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Syntheses, structures, and photoluminescent properties of a series of coordination polymers based on a new 2'-carboxybiphenyl-4-ylmethylaminodiacetic acid and different N-donor ligands

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

Co(1)-O(5)#1	2.0271(19)	Co(1)-O(3)#1	2.063(2)
Co(1)-O(4)#2	2.0960(19)	Co(1)-O(2)	2.1511(19)
Co(1)-N(1)#1	2.204(2)	Co(1)-O(1)	2.203(2)
Co(2)-O(1W)	1.943(3)	Co(2)-O(6)	1.993(2)
Co(2)-O(6)#3	1.993(2)	Co(2)-O(2W)	2.109(2)
Co(2)-O(2W)#3	2.109(2)		
O(5)#1-Co(1)-O(3)#1	108.77(8)	O(5)#1-Co(1)-O(4)#2	96.43(8)
O(3)#1-Co(1)-O(4)#2	93.61(8)	O(5)#1-Co(1)-O(2)	161.10(8)
O(3)#1-Co(1)-O(2)	90.11(8)	O(4)#2-Co(1)-O(2)	82.93(8)
O(5)#1-Co(1)-N(1)#1	78.36(8)	O(3)#1-Co(1)-N(1)#1	79.76(8)
O(4)#2-Co(1)-N(1)#1	169.59(8)	O(2)-Co(1)-N(1)#1	104.93(8)
O(5)#1-Co(1)-O(1)	101.60(8)	O(3)#1-Co(1)-O(1)	147.09(8)
O(4)#2-Co(1)-O(1)	95.33(8)	O(2)-Co(1)-O(1)	59.80(8)
N(1)#1-Co(1)-O(1)	94.55(10)	O(5)#1-Co(1)-C(1)	130.90(11)
O(1W)-Co(2)-O(6)	116.19(7)	O(1W)-Co(2)-O(6)#3	116.19(7)
O(6)-Co(2)-O(6)#3	127.62(14)	O(1W)-Co(2)-O(2W)	93.36(6)
O(6)-Co(2)-O(2W)	91.28(9)	O(6)#3-Co(2)-O(2W)	85.75(8)
O(1W)-Co(2)-O(2W)#3	93.36(6)	O(6)-Co(2)-O(2W)#3	85.90(7)
O(6)#3-Co(2)-O(2W)#3	91.28(9)	O(2W)-Co(2)-O(2W)#3	173.28(12)

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

Table S2. Selected bond distances (Å) and angles (°) for **2**

Zn(1)-O(4)#1	2.03330(18)	Zn(1)-O(5)#1	2.0744(19)
Zn(1)-O(6)#2	2.0785(18)	Zn(1)-O(1)	2.122(2)
Zn(1)-N(1)#1	2.219(2)	Zn(1)-O(2)	2.2742)
Zn(2)-O(2W)	1.959(3)	Zn(2)-O(3)#3	1.9976(18)
Zn(2)-O(3)	1.9976(18)	Zn(2)-O(1W)#3	2.0903(2)
O(4)#1-Zn(1)-O(5)#1	109.67(8)	O(4)#1-Zn(1)-O(6)#2	95.21(7)
O(5)#1-Zn(1)-O(6)#2	92.32(7)	O(4)#1-Zn(1)-O(1)	158.26(8)

O(5)#1-Zn(1)-O(1)	92.02(8)	O(6)#2-Zn(1)-O(1)	85.01(8)
O(4)#1-Zn(1)-N(1)#1	78.50(7)	O(5)#1-Zn(1)-N(1)#1	79.87(7)
O(6)#2-Zn(1)-N(1)#1	167.521(8)	O(1)-Zn(1)-N(1)#1	104.86(8)
O(4)#1-Zn(1)-O(2)	99.56(8)	O(5)#1-Zn(1)-O(2)	148.46(8)
O(6)#2-Zn(1)-O(2)	96.67(8)	O(1)-Zn(1)-O(2)	58.95(8)
N(1)#1-Zn(1)-O(2)	95.03(8)	O(2W)-Zn(2)-O(3)#3	117.18(6)
O(2W)-Zn(2)-O(3)	117.18(6)	O(3)#3-Zn(2)-O(3)	125.63(12)
O(2W)-Zn(2)-O(1W)#3	94.15(6)	O(3)#3-Zn(2)-O(1W)#3	85.55(8)
O(3)-Zn(2)-O(1W)#3	90.66(8)	O(2W)-Zn(2)-O(1W)	94.15(6)
O(3)#3-Zn(2)-O(1W)	90.66(8)	O(3)-Zn(2)-O(1W)	85.55(8)

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

Table S3. Selected bond distances (Å) and angles (°) for **3**

Co(2)-O(2W)	2.062(2)	Co(2)-O(2W)#1	2.062(2)
Co(2)-O(5)	2.119(2)	Co(2)-O(5)#1	2.119(2)
Co(2)-N(2)	2.166(2)	Co(2)-N(2)#1	2.166(2)
Co(1)-O(6)	2.048(2)	Co(1)-O(4)	2.076(2)
Co(1)-O(2)#2	2.097(2)	Co(1)-O(1W)	2.146(3)
Co(1)-N(3)#3	2.150(3)	Co(1)-N(1)	2.199(2)
O(2W)-Co(2)-O(2W)#1	180.00(1)	O(2W)-Co(2)-O(5)	91.03(10)
O(2W)#1-Co(2)-O(5)	88.97(10)	O(2W)-Co(2)-O(5)#1	88.97(10)
O(2W)#1-Co(2)-O(5)#1	91.03(10)	O(5)-Co(2)-O(5)#1	180.00(11)
O(2W)-Co(2)-N(2)	88.57(10)	O(2W)#1-Co(2)-N(2)	91.43(10)
O(5)-Co(2)-N(2)	89.58(9)	O(5)#1-Co(2)-N(2)	90.42(9)
O(2W)-Co(2)-N(2)#1	91.43(10)	O(2W)#1-Co(2)-N(2)#1	88.57(10)
O(5)-Co(2)-N(2)#1	90.42(9)	O(5)#1-Co(2)-N(2)#1	89.58(9)
O(6)-Co(1)-O(2)#2	89.57(9)	O(4)-Co(1)-O(2)#2	175.15(10)
O(6)-Co(1)-O(1W)	170.25(10)	O(4)-Co(1)-O(1W)	88.21(12)
O(2)#2-Co(1)-O(1W)	88.14(8)	O(6)-Co(1)-N(3)#3	92.54(9)

O(4)-Co(1)-N(3)#3	90.43(10)	O(2)#2-Co(1)-N(3)#3	93.18(10)
O(1W)-Co(1)-N(3)#3	97.02(11)	O(6)-Co(1)-N(1)	80.75(9)
O(4)-Co(1)-N(1)	79.77(9)	O(2)#2-Co(1)-N(1)	97.05(9)
O(1W)-Co(1)-N(1)	90.06(8)	N(3)#3-Co(1)-N(1)	167.71(4)

