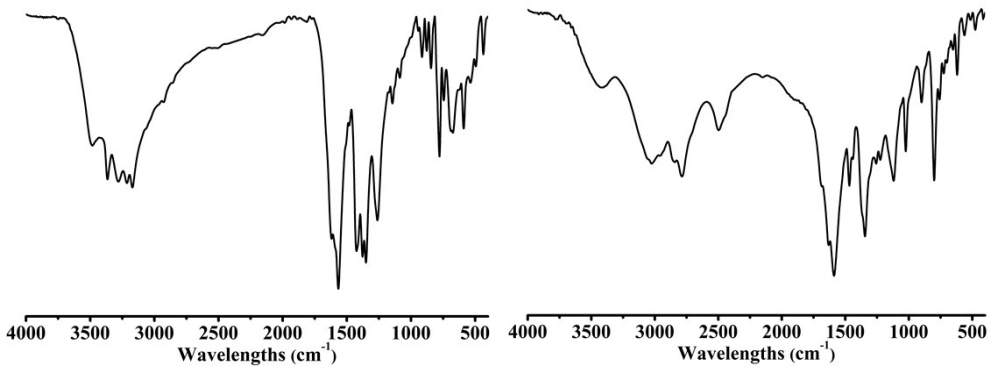
Cd(1)-O(5)#3	2.382(7)	O(7)#4-Cd(2)-O(10)	91.4(4)
Cd(1)-O(6)#3	2.454(8)	O(1)-Cd(2)-O(10)	175.7(4)
Cd(2)-O(7)#4	2.220(9)	O(7)#4-Cd(2)-O(5)#3	151.4(3)
Cd(2)-O(1)	2.272(11)	O(1)-Cd(2)-O(5)#3	87.8(4)
Cd(2)-O(10)	2.312(10)	O(10)-Cd(2)-O(5)#3	89.3(3)
Cd(2)-O(5)#3	2.318(7)	O(7)#4-Cd(2)-O(4)#5	133.0(4)
Cd(2)-O(4)#5	2.359(9)	O(1)-Cd(2)-O(4)#5	84.0(4)
Cd(2)-O(11)	2.431(17)	O(10)-Cd(2)-O(4)#5	92.2(4)
Cd(2)-O(3)#5	2.610(9)	O(5)#3-Cd(2)-O(4)#5	75.5(3)
O(2)-Cd(1)-O(3)#1	104.2(4)	O(7)#4-Cd(2)-O(11)	74.6(5)
O(2)-Cd(1)-O(8)#2	84.1(4)	O(1)-Cd(2)-O(11)	85.2(5)
O(3)#1-Cd(1)-O(8)#2	105.2(3)	O(10)-Cd(2)-O(11)	97.2(6)
O(2)-Cd(1)-O(9)	91.5(4)	O(5)#3-Cd(2)-O(11)	76.9(4)
O(3)#1-Cd(1)-O(9)	92.6(3)	O(4)#5-Cd(2)-O(11)	150.8(5)
O(8)#2-Cd(1)-O(9)	162.1(3)	O(7)#4-Cd(2)-O(3)#5	83.3(3)
O(2)-Cd(1)-O(5)#3	118.1(3)	O(1)-Cd(2)-O(3)#5	94.1(4)
O(3)#1-Cd(1)-O(5)#3	137.0(3)	O(10)-Cd(2)-O(3)#5	85.1(3)
O(8)#2-Cd(1)-O(5)#3	87.2(3)	O(5)#3-Cd(2)-O(3)#5	125.2(3)
O(9)-Cd(1)-O(5)#3	79.6(3)	O(4)#5-Cd(2)-O(3)#5	50.4(3)
O(2)-Cd(1)-O(6)#3	171.0(3)	O(11)-Cd(2)-O(3)#5	157.8(4)
O(3)#1-Cd(1)-O(6)#3	84.0(3)		

Symmetry codes: #1: x, y, z+1; #2: -x+1, y+1/2, -z; #3: -x+2, y+1/2, -z+1; #4: -x+2, y+1/2, -z; #5: x+1, y, z+1.

