Supplementary Material for CrystEngComm

Ten new coordination polymers based on 3-carboxy-1-(4'-carboxybenzyl)-2-oxidopyridinium and different N-donor ligands: syntheses, structures, and photoluminescent properties

Jia-Zhen Gao, Jin Yang,* Ying-Ying Liu and Jian-Fang Ma*

Key Lab of Polyoxometalate Science, Department of Chemistry, Northeast Normal University, Changchun 130024, People's Republic of China

* Correspondence authors

E-mail: yangjinnenu@yahoo.com.cn (J. Yang)

E-mail: jianfangma@yahoo.com.cn (J.-F. Ma)

Fax: +86-431-85098620 (J.-F. Ma)

Table S1a. Selected bond distances (Å) and angles (°) for **1**

Zn(1)-O(1)$^{\#1}$	1.945(2)	Zn(1)-O(3)	2.023(2)
Zn(1)-O(4)	2.053(2)	Zn(1)-O(5)$^{\#2}$	2.075(2)
Zn(1)-O(1W)	2.078(3)		
O(1)$^{\#1}$-Zn(1)-O(3)	109.30(10)	O(1)$^{\#1}$-Zn(1)-O(4)	116.04(11)
O(3)-Zn(1)-O(4)	86.51(9)	O(1)$^{\#1}$-Zn(1)-O(5)$^{\#2}$	99.89(10)
O(3)-Zn(1)-O(5)$^{\#2}$	150.56(10)	O(4)-Zn(1)-O(5)$^{\#2}$	84.11(9)
O(1)$^{\#1}$-Zn(1)-O(1W)	96.33(11)	O(3)-Zn(1)-O(1W)	87.12(10)
O(5)$^{\#2}$-Zn(1)-O(1W)	85.89(10)	O(4)-Zn(1)-O(1W)	147.29(11)

Table S1b. Hydrogen bonds for **1** (Å and °)

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(1W)-H(1A)···O(2)$^{\#4}$	0.8991(10)	1.771(15)	2.649(4)	165(4)
O(1W)-H(1B)···O(4)$^{\#2}$	0.890(10)	2.16(3)	2.814(4)	130(3)

Symmetry transformations used to generate equivalent atoms: $^{\#1}$ -x+1, -y+1, -z+1; $^{\#2}$ -x+3/2, y-1/2, -z+1/2; $^{\#3}$ -x+3/2, y+1/2, -z+1/2; $^{\#4}$ -x+1, -y, -z+1.

Table S2a. Selected bond distances (Å) and angles (°) for **2**

Zn(1)-O(4)	1.971(3)	Zn(1)-N(2)	1.984(4)
Zn(1)-O(3)	2.004(3)	Zn(1)-O(1)$^{\#1}$	2.011(3)
Zn(1)-O(2)$^{\#1}$	2.392(3)		
O(4)-Zn(1)-N(2)	104.29(15)	O(4)-Zn(1)-O(3)	90.23(12)
N(2)-Zn(1)-O(3)	107.98(13)	O(4)-Zn(1)-O(1)$^{\#1}$	107.04(14)
N(2)-Zn(1)-O(1)$^{\#1}$	133.20(14)	O(3)-Zn(1)-O(1)$^{\#1}$	105.77(14)
O(4)-Zn(1)-O(2)$^{\#1}$	165.27(14)	N(2)-Zn(1)-O(2)$^{\#1}$	89.65(13)
O(3)-Zn(1)-O(2)$^{\#1}$	89.96(13)	O(1)$^{\#1}$-Zn(1)-O(2)$^{\#1}$	58.84(12)

Table S2b. Hydrogen bonds for **2** (Å and °)

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(1W)-H(1A)···O(1W)$^{\#3}$	0.90	2.44	3.148(13)	135.4
O(2W)-H(2B)···O(1W)$^{\#4}$	0.93	2.15	2.996(10)	150.5

O(1W)-H(1B)···O(5)[#4]	0.91	1.98	2.818(7)	153.2

Symmetry transformations used to generate equivalent at: [#1] -x+3, -y+1, -z; [#2] –x+1, -y+1, -z+1; [#3] -x+4, -y+1, -z-1; [#4] -x+3, -y, -z.

Table S3a. Selected bond distances (Å) and angles (°) for **3**

Zn(1)-O(4)	1.966(3)	Zn(1)-N(2)	1.993(4)
Zn(1)-O(3)	1.974(3)	Zn(1)-O(1)[#1]	2.044(3)
Zn(1)-O(2)[#1]	2.328(3)		
O(4)-Zn(1)-N(2)	101.50(14)	O(4)-Zn(1)-O(3)	92.94(12)
O(3)-Zn(1)-N(2)	112.34(14)	O(4)-Zn(1)-O(1)[#1]	101.95(13)
N(2)-Zn(1)-O(1)[#1]	132.32(13)	O(3)-Zn(1)-O(1)[#1]	107.23(13)
O(4)-Zn(1)-O(2)[#1]	161.41(13)	N(2)-Zn(1)-O(2)[#1]	90.96(13)
O(3)-Zn(1)-O(2)[#1]	95.01(12)	O(1)[#1]-Zn(1)-O(2)[#1]	59.62(12)

Table S3b. Hydrogen bonds for **3** (Å and °)

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(1W)-H(1B)···O(2W)[#3]	0.92	1.88	2.748(7)	157.6
O(1W)-H(1A)···O(2) [#4]	0.92	2.03	2.938(6)	170.0
O(2W)-H(2B)···O(1W)	0.91	2.04	2.764(7)	135.7
O(2W)-H(2A)···O(5)	0.90	1.92	2.728(6)	148.9

Symmetry transformations used to generate equivalent at: [#1] -x, -y, -z+2; [#2] -x+2, -y, -z+1; [#3] –x+1, -y+1, -z+1; [#4] x+1, y+1, z-1.

