Supporting Information

Four new Zn(II) and Cd(II) coordination polymers using two amide-liked aromatic multi-carboxylate ligands: synthesis, structures and electrochemical properties

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Contents

Table S1. Selected Bond Distances (Å) and Angles (°) for compounds **1-4**

compound **1**

Zn(1)-O(4)#1	1.956(4)	O(4)#1-Zn(1)-O(1W)	117.97(15)
Zn(1)-O(1W)	1.972(4)	O(4)#1-Zn(1)-O(2)#2	96.17(15)
Zn(1)-O(2)#2	1.968(4)	O(1W)-Zn(1)-O(2)#2	114.45(16)
Zn(1)-N(2)	2.043(5)	O(4)#1-Zn(1)-N(2)	106.25(16)
Zn(1)-C(1)#2	2.577(5)	O(1W)-Zn(1)-N(2)	101.98(17)
C(1)-Zn(1)#2	2.577(5)	O(2)#2-Zn(1)-N(2)	120.71(17)
O(2)-Zn(1)#2	1.968(4)	O(4)#1-Zn(1)-C(1)#2	124.89(17)
O(4)-Zn(1)#1	1.956(3)	O(1W)-Zn(1)-C(1)#2	97.29(16)
N(2)-Zn(1)-C(1)#2	105.86(17)	O(2)#2-Zn(1)-C(1)#2	28.74(17)
O(1)-C(1)-Zn(1)#2	73.9(3)	C(18)-N(2)-Zn(1)	119.7(3)
O(2)-C(1)-Zn(1)#2	48.0(2)	C(17)-N(2)-Zn(1)	122.5(3)
C(5)-C(1)-Zn(1)#2	164.6(4)	C(1)-O(2)-Zn(1)#2	103.2(3)
C(2)-O(4)-Zn(1)#1	114.8(3)	Zn(1)-O(1W)-H(6B)	120.0
Zn(1)-O(1W)-H(6C)	120.0		

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

compound **2**

Cd(1)-O(4)#1	2.272(4)	O(4)#1-Cd(1)-O(3)#2	127.92(14)
Cd(1)-O(3)#2	2.282(4)	O(4)#1-Cd(1)-O(6)	80.88(17)
Cd(1)-O(6)	2.314(4)	O(3)#2-Cd(1)-O(6)	88.42(17)
Cd(1)-N(2)#3	2.323(5)	O(4)#1-Cd(1)-N(2)#3	93.59(17)
Cd(1)-O(2)	2.391(3)	O(3)#2-Cd(1)-N(2)#3	92.32(17)
Cd(1)-O(1)	2.420(4)	O(6)-Cd(1)-N(2)#3	173.47(17)
Cd(1)-C(1)	2.729(5)	O(4)#1-Cd(1)-O(2)	89.53(14)
N(2)-Cd(1)#4	2.323(5)	O(3)#2-Cd(1)-O(2)	141.46(14)
O(3)-Cd(1)#2	2.282(4)	O(6)-Cd(1)-O(2)	89.26(16)
O(4)-Cd(1)#5	2.272(4)	N(2)#3-Cd(1)-O(2)	94.18(15)
O(6)-Cd(1)-O(1)	97.64(15)	O(4)#1-Cd(1)-O(1)	143.50(14)
N(2)#3-Cd(1)-O(1)	88.88(15)	O(3)#2-Cd(1)-O(1)	88.27(13)
O(2)-Cd(1)-O(1)	53.98(13)	O(4)#1-Cd(1)-C(1)	116.28(16)
N(2)#3-Cd(1)-C(1)	90.26(16)	O(3)#2-Cd(1)-C(1)	115.38(16)
O(2)-Cd(1)-C(1)	26.83(13)	O(6)-Cd(1)-C(1)	95.29(16)
O(1)-Cd(1)-C(1)	27.23(13)	O(2)-C(1)-Cd(1)	61.1(3)
C(19)-N(2)-Cd(1)#4	124.9(4)	O(1)-C(1)-Cd(1)	62.5(3)
C(20)-N(2)-Cd(1)#4	117.9(4)	C(5)-C(1)-Cd(1)	173.5(4)
C(1)-O(1)-Cd(1)	90.3(3)	C(2)-O(3)-Cd(1)#2	163.5(4)
C(1)-O(2)-Cd(1)	92.0(3)	C(2)-O(4)-Cd(1)#5	106.1(4)
		C(21)-O(6)-Cd(1)	121.4(5)