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

Table S4. Selected bond distances (Å) and angles (°) for **4**

Ni(1)-O(4)	2.049(3)	Ni(1)-O(5)	2.053(3)
Ni(1)-N(2)	2.068(4)	Ni(1)-O(2)#1	2.073(3)
Ni(1)-O(1W)	2.105(4)	Ni(1)-N(1)	2.144(3)
Ni(2)-N(6)#2	2.105(3)	Ni(2)-N(6)	2.105(3)
Ni(2)-O(3)	2.108(3)	Ni(2)-O(3)#2	2.108(3)
Ni(2)-N(5)#3	2.110(3)	Ni(2)-N(5)#4	2.110(3)
O(4)-Ni(1)-O(5)	88.04(12)	O(4)-Ni(1)-N(2)	91.24(13)
O(5)-Ni(1)-N(2)	93.18(14)	O(4)-Ni(1)-O(2)#1	93.21(12)
O(5)-Ni(1)-O(2)#1	176.93(12)	N(2)-Ni(1)-O(2)#1	89.60(13)
O(4)-Ni(1)-O(1W)	172.93(13)	O(5)-Ni(1)-O(1W)	88.72(16)
N(2)-Ni(1)-O(1W)	95.22(16)	O(2)#1-Ni(1)-O(1W)	89.72(16)
O(4)-Ni(1)-N(1)	83.12(12)	O(5)-Ni(1)-N(1)	81.21(13)
N(2)-Ni(1)-N(1)	172.15(13)	O(2)#1-Ni(1)-N(1)	96.16(12)
O(1W)-Ni(1)-N(1)	90.17(15)	N(6)#2-Ni(2)-N(6)	180.00(12)
N(6)#2-Ni(2)-O(3)	93.90(11)	N(6)-Ni(2)-O(3)	86.10(11)
N(6)#2-Ni(2)-O(3)#2	86.10(10)	N(6)-Ni(2)-O(3)#2	93.90(11)
O(3)-Ni(2)-O(3)#2	180.00(16)	N(6)#2-Ni(2)-N(5)#3	85.73(12)
N(6)-Ni(2)-N(5)#3	94.27(12)	O(3)-Ni(2)-N(5)#3	87.80(11)
O(3)#2-Ni(2)-N(5)#3	92.20(11)	N(6)#2-Ni(2)-N(5)#4	94.27(12)
N(6)-Ni(2)-N(5)#4	85.73(12)	O(3)-Ni(2)-N(5)#4	92.20(11)
O(3)#2-Ni(2)-N(5)#4	87.80(15)	N(5)#3-Ni(2)-N(5)#4	180.00(15)

Symmetry transformations used to generate equivalent atoms: #1 -x+2, -y-1, -z-1; #2 -x+1, -y-1, -z; #3 -x+1, -y, -z; #4 x, y-1, z; #5 -x+2, -y-2, -z; #6 x, y+1, z.

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

Co(1)-O(5)	2.065(2)	Co(1)-O(2)#1	2.0934(19)
Co(1)-O(4)	2.0934(19)	Co(1)-N(2)	2.105(2)
Co(1)-O(1W)	2.104(2)	Co(1)-N(1)	2.180(2)
Co(2)-O(3W)#2	2.070(2)	Co(2)-O(3W)	2.070(2)
Co(2)-O(4W)	2.087(2)	Co(2)-O(4W)#2	2.087(2)
Co(2)-N(7)#2	2.133(3)	Co(2)-N(7)	2.138(3)
O(5)-Co(1)-O(2)#1	88.14(8)	O(5)-Co(1)-O(4)	92.72(9)
O(2)#1-Co(1)-O(4)	179.04(9)	O(5)-Co(1)-N(2)	95.20(9)
O(2)#1-Co(1)-N(2)	90.24(9)	O(4)-Co(1)-N(2)	89.21(9)
O(5)-Co(1)-O(1W)	169.73(9)	O(2)#1-Co(1)-O(1W)	89.66(9)
O(4)-Co(1)-O(1W)	89.61(7)	N(2)-Co(1)-O(1W)	94.91(8)
O(5)-Co(1)-N(1)	80.72(8)	O(2)#1-Co(1)-N(1)	101.49(8)
O(4)-Co(1)-N(1)	79.13(8)	N(2)-Co(1)-N(1)	167.39(9)
O(1W)-Co(1)-N(1)	89.89(9)	O(3W)#2-Co(2)-O(3W)	180.00(9)
O(3W)#2-Co(2)-O(4W)	89.56(10)	O(3W)-Co(2)-O(4W)	90.44(10)
O(3W)#2-Co(2)-O(4W)#2	90.44(10)	O(3W)-Co(2)-O(4W)#2	89.56(10)
O(4W)-Co(2)-O(4W)#2	180.00(14)	O(3W)#2-Co(2)-N(7)#2	91.92(12)
O(3W)-Co(2)-N(7)#2	88.08(12)	O(4W)-Co(2)-N(7)#2	86.75(12)
O(4W)#2-Co(2)-N(7)#2	93.25(12)	O(3W)#2-Co(2)-N(7)	88.08(12)
O(3W)-Co(2)-N(7)	91.92(12)	O(4W)-Co(2)-N(7)	93.25(12)
O(4W)#2-Co(2)-N(7)	86.75(12)	N(7)#2-Co(2)-N(7)	180.00(14)

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

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

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(2W)-H(2A)···O(1)	0.84(5)	1.94(5)	2.778(4)	171(4)
O(3W)-H(3A)···O(3)	0.76(5)	1.94(5)	2.684(3)	165(5)

C(23)-H(23) ⋯ N(4)	0.93	2.53	2.870(4)	101.8
O(1W)-H(1A)⋯O(2W)#5	0.87(4)	1.86(4)	2.729(4)	173(4)
O(1W)-H(1B)⋯O(1)#1	0.79(4)	1.85(4)	2.628(3)	166(4)
O(2W)-H(2B)⋯N(3)#6	0.90(5)	2.07(5)	2.948(4)	166(4)
O(3W)-H(3B)⋯O(5)#7	0.81(5)	1.88(5)	2.670(3)	163(4)
O(4W)-H(4A)⋯O(6)#7	0.95(5)	1.73(5)	2.633(3)	157(4)
O(4W)-H(4B)⋯O(3)#2	0.77(5)	1.98(5)	2.714(3)	158(5)

