Supporting information

Syntheses, Structures, and Properties of Six New Coordination polymers Constructed by N-heterocyclic Multicarboxylic Acids

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Table S1 Selected bond lengths (Å) and angles (°) for {[Zn_2(Hpdtc)$_2$(Hbpe)$_2$]·5H_2O} (**1**)

Zn(1)-O(9)	1.959(2)	Zn(2)-O(3)	1.971(2)
Zn(1)-N(3)	2.024(2)	Zn(2)-N(5)	2.025(2)
Zn(1)-N(1)	2.048(2)	Zn(2)-N(2)	2.048(2)
Zn(1)-O(1)	2.133(2)	Zn(2)-O(14)	2.102(2)
Zn(1)-O(8)	2.144(2)	Zn(2)-O(15)	2.132(2)
O(9)-Zn(1)-N(3)	102.05(9)	O(9)-Zn(1)-N(1)	124.34(9)
N(3)-Zn(1)-N(1)	133.59(10)	O(9)-Zn(1)-O(1)	103.38(9)
N(3)-Zn(1)-O(1)	94.37(9)	N(1)-Zn(1)-O(1)	77.37(9)
O(9)-Zn(1)-O(8)	93.11(9)	N(3)-Zn(1)-O(8)	102.61(9)
N(1)-Zn(1)-O(8)	76.02(9)	O(1)-Zn(1)-O(8)	153.33(8)
O(3)-Zn(2)-N(5)	103.86(9)	O(3)-Zn(2)-N(2)	131.20(9)
N(5)-Zn(2)-N(2)	124.89(10)	O(3)-Zn(2)-O(14)	94.16(9)
N(5)-Zn(2)-O(14)	100.04(9)	N(2)-Zn(2)-O(14)	76.80(9)
O(3)-Zn(2)-O(15)	102.72(8)	N(5)-Zn(2)-O(15)	95.12(9)
N(2)-Zn(2)-O(15)	77.10(9)	O(14)-Zn(2)-O(15)	153.90(8)
C(1)-O(1)-Zn(1)	116.47(18)	C(8)-O(3)-Zn(2)	132.06(19)
C(7)-O(8)-Zn(1)	116.04(18)	C(18)-O(9)-Zn(1)	138.01(19)
C(10)-O(14)-Zn(2)	116.45(18)	C(16)-O(15)-Zn(2)	115.97(18)
C(6)-N(1)-Zn(1)	120.02(19)	C(15)-N(2)-Zn(2)	117.8(2)
C(2)-N(1)-Zn(1)	116.77(19)	C(11)-N(2)-Zn(2)	118.9(2)
C(19)-N(3)-Zn(1)	123.1(2)	C(31)-N(5)-Zn(2)	122.5(2)
C(23)-N(3)-Zn(1)	119.6(2)	C(35)-N(5)-Zn(2)	120.1(2)

Table S2 Selected bond lengths (Å) and angles (°) for $[Zn_2(pdtc)(bpe)_{1.5}]_n$ (**2**)

Zn(1)-O(5)#1	1.976(2)	Zn(2)-O(4)#1	1.947(2)
Zn(1)-N(2)	1.988(3)	Zn(2)-O(7)	1.9732(19)
Zn(1)-N(1)	2.012(2)	Zn(2)-O(6)#2	1.9802(19)
Zn(1)-O(1)	2.072(2)	Zn(2)-N(4)	2.027(3)
Zn(1)-O(8)	2.2623(19)	O(5)#1-Zn(1)-N(2)	116.85(10)
O(5)#1-Zn(1)-N(1)	111.64(9)	N(2)-Zn(1)-N(1)	131.48(10)
O(5)#1-Zn(1)-O(1)	92.58(9)	N(2)-Zn(1)-O(1)	99.21(9)
N(1)-Zn(1)-O(1)	79.81(8)	O(5)#1-Zn(1)-O(8)	101.63(8)
N(2)-Zn(1)-O(8)	93.90(8)	N(1)-Zn(1)-O(8)	74.52(8)
O(1)-Zn(1)-O(8)	153.79(8)	O(4)#1-Zn(2)-O(7)	123.77(8)
O(4)#1-Zn(2)-O(6)#2	101.22(8)	O(7)-Zn(2)-O(6)#2	102.18(8)
O(4)#1-Zn(2)-N(4)	99.93(10)	O(7)-Zn(2)-N(4)	112.73(9)
O(6)#2-Zn(2)-N(4)	117.54(9)	C(1)-O(1)-Zn(1)	114.18(17)
C(7)-O(4)-Zn(2)#1	130.19(19)	C(8)-O(5)-Zn(1)#1	135.8(2)
C(8)-O(6)-Zn(2)#2	119.42(18)	C(9)-O(7)-Zn(2)	116.15(19)
C(9)-O(8)-Zn(1)	113.76(17)	C(2)-N(1)-C(6)	122.1(3)
C(2)-N(1)-Zn(1)	114.95(19)	C(6)-N(1)-Zn(1)	122.30(19)
C(10)-N(2)-Zn(1)	119.8(2)	C(14)-N(2)-Zn(1)	121.9(2)
C(26)-N(4)-Zn(2)	119.9(2)	C(22)-N(4)-Zn(2)	122.5(2)