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

compound **3**			
Zn(1)-O(1)	1.912(4)	O(1)-Zn(1)-O(3)#1	113.40(18)
Zn(1)-O(3)#1	1.967(4)	O(1)-Zn(1)-N(1)#2	123.5(2)
Zn(1)-N(1)#2	2.007(6)	O(3)#1-Zn(1)-N(1)#2	122.2(2)
Zn(1)-O(10)#3	2.124(5)	O(1)-Zn(1)-O(10)#3	94.6(2)
Zn(1)-O(9)	2.317(7)	O(3)#1-Zn(1)-O(10)#3	90.5(2)
Zn(1)-Zn(3)	3.0674(11)	N(1)#2-Zn(1)-O(10)#3	93.9(3)
Zn(1)-Zn(2)	3.0883(11)	O(1)-Zn(1)-O(9)	88.7(2)
Zn(2)-O(1)	1.906(4)	O(3)#1-Zn(1)-O(9)	84.7(2)
Zn(2)-O(11)#3	1.985(5)	N(1)#2-Zn(1)-O(9)	87.4(3)
Zn(2)-N(3)#4	2.013(6)	O(10)#3-Zn(1)-O(9)	175.0(2)
Zn(2)-O(13)#5	2.060(5)	O(1)-Zn(1)-Zn(3)	38.14(12)
Zn(3)-O(1)	1.959(4)	O(3)#1-Zn(1)-Zn(3)	77.92(14)
Zn(3)-O(4)#1	1.987(4)	N(1)#2-Zn(1)-Zn(3)	159.51(19)
Zn(3)-O(15)	1.992(4)	O(10)#3-Zn(1)-Zn(3)	81.25(18)
Zn(3)-O(5)	1.994(5)	O(9)-Zn(1)-Zn(3)	99.16(16)
Zn(4)-O(14)#5	2.004(4)	O(1)-Zn(1)-Zn(2)	35.94(11)
Zn(4)-O(8)	2.009(5)	O(3)#1-Zn(1)-Zn(2)	139.74(15)
Zn(4)-O(1)	2.031(4)	N(1)#2-Zn(1)-Zn(2)	95.92(19)
Zn(4)-O(16)	2.046(5)	O(10)#3-Zn(1)-Zn(2)	73.04(14)
Zn(4)-N(5)#6	2.190(6)	O(9)-Zn(1)-Zn(2)	111.61(18)
N(1)-Zn(1)#7	2.007(6)	Zn(3)-Zn(1)-Zn(2)	63.61(3)
N(3)-Zn(2)#8	2.013(5)	O(1)-Zn(2)-O(11)#3	109.03(17)
N(5)-Zn(4)#9	2.190(6)	O(1)-Zn(2)-N(3)#4	139.2(2)
O(3)-Zn(1)#3	1.967(4)	O(11)#3-Zn(2)-N(3)#4	105.9(2)
O(4)-Zn(3)#3	1.987(4)	O(1)-Zn(2)-O(13)#5	102.19(19)
O(10)-Zn(1)#1	2.124(5)	O(11)#3-Zn(2)-O(13)#5	99.6(2)
O(11)-Zn(2)#1	1.985(5)	N(3)#4-Zn(2)-O(13)#5	92.1(2)
O(13)-Zn(2)#10	2.060(5)	O(1)-Zn(2)-Zn(1)	36.09(11)
O(14)-Zn(4)#10	2.004(4)	O(11)#3-Zn(2)-Zn(1)	77.07(14)
C(1)-N(1)-Zn(1)#7	123.6(5)	N(3)#4-Zn(2)-Zn(1)	174.78(19)
C(5)-N(1)-Zn(1)#7	117.9(6)	O(13)#5-Zn(2)-Zn(1)	91.67(15)
C(25)-N(3)-Zn(2)#8	123.6(5)	O(1)-Zn(3)-O(4)#1	107.59(18)
C(21)-N(3)-Zn(2)#8	117.8(5)	O(1)-Zn(3)-O(15)	105.58(16)
C(45)-N(5)-Zn(4)#9	119.3(6)	O(4)#1-Zn(3)-O(15)	114.41(19)
C(41)-N(5)-Zn(4)#9	124.8(6)	O(1)-Zn(3)-O(5)	128.79(17)
Zn(2)-O(1)-Zn(1)	107.98(18)	O(4)#1-Zn(3)-O(5)	98.12(17)
Zn(2)-O(1)-Zn(3)	114.2(2)	O(15)-Zn(3)-O(5)	102.6(2)
Zn(1)-O(1)-Zn(3)	104.80(17)	O(1)-Zn(3)-Zn(1)	37.07(11)
Zn(2)-O(1)-Zn(4)	108.10(17)	O(4)#1-Zn(3)-Zn(1)	76.34(14)
Zn(1)-O(1)-Zn(4)	116.4(2)	O(15)-Zn(3)-Zn(1)	138.27(13)

