Electronic supplementary information (ESI)

Structural Modulation and Properties of Four Cadmium (II) Coordination Architectures Based on 3-(pyridin-4-yl)-5-(pyrazin-2-yl)-1H- 1, 2, 4-triazole and Aromatic Polycarboxylate Ligands

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

Cd(1)-N(4)	2.293(4)□	Cd(1)-O(3)	2.430(4)□
Cd(1)-O(1)	2.310(4)□	Cd(1)-O(4)	2.483(4)□
Cd(1)-O(2)	2.315(4)□	N(4)-N(5)	1.373(6)□
Cd(1)-N(6)#2	2.329(4)□	N(6)-Cd(1)#3	2.329(4)
O(1)-Cd(1)-N(6)#2	92.52(16)□	N(4)-Cd(1)-O(4)	144.39(15)□
O(2)-Cd(1)-N(6)#2	88.02(15)□	O(1)-Cd(1)-O(4)	92.93(16)□
N(4)-Cd(1)-O(3)	91.65(14)□	O(2)-Cd(1)-O(4)	89.88(15)□
O(1)-Cd(1)-O(3)	90.58(14)□	N(6)#2-Cd(1)-O(4)	77.85(15)□
O(2)-Cd(1)-O(3)	91.16(13)□	O(3)-Cd(1)-O(4)	52.93(14)
N(6)#2-Cd(1)-O(3)	130.77(14)□	C(5)-N(4)-Cd(1)	126.3(3)□
C(9)-N(6)-Cd(1)#3	123.2(4)	N(5)-N(4)-Cd(1)	127.3(3)

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

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

Cd(1)-N(9)	2.233(3)□	Cd(3)-N(7)#3	2.359(3)□
Cd(1)-O(4)	2.251(3)□	Cd(3)-N(1)#4	2.361(3)□
Cd(1)-N(12)#1	2.267(3)□	Cd(3)-O(7)#2	2.415(3)□
Cd(1)-O(6)	2.269(3)□	Cd(3)-C(30)#2	2.705(4)□
Cd(1)-O(3)	2.391(3)□	O(2)-Cd(3)#2	2.282(3)□
Cd(1)-N(8)	2.514(3)□	O(7)-Cd(3)#2	2.415(3)□
Cd(1)-C(38)	2.660(4)□	O(8)-C(30)	1.258(4)□
Cd(2)-N(3)	2.240(3)□	O(8)-Cd(3)#2	2.304(3)□
Cd(2)-N(6)#1	2.242(3)□	N(1)-Cd(3)#4	2.361(3)□
Cd(2)-O(5)	2.286(2)□	N(6)-Cd(2)#5	2.242(3)□
Cd(2)-O(11)	2.314(3)□	N(7)-Cd(3)#6	2.359(3)□
Cd(2)-N(2)	2.388(3)□	N(12)-Cd(1)#5	2.267(3)
Cd(2)-O(6)	2.619(3)□	Cd(3)-O(2)#2	2.282(3)□
Cd(3)-O(1)	2.271(2)□	Cd(3)-O(8)#2	2.304(3)□
N(9)-Cd(1)-O(4)	140.93(11)□	N(9)-Cd(1)-O(6)	98.89(10)□
N(9)-Cd(1)-N(12)#1	106.38(11)□	O(4)-Cd(1)-O(6)	105.62(9)□
O(4)-Cd(1)-N(12)#1	102.04(12)□	N(12)#1-Cd(1)-O(6)	93.47(11)□
O(4)-Cd(1)-O(3)	56.09(9)□	N(6)#1-Cd(2)-N(2)	172.12(11)□
N(12)#1-Cd(1)-O(3)	101.21(12)□	O(5)-Cd(2)-N(2)	88.03(10)□
O(6)-Cd(1)-O(3)	158.46(10)□	O(11)-Cd(2)-N(2)	86.67(10)□
N(9)-Cd(1)-N(8)	70.70(10)□	N(3)-Cd(2)-O(6)	123.98(10)□
O(4)-Cd(1)-N(8)	85.51(11)□	N(6)#1-Cd(2)-O(6)	87.68(10)□
N(12)#1-Cd(1)-N(8)	169.37(10)□	O(5)-Cd(2)-O(6)	52.34(8)□
O(6)-Cd(1)-N(8)	77.16(10)□	O(11)-Cd(2)-O(6)	139.59(9)□
O(3)-Cd(1)-N(8)	89.19(11)□	N(2)-Cd(2)-O(6)	88.82(9)□
N(9)-Cd(1)-C(38)	117.12(12)□	O(1)-Cd(3)-O(2)#2	123.54(10)□