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

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

Ni(1)-O(4)	2.047(2)	Ni(1)-O(5)	2.060(2)
Ni(1)-N(2)	2.062(3)	Ni(1)-O(3W)	2.068(3)
Ni(1)-O(2)#1	2.072(2)	Ni(1)-N(1)	2.125(2)
Ni(2)-O(2W)#2	2.045(2)	Ni(2)-O(2W)	2.045(2)
Ni(2)-O(1W)	2.047(2)	Ni(2)-O(1W)#2	2.047(2)
Ni(2)-N(5)#2	2.094(4)	Ni(2)-N(5)	2.094(4)
O(4)-Ni(1)-O(5)	91.12(10)	O(4)-Ni(1)-N(2)	93.71(10)
O(5)-Ni(1)-N(2)	88.55(10)	O(4)-Ni(1)-O(3W)	171.68(10)
O(5)-Ni(1)-O(3W)	90.20(11)	N(2)-Ni(1)-O(3W)	94.54(11)
O(4)-Ni(1)-O(2)#1	87.57(9)	O(5)-Ni(1)-O(2)#1	178.48(10)
N(2)-Ni(1)-O(2)#1	90.77(10)	O(3W)-Ni(1)-O(2)#1	91.21(10)
O(4)-Ni(1)-N(1)	82.49(9)	O(5)-Ni(1)-N(1)	81.22(10)
N(2)-Ni(1)-N(1)	168.98(11)	O(3W)-Ni(1)-N(1)	89.59(10)
O(2)#1-Ni(1)-N(1)	99.36(10)	O(2W)#2-Ni(2)-O(2W)	180.00(17)
O(2W)#2-Ni(2)-O(1W)	90.40(11)	O(2W)-Ni(2)-O(1W)	89.60(11)
O(2W)#2-Ni(2)-O(1W)#2	89.60(11)	O(2W)-Ni(2)-O(1W)#2	89.60(11)
O(1W)-Ni(2)-O(1W)#2	180.0	O(2W)#2-Ni(2)-N(5)#2	87.58(14)
O(2W)-Ni(2)-N(5)#2	92.42(13)	O(1W)-Ni(2)-N(5)#2	86.96(13)
O(1W)#2-Ni(2)-N(5)#2	93.04(13)	O(2W)#2-Ni(2)-N(5)	92.42(14)

O(2W)-Ni(2)-N(5)	87.58(14)	O(2W)-Ni(2)-N(5)#2	92.42(14)
O(1W)-Ni(2)-N(5)#2	86.96(13)	O(1W)#2-Ni(2)-N(5)#2	93.04(13)
O(2W)#2-Ni(2)-N(5)	92.42(14)	O(2W)-Ni(2)-N(5)	87.58(14)
O(1W)-Ni(2)-N(5)	93.04(13)	O(1W)#2-Ni(2)-N(5)	86.96(13)
N(5)#2-Ni(2)-N(5)	180.00(17)		

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

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

D-H⋯A	d(D-H)	d(H⋯A)	d(D⋯A)	<(DHA)
O(3W)-H(3B)⋯O(4W)	0.85(4)	1.89(4)	2.732(4)	171(4)
O(1W)-H(1A)⋯O(3)#5	0.96(5)	1.73(5)	2.627(4)	153(4)
O(1W)-H(1B)⋯O(6)#2	0.81(5)	1.92(5)	2.705(4)	163(5)
O(2W)-H(2B)⋯O(4)#6	0.87(5)	1.84(5)	2.659(3)	156(5)
O(4W)-H(4A)⋯N(3)#5	0.81(5)	2.16(5)	2.954(4)	165(5)
O(4W)-H(4B)⋯O(1)#7	0.83(5)	1.95(5)	2.785(4)	175(5)

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

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

Zn(1)-O(2)#1	2.085(2)	Zn(1)-O(4)	2.092(2)
Zn(1)-N(2)	2.096(3)	Zn(1)-O(1W)	2.120(2)
Zn(1)-O(5)	2.153(2)	Zn(1)-N(1)	2.183(2)
Zn(2)-O(2W)	2.086(2)	Zn(2)-O(2W)#2	2.086(2)
Zn(2)-O(3W)#2	2.096(3)	Zn(2)-O(3W)	2.096(3)
Zn(2)-N(5)	2.148(3)	Zn(2)-N(5)#2	2.148(3)
O(2)#1-Zn(1)-O(4)	87.95(9)	O(2)#1-Zn(1)-N(2)	91.86(10)
O(4)-Zn(1)-O(1W)	168.68(8)	N(2)-Zn(1)-O(1W)	95.77(10)
O(2)#1-Zn(1)-O(5)	179.13(8)	O(4)-Zn(1)-O(5)	92.14(10)
N(2)-Zn(1)-O(5)	87.28(9)	O(1W)-Zn(1)-O(5)	89.80(10)

O(2)#1-Zn(1)-N(1)	103.11(9)	O(4)-Zn(1)-N(1)	80.63(9)
N(2)-Zn(1)-N(1)	164.32(10)	O(1W)-Zn(1)-N(1)	88.90(9)
O(5)-Zn(1)-N(1)	77.76(9)	O(2W)-Zn(2)-O(2W)#2	180.00(17)
O(2W)-Zn(2)-O(3W)#2	90.37(11)	O(2W)#2-Zn(2)-O(3W)#2	89.63(11)
O(2W)-Zn(2)-O(3W)	89.63(11)	O(2W)#2-Zn(2)-O(3W)	90.37(11)
O(3W)#2-Zn(2)-O(3W)	180.00(13)	O(2W)-Zn(2)-N(5)	92.65(13)
O(2W)#2-Zn(2)-N(5)	87.35(13)	O(3W)#2-Zn(2)-N(5)	93.61(12)
O(3W)-Zn(2)-N(5)	86.39(12)	O(2W)-Zn(2)-N(5)#2	87.35(13)
O(2W)#2-Zn(2)-N(5)#2	92.65(13)	O(3W)#2-Zn(2)-N(5)#2	86.39(12)
O(3W)-Zn(2)-N(5)#2	93.6112)	N(5)-Zn(2)-N(5)#2	180.00(15)

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

Table S7b. Hydrogen bonds for **7** (Å and °).

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(1W)-H(1B)···O(4W)	0.81(4)	1.93(4)	2.744(4)	179(4)
O(2W)-H(2A)···O(6)	0.75(5)	1.94(5)	2.676(3)	168(5)
O(3W)-H(3A)···O(6)	0.82(5)	1.94(5)	2.721(4)	161(5)
O(1W)-H(1A)···O(1)#1	0.85(4)	1.83(5)	2.629(4)	155(4)
O(2W)-H(2B)···O(4)#5	0.80(5)	1.91(5)	2.670(3)	160(5)
O(4W)-H(4A)···N(3)#5	0.895(10)	2.065(15)	2.944(4)	167(4)

Symmetry transformations used to generate equivalent atoms: #1 -x, -y+1, -z+1; #2 -x+1, -y+1, -z; #3 -x-1, -y, -z; #4 -x, -y+2, -z; #5 x+1, y, z.