Table S4a. Selected bond distances (Å) and angles (°) for **4**

Zn(1)-O(1)[#1]	2.028(2)	Zn(1)-O(4)	2.031(3)
Zn(1)-N(2)	2.038(3)	Zn(1)-O(3)	2.107(3)
Zn(1)-O(2W)	2.119(3)	Zn(1)-O(2)[#1]	2.417(3)
O(1)[#1]-Zn(1)-O(4)	109.91(11)	O(1)[#1]-Zn(1)-N(2)	150.02(12)
O(4)-Zn(1)-N(2)	99.88(12)	O(1)[#1]-Zn(1)-O(3)	94.10(11)
O(4)-Zn(1)-O(3)	85.08(11)	N(2)-Zn(1)-O(3)	91.64(12)
O(1)[#1]-Zn(1)-O(2W)	87.36(10)	O(4)-Zn(1)-O(2W)	91.18(12)

N(2)-Zn(1)-O(2W)	88.79(11)	O(3)-Zn(1)-O(2W)	176.25(11)
O(1)$^{\#1}$-Zn(1)-O(2)$^{\#1}$	58.08(9)	O(4)-Zn(1)-O(2)$^{\#1}$	165.00(10)
N(2)-Zn(1)-O(2)$^{\#1}$	92.97(11)	O(3)-Zn(1)-O(2)$^{\#1}$	86.87(10)
O(2W)-Zn(1)-O(2)$^{\#1}$	96.82(11)		

Table S4b. Hydrogen bonds for **4** (Å and °)

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(2W)-H(2B)···N(4)$^{\#5}$	0.89	2.01	2.898(4)	177.1
O(1W)-H(1A)···O(2)$^{\#3}$	0.89	1.96	2.854(4)	177.3
O(2W)-H(2A)···O(4)$^{\#4}$	0.89	1.92	2.797(4)	167.4
O(1W)-H(1B)···O(5)	0.89	1.96	2.808(4)	159.1

Symmetry transformations used to generate equivalent atoms: $^{\#1}$ -x+1/2, -y+3/2, -z+1; $^{\#2}$ -x, y, -z+1/2; $^{\#3}$ -x+1/2, y+1/2, -z+3/2; $^{\#4}$ -x, -y+2, -z+1; $^{\#5}$ x, y-1, z.

Table S5a. Selected bond distances (Å) and angles (°) for **5**

Zn(1)-O(1)	1.948(2)	Zn(1)-O(4)$^{\#1}$	2.004(2)
Zn(1)-O(3)$^{\#1}$	2.045(2)	Zn(1)-N(2)	2.115(2)
Zn(1)-N(3)	2.139(2)		
O(1)-Zn(1)-O(4)$^{\#1}$	94.84(9)	O(1)-Zn(1)-O(3)$^{\#1}$	107.59(9)
O(4)$^{\#1}$-Zn(1)-O(3)$^{\#1}$	87.63(8)	O(1)-Zn(1)-N(2)	116.74(9)
O(4)$^{\#1}$-Zn(1)-N(2)	148.10(10)	O(1)-Zn(1)-N(3)	105.53(9)
O(3)$^{\#1}$-Zn(1)-N(2)	87.00(8)	O(4)$^{\#1}$-Zn(1)-N(3)	89.69(8)
O(3)$^{\#1}$-Zn(1)-N(3)	146.87(9)	N(2)-Zn(1)-N(3)	78.11(9)

Table S5b. Hydrogen bonds for **5** (Å and °)

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(1W)-H(1A)···O(5)	0.89	2.15	3.020(3)	165.8
O(1W)-H(1B)···O(4)$^{\#3}$	0.89	2.29	3.152(3)	162.9
C(11)-H(11)···O(2)$^{\#4}$	0.93	2.49	3.121(5)	125.5
C(8)-H(8A)···O(5)$^{\#5}$	0.97	2.62	3.404(4)	138.3

Symmetry transformations used to generate equivalent at: $^{\#1}$ x+1/2, -y+1/2, z-1/2; $^{\#2}$

x-1/2, -y+1/2, z+1/2; [#3] -x-1, -y+1, -z+1; [#4] x-1, y, z; [#5] x+1/2, -y+1/2, z+1/2.

Table S6a. Selected bond distances (Å) and angles (°) for **6**

Cu(1)-O(4)	1.9262(18)	Cu(1)-O(3)	1.9501(17)
Cu(1)-N(2)	2.015(2)	Cu(1)-N(3)	2.032(2)
Cu(1)-O(1)$^{\#1}$	2.120(2)		
O(4)-Cu(1)-O(3)	91.87(7)	O(4)-Cu(1)-N(2)	159.80(9)
O(3)-Cu(1)-N(2)	89.82(8)	O(4)-Cu(1)-N(3)	90.51(8)
O(3)-Cu(1)-N(3)	160.46(9)	N(2)-Cu(1)-N(3)	81.46(8)
O(4)-Cu(1)-O(1)$^{\#1}$	91.14(9)	O(3)-Cu(1)-O(1)$^{\#1}$	99.66(8)
N(2)-Cu(1)-O(1)$^{\#1}$	108.42(9)	N(3)-Cu(1)-O(1)$^{\#1}$	99.68(8)

Table S6b. Hydrogen bonds for **6** (Å and °)

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(1W)-H(1B)···O(1)$^{\#3}$	0.89	2.33	3.108(3)	146.3
O(1W)-H(1A)···O(5)	0.89	2.16	3.018(3)	163.0
C(10)-H(10)···O(2)$^{\#4}$	0.93	2.73	3.218(4)	114.0

Symmetry transformations used to generate equivalent atoms: [#1] x+1/2, -y+1/2, z-1/2; [#2] x-1/2, -y+1/2, z+1/2; [#3] -x+3/2, y+1/2, -z+3/2; [#4] x+1, y, z.