O(4)-Cd(1)-C(38)	28.10(10)□	O(1)-Cd(3)-O(8)#2	91.00(9)□
N(12)#1-Cd(1)-C(38)	103.68(12)□	O(2)#2-Cd(3)-O(8)#2	144.30(9)□
O(6)-Cd(1)-C(38)	132.72(10)□	O(1)-Cd(3)-N(7)#3	89.16(11)□
O(3)-Cd(1)-C(38)	27.99(10)□	O(2)#2-Cd(3)-N(7)#3	87.36(11)□
N(8)-Cd(1)-C(38)	86.52(11)□	O(8)#2-Cd(3)-N(7)#3	103.30(11)□
N(3)-Cd(2)-N(6)#1	104.58(11)□	O(1)-Cd(3)-N(1)#4	92.90(10)□
N(3)-Cd(2)-O(5)	159.70(10)□	O(2)#2-Cd(3)-N(1)#4	83.22(11)□
N(6)#1-Cd(2)-O(5)	95.40(11)□	O(8)#2-Cd(3)-N(1)#4	86.61(11)□
N(3)-Cd(2)-O(11)	92.38(11)□	N(7)#3-Cd(3)-N(1)#4	169.86(10)□
N(6)#1-Cd(2)-O(11)	100.55(11)□	O(1)-Cd(3)-O(7)#2	144.38(9)□
O(5)-Cd(2)-O(11)	87.36(9)□	O(2)#2-Cd(3)-O(7)#2	91.89(9)□
N(3)-Cd(2)-N(2)	71.70(10)□	O(8)#2-Cd(3)-O(7)#2	55.01(9)□
N(1)#4-Cd(3)-O(7)#2	95.06(10)	N(7)#3-Cd(3)-O(7)#2	88.99(10)□

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

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

Cd(1)-O(4)#1	2.1738(18)	Cd(2)-O(10)	2.3305(19)□
Cd(1)-O(1)	2.2196(19)	Cd(2)-O(5A)#2	2.36(2)□
Cd(1)-O(8)	2.306(2)□	Cd(2)-N(6)#3	2.361(2)□
Cd(1)-O(7)	2.323(2)□	Cd(2)-O(9)	2.409(2)□
Cd(1)-N(1)	2.339(2)□	Cd(2)-O(6A)#2	2.41(2)□
Cd(1)-O(2)	2.5812(17)	Cd(2)-N(2)	2.548(2)□
Cd(2)-O(6)#2	2.281(5)□	N(6)-Cd(2)#4	2.361(2)□
Cd(2)-N(3)	2.312(2)□	O(4)-Cd(1)#5	2.1738(18)□
O(6A)-Cd(2)#6	2.41(2)	O(6)-Cd(2)#6	2.281(5)□
O(5A)-Cd(2)#6	2.36(2)□		
O(4)#1-Cd(1)-O(1)	117.11(8)□	N(3)-Cd(2)-O(9)	83.28(8)□