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

Co(1)-O(4W)#1	2.098(2)	Co(1)-O(4W)	2.098(2)
Co(1)-N(5)	2.121(2)	Co(1)-N(5)#1	2.12(2)
Co(1)-O(3W)	2.1314(19)	Co(1)-O(3W)#1	2.1314(19)
Co(2)-O(4)	2.007(2)	Co(2)-O(1)#2	2.012(2)
Co(2)-O(6)	2.0399(19)	Co(2)-N(2)	2.067(2)
Co(2)-N(1)	2.2127(19)		

O(4W)#1-Co(1)-O(4W)	180.00(12)	O(4W)#1-Co(1)-N(5)	88.61(9)
O(4W)-Co(1)-N(5)	91.39(9)	O(4W)#1-Co(1)-N(5)#1	91.39(9)
O(4W)-Co(1)-N(5)#1	88.61(9)	N(5)-Co(1)-N(5)#1	180.00(9)
O(4W)#1-Co(1)-O(3W)	89.63(8)	O(4W)-Co(1)-O(3W)	90.37(8)
N(5)-Co(1)-O(3W)	90.10(8)	N(5)#1-Co(1)-O(3W)	89.90(8)
O(4W)#1-Co(1)-O(3W)#1	90.37(8)	O(4W)-Co(1)-O(3W)#1	89.63(8)
N(5)-Co(1)-O(3W)#1	89.90(8)	N(5)#1-Co(1)-O(3W)#1	90.10(8)
O(3W)-Co(1)-O(3W)#1	180.00(13)	O(4)-Co(2)-O(1)#2	151.57(10)
O(4)-Co(2)-O(6)	102.85(9)	O(1)#2-Co(2)-O(6)	102.21(9)
O(4)-Co(2)-N(2)	95.95(8)	O(1)#2-Co(2)-N(2)	95.03(8)
O(6)-Co(2)-N(2)	97.17(8)	O(4)-Co(2)-N(1)	80.32(8)
O(1)#2-Co(2)-N(1)	91.24(8)	O(6)-Co(2)-N(1)	79.58(7)
N(2)-Co(2)-N(1)	173.44(8)		

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

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

D-H···A		d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(1W)-H(1A)	O(2W)	0.92(1)	1.91(3)	2.752(6)	151(4)
O(2W)-H(2A)	O(2)	0.918(10)	2.01(4)	2.849(5)	152(7)
O(3W)-H(3B)	O(3)	0.79(3)	2.19(4)	2.900(3)	150(3)
O(1W)-H(1B)	O(4)#5	0.907(10)	2.031(18)	2.918(4)	165(5)
O(2W)-H(2B)	O(2)#6	0.912(10)	2.091(14)	2.999(5)	173(6)
O(3W)-H(3A)	O(6)#7	0.77(4)	2.03(4)	2.778(3)	165(4)
O(4W)-H(4A)	O(3)#1	0.73(4)	2.11(4)	2.810(3)	161(4)
O(4W)-H(4B)	O(5)#7	0.80(4)	1.90(4)	2.701(3)	174(4)

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

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

Co(1)-O(3)#1	2.0261(17)	Co(1)-O(2)	2.0480(18)

Co(1)-O(5)#1	2.0541(18)	Co(1)-N(2)	2.0746(17)
Co(1)-N(1)#1	2.2046(18)	Co(2)-N(4)#2	2.1189(19)
Co(2)-N(4)	2.1189(19)	Co(2)-O(1W)	2.1274(18)
Co(2)-O(1W)#2	2.1274(18)	Co(2)-O(2W)#2	2.1390(18)
Co(2)-O(2W)	2.1390(18)		
O(3)#1-Co(1)-O(2)	151.43(8)	O(3)#1-Co(1)-O(5)#1	107.03(8)
O(2)-Co(1)-O(5)#1	97.73(8)	O(3)#1-Co(1)-N(2)	93.27(7)
O(2)-Co(1)-N(2)	97.26(7)	O(5)#1-Co(1)-N(2)	97.93(7)
O(3)#1-Co(1)-N(1)#1	79.62(7)	O(2)-Co(1)-N(1)#1	92.20(7)
O(5)#1-Co(1)-N(1)#1	77.85(7)	N(2)-Co(1)-N(1)#1	170.11(7)
N(4)#2-Co(2)-N(4)	180.00(11)	N(4)#2-Co(2)-O(1W)	89.43(7)
N(4)-Co(2)-O(1W)	90.57(7)	N(4)#2-Co(2)-O(1W)#2	90.57(7)
N(4)-Co(2)-O(1W)#2	89.43(7)	O(1W)-Co(2)-O(1W)#2	180.00(10)
N(4)#2-Co(2)-O(2W)#2	88.16(7)	N(4)-Co(2)-O(2W)#2	91.84(7)
O(1W)-Co(2)-O(2W)#2	87.89(7)	O(1W)#2-Co(2)-O(2W)#2	92.11(7)
N(4)#2-Co(2)-O(2W)	91.82(7)	N(4)-Co(2)-O(2W)	88.16(7)
O(1W)-Co(2)-O(2W)	92.11(8)	O(1W)#2-Co(2)-O(2W)	87.89(8)

Symmetry transformations used to generate equivalent atoms:#1 -x+1, -y, -z; #2 -x+1, -y+1, -z-1; #3 -x+2, -y+1, -z+1; #4 -x, -y+2, -z-1; #5 -x+1, -y+1, -z-2.

Table S9b. Hydrogen bonds for **9** (Å and °).

D-H⋯A	d(D-H)	d(H⋯A)	d(D⋯A)	<(DHA)
O(1W)-H(1A)⋯O(3W)	0.81(3)	1.98(4)	2.759(17)	162(3)
O(2W)-H(2A)⋯O(6)	0.74(5)	2.09(3)	2.824(3)	169(3)
O(3W)-H(3A)⋯O(4W)	0.76(3)	1.98(3)	2.724(3)	168(3)
O(2W)-H(2B)⋯O(4)#6	0.82(3)	1.86(3)	2.671(3)	169(3)

Symmetry transformations used to generate equivalent atoms:#1 -x+1, -y, -z; #2 -x+1, -y+1, -z-1; #3 -x+2, -y+1, -z+1; #4 -x, -y+2, -z-1; #5 -x+1, -y+1, -z-2; #6 -x+1, -y, -z-1.

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

Ni(1)-O(4)#1	2.0109(11)	Ni(1)-O(6)	2.0302(12)

Ni(1)-O(5)#1	2.0330(11)	Ni(1)-O(2W)	2.0531(12)
Ni(1)-O(1W)	2.0736(14)	Ni(1)-N(1)#1	2.1371(14)
O(4)#1-Ni(1)-O(6)	174.18(5)	O(4)#1-Ni(1)-O(5)#1	88.93(5)
O(6)-Ni(1)-O(5)#1	92.49(5)	O(4)#1-Ni(1)-O(2W)	90.38(5)
O(6)-Ni(1)-O(2W)	87.98(5)	O(5)#1-Ni(1)-O(2W)	177.67(5)
O(4)#1-Ni(1)-O(1W)	92.72(5)	O(6)-Ni(1)-O(1W)	92.91(5)
O(5)#1-Ni(1)-O(1W)	90.56(5)	O(2W)-Ni(1)-O(1W)	91.69(6)
O(4)#1-Ni(1)-N(1)#1	83.69(5)	O(6)-Ni(1)-N(1)#1	90.97(5)
O(5)#1-Ni(1)-N(1)#1	80.48(5)	O(2W)-Ni(1)-N(1)#1	97.24(5)
O(1W)-Ni(1)-N(1)#1	170.39(18)		

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

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

D-H⋯A	d(D-H)	d(H⋯A)	d(D⋯A)	<(DHA)
O(2)-H(2)⋯O(3W)	0.86(3)	1.80(3)	2.656(2)	177(3)
O(1W)-H(1A)⋯O(3)#3	0.84(3)	1.88(3)	2.695(2)	165(2)
O(2W)-H(2B)⋯O(1)#4	0.78(2)	2.04(2)	2.778(2)	158(2)
O(3W)-H(3A)⋯O(5)#1	0.79(3)	1.97(3)	2.758(2)	172(3)
O(3W)-H(3B)⋯O(4)#3	0.82(3)	1.96(3)	2.783(6)	175(3)

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

.