The symmetry code: #1 -x+1, -y+1, -z+2; #2 -x, -y+1, -z+2.

Table S3 Selected bond lengths (Å) and angles (°) for Zn(Hpztc)(Hbpe)(H_2O)] (**3**)

Zn(1)-N(3)	2.0572(19)	Zn(1)-N(1)	2.0886(18)
Zn(1)-O(1)	2.0640(17)	Zn(1)-O(4)	2.1172(17)
Zn(1)-O(9)	2.1313(18)	Zn(1)-O(8)	2.2619(16)
O(1)-Zn(1)-N(3)	118.15(7)	N(3)-Zn(1)-N(1)	163.31(7)
O(1)-Zn(1)-N(1)	78.48(7)	N(3)-Zn(1)-O(4)#1	85.57(7)
O(1)-Zn(1)-O(4) #1	100.67(6)	C(1)-O(1)-Zn(1)	117.03(14)
N(1)-Zn(1)-O(4) #1	90.03(7)	C(4)-O(4)-Zn(1)#1	142.75(15)
N(3)-Zn(1)-O(9)	88.29(7)	C(8)-O(8)-Zn(1)	116.30(14)
O(1)-Zn(1)-O(9)	88.31(7)	Zn(1)-O(9)-H(9A)	114.4(17)
N(1)-Zn(1)-O(9)	93.93(7)	Zn(1)-O(9)-H(9B)	108(2)
O(4)#1-Zn(1)-O(9)	170.77(6)	C(2)-N(1)-Zn(1)	114.71(14)
N(3)-Zn(1)-O(8)	91.21(7)	C(7)-N(1)-Zn(1)	122.73(15)
O(1)-Zn(1)-O(8)	150.46(6)	C(13)-N(3)-Zn(1)	122.99(16)
N(1)-Zn(1)-O(8)	72.30(7)	C(9)-N(3)-Zn(1)	119.27(15)
O(4)#1-Zn(1)-O(8)	83.81(6)	O(9)-Zn(1)-O(8)	89.44(6)

The symmetry code: #1 -x+1, -y, -z.

Table S4 Selected bond lengths (Å) and angles (°) for {[Zn2(pztc)(bpe)2(H2O]·9H2O}$_n$ (**4**)

Zn(1)-O(3)	2.0629(19)	Zn(1)-O(3)#1	2.0629(19)
Zn(1)-N(2)#1	2.123(2)	Zn(1)-N(2)	2.123(2)
Zn(1)-N(1)#1	2.342(2)	Zn(1)-N(1)	2.342(2)
Zn(2)-O(5)#2	2.043(2)	Zn(2)-O(5)	2.043(2)
Zn(2)-O(4)	2.1220(17)	Zn(2)-O(4)#2	2.1220(17)
Zn(2)-N(3)	2.144(2)	Zn(2)-N(3)#2	2.144(2)
O(3)-Zn(1)-O(3)#1	180.000(1)	O(3)-Zn(1)-N(2)#1	89.95(9)
O(3)#1-Zn(1)-N(2)#1	90.05(9)	O(3)-Zn(1)-N(2)	90.05(9)
O(3)#1-Zn(1)-N(2)	89.95(9)	N(2)#1-Zn(1)-N(2)	180.0
O(3)-Zn(1)-N(1)#1	103.80(7)	O(3)#1-Zn(1)-N(1)#1	76.20(7)
N(2)#1-Zn(1)-N(1)#1	92.47(8)	N(2)-Zn(1)-N(1)#1	87.53(8)
O(3)-Zn(1)-N(1)	76.20(7)	O(3)#1-Zn(1)-N(1)	103.80(7)
N(2)#1-Zn(1)-N(1)	87.53(8)	N(2)-Zn(1)-N(1)	92.47(8)
N(1)#1-Zn(1)-N(1)	180.0	O(5)#2-Zn(2)-O(5)	180.0
O(5)#2-Zn(2)-O(4)	86.64(8)	O(5)-Zn(2)-O(4)	93.36(8)
O(5)#2-Zn(2)-O(4)#2	93.36(8)	O(5)-Zn(2)-O(4)#2	86.64(8)
O(4)-Zn(2)-O(4)#2	180.0	O(5)#2-Zn(2)-N(3)	89.38(13)
O(5)-Zn(2)-N(3)	90.63(13)	O(4)-Zn(2)-N(3)	91.42(8)
O(4)#2-Zn(2)-N(3)	88.58(8)	O(5)#2-Zn(2)-N(3)#2	90.63(13)
O(5)-Zn(2)-N(3)#2	89.37(13)	O(4)-Zn(2)-N(3)#2	88.58(8)
O(4)#2-Zn(2)-N(3)#2	91.42(8)	N(3)-Zn(2)-N(3)#2	180.0
C(4)-O(3)-Zn(1)	119.99(15)	C(4)-O(4)-Zn(2)	132.01(16)
Zn(2)-O(5)-H(5A)	122(2)	Zn(2)-O(5)-H(5B)	116(2)
C(3)-N(1)-Zn(1)	107.51(15)	C(2)-N(1)-Zn(1)	133.72(17)
C(5)-N(2)-Zn(1)	122.53(18)	C(9)-N(2)-Zn(1)	119.74(18)
C(15)-N(3)-Zn(2)	120.73(19)	C(11)-N(3)-Zn(2)	121.7(2)