O(4)#1-Cd(1)-O(8)	87.96(8)□	O(10)-Cd(2)-O(9)	175.77(7)□
O(1)-Cd(1)-O(8)	92.27(9)□	O(5A)#2-Cd(2)-O(9)	87.5(11)□
O(4)#1-Cd(1)-O(7)	95.78(8)□	N(6)#3-Cd(2)-O(9)	94.47(8)□
O(1)-Cd(1)-O(7)	90.87(9)□	O(6)#2-Cd(2)-O(6A)#2	20.8(6)□
O(8)-Cd(1)-O(7)	173.39(7)□	N(3)-Cd(2)-O(6A)#2	134.1(5)□
O(4)#1-Cd(1)-N(1)	102.02(8)□	O(10)-Cd(2)-O(6A)#2	107.8(12)□
O(1)-Cd(1)-N(1)	140.87(7)□	O(5A)#2-Cd(2)-O(6A)#2	52.5(4)□
O(8)-Cd(1)-N(1)	88.76(8)□	N(6)#3-Cd(2)-O(6A)#2	72.7(3)□
O(7)-Cd(1)-N(1)	85.13(8)□	O(9)-Cd(2)-O(6A)#2	73.6(12)□
O(4)#1-Cd(1)-O(2)	170.74(7)□	O(6)#2-Cd(2)-N(2)	157.7(3)□
O(1)-Cd(1)-O(2)	54.11(6)□	N(3)-Cd(2)-N(2)	69.35(7)□
O(8)-Cd(1)-O(2)	95.05(7)□	O(10)-Cd(2)-N(2)	89.37(7)□
O(7)-Cd(1)-O(2)	82.10(7)□	O(5A)#2-Cd(2)-N(2)	157.4(6)□
N(1)-Cd(1)-O(2)	86.83(6)□	N(6)#3-Cd(2)-N(2)	80.49(7)□
O(6)#2-Cd(2)-O(10)	87.8(5)□	O(9)-Cd(2)-N(2)	91.28(8)□
N(3)-Cd(2)-O(10)	93.05(8)□	O(6A)#2-Cd(2)-N(2)	147.7(7)
O(6)#2-Cd(2)-O(5A)#2	44.8(5)□	N(3)-Cd(2)-N(6)#3	149.66(7)□
N(3)-Cd(2)-O(5A)#2	88.2(7)□	O(10)-Cd(2)-N(6)#3	89.76(7)□
O(10)-Cd(2)-O(5A)#2	90.3(11)□	O(5A)#2-Cd(2)-N(6)#3	122.1(6)□
O(6)#2-Cd(2)-N(6)#3	77.3(3)□	O(6)#2-Cd(2)-O(9)	93.2(5)□

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

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

Cd(1)-O(1)	2.2349(18)□	Cd(2)-O(8)	2.465(2)□
Cd(1)-O(5)	2.299(2)□	Cd(2)-N(7)	2.475(2)□
Cd(1)-N(10)	2.323(2)□	Cd(2)-N(4)	2.339(2)□
Cd(1)-N(3)	2.328(2)□	Cd(3)-O(2)#1	2.2455(19)□
Cd(1)-O(6)	2.359(2)□	Cd(3)-N(12)#2	2.246(2)□