Complex **7**

Pb(1)-O(1)	2.388(12)	O(1)-Pb(1)-O(5)	75.0(5)
Pb(1)-O(3)#1	2.409(14)	O(3)#1-Pb(1)-O(5)	74.4(5)
Pb(1)-O(5)	2.568(15)	O(1)-Pb(1)-O(2)	50.7(4)
Pb(1)-O(2)	2.721(14)	O(3)#1-Pb(1)-O(2)	72.2(5)
O(1)-Pb(1)-O(3)#1	82.4(5)	O(5)-Pb(1)-O(2)	118.5(5)

Symmetry code: #1: x, y+1, z.



(a) **(b)**

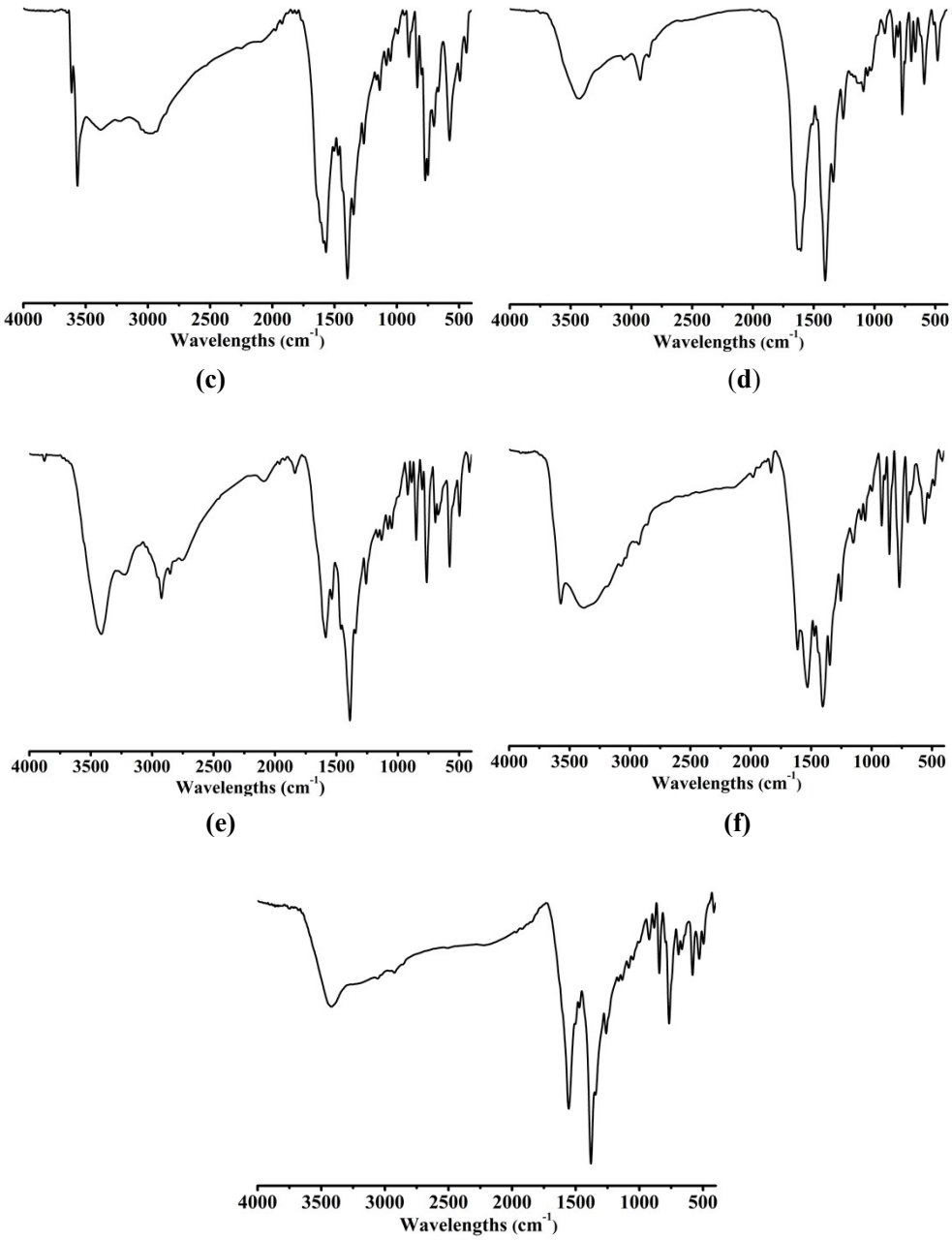


Fig. S1 The FT-IR spectra of **1-(a)**; **2-(b)**; **3-(c)**; **4-(d)**; **5-(e)**; **6-(f)**; **7-(g)**.