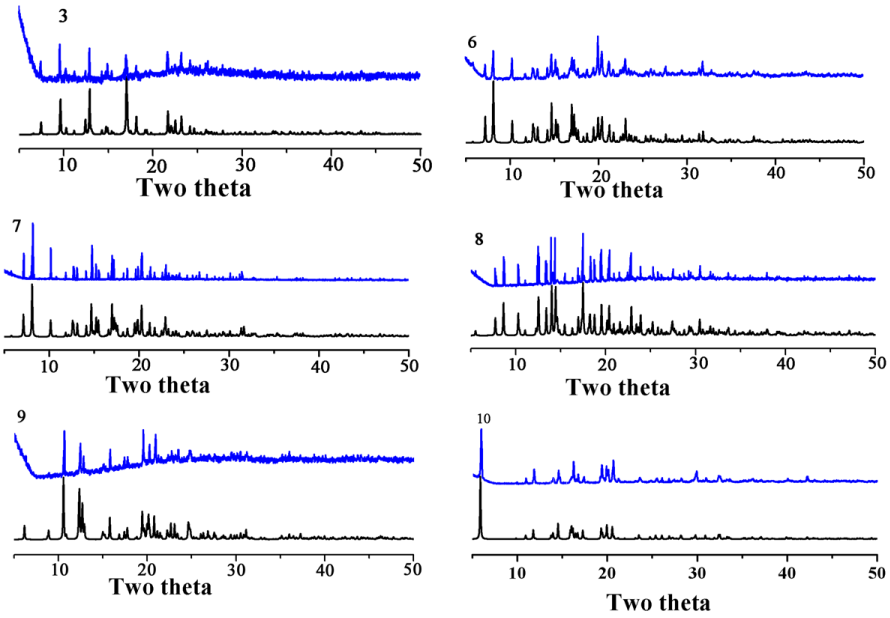


Fig. S2 Simulated (black) and experimental (blue) PXRD patterns of **3**, **6** and **7**–**10**.

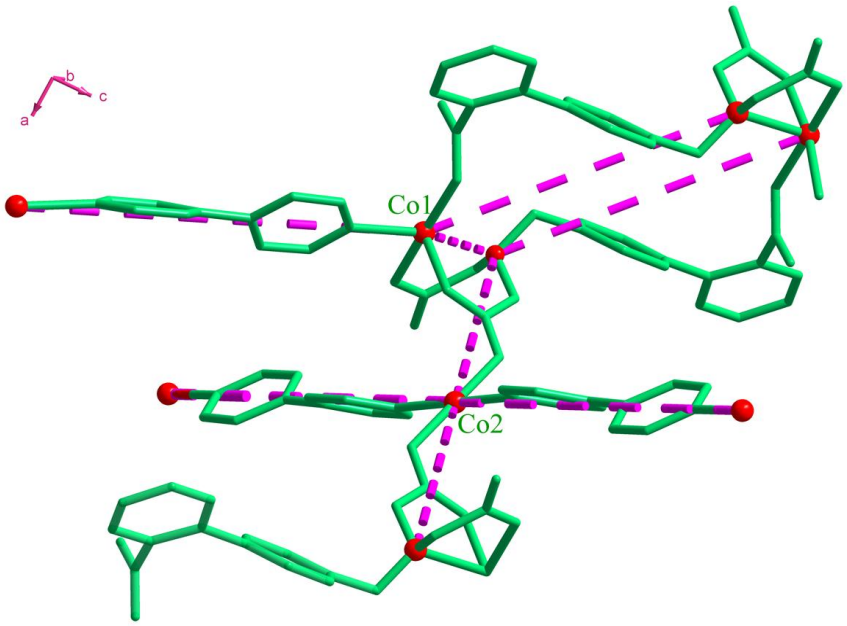
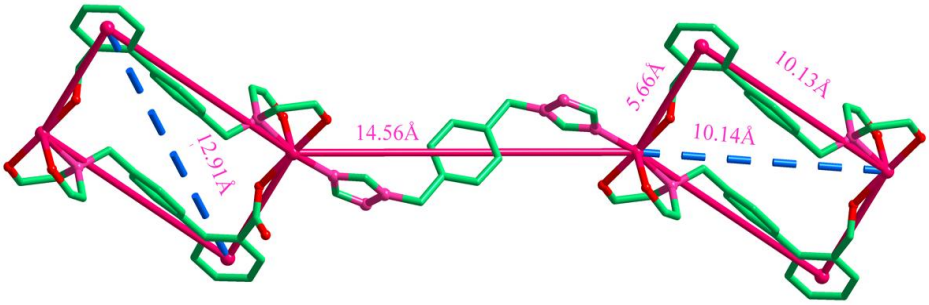
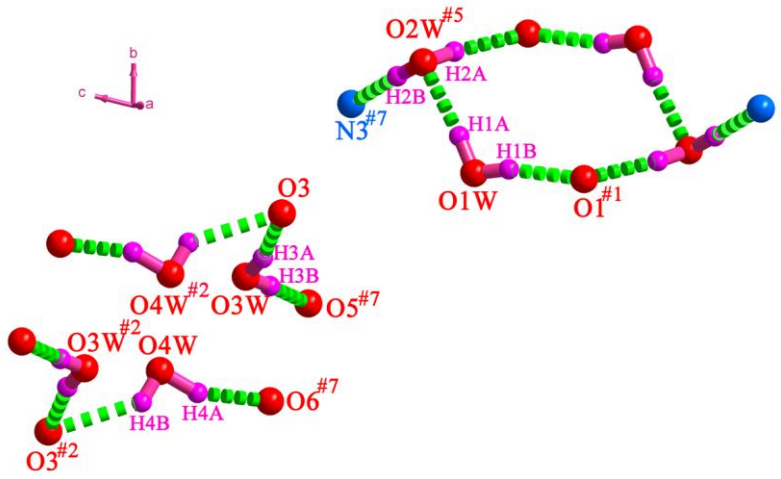


Fig. S3 View of the unit of the 3D framework in **3**.



(a)



(b)

Fig. S4 (a) View of the length of the unit $[Co_2(L)_2(bbtz)]$. (b) View of the hydrogen-bonding interactions among the water molecules and carboxylate anions.