Zn(3)-O(1)-Zn(4)	105.61(17)	O(5)-Zn(3)-Zn(1)	116.06(15)
C(19)-O(3)-Zn(1)#3	127.2(4)	O(14)#5-Zn(4)-O(8)	133.9(2)
C(19)-O(4)-Zn(3)#3	128.3(4)	O(14)#5-Zn(4)-O(1)	99.60(16)
C(20)-O(5)-Zn(3)	106.3(4)	O(8)-Zn(4)-O(1)	94.57(18)
C(39)-O(8)-Zn(4)	110.0(5)	O(14)#5-Zn(4)-O(16)	104.5(2)
C(39)-O(9)-Zn(1)	117.0(5)	O(8)-Zn(4)-O(16)	119.3(2)
C(40)-O(10)-Zn(1)#1	125.1(5)	O(1)-Zn(4)-O(16)	89.30(19)
C(40)-O(11)-Zn(2)#1	118.7(4)	O(14)#5-Zn(4)-N(5)#6	85.2(2)
C(59)-O(13)-Zn(2)#10	126.0(4)	O(8)-Zn(4)-N(5)#6	84.0(2)
C(59)-O(14)-Zn(4)#10	136.1(4)	O(1)-Zn(4)-N(5)#6	174.5(2)
C(60)-O(15)-Zn(3)	122.4(4)	O(16)-Zn(4)-N(5)#6	86.7(3)
C(60)-O(16)-Zn(4)	124.1(4)		

