ESI

Zn(II) and Cd(II) Coordination Polymers Assembled by di(1*H*-imidazol-1-yl)methane and Carboxylic Acid Ligands

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Table S1. Selected bond lengths [Å] and angles [°] for complex **1**.

Zn(1)-N(1)	1.999(4)	Zn(1)-O(1)	2.064(3)
Zn(1)-N(4)#1	2.001(4)	Zn(1)-O(2)	2.481(3)
Zn(1)-O(7)	2.040(3)	Zn(1)-O(8)	2.547(3)
N(1)-Zn(1)-N(4)#1	139.31(15)	N(1)-Zn(1)-O(2)	85.34(12)
N(1)-Zn(1)-O(7)	106.43(13)	N(4)#1-Zn(1)-O(2)	86.44(13)
N(4)#1-Zn(1)-O(7)	98.28(14)	O(7)-Zn(1)-O(2)	153.68(11)
N(1)-Zn(1)-O(1)	106.48(13)	O(1)-Zn(1)-O(2)	56.66(10)
N(4)#1-Zn(1)-O(1)	101.83(14)	O(1)-Zn(1)-O(8)	152.58(12)
O(7)-Zn(1)-O(1)	97.11(11)	O(7)-Zn(1)-O(8)	55.49(12)

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

Table S2. Selected bond lengths [Å] and angles [°] for complex **2**.

Zn(1)-O(4)#3	2.012(7)	Zn(1)-N(4)#4	2.012(7)
Zn(1)-O(1)	2.015(6)	Zn(1)-N(1)	2.055(7)
O(4)#3-Zn(1)-O(1)	94.9(3)	O(4)#3-Zn(1)-N(1)	133.9(3)
O(4)#3-Zn(1)-N(4)#	96.7(3)	O(1)-Zn(1)-N(1)	103.4(3)
O(1)-Zn(1)-N(4)#4	125.4(3)	N(4)#4-Zn(1)-N(1)	105.8(3)

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

Table S3. Selected bond lengths [Å] and angles [°] for complex **3**.

Cd(1)-N(5)#4	2.255(4)	Cd(2)-O(3)#5	2.456(3)
Cd(1)-N(5)	2.255(4)	Cd(2)-O(2)	2.622(3)
Cd(1)-O(8)	2.262(4)	Cd(3)-N(8)	2.257(4)
Cd(1)-O(8)#4	2.262(4)	Cd(3)-N(8)#6	2.257(4)
Cd(1)-O(7)	2.520(5)	Cd(3)-O(6)#6	2.296(4)
Cd(1)-O(7)#4	2.520(5)	Cd(3)-O(6)	2.296(4)
Cd(2)-O(1)	2.224(3)	Cd(3)-O(5)#6	2.442(4)
Cd(2)-N(3)	2.236(4)	Cd(3)-O(5)	2.442(4)

Cd(2)-N(1)	2.252(4)	Cd(2)-O(3)#5	2.456(3)
Cd(2)-O(4)#5	2.311(4)		
N(5)#4-Cd(1)-N(5)	93.5(2)	N(1)-Cd(2)-O(3)#5	92.16(15)
N(5)#4-Cd(1)-O(8)	136.11(15)	O(4)#5-Cd(2)-O(3)#	54.73(13)
N(5)-Cd(1)-O(8)	104.36(14)	O(1)-Cd(2)-O(2)	52.77(13)
N(5)#4-Cd(1)-O(8)#	104.36(14)	N(3)-Cd(2)-O(2)	84.59(14)
N(5)-Cd(1)-O(8)#4	136.11(15)	N(1)-Cd(2)-O(2)	94.32(14)
O(8)-Cd(1)-O(8)#4	90.05(18)	O(4)#5-Cd(2)-O(2)	124.15(13)
N(5)#4-Cd(1)-O(7)	86.39(15)	O(3)#5-Cd(2)-O(2)	170.90(13)
N(5)-Cd(1)-O(7)	89.17(15)	N(8)-Cd(3)-N(8)#6	104.5(2)
O(8)-Cd(1)-O(7)	54.79(12)	N(8)-Cd(3)-O(6)#6	96.87(16)
O(8)#4-Cd(1)-O(7)	131.02(14)	N(8)#6-Cd(3)-O(6)#	136.42(16)
N(5)#4-Cd(1)-O(7)#	89.17(15)	N(8)-Cd(3)-O(6)	136.42(16)
N(5)-Cd(1)-O(7)#4	86.39(15)	N(8)#6-Cd(3)-O(6)	96.87(16)
O(8)-Cd(1)-O(7)#4	131.02(14)	O(6)#6-Cd(3)-O(6)	92.83(19)

Symmetry Codes: #1 -x+2,y,-z+5/2; #2 -x+1,y,-z+5/2; #3 x,y,z-1; #4 -x+2,y,-z+1/2; #5 x,y,z+1; #6 -x+1,y,-z+1/2; #7 -x+1,y,-z+3/2; #8 -x+2,y,-z-1/2.

Table S4. Selected bond lengths [Å] and angles [°] for complex **4**.