The symmetry code: #1 -x+2, -y+1, -z; #2 -x+1, -y+2, -z.

Table S5 Selected bond lengths (Å) and angles (°) for {[Cu_2(pdtc)(bpy)(H_2O)$_2$]·3H_2O}$_n$ (**5**)

Cu(1)-N(1)	1.916(4)	Cu(1)-N(2)	1.952(4)
Cu(1)-O(2)	2.012(3)	Cu(1)-O(3)	2.028(3)
Cu(1)-O(9)	2.289(4)	Cu(2)-O(10)	1.952(3)
Cu(2)-O(6)#1	1.961(3)	Cu(2)-O(7)	1.968(3)
Cu(2)-N(3)#2	2.006(3)	O(6)-Cu(2)#3	1.961(3)
N(1)-Cu(1)-N(2)	167.88(19)	N(1)-Cu(1)-O(2)	80.89(13)
N(2)-Cu(1)-O(2)	102.13(13)	N(1)-Cu(1)-O(3)	80.33(13)
N(2)-Cu(1)-O(3)	94.42(13)	O(2)-Cu(1)-O(3)	159.01(13)
N(1)-Cu(1)-O(9)	101.14(15)	N(2)-Cu(1)-O(9)	90.53(16)
O(2)-Cu(1)-O(9)	92.13(13)	O(3)-Cu(1)-O(9)	100.62(13)
O(10)-Cu(2)-O(6)#1	87.02(13)	O(10)-Cu(2)-O(7)	89.19(12)
O(6)#1-Cu(2)-O(7)	170.83(15)	O(10)-Cu(2)-N(3)#2	171.64(18)
O(6)#1-Cu(2)-N(3)#2	89.69(13)	O(7)-Cu(2)-N(3)#2	92.91(13)
C(1)-O(2)-Cu(1)	114.3(2)	C(7)-O(3)-Cu(1)	114.9(2)

C(9)-O(6)-Cu(2)#3	120.5(3)	C(8)-O(7)-Cu(2)	116.3(3)
C(8)-O(7)-Cu(2)	116.3(3)	Cu(1)-O(9)-H(9A)	120.2
Cu(1)-O(9)-H(9B)	119.8	Cu(2)-O(10)-H(10A)	120.0
Cu(2)-O(10)-H(10B)	120.0	C(6)-N(1)-Cu(1)	117.0(3)
C(2)-N(1)-Cu(1)	118.2(3)	C(10)-N(2)-Cu(1)	119.2(3)
C(14)-N(2)-Cu(1)	122.7(3)	C(17)-N(3)-Cu(2)#4	120.5(3)
C(18)-N(3)-Cu(2)#4	122.7(3)		

The symmetry code: #1 x+1/2, -y+5/2, z+1/2; #2 x+1/2, -y+3/2, z+1/2; #3 x-1/2, -y+5/2, z-1/2; #4 x-1/2, -y+3/2, z-1/2.