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

compound **4**			
Cd(4)-O(13)#1	2.243(8)	O(13)#1-Cd(4)-N(8)#2	87.8(3)
Cd(4)-N(8)#2	2.318(9)	O(13)#1-Cd(4)-O(12)	170.0(4)
Cd(4)-O(12)	2.344(8)	N(8)#2-Cd(4)-O(12)	86.3(3)
Cd(4)-O(17)	2.348(8)	O(13)#1-Cd(4)-O(17)	88.9(3)
Cd(4)-O(11)	2.350(7)	N(8)#2-Cd(4)-O(17)	99.0(3)
Cd(4)-O(5W)	2.358(9)	O(12)-Cd(4)-O(17)	100.0(3)
Cd(4)-C(41)	2.691(11)	O(13)#1-Cd(4)-O(11)	128.8(3)
Cd(3)-O(16)#1	2.270(8)	N(8)#2-Cd(4)-O(11)	140.5(3)
Cd(3)-N(6)#2	2.298(9)	O(12)-Cd(4)-O(11)	55.2(3)
Cd(3)-O(6W)	2.306(10)	O(17)-Cd(4)-O(11)	96.3(3)
Cd(3)-O(19)	2.340(8)	O(13)#1-Cd(4)-O(5W)	84.5(3)
Cd(3)-O(14)#3	2.341(9)	N(8)#2-Cd(4)-O(5W)	91.5(3)
Cd(3)-O(18)	2.353(8)	O(12)-Cd(4)-O(5W)	87.6(3)
Cd(3)-C(62)	2.689(11)	O(17)-Cd(4)-O(5W)	167.4(3)
Cd(1)-O(2)	2.229(8)	O(11)-Cd(4)-O(5W)	79.6(3)
Cd(1)-O(1W)	2.304(10)	O(13)#1-Cd(4)-C(41)	155.3(4)
Cd(1)-N(4)	2.314(10)	N(8)#2-Cd(4)-C(41)	112.9(4)
Cd(1)-O(2W)	2.353(11)	O(12)-Cd(4)-C(41)	27.2(3)
Cd(1)-O(3)#1	2.390(9)	O(17)-Cd(4)-C(41)	100.5(3)
Cd(1)-O(4)#1	2.419(7)	O(11)-Cd(4)-C(41)	28.0(3)
Cd(1)-C(2)#1	2.756(12)	O(5W)-Cd(4)-C(41)	81.6(3)
Cd(2)-O(9)	2.246(8)	O(16)#1-Cd(3)-N(6)#2	89.5(3)
Cd(2)-N(2)#4	2.318(9)	O(16)#1-Cd(3)-O(6W)	81.8(3)