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

Cd(1)-O(2')	2.166(6)	Cd(1)-O(5)$^{\#2}$	2.360(3)
Cd(1)-N(3)	2.424(3)	Cd(1)-N(2)	2.386(3)
Cd(1)-O(1)	2.397(9)	Cd(1)-O(3)$^{\#1}$	2.459(2)
Cd(1)-O(4)$^{\#1}$	2.315(2)		
O(2')-Cd(1)- O(4)$^{\#1}$	93.72(18)	O(4)$^{\#1}$-Cd(1)-O(5)$^{\#2}$	101.77(9)
O(2')-Cd(1)-O(5)$^{\#2}$	120.86(18)	O(4)$^{\#1}$-Cd(1)-N(2)	145.46(16)
O(2')-Cd(1)-N(2)	105.84(18)	O(5)$^{\#2}$-Cd(1)-N(2)	92.33(9)
O(4)$^{\#1}$-Cd(1)-N(3)	81.14(9)	O(2')-Cd(1)-N(3)	155.38(18)
O(5)$^{\#2}$-Cd(1)-N(3)	83.73(9)	N(2)-Cd(1)-N(3)	69.20(10)

O(4)$^{\#1}$-Cd(1)-O(3)$^{\#1}$	72.17(8)	O(2')-Cd(1)-O(3)$^{\#1}$	77.68(18)
O(5)$^{\#2}$-Cd(1)-O(3)$^{\#1}$	161.24(9)	N(2)-Cd(1)-O(3)$^{\#}$1	84.40(9)
N(3)-Cd(1)-O(3)$^{\#1}$	77.83(9)	O(4)$^{\#1}$-Cd(1)-O(1)	126.0(3)
O(2)-Cd(1)-O(1)	52.21(18)	O(5)$^{\#2}$-Cd(1)-O(1)	88.7(3)
N(2)-Cd(1)-O(1)	85.1(3)	O(1)-Cd(1)-O(2)	52.0(3)
O(3)$^{\#1}$-Cd(1)-O(2)	72.07(15)	O(1)-Cd(1)-N(3)	152.8(3)
O(1)-Cd(1)-O(3)#1	109.3(3)	O(2')-Cd(1)-O(2)	13.04(19)
O(4)#1-Cd(1)-O(2)	80.80(15)	O(5)#2-Cd(1)-O(2)	125.32(15)
N(2)-Cd(1)-O(2)	116.12(15)	N(3)-Cd(1)-O(2)	148.42(15)

Symmetry transformations used to generate equivalent atoms: $^{\#1}$ x+1/2, y+1/2, z; $^{\#2}$ -x+1/2, -y+1/2, -z+1; $^{\#3}$ x-1/2, y-1/2, z.

Table S8a. Selected bond distances (Å) and angles (°) for **8**

Cd(1)-N(4)	2.238(5)	Cd(1)-O(7)$^{\#1}$	2.292(4)
Cd(1)-O(5)$^{\#1}$	2.303(4)	Cd(1)-O(1)	2.381(4
Cd(1)-O(8)$^{\#1}$	2.393(4)	Cd(1)-O(2)	2.426(4)
Cd(2)-N(15)$^{\#2}$	2.235(5)	Cd(2)-O(6)	2.294(5)
Cd(2)-O(4)	2.293(4)	Cd(2)-O(10)	2.321(4)
Cd(2)-O(3)	2.412(4)	Cd(2)-O(9)	2.540(4)
Cd(3)-N(8)	2.231(5)	Cd(3)-O(20)	2.264(4)
Cd(3)-O(13)	2.273(4)	Cd(3)-O(15)	2.423(5)
Cd(3)-O(16)	2.270(4)	Cd(3)-O(19)	2.612(4)
Cd(4)-O(17)	2.274(4)	Cd(4)-N(7)$^{\#3}$	2.234(5)
Cd(4)-O(11)	2.352(4)	Cd(4)-O(14)	2.289(5)
Cd(4)-O(12)	2.418(4)	Cd(4)-O(18)	2.405(5)
Cd(5)-N(12)	2.224(5)	Cd(5)-O(22)$^{\#4}$	2.256(4)
Cd(5)-O(23)	2.262(5)	Cd(5)-O(25)	2.271(4)
Cd(5)-O(21)$^{\#4}$	2.423(4)	Cd(5)-O(24)	2.562(5)
N(4)-Cd(1)-O(7)$^{\#1}$	116.91(16)	N(4)-Cd(1)-O(5)$^{\#1}$	86.55(17)
O(7)$^{\#1}$-Cd(1)-O(5)$^{\#1}$	93.99(15)	N(4)-Cd(1)-O(1)	140.77(18)