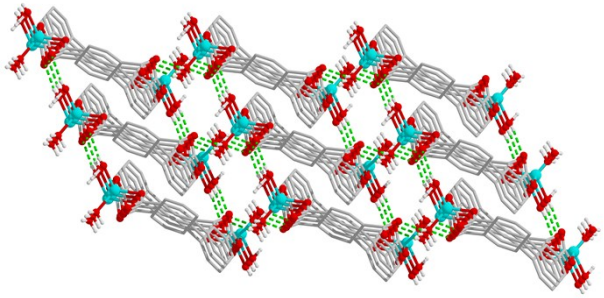


Fig. S2 The 3D supramolecular framework of **1**.

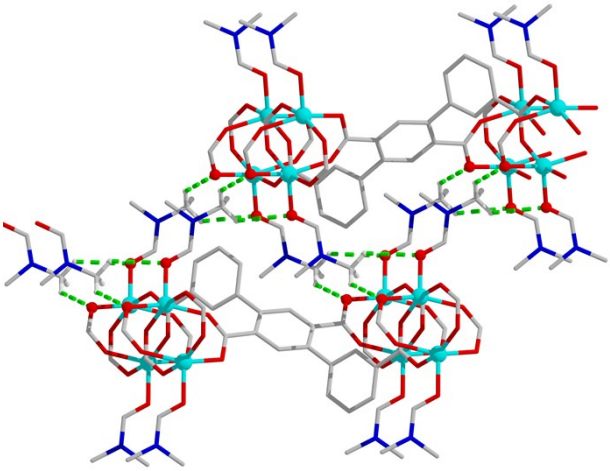


Fig. S3 The C13-H13C···O5 (2.67 Å) and C13-H13B···O4 (2.8 Å) H-bonds exist between the neighboring layers.

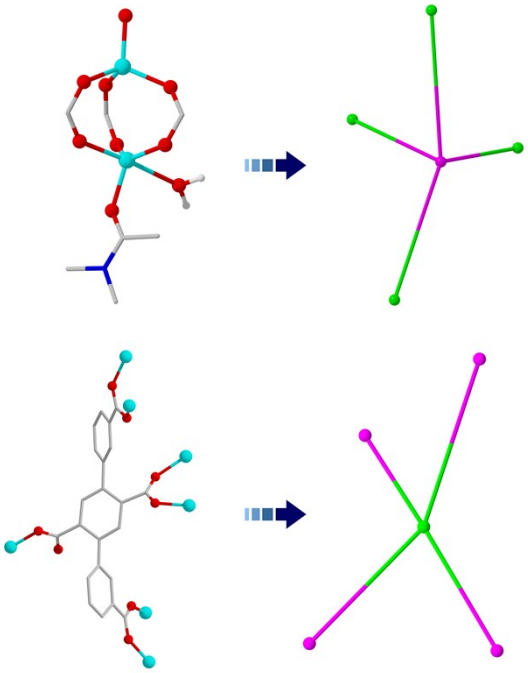


Fig. S4 Both metal ions and organic linkers are viewed as 4-connected nodes in **4**.

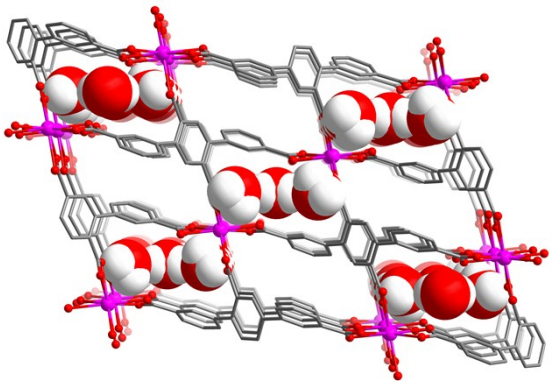


Fig. S5 The space-filling structure for **5**.