Cd(2)-O(4W)	2.341(11)	N(6)#2-Cd(3)-O(6W)	91.3(3)
Cd(2)-O(7)#5	2.374(7)	O(16)#1-Cd(3)-O(19)	168.1(4)
Cd(2)-O(3W)	2.406(9)	N(6)#2-Cd(3)-O(19)	85.5(3)
Cd(2)-O(6)#5	2.431(8)	O(6W)-Cd(3)-O(19)	87.5(3)
Cd(2)-O(8)	2.603(9)	O(16)#1-Cd(3)-O(14)#3	87.5(3)
Cd(2)-C(21)#5	2.742(12)	N(6)#2-Cd(3)-O(14)#3	97.9(3)
C(2)-Cd(1)#6	2.756(12)	O(6W)-Cd(3)-O(14)#3	165.8(3)
C(21)-Cd(2)#7	2.743(12)	O(19)-Cd(3)-O(14)#3	103.9(3)
N(2)-Cd(2)#8	2.318(9)	O(16)#1-Cd(3)-O(18)	128.4(3)
N(6)-Cd(3)#2	2.298(9)	N(6)#2-Cd(3)-O(18)	140.2(3)
N(8)-Cd(4)#2	2.318(9)	O(6W)-Cd(3)-O(18)	83.7(3)
O(3)-Cd(1)#6	2.390(9)	O(19)-Cd(3)-O(18)	54.9(3)
O(4)-Cd(1)#6	2.419(7)	O(14)#3-Cd(3)-O(18)	95.9(3)
O(6)-Cd(2)#7	2.431(8)	O(16)#1-Cd(3)-C(62)	153.9(4)
O(7)-Cd(2)#7	2.374(7)	N(6)#2-Cd(3)-C(62)	113.1(4)
O(13)-Cd(4)#6	2.243(8)	O(6W)-Cd(3)-C(62)	84.6(4)
O(14)-Cd(3)#9	2.341(9)	O(19)-Cd(3)-C(62)	27.7(3)
O(16)-Cd(3)#6	2.270(8)	O(14)#3-Cd(3)-C(62)	101.5(3)
O(3)-C(2)-Cd(1)#6	60.0(7)	O(18)-Cd(3)-C(62)	27.2(3)
O(4)-C(2)-Cd(1)#6	61.3(6)	O(2)-Cd(1)-O(1W)	92.1(4)
C(3)-C(2)-Cd(1)#6	179.1(10)	O(2)-Cd(1)-N(4)	87.5(4)
O(6)-C(21)-Cd(2)#7	62.4(7)	O(1W)-Cd(1)-N(4)	96.3(4)
O(7)-C(21)-Cd(2)#7	59.8(6)	O(2)-Cd(1)-O(2W)	85.2(4)
C(23)-C(21)-Cd(2)#7	178.1(10)	O(1W)-Cd(1)-O(2W)	173.2(4)
O(12)-C(41)-Cd(4)	60.5(6)	N(4)-Cd(1)-O(2W)	89.8(4)
O(11)-C(41)-Cd(4)	60.8(6)	O(2)-Cd(1)-O(3)#1	172.8(4)
C(43)-C(41)-Cd(4)	175.4(9)	O(1W)-Cd(1)-O(3)#1	91.9(4)
O(18)-C(62)-Cd(3)	61.0(6)	N(4)-Cd(1)-O(3)#1	86.1(3)
O(19)-C(62)-Cd(3)	60.5(6)	O(2W)-Cd(1)-O(3)#1	91.5(4)
C(67)-C(62)-Cd(3)	177.9(11)	O(2)-Cd(1)-O(4)#1	132.3(3)
C(18)-N(2)-Cd(2)#8	122.8(8)	O(1W)-Cd(1)-O(4)#1	91.5(3)
C(19)-N(2)-Cd(2)#8	121.8(8)	N(4)-Cd(1)-O(4)#1	139.2(3)
C(39)-N(4)-Cd(1)	122.3(8)	O(2W)-Cd(1)-O(4)#1	85.8(3)
C(38)-N(4)-Cd(1)	121.2(8)	O(3)#1-Cd(1)-O(4)#1	53.6(3)
C(58)-N(6)-Cd(3)#2	121.8(8)	O(2)-Cd(1)-C(2)#1	159.2(4)
C(59)-N(6)-Cd(3)#2	122.4(8)	O(1W)-Cd(1)-C(2)#1	91.3(4)
C(79)-N(8)-Cd(4)#2	121.9(8)	N(4)-Cd(1)-C(2)#1	112.6(4)
C(78)-N(8)-Cd(4)#2	122.1(8)	O(2W)-Cd(1)-C(2)#1	89.1(4)
C(1)-O(2)-Cd(1)	105.0(8)	O(3)#1-Cd(1)-C(2)#1	26.6(3)
C(2)-O(3)-Cd(1)#6	93.4(8)	O(4)#1-Cd(1)-C(2)#1	27.0(3)
C(2)-O(4)-Cd(1)#6	91.7(7)	O(9)-Cd(2)-N(2)#4	86.4(3)
C(21)-O(6)-Cd(2)#7	91.0(8)	O(9)-Cd(2)-O(4W)	91.5(4)
C(21)-O(7)-Cd(2)#7	92.9(7)	N(2)#4-Cd(2)-O(4W)	93.3(4)
C(22)-O(8)-Cd(2)	83.8(7)	O(9)-Cd(2)-O(7)#5	134.8(3)