Cd(1)-O(4)#1	2.237(3)	Cd(1)-N(3)	2.360(3)
Cd(1)-N(1)#2	2.276(3)	Cd(1)-O(1)#3	2.519(3)
Cd(1)-O(2)	2.348(3)	Cd(1)-O(1)	2.580(3)
O(4)#1-Cd(1)-N(1)#	133.09(11)	O(2)-Cd(1)-O(1)#3	93.68(10)
O(4)#1-Cd(1)-O(2)	88.72(10)	N(3)-Cd(1)-O(1)#3	171.88(10)
N(1)#2-Cd(1)-O(2)	138.15(10)	O(4)#1-Cd(1)-O(1)	131.13(9)
O(4)#1-Cd(1)-N(3)	102.73(11)	N(1)#2-Cd(1)-O(1)	89.35(10)
N(1)#2-Cd(1)-N(3)	88.37(11)	O(2)-Cd(1)-O(1)	53.13(9)
O(2)-Cd(1)-N(3)	82.54(11)	N(3)-Cd(1)-O(1)	101.11(10)
O(4)#1-Cd(1)-O(1)#	84.30(10)	O(1)#3-Cd(1)-O(1)	70.97(9)

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

Table S5. Selected bond lengths [Å] and angles [°] for complex **5**.

Cd(1)-O(4)#1	2.2563(18)	Cd(1)-N(4)#2	2.351(2)
Cd(1)-N(1)	2.290(2)	Cd(1)-O(2)	2.373(2)
Cd(1)-O(3)	2.2959(18)	Cd(1)-O(1)	2.490(2)
O(4)#1-Cd(1)-N(1)	93.92(7)	O(3)-Cd(1)-O(2)	89.35(7)
O(4)#1-Cd(1)-O(3)	102.72(7)	N(4)#2-Cd(1)-O(2)	90.28(8)
N(1)-Cd(1)-O(3)	97.60(7)	O(4)#1-Cd(1)-O(1)	112.10(7)

O(4)#1-Cd(1)-N(4)#	84.39(7)	N(1)-Cd(1)-O(1)	98.54(7)
N(1)-Cd(1)-N(4)#2	177.84(7)	O(3)-Cd(1)-O(1)	140.24(6)
O(3)-Cd(1)-N(4)#2	81.48(7)	N(4)#2-Cd(1)-O(1)	83.37(7)
O(4)#1-Cd(1)-O(2)	165.88(6)	O(2)-Cd(1)-O(1)	54.15(7)
N(1)-Cd(1)-O(2)	91.66(8)		

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

Table S6. Hydrogen-bond parameters in complex **1**.

D–H…A	D–H [Å]	H…A [Å]	D…A [Å]	< D–H…A[°]
O(3)-H(3)...O(4E)	0.8200	1.8100	2.616(5)	166.00
O(5)-H(5)...O(8D)	0.8200	1.7900	2.563(5)	158.00
O(9)-H(9)...O(2I)	0.8200	1.8700	2.624(5)	152.00
O(11)-H(11)...O(12L)	0.8200	1.8000	2.610(5)	170.00

Symmetry Codes : D -x,-1/2+y,1/2-z; E -1-x,-y,-1-z; I -x,1/2+y,1/2-z; L -1-x,1-y,-1-z.

Table S7. Hydrogen-bond parameters in complex **2**.

D–H…A	D–H [Å]	H…A [Å]	D…A [Å]	< D–H…A[°]
O(1W)-H(1WA)...O(3)	0.9000	1.8800	2.721(12)	154.00
C(14)-H(14A)...O(1W)	0.9300	2.4900	3.379(12)	160.00
C(15)-H(15A)...O(2)	0.9300	2.4700	3.069(12)	122.00
C(17)-H(17A)...O(3B)	0.9300	2.4900	3.056(12)	120.00
C(18)-H(18B)...O(1Q)	0.9300	2.4800	3.443(11)	171.00
C(19)-H(19A)...O(1WP)	0.9300	2.4800	3.312(13)	149.00
C(19)-H(19A)...O(2D)	0.9300	2.3500	2.988(11)	126.00

Symmetry Codes: B x,1+y,z; D 1/2+x,5/2-y,-1/2+z; P 1-x,2-y,1-z; Q 1+x,y,z.

Table S8. Hydrogen-bond parameters in complex **3**.

D–H…A	D–H [Å]	H…A [Å]	D…A [Å]	< D–H…A[°]
C(40)-H(40B)...O(1S)	0.9700	2.3000	3.134(7)	144.00

Symmetry Code: S 3/2-x,1/2+y,1/2-z.

Table S9. Hydrogen-bond parameters in complex **4**.