Cd(1)-N(1)	2.449(2)□	Cd(3)-O(3)#3	2.2611(19)□
Cd(2)-O(7)	2.238(3)□	Cd(3)-O(11)	2.2941(19)□
Cd(2)-N(9)	2.310(2)□	Cd(3)-O(10)	2.460(2)□
Cd(2)-O(9)	2.321(2)□	Cd(3)-O(4)#3	2.484(2)
O(1)-Cd(1)-O(5)	92.74(8)□	O(2)#1-Cd(3)-N(12)#2	111.96(7)□
O(1)-Cd(1)-N(10)	88.61(7)□	O(2)#1-Cd(3)-O(3)#3	84.69(7)□
O(5)-Cd(1)-N(10)	104.18(8)□	N(12)#2-Cd(3)-O(3)#3	142.54(7)□
O(1)-Cd(1)-N(3)	171.74(8)□	O(2)#1-Cd(3)-O(11)	93.26(7)□
O(5)-Cd(1)-N(3)	92.61(8)□	N(12)#2-Cd(3)-O(11)	111.22(8)□
N(10)-Cd(1)-N(3)	96.17(8)□	O(3)#3-Cd(3)-O(11)	100.51(7)□
O(1)-Cd(1)-O(6)	86.46(7)□	O(2)#1-Cd(3)-O(10)	146.45(6)□
O(5)-Cd(1)-O(6)	164.79(8)□	N(12)#2-Cd(3)-O(10)	92.18(7)□
N(10)-Cd(1)-O(6)	90.99(8)□	O(3)#3-Cd(3)-O(10)	89.86(7)□
O(1)-Cd(1)-N(1)	103.80(7)□	O(2)#1-Cd(3)-O(4)#3	110.10(7)□
O(5)-Cd(1)-N(1)	78.72(8)□	N(12)#2-Cd(3)-O(4)#3	87.49(7)□
N(10)-Cd(1)-N(1)	167.20(7)□	O(3)#3-Cd(3)-O(4)#3	55.04(6)□
N(3)-Cd(1)-N(1)	71.13(8)□	O(11)-Cd(3)-O(4)#3	142.39(7)□
O(6)-Cd(1)-N(1)	86.72(8)□	O(10)-Cd(3)-O(4)#3	93.26(7)□
N(9)-Cd(2)-O(9)	129.70(8)□	O(7)-Cd(2)-N(7)	104.08(10)□
O(7)-Cd(2)-N(4)	97.68(10)□	N(9)-Cd(2)-N(7)	69.44(7)□
O(7)-Cd(2)-O(8)	87.11(8)□	O(8)-Cd(2)-N(7)	83.81(7)□

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

Table S5. Hydrogen bonds for **1-4**

1

D-H...A	d(D-H)	d(H...A)	d(D...A)	∠(DHA)
O(2)-H(4W)...O(3)#4	0.85	1.92	2.731(5)	159.4□
O(2)-H(3W)...N(5)#4	0.85	1.91	2.743(6)	168.0□
O(1)-H(2W)...N(3)#5	0.85	2.05	2.816(6)	148.7□

O(1)-H(1W)...O(5)#6	0.85	1.94	2.719(6)	151.6□
O(5)-H(5W)...O(3)#7	0.94	1.93	2.869(7)	175.1□
O(5)-H(6W)...N(2)#8	0.82	2.21	3.007(7)	162.2
2				
O(11)-H(6W)...N(11)#10	0.85	1.92	2.741(4)	161.8□
O(11)-H(5W)...O(1)#11	0.85	2.47	3.285(4)	161.0□
O(10)-H(10A)...O(11)#12	0.85	2.68	2.935(15)	99.3
3				
O(10)-H(7W)...O(2)#7	0.85	1.91	2.759(2)	172.5□
O(10)-H(8W)...N(5)#7	0.85	2.00	2.851(3)	176.9□
O(9)-H(6W)...O(5)#8	0.85	2.10	2.852(13)	147.7□
O(9)-H(5W)...N(4)#9	0.85	2.51	3.259(3)	148.3□
O(8)-H(4W)...O(9)#10	0.85	2.08	2.927(3)	172.4□
O(8)-H(3W)...O(3)#8	0.85	1.75	2.602(3)	175.7□
O(7)-H(2W)...N(4)#7	0.85	2.05	2.874(3)	162.7□
O(7)-H(1W)...O(5A)#11	0.85	1.94	2.715(17)	150.1□
O(7)-H(1W)...O(5)#11	0.85	1.91	2.636(8)	142.2
4				
O(14)-H(12W)...O(2)#8	0.85	2.50	3.046(3)□	123.0
O(14)-H(12W)...O(3)	0.85	2.14	2.917(3)	152.0□
O(14)-H(11W)...O(6)#8	0.85	2.10	2.945(4)	179.6□
O(13)-H(10W)...O(9)#8	0.85	1.96	2.796(3)	167.8□
O(13)-H(9W)...N(2)#9	0.85	2.00	2.822(4)	163.7□
O(12)-H(8W)...O(10)#8	0.85	2.32	3.118(4)	157.3□
O(12)-H(7W)...N(6)#10	0.85	2.04	2.840(4)	156.1□
O(7)-H(5W)...O(12)	0.85	1.80	2.644(4)	170.9□
O(6)-H(4W)...N(8)#11	0.85	1.96	2.766(3)	158.0□
O(6)-H(3W)...O(13)#12	0.85	2.06	2.843(3)	152.2□
O(5)-H(2W)...N(5)#9	0.85	2.06	2.900(3)	171.4□