O(7)$^{\#1}$-Cd(1)-O(1)	90.24(15)	O(5)$^{\#1}$-Cd(1)-O(1)	121.19(15)
N(4)-Cd(1)-O(8)$^{\#1}$	82.05(17)	O(7)$^{\#1}$-Cd(1)-O(8)$^{\#1}$	72.85(14)
O(5)$^{\#1}$-Cd(1)-O(8)$^{\#1}$	156.02(14)	O(1)-Cd(1)-O(8)$^{\#1}$	79.71(15)
N(4)-Cd(1)-O(2)	101.93(16)	O(7)$^{\#1}$-Cd(1)-O(2)	140.88(15)
O(5)$^{\#1}$-Cd(1)-O(2)	92.80(16)	O(1)-Cd(1)-O(2)	53.94(16)
O(8)$^{\#1}$-Cd(1)-O(2)	110.14(15)	N(15)$^{\#2}$-Cd(2)-O(6)	86.76(18)
N(15)$^{\#2}$-Cd(2)-O(4)	117.37(16)	O(4) -Cd(2)- O(6)	93.24(15)
N(15)$^{\#2}$-Cd(2)-O(10)	141.54 (18)	O(6)-Cd(2)-O(10)	120.03(16)
N(15)#2-Cd(2)-O(6)	86.76(18)	N(15)$^{\#2}$-Cd(2)-O(3)	82.45(18)
O(4)-Cd(2)-O(10)	90.03(15)	O(4)-Cd(2)-O(3)	72.87(14)
O(6)-Cd(2)-O(3)	155.72(15)	N(15)$^{\#2}$-Cd(2)-O(9)	102. 62(17)
O(10)-Cd(2)-O(3)	80.66(16)	O(4)-Cd(2)-O(9)	139.80(15)
O(6)-Cd(2)-O(9)	92.89(18)	O(3)-Cd(2)-O(9)	110.65(16)
O(10)-Cd(2)-O(9)	53.13(16)	N(8)-Cd(3)-O(13)	115.64(15)
N(8)-Cd(3)-O(20)	142.56(17)	N(8)-Cd(3)-O(16)	88.26(17)
O(20)-Cd(3)-O(13)	92.92(15)	O(16) -Cd(3)- O(13)	92.11(14)
O(20)-Cd(3)-O(16)	115.74(16)	O(16)-Cd(3)-O(15)	158.34(14)
N(8)-Cd(3)-O(15)	84.08(17)	O(20)-Cd(3)-O(15)	81.59(15)
O(13)-Cd(3)-O(15)	73.24(14)	O(20)-Cd(3)-O(19)	53.06(16)
N(8)-Cd(3)-O(19)	101.52(16)	O(13)-Cd(3)-O(19)	142.80(14)
O(15)-Cd(3)-O(19)	110.61(16)	O(16)-Cd(3)-O(19)	90.75(16)
N(7)$^{\#3}$-Cd(4)-O(14)	87.83(18)	N(7)$^{\#3}$-Cd(4)-O(17)	115.33(16)
N(7)$^{\#3}$-Cd(4)-O(11)	142.19(18)	O(17)-Cd(4)-O(14)	92.46(15)
O(14)-Cd(4)-O(11)	117.10(17)	O(17)-Cd(4)-O(11)	92.81(15)
O(17)-Cd(4)-O(18)	73.09(14)	N(7)$^{\#3}$-Cd(4)-O(18)	84.48(18)
O(11)-Cd(4)-O(18)	80.05(16)	O(14)-Cd(4)-O(18)	158.64(16)
O(17)-Cd(4)-O(12)	144.37(15)	N(7)$^{\#3}$-Cd(4)-O(12)	100.23(15)
O(11)-Cd(4)-O(12)	54.65(17)	O(14)-Cd(4)-O(12)	90.97(17)
N(12)-Cd(5)-O(22)$^{\# 4}$	114.34(16)	O(18)-Cd(4)-O(12)	109.99(16)

O(22)$^{\#4}$-Cd(5)-O(23)	91.99 (16)	N(12)-Cd(5)-O(23)	88.11(28)
O(22)$^{\#4}$-Cd(5)-O(25)	95.52(17)	N(12)-Cd(5)-O(25)	142.99(18)
O(21)$^{\#4}$-Cd(5)-O(24)	110.02(18)	O(23)-Cd(5)-O(25)	113.29(18)
N(12)-Cd(5)-O(21)$^{\#4}$	85.86(17)	O(22)$^{\#4}$-Cd(5)-O(21)$^{\#4}$	73.52(15)
O(23)-Cd(5)-O(21)$^{\#4}$	160.22(15)	O(25)-Cd(5)-O(21)$^{\#4}$	82.09 (17)
N(12)-Cd(5)-O(24)	99.79(17)	O(22)$^{\#4}$-Cd(5)-O(24)	145.87(15)
O(23)-Cd(5)-O(24)	89.56(19)	O(25)-Cd(5)-O(24)	53.18(18)

Table S8b. Hydrogen bonds for **8** (Å and °)

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(1W)-H(1B)···O(5)	0.89	2.35	2.888(6))	119.0
O(2W)-H(2A)···O(6)$^{\#6}$	0.90	2.38	2.935(7)	119.9
O(2W)-H(2B)···O(9)	0.89	2.32	3.189(8)	164.9
O(4W)-H(4A)···O(25)	0.91	2.91	3.324(11)	108.5
O(4W)-H(4B)···O(23)$^{\#4}$	0.91	2.51	2.923(10)	108.0
O(5W)-H(5A)···O(16)$^{\#7}$	0.93	2.08	2.936(7)	153.3

Symmetry transformations used to generate equivalent atoms: $^{\#1}$ -x, -y+2, -z+2; $^{\#2}$ x, y+1, z+1; $^{\#3}$ x, y-1, z-1; $^{\#4}$ -x, -y-1, -z+1; $^{\#5}$ -x, -y, -z+2; $^{\#6}$ -x, -y+1, -z+2; $^{\#7}$ -x, -y, -z+1.

Table S9a. Selected bond distances (Å) and angles (°) for **9**

Co(1)-O(4)	2.005(3)	Co(1)-N(2)	2.055(4)
Co(1)-O(1W)	2.093(3)	Co(1)-O(3)	2.135(2)
Co(1)-O(2)$^{\#1}$	2.180(3)	Co(1)-O(1)$^{\#1}$	2.200(3)
O(4)-Co(1)-N(2)	112.31(14)	O(4)-Co(1)-O(1W)	84.78(11)
N(2)-Co(1)-O(1W)	94.04(14)	O(4)-Co(1)-O(3)	84.80(10)
N(2)-Co(1)-O(3)	88.83(14)	O(1W)-Co(1)-O(3)	169.51(10)
O(4)-Co(1)-O(2)$^{\#1}$	97.44(11)	N(2)-Co(1)-O(2)$^{\#1}$	149.78(12)
O(1W)-Co(1)-O(2)$^{\#1}$	93.83(10)	O(3)-Co(1)-O(2)$^{\#1}$	88.68(10)
O(4)-Co(1)-O(1)$^{\#1}$	156.89(11)	N(2)-Co(1)-O(1)$^{\#1}$	90.81(13)
O(1W)-Co(1)-O(1)$^{\#1}$	93.59(11)	O(3)-Co(1)-O(1)$^{\#1}$	96.46(10)

O(2)$^{\#1}$-Co(1)-O(1)$^{\#1}$	59.60(9)

Symmetry transformations used to generate equivalent atoms: $^{\#1}$ x, -y+1, z+1/2; $^{\#2}$ -x+3/2, -y+1/2, -z+1; $^{\#3}$ x, -y+1, z-1/2.