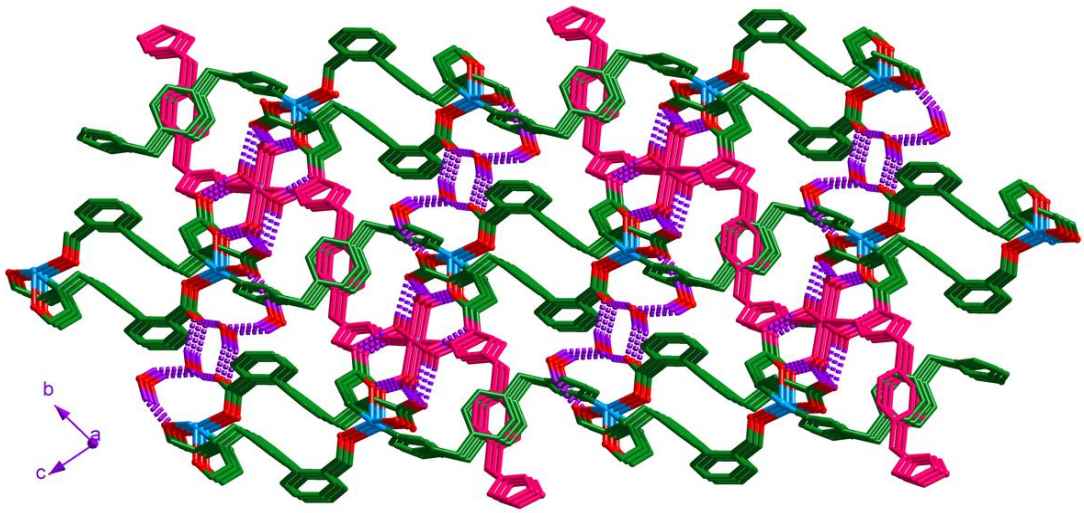


Fig. S5 View of the 3D supramolecular structure of **8** linked by hydrogen-bonding interactions (H-bonds purple lines).