Table S6 Selected bond lengths (Å) and angles (°) for $\{[Cu_2(pdtc)(bpy)(H_2O)_2]\cdot 2H_2O\}_n$ (**6**)

Cu(1)-N(1)	1.9141(18)	Cu(1)-N(3)#1	1.9537(18)
Cu(1)-O(1)	2.0288(16)	Cu(1)-O(8)	2.0300(17)
Cu(1)-O(3)#2	2.1848(17)	Cu(2)-O(6)	1.9412(16)
Cu(2)-O(4)#3	1.9463(15)	Cu(2)-N(2)	2.0183(19)
Cu(2)-O(9)	2.0443(17)	Cu(2)-O(10)	2.2158(18)
O(3)-Cu(1)#2	2.1848(17)	O(4)-Cu(2)#4	1.9463(15)
N(3)-Cu(1)#5	1.9537(18)	N(1)-Cu(1)-N(3)#1	169.09(8)
N(1)-Cu(1)-O(1)	80.42(7)	N(3)#1-Cu(1)-O(1)	97.11(7)
N(3)#1-Cu(1)-O(8)	99.97(7)	O(1)-Cu(1)-O(8)	159.52(6)
N(1)-Cu(1)-O(3)#2	97.66(7)	N(3)#1-Cu(1)-O(3)#2	93.24(7)
O(1)-Cu(1)-O(3)#2	100.39(6)	O(1)-Cu(1)-O(3)#2	100.39(6)
O(8)-Cu(1)-O(3)#2	89.87(7)	O(6)-Cu(2)-O(4)#3	163.67(7)
O(6)-Cu(2)-N(2)	91.14(7)	O(4)#3-Cu(2)-N(2)	94.58(7)
O(6)-Cu(2)-O(9)	89.42(7)	O(4)#3-Cu(2)-O(9)	84.59(7)
N(2)-Cu(2)-O(9)	178.77(8)	O(6)-Cu(2)-O(10)	90.80(7)
O(4)#3-Cu(2)-O(10)	103.37(7)	N(2)-Cu(2)-O(10)	98.84(7)
O(9)-Cu(2)-O(10)	82.25(7)	C(1)-O(1)-Cu(1)	115.06(14)
C(8)-O(3)-Cu(1)#2	144.33(15)	C(8)-O(4)-Cu(2)#4	120.02(14)
C(9)-O(6)-Cu(2)	114.14(14)	C(7)-O(8)-Cu(1)	114.46(14)
Cu(2)-O(9)-H(9A)	109(2)	Cu(2)-O(9)-H(9B)	105(2)
Cu(2)-O(10)-H(10A)	110(2)	Cu(2)-O(10)-H(10B)	108(2)
C(6)-N(1)-Cu(1)	118.26(15)	C(2)-N(1)-Cu(1)	118.03(15)
C(10)-N(2)-Cu(2)	123.52(15)	C(14)-N(2)-Cu(2)	119.07(15)
C(18)-N(3)-Cu(1)#5	119.54(15)	C(17)-N(3)-Cu(1)#5	122.12(16)

The symmetry code: #1 -x+1/2, y-1/2, -z-1/2; #2 -x+2, -y, -z; #3 -x+3/2, y+1/2, -z+1/2; #4 -x+3/2, y-1/2, -z+1/2; #5 -x+1/2 ,y+1/2, -z-1/2.