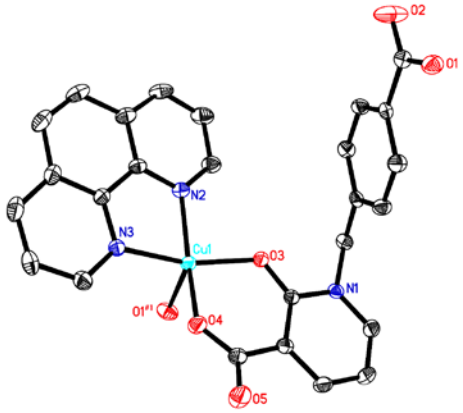
Table S10a. Selected bond distances (Å) and angles (°) for **10**

Ni(1)-O(4)	1.989(2)	Ni(1)-O(4)#1	1.989(2)
Ni(1)-O(3)	2.058(2)	Ni(1)-N(2)	2.085(3)
Ni(1)-O(3)#1	2.058(2)	Ni(1)-N(2)#1	2.086(3)
Ni(2)-O(5)#3	2.058(2)	Ni(2)-O(1)	2.054(3)
Ni(2)-O(5)#4	2.058(2)	Ni(2)-O(1)#2	2.054(3)
Ni(2)-O(3W)	2.091(2)	Ni(2)-O(3W)#2	2.091(2)
O(4)#1-Ni(1)-O(3)	91.59(9)	O(4)-Ni(1)-O(3)	88.41(9)
O(4)#1-Ni(1)-O(3)#1	88.41(9)	O(4)-Ni(1)-O(3)#1	91.59(9)
O(4)-Ni(1)-N(2)#1	90.54(11)	O(4)#1-Ni(1)-N(2)#1	89.46(11)
O(3)-Ni(1)-N(2)#1	87.11(11)	O(3)#1-Ni(1)-N(2)#1	92.89(11)
O(3)#1-Ni(1)-N(2)	87.11(11)	O(3)-Ni(1)-N(2)	92.89(11)
O(4)-Ni(1)-N(2)	89.46(11)	O(4)#1-Ni(1)-N(2)	90.54(11)
O(1)#2-Ni(2)-O(5)#3	88.90(12)	O(1)-Ni(2)-O(5)#4	88.90(12)
O(1)#2-Ni(2)-O(3W)	86.99(11)	O(1)-Ni(2)-O(5)#3	91.10(12)
O(5)#3-Ni(2)-O(3W)	96.20(10)	O(1)-Ni(2)-O(3W)	93.01(11)
O(5)#4-Ni(2)-O(3W)#2	96.20(10)	O(5)#4-Ni(2)-O(3W)	83.80(10)
O(5)#3-Ni(2)-O(3W)#2	83.80(10)	O(1)#2-Ni(2)-O(5)#4	91.10(12)

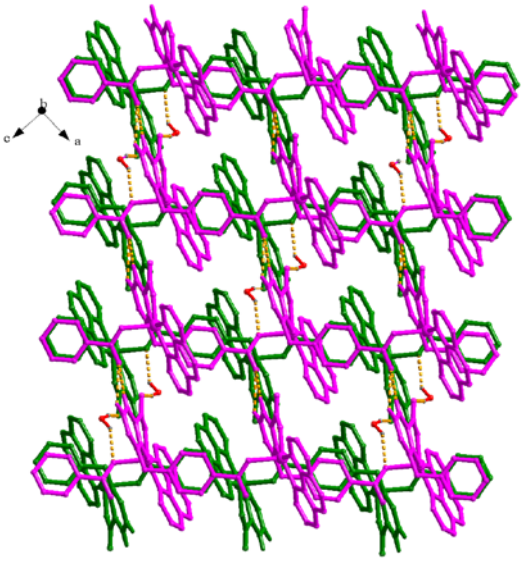
Table S10b. Hydrogen bonds for **10** (Å and °)

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(3W)-H(3A)···O(4)#3	0.90	1.78	2.674(3)	171.7
O(3W)-H(3B)···O(2)	0.89	1.74	2.629(4)	174.0
O(2W)-H(2A)···O(1W)#7	0.90	2.27	3.044(9)	143.8

Symmetry transformations used to generate equivalent atoms: $^{\#1}$ -x+2, -y, -z+1; $^{\#2}$ -x+2, -y-1, -z+3; $^{\#3}$ -x+2, -y, -z+2; $^{\#4}$ x, y-1, z+1; $^{\#5}$ -x+2, -y, -z; $^{\#6}$ x, y+1, z-1; $^{\#7}$ x, y, z-1.



(a)



(b)

Fig. S1 (a) ORTEP view of **6** showing the local coordination environment of Cu(II) atom with hydrogen atoms and lattice water molecule omitted for clarity (30% probability displacement ellipsoids). Symmetry codes: $^{\#1}$ x+1/2, -y+1/2, z-1/2. (b) The 3D hydrogen-bonding structure of **6**.