D–H…A	D–H [Å]	H…A [Å]	D…A [Å]	< D–H…A[°]
O(1W)-H(1WA)...O(2R)	0.8500	2.4000	3.131(6)	144.00
O(1W)-H(1WB)...O(4S)	0.8500	1.9900	2.758(5)	151.00
C(10)-H(10A)...O(3P)	0.9300	2.5400	3.471(5)	177.00
C(14)-H(14A)...O(2)	0.9300	2.5800	3.107(4)	116.00

C(14)-H(14A)...O(1WM)	0.9300	2.3500	3.126(6)	141.00
C(15)-H(15A)...O(1WM)	0.9700	2.4200	3.198(6)	137.00
C(15)-H(15B)...O(1P)	0.9700	2.3600	3.248(4)	151.00

Symmetry Codes: M 1-x,1-y,1-z; P 2-x,-1/2+y,1/2-z; R -1+x,y,1+z; S x,y,1+z.

Table S10. Hydrogen-bond parameters in complex **5**.

D–H…A	D–H [Å]	H…A [Å]	D…A [Å]	< D–H…A[°]
C(1)-H(1A)...O(2G)	0.9300	2.4700	3.234(3)	139.00
C(3)-H(3A)...O(1G)	0.9300	2.4500	3.342(4)	161.00
C(4)-H(4A)...O(2G)	0.9700	2.2100	3.144(3)	161.00

Symmetry Code: G -x,1-y,1-z.

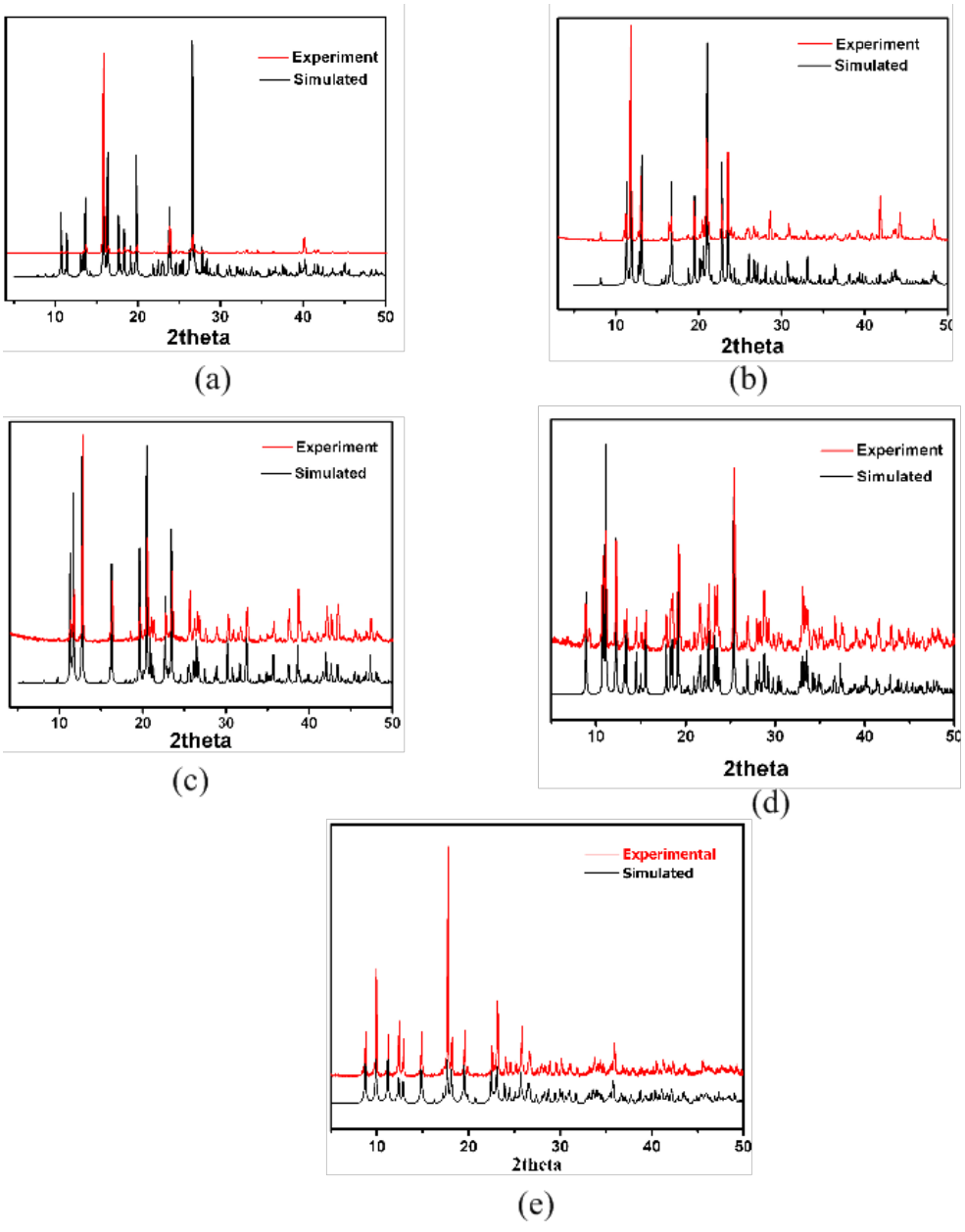

Fig. S1 The XRPD diagrams for complexes **1**: (a), **2**: (b), **3**: (c), **4**: (d), **5**: (e).