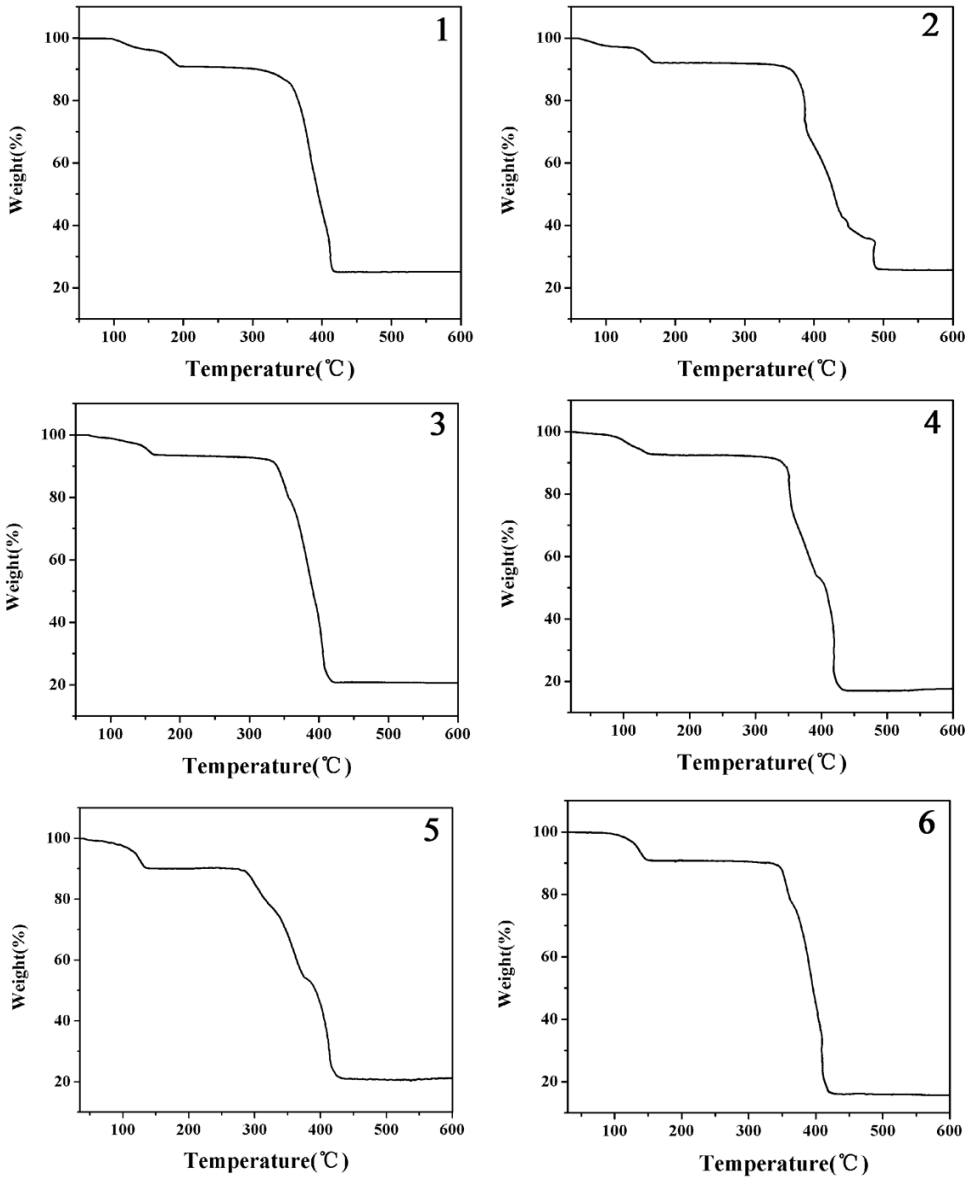


Fig. S6 The TGA curves of compounds **1-6.**

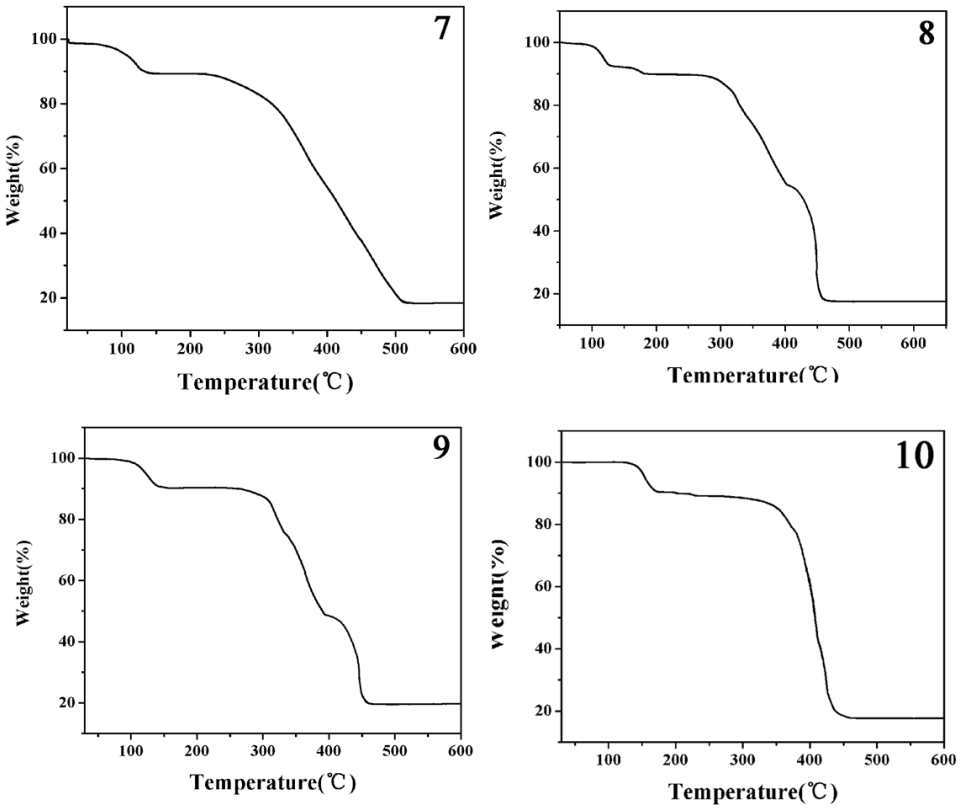


Fig. S7 The TGA curves of compounds **7**-**10.**

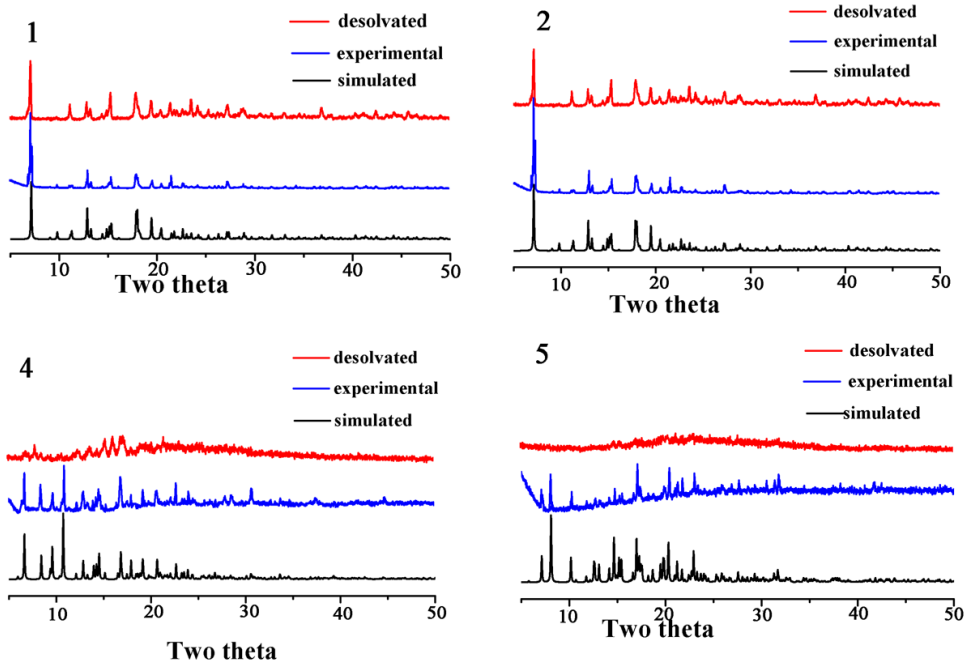


Fig. S8 Simulated, experimental and desolvated PXRD patterns of **1**, **2**, **4** and **5** (**1**, **2**, **4** and **5** were heated to 200, 170, 160 and 130 ℃ under vacuum, respectively).

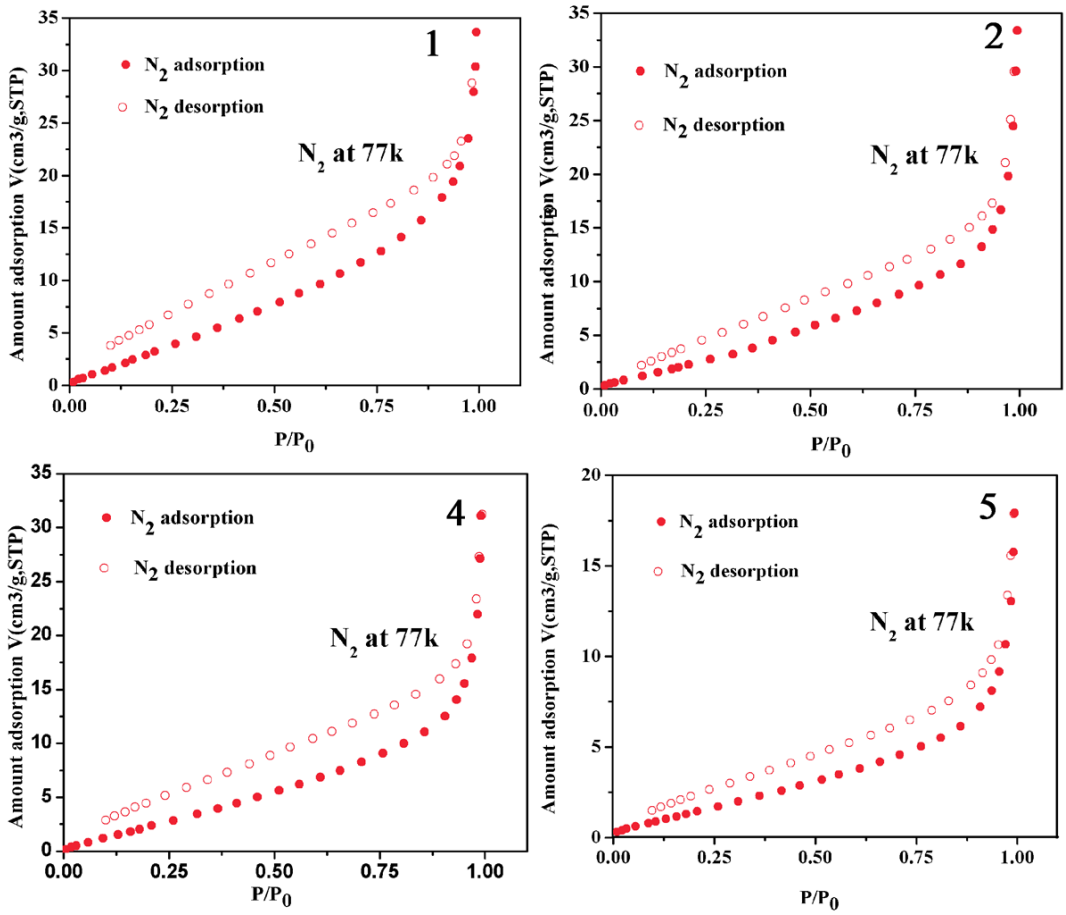


Fig. S9 Adsorption isotherms of N_2 for anhydrous compounds **1**, **2**, **4**, and **5**.