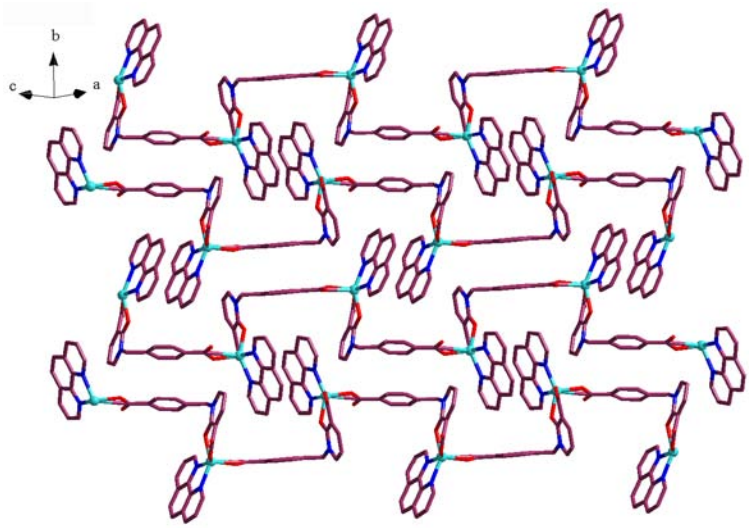
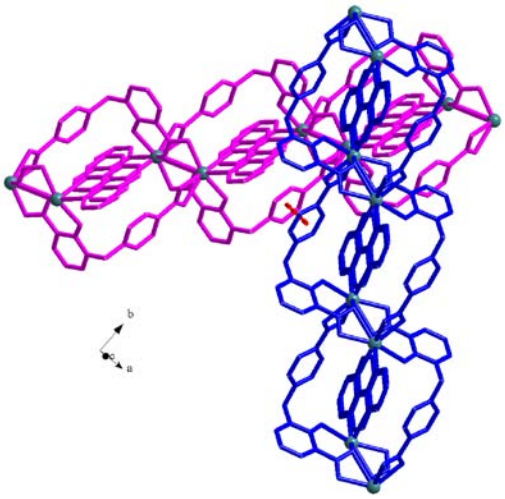
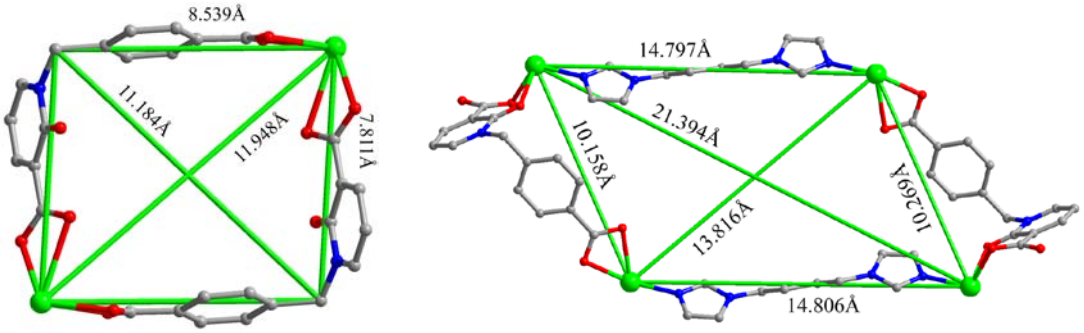


Fig. S2 View of the 2D supramolecular layer connected by π–π interactions of compound **5**.



(d)

Fig. S3 View of the π–π interactions of **7**.



(a) (b)

Fig. S4 (a) Ball-and-stick representation of the $[Cd(L)_2Cd]$ 26-membered ring. (b) Ball-and-stick representation of the large rectangular 44-membered ring $[Cd_4(L)_2(biim\text{-}4)_2]$.

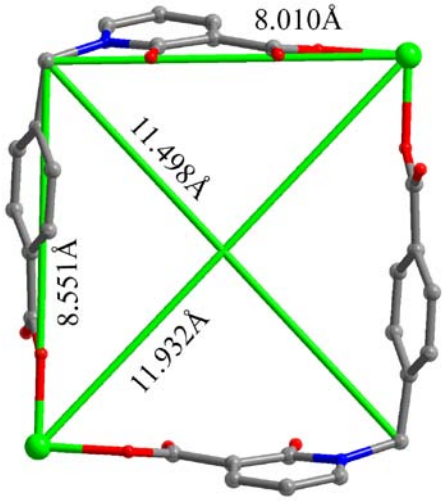
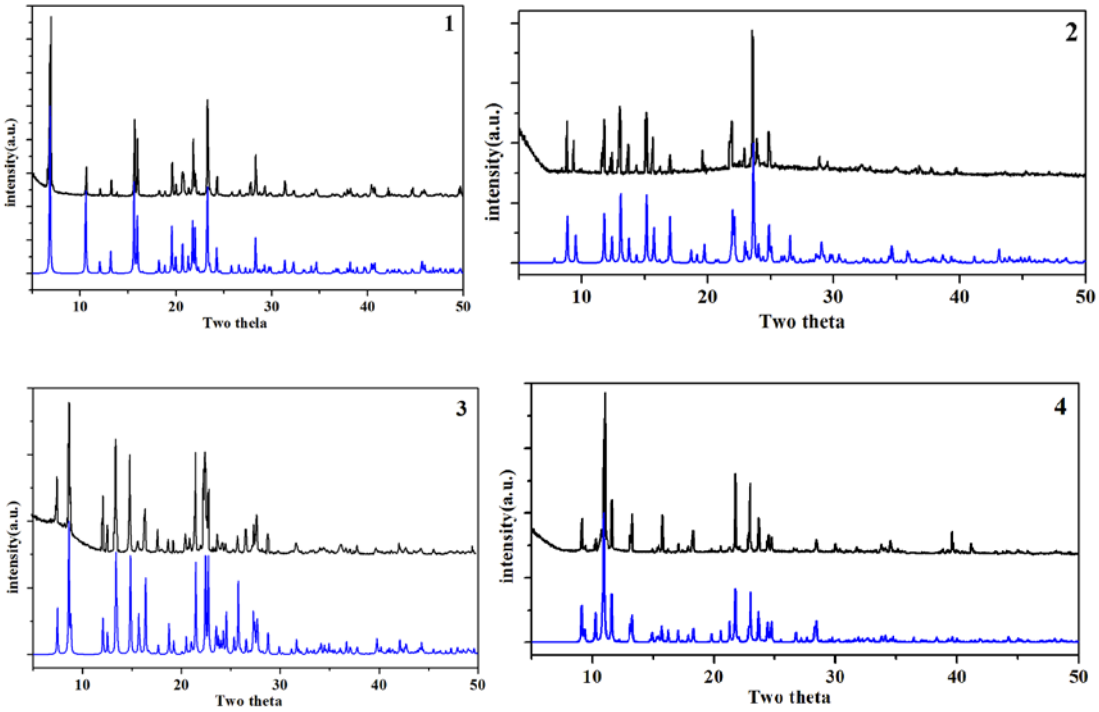