O(5)-H(1W)...O(14)	0.85	1.80	2.647(3)	172.3

Symmetry codes for **1**: #4 -x+1/2, -y-1/2, -z; #5 -x+1/2, -y+1/2, -z; #6 -x+1, -y+1, -z; #7 x, y+1, z; #8 -x+1/2, -y+3/2, -z; for **2**: #10 x+1, y, z; #11 x, y, z-1; #12 x-1, -y+3/2, z+1/2; for **3:** #7 -x+1, -y, -z; #8 -x, -y, -z; #9 -x+1, -y-1, -z; #10 -x+1/2, y+1/2, -z+1/2; #11 -x, -y+1, -z; for **4:** #8 x-1, y, z; #9 -x+1, -y+1, -z+2; #10 -x+1, -y, -z+2; #11 -x+2, -y+1, -z+1; #12 x+1, y, z.

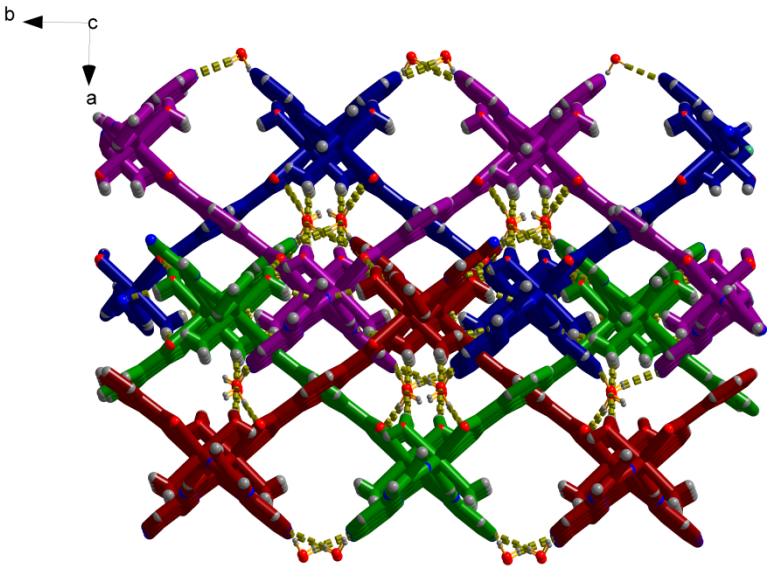


Fig. S1 View of 3D supramolecular structure of **1**.