C(22)-O(9)-Cd(2)	101.5(8)	N(2)#4-Cd(2)-O(7)#5	138.7(3)
C(41)-O(11)-Cd(4)	91.2(7)	O(4W)-Cd(2)-O(7)#5	86.9(3)
C(41)-O(12)-Cd(4)	92.3(7)	O(9)-Cd(2)-O(3W)	88.5(3)
C(42)-O(13)-Cd(4)#6	104.8(7)	N(2)#4-Cd(2)-O(3W)	95.3(3)
C(42)-O(14)-Cd(3)#9	117.0(8)	O(4W)-Cd(2)-O(3W)	171.4(3)
C(61)-O(16)-Cd(3)#6	106.9(8)	O(7)#5-Cd(2)-O(3W)	87.1(3)
C(61)-O(17)-Cd(4)	116.5(7)	O(9)-Cd(2)-O(6)#5	170.6(3)
C(62)-O(18)-Cd(3)	91.8(7)	N(2)#4-Cd(2)-O(6)#5	85.0(3)
C(62)-O(19)-Cd(3)	91.8(8)	O(4W)-Cd(2)-O(6)#5	92.8(4)
O(6)#5-Cd(2)-O(8)	136.2(3)	O(7)#5-Cd(2)-O(6)#5	53.8(3)
O(9)-Cd(2)-C(21)#5	162.0(4)	O(3W)-Cd(2)-O(6)#5	88.5(3)
N(2)#4-Cd(2)-C(21)#5	111.5(4)	O(9)-Cd(2)-O(8)	52.7(3)
O(4W)-Cd(2)-C(21)#5	89.0(4)	N(2)#4-Cd(2)-O(8)	138.7(3)
O(7)#5-Cd(2)-C(21)#5	27.3(3)	O(4W)-Cd(2)-O(8)	83.8(3)
O(3W)-Cd(2)-C(21)#5	88.4(3)	O(7)#5-Cd(2)-O(8)	82.3(3)
O(6)#5-Cd(2)-C(21)#5	26.6(3)	O(3W)-Cd(2)-O(8)	89.4(3)
O(8)-Cd(2)-C(21)#5	109.6(3)		

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

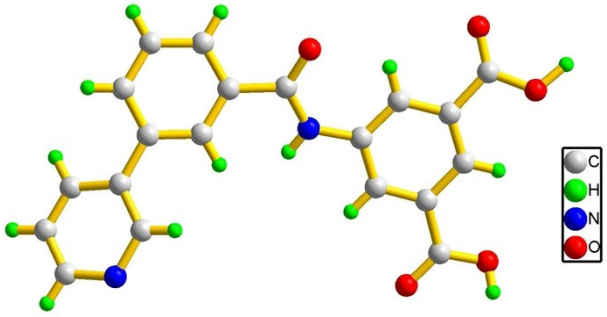

Fig. S1. Crystal structure of 3-H_2PBI ligand.

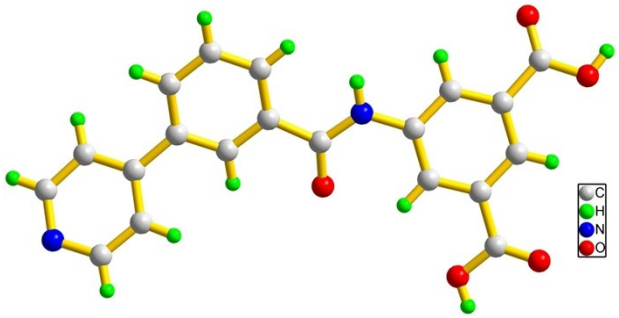

Fig. S2. Crystal structure of 4-H_2PBI ligand.