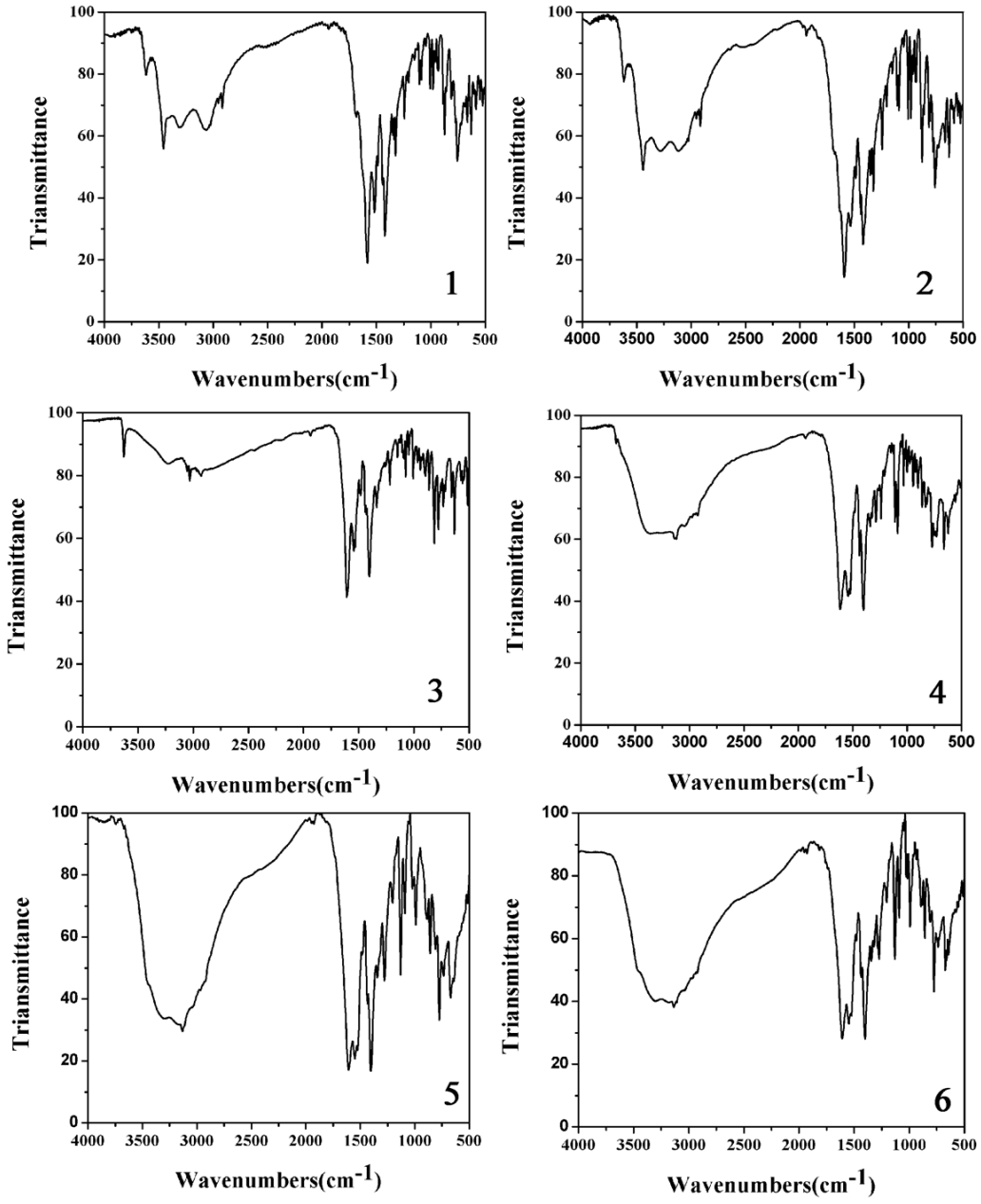


Fig. S10 IR spectra of compounds **1-6**.

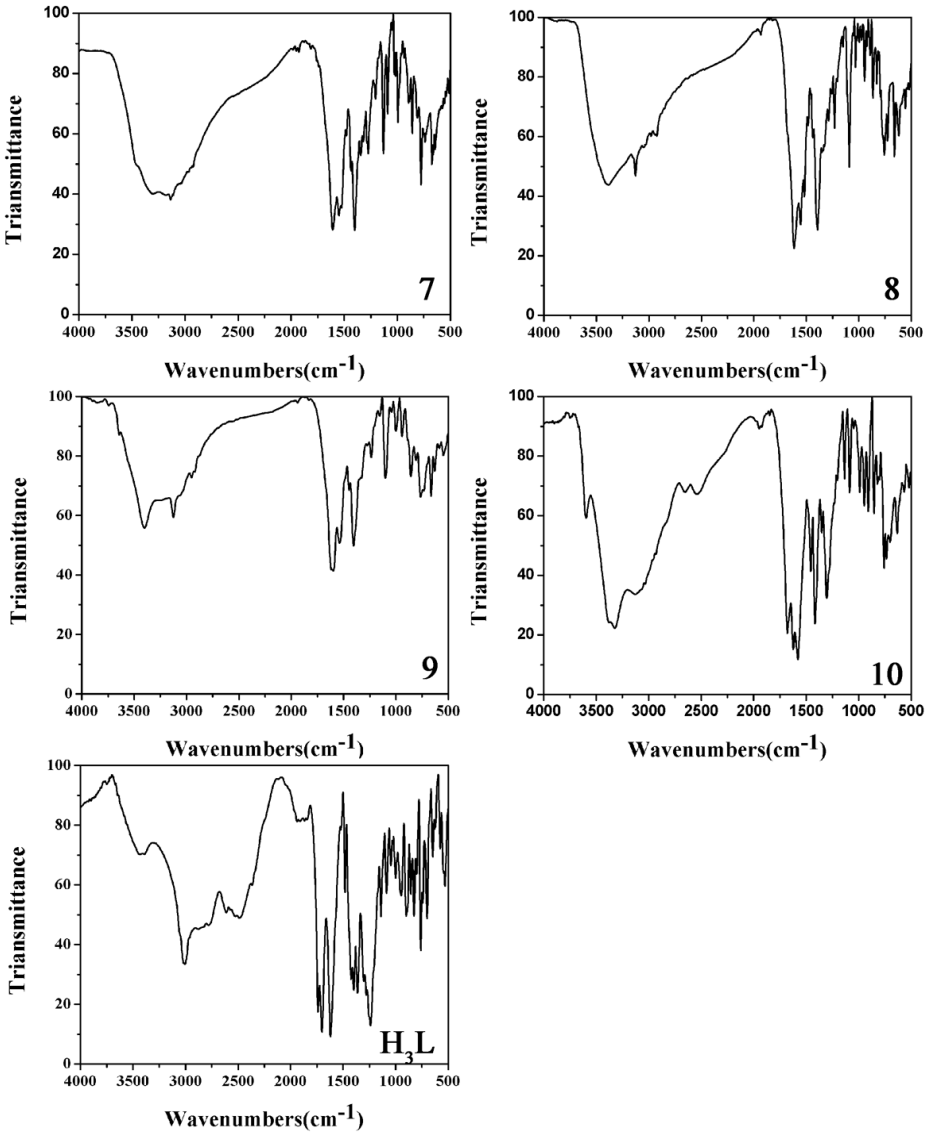


Fig. S11 IR spectra of compounds **7-10** and H_3L.