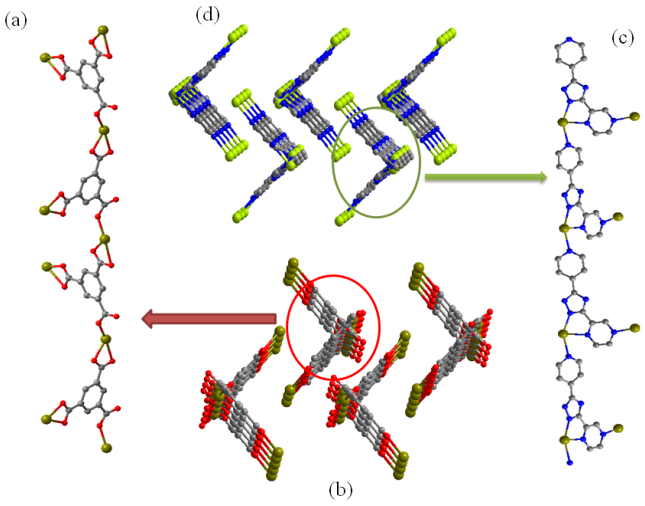
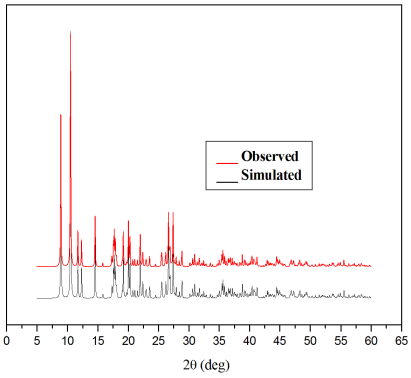
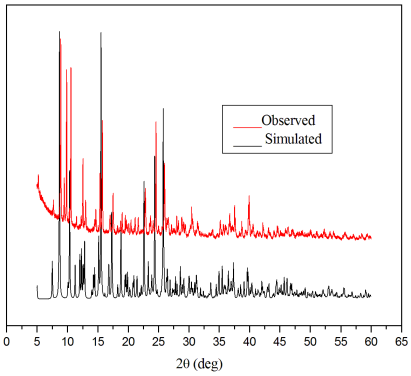


Fig. S2 (a) 1D chain of **3** formed by Cd–btc^{3-}; (b) Packing of 1D Cd–btc^{3-} chains; (c) 1D chain of **3** formed by Cd–ppt^{-};(d) Packing of 1D Cd–ppt^{-} chains.



(a)



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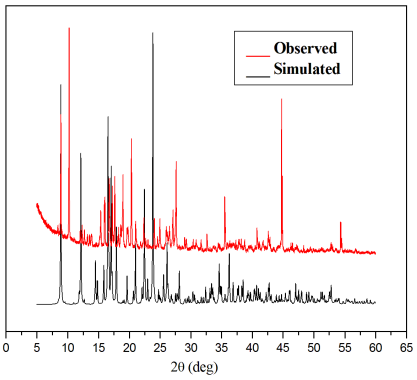

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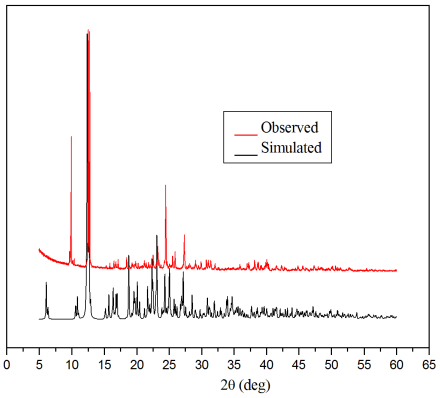

(d)

Fig. S3. Experimental and simulated powder X-ray diffraction (PXRD) patterns for complexes **1**–**4** (a–d).

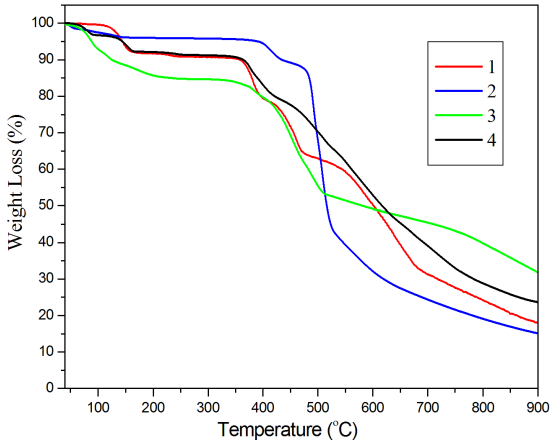

Fig. S4 TGA curves for complexes **1**–**4**.