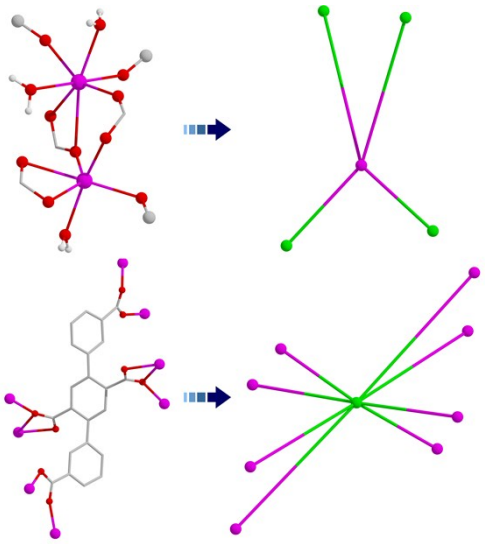


Fig. S6 The dinuclear metal ions and organic linkers can be acted as 4,8-connected nodes in **6**.

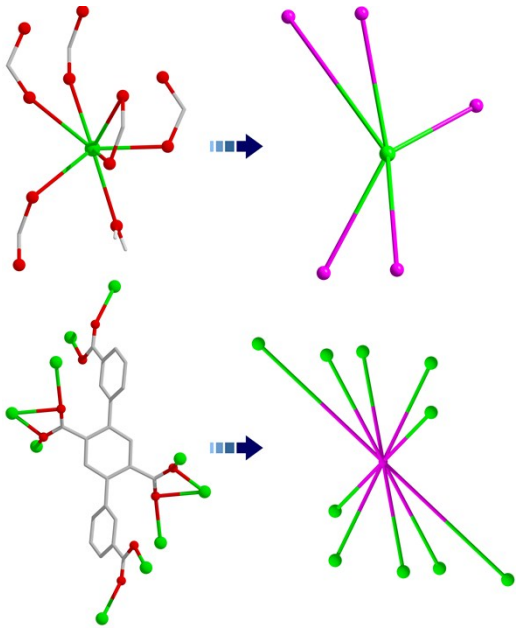
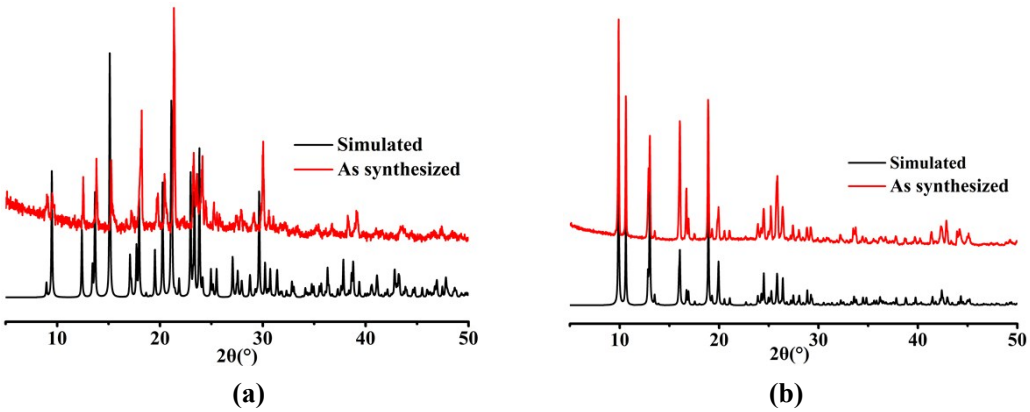


Fig. S7 The dinuclear metal ions and organic linkers can be acted as 5,10-connected nodes in **7**.