Fig. S5 View of the $[Ni_2(L)_2]$ ring in **10**.



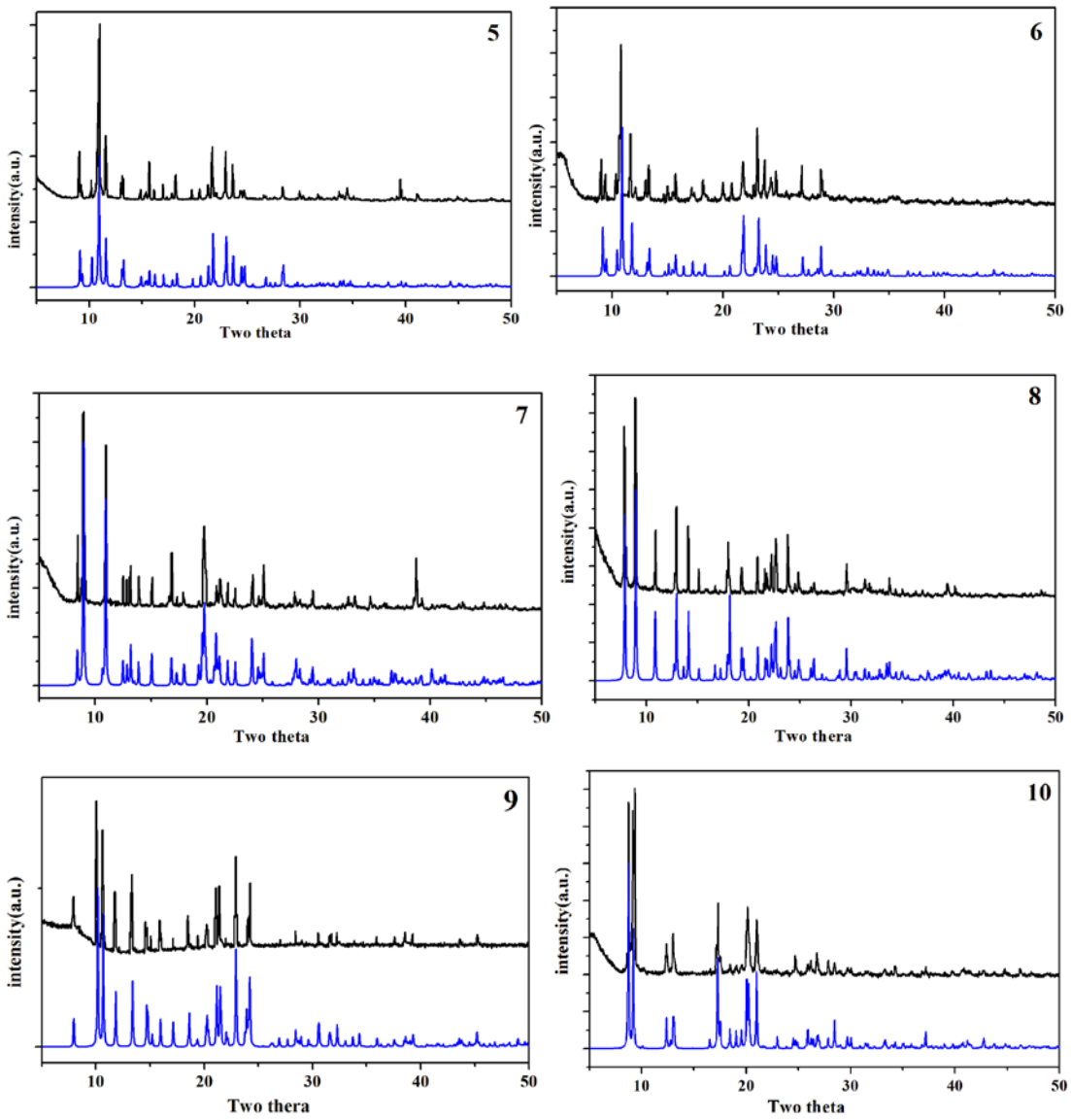


Fig. S6 The simulated (blue) and experimental (black) PXRD patterns of **1**–**10**.