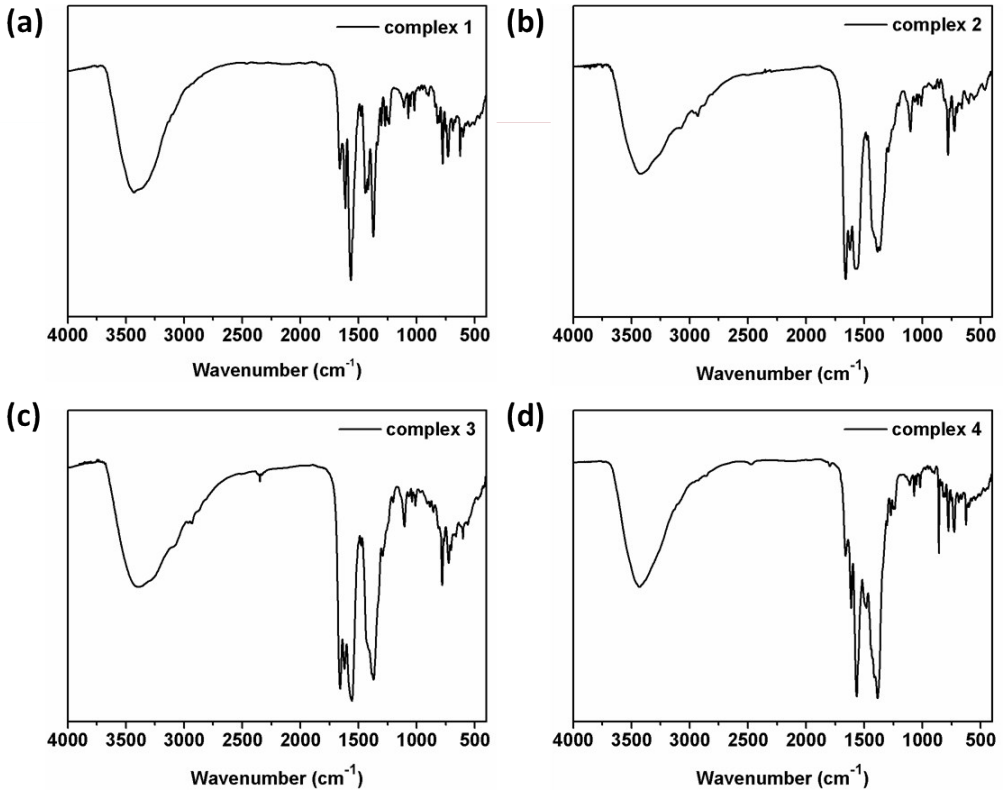

Fig. S3. FT-IR spectrum of the obtained compounds **1**-**4**.

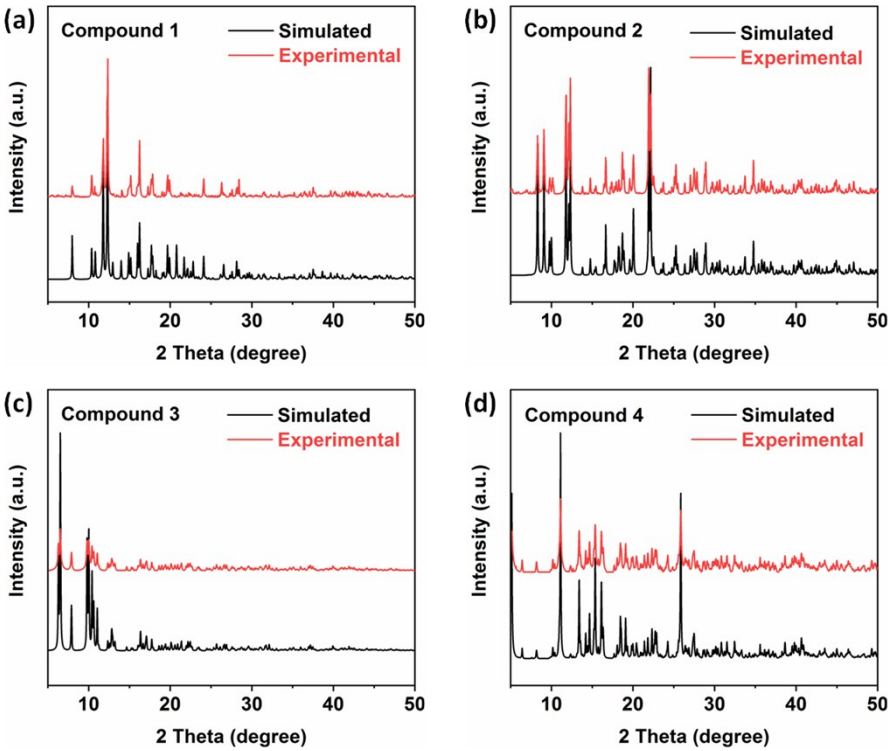

Fig. S4. PXRD patterns of compounds **1**-**4**.