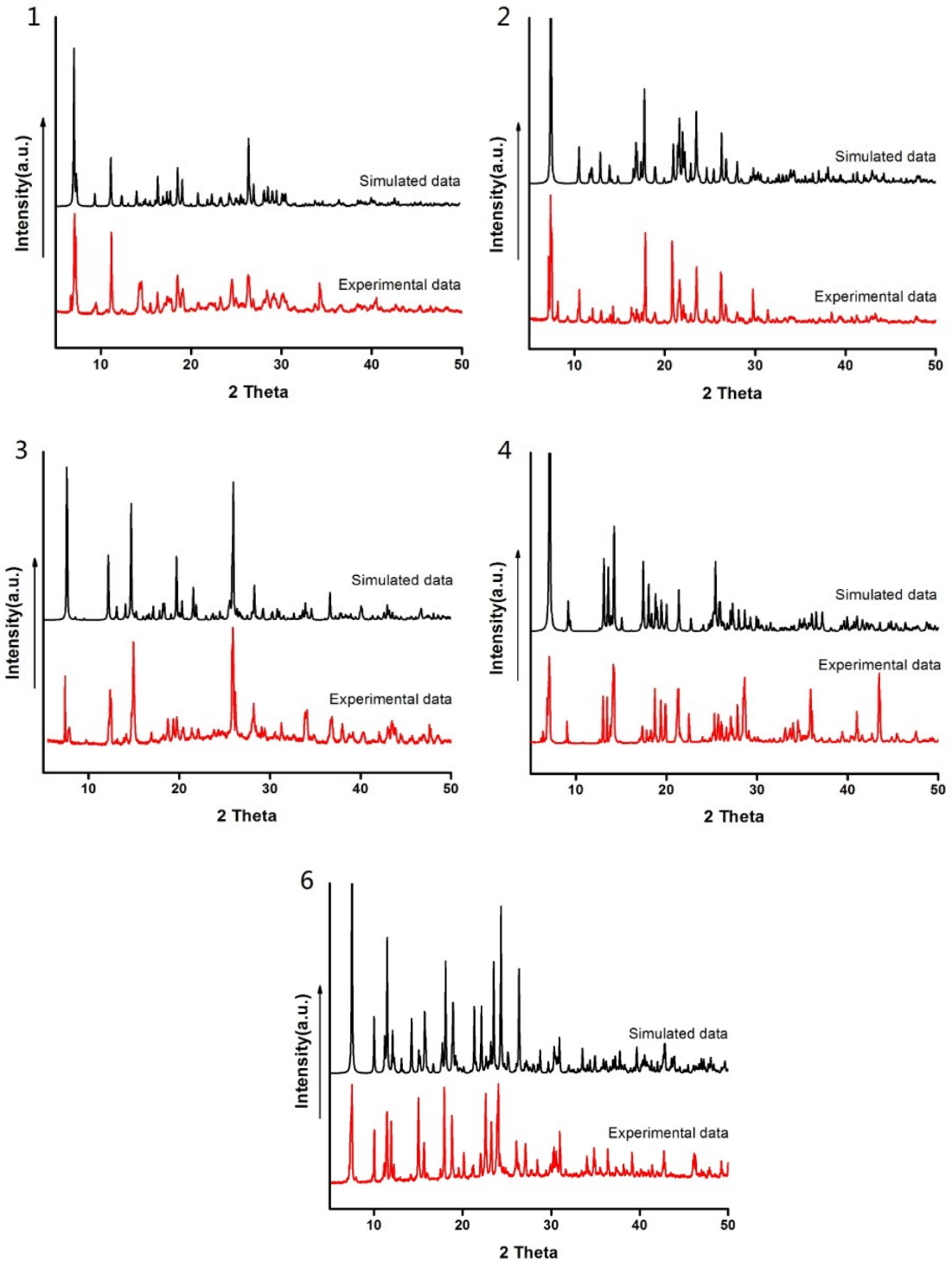

Fig. S1 PXRD patterns of compounds **1**, **2**, **3**, **4** and **6**.

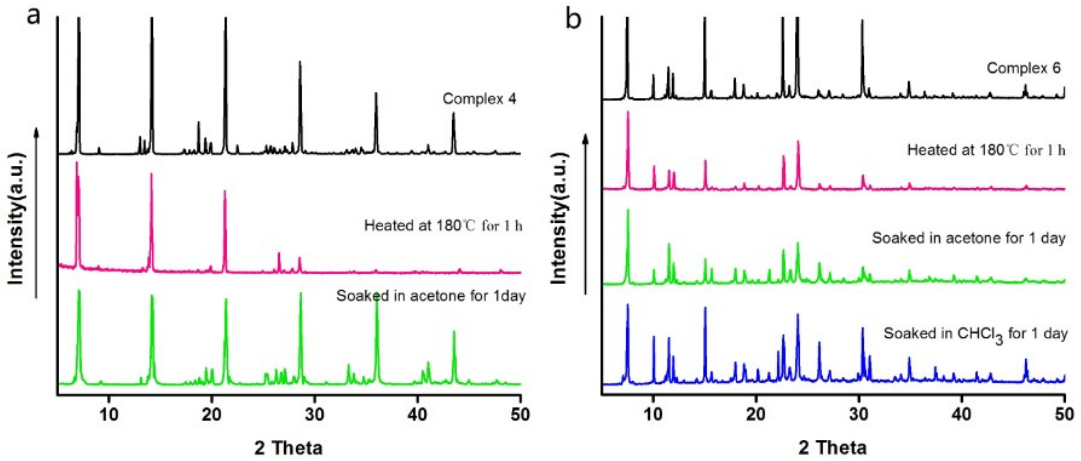

Fig. S2(a) PXRD patterns of **4** and heated at 180 ºC for 1 h and after being soaked in acetone for 1 day. **(b)** PXRD patterns of **6** and after being heated at 180 ºC for 1 h and soaked in acetone or chloroform for 1 day.