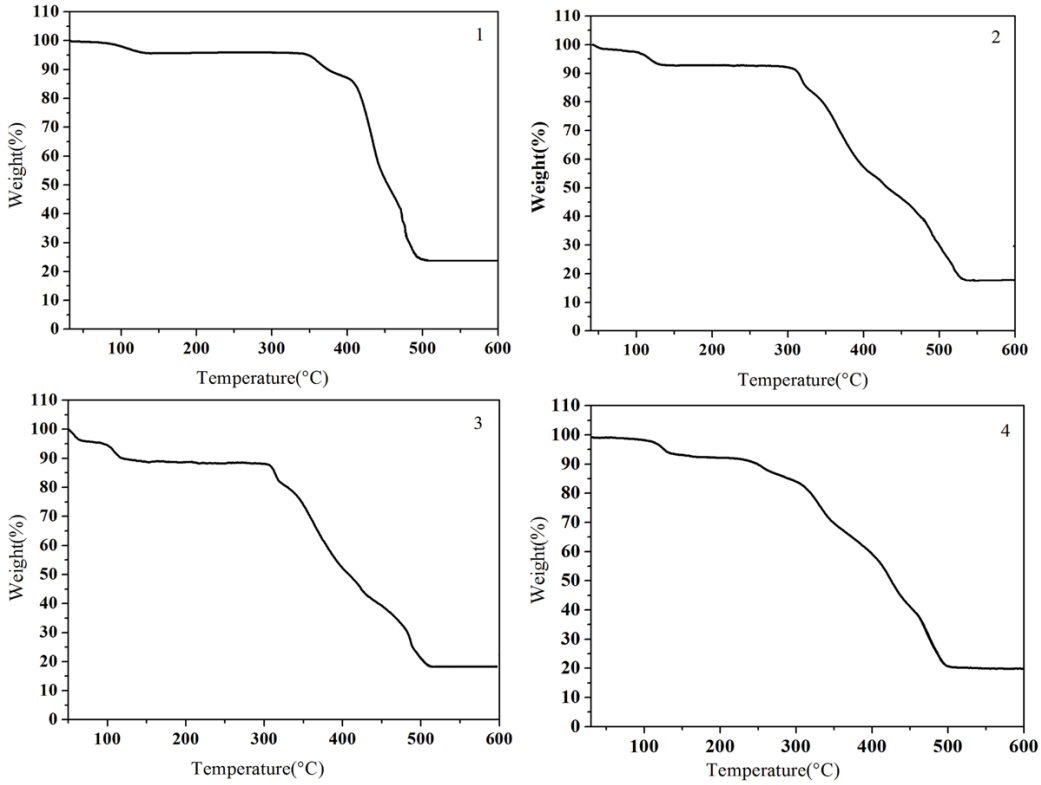


Fig. S7 The TGA curves of compounds **1**–**4**.

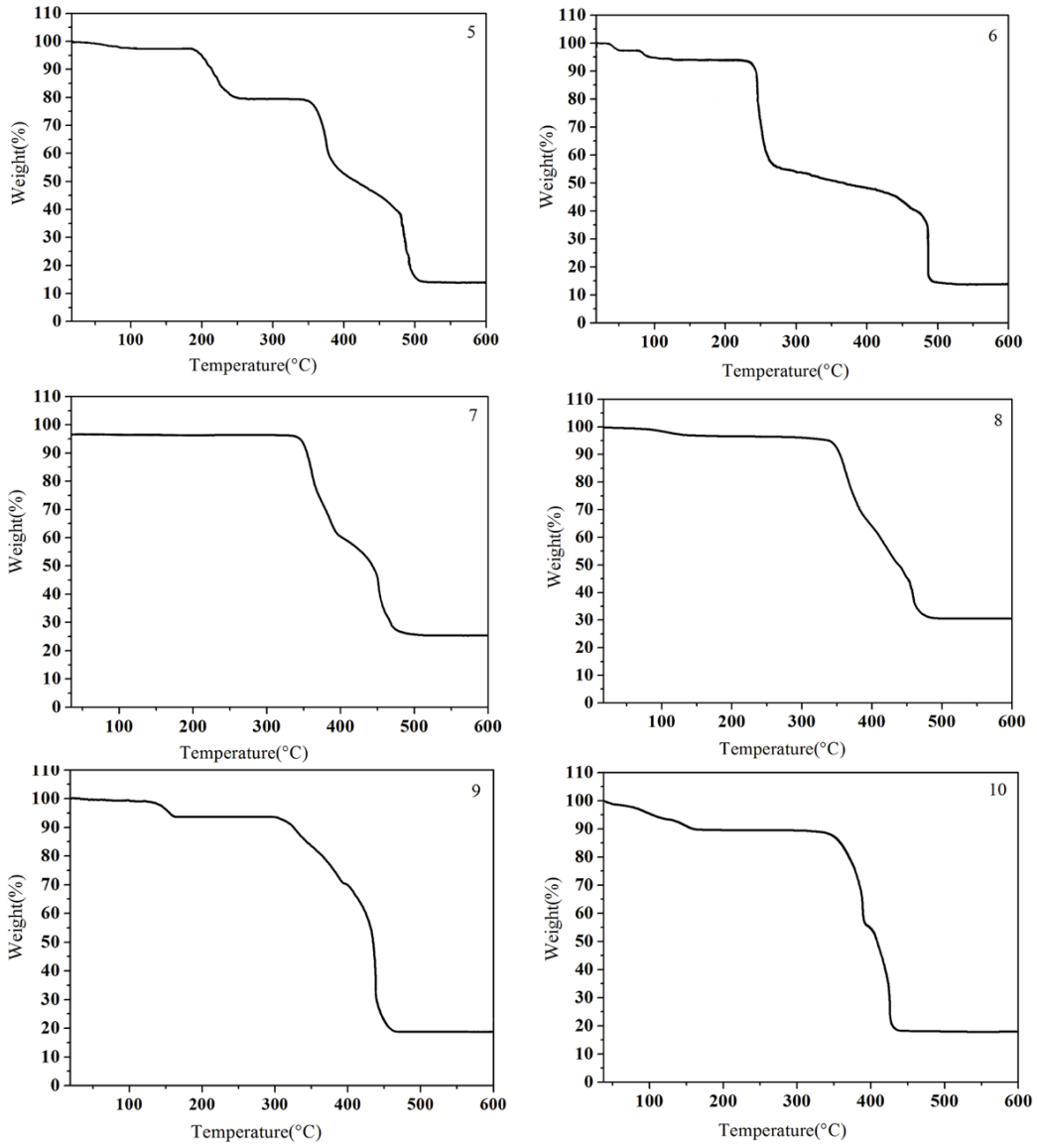


Fig. S8 The TGA curves of compounds **5**–**10**.