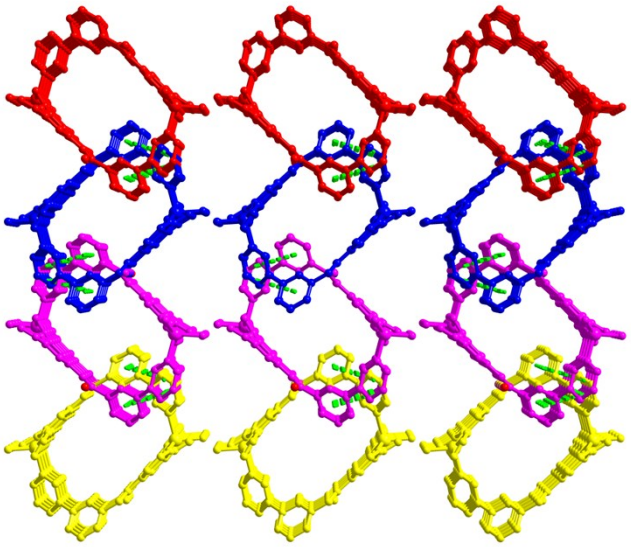

Fig. S5. Schematic view of the 2D layers in compound **1**.

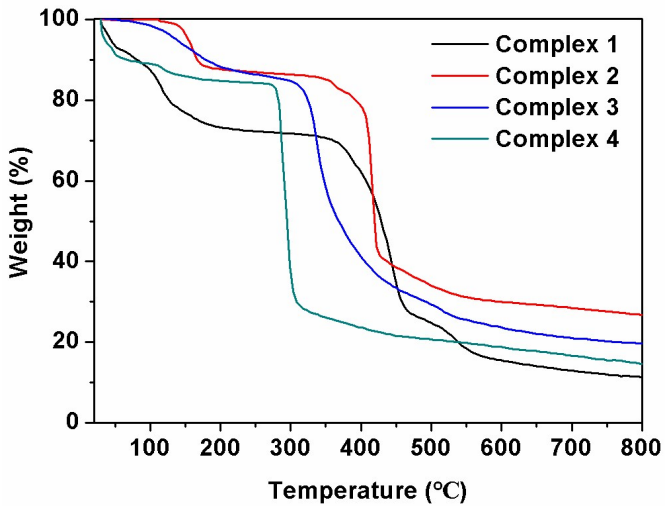

Fig. S6. TG curves of compounds **1-4**.

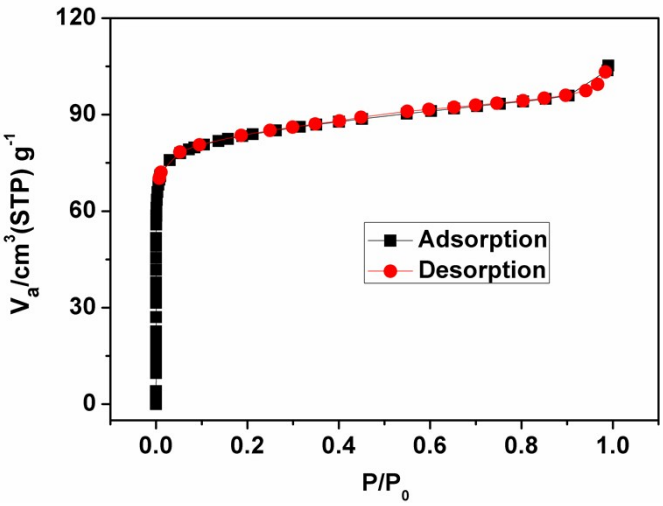

Fig. S7. N_2 adsorption/desorption isotherms of Cd-CP at 77 K.