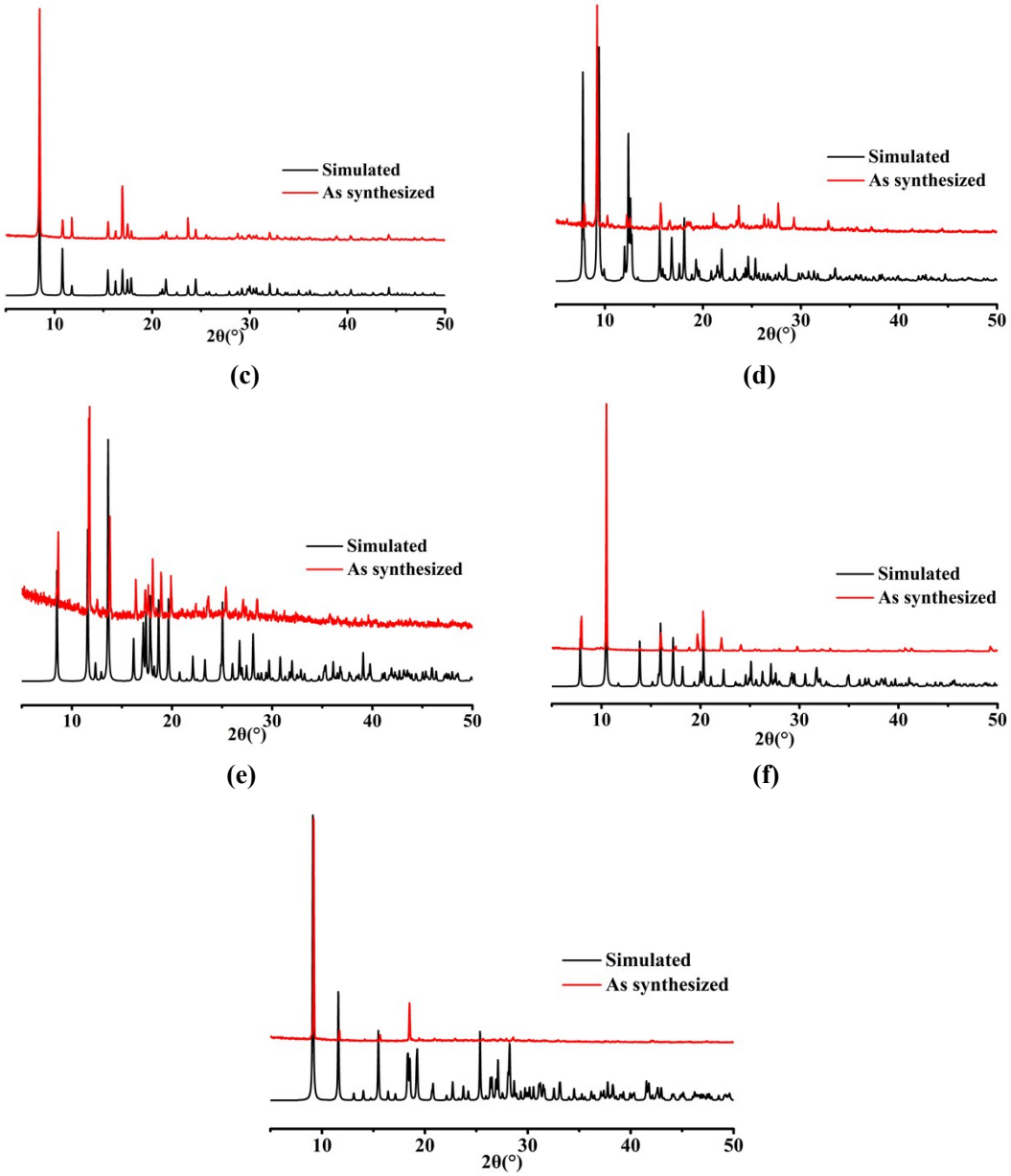


Fig. S8 PXRD patterns of complex after experimented well matched with the synthesized and simulated: **1-(a)**; **2-(b)**; **3-(c)**; **4-(d)**; **5-(e)**; **6-(f)**; **7-(g)**.

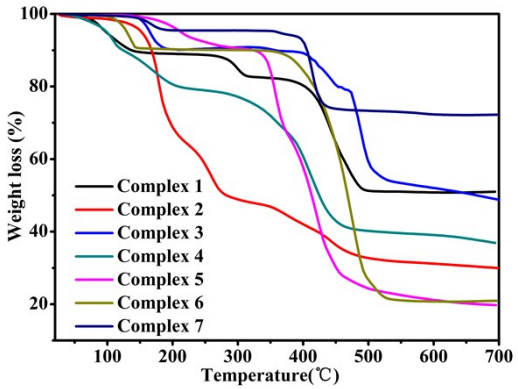


Fig. S9 TGA curves for the complexes.