Electronic Supplementary Material (ESI) for CrystEngComm

Synthetic Methods and Structural Study of Coordination Polymers of Cd(II) and Co(II) with Tetrathiafulvalene–Tetracarboxylate

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Table S1. Selected Bond Lengths (Å) and Angles (deg) of **1**–**3**[a]

		1	
Cd1–O2	2.253(3)	Cd1–O6	2.333(4)
Cd1–O4#1	2.307(3)	Cd1–N1	2.351(3)
Cd1–O5	2.347(3)	Cd1–N2	2.355(4)
O2–Cd1–O4#1	94.87(12)	O6–Cd1–N1	85.83(12)
O2–Cd1–O6	85.83(13)	O5–Cd1–N1	150.11(12)
O4#1–Cd1–O6	163.53(11)	O2–Cd1–N2	155.13(13)
O2–Cd1–O5	119.22(12)	O4#1–Cd1–N2	90.21(12)
O4#1–Cd1–O5	85.53(11)	O6–Cd1–N2	96.05(13)
O6–Cd1–O5	79.82(13)	O5–Cd1–N2	85.41(13)
O2–Cd1–N1	85.36(12)	N1–Cd1–N2	70.10(13)
O4#1–Cd1–N1	110.64(11)		
		2	
Cd1–O6	2.270(5)	Cd1–O5	2.324(5)
Cd1–N2	2.301(6)	Cd1–N1	2.363(6)
Cd1–O1#2	2.309(5)	Cd1–O1	2.460(5)
O6–Cd1–N2	162.6(2)	O1#2–Cd1–N1	166.2(2)
O6–Cd1–O1#2	86.7(2)	O5–Cd1–N1	85.1(2)
N2–Cd1–O1#2	105.87(19)	O6–Cd1–O1	77.38(19)
O6–Cd1–O5	79.8(2)	N2–Cd1–O1	94.48(19)
N2–Cd1–O5	106.6(2)	O1–Cd1–O1#2	73.36(18)
O1#2–Cd1–O5	108.50(19)	O5–Cd1–O1	157.01(19)
O6–Cd1–N1	94.0(2)	N1–Cd1–O1	93.3(2)
N2–Cd1–N1	70.9(2)		
		3	
Cd1–O6	2.286(6)	Cd1–N2	2.320(7)
Cd1–O5	2.309(6)	Cd1–N1	2.355(8)
Cd1–O1	2.314(6)	Cd1–O1#2	2.468(6)
O6–Cd1–O5	82.9(2)	O1–Cd1–N1	166.7(2)
O6–Cd1–O1	85.2(2)	N2–Cd1–N1	71.3(3)
O5–Cd1–O1	105.7(2)	O6–Cd1–O1#2	77.7(2)
O6–Cd1–N2	160.3(3)	O5–Cd1–O1#2	160.6(2)
O5–Cd1–N2	106.1(2)	O1–Cd1–O1#2	73.7(2)
O1–Cd1–N2	108.3(2)	N2–Cd1–O1#2	92.2(2)
O6–Cd1–N1	92.2(2)	N1–Cd1–O1#2	93.0(2)
O5–Cd1–N1	86.8(2)		

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

Table S2. Selected Bond Lengths (Å) and Angles (deg) of **4**–**6**[b]

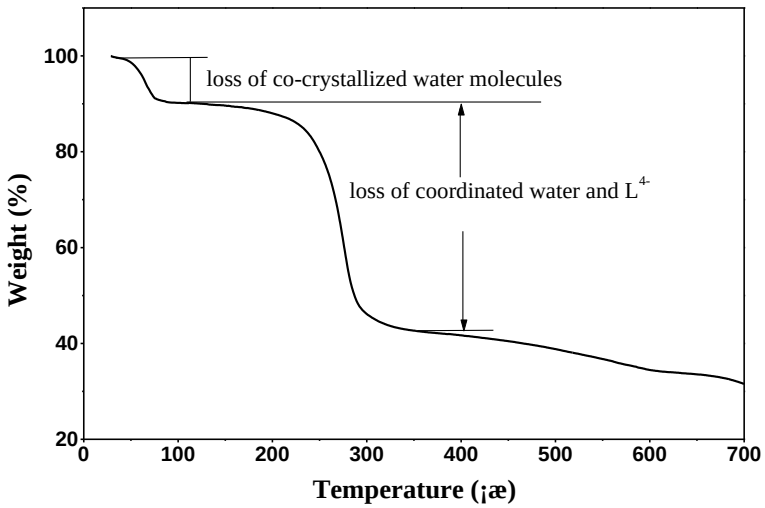
		4	
Co1–O3#3	2.331(4)	Co1–O2	2.380(4)
Co1–O6	2.363(4)	Co1–N1	2.548(6)
Co1–O5	2.368(5)	Co1–N2	2.548(5)
Co1–O2#3	2.478(5)		
O3#3–Co1–O6	152.99(15)	O3#3–Co1–O2	84.47(15)
O3#3–Co1–O5	75.92(16)	O6–Co1–O2	85.68(16)
O6–Co1–O5	79.99(16)	O5–Co1–O2	95.06(16)
N1–Co1–N2	64.74(16)	O3#3–Co1–O2#3	71.01(16)
		5	
Co1–O2	2.070(6)	Co1–N1	2.118(7)
Co1–O4#4	2.089(7)	Co1–N2	2.145(7)
Co1–O6	2.111(8)	Co1–O5	2.162(7)
O2–Co1–O4#4	84.7(3)	O6–Co1–N2	92.7(3)
O2–Co1–O6	84.6(3)	N1–Co1–N2	78.4(3)
O4#4–Co1–O6	169.0(3)	O2–Co1–O5	93.3(3)
O2–Co1–N1	93.6(3)	O4#4–Co1–O5	88.6(3)
O4#4–Co1–N1	96.1(3)	O6–Co1–O5	89.4(3)
O6–Co1–N1	87.3(3)	N1–Co1–O5	172.0(3)
O2–Co1–N2	171.7(3)	N2–Co1–O5	94.5(3)
O4#4–Co1–N2	98.2(3)		
		6	
Co1–O2	Co1–O2	Co1–O2	Co1–O2
Co1–O3	Co1–O3	Co1–O3	Co1–O3
Co1–O5	Co1–O5	Co1–O5	Co1–O5
O2–Co1–O3	O2–Co1–O3	O2–Co1–O3	O2–Co1–O3
O2–Co1–O5	O2–Co1–O5	O2–Co1–O5	O2–Co1–O5
O3–Co1–O5	O3–Co1–O5	O3–Co1–O5	O3–Co1–O5
O2–Co1–O4#5	O2–Co1–O4#5	O2–Co1–O4#5	O2–Co1–O4#5
O3–Co1–O4#5	O3–Co1–O4#5	O3–Co1–O4#5	O3–Co1–O4#5
O5–Co1–O4#5	O5–Co1–O4#5	O5–Co1–O4#5	O5–Co1–O4#5
O2–Co1–N2	O2–Co1–N2	O2–Co1–N2	O2–Co1–N2
O3–Co1–N2	O3–Co1–N2	O3–Co1–N2	O3–Co1–N2

b: Symmetry transformations used to generate equivalent atoms: #3: 1-x, -y, 1-z; #4: 0.5+x, -0.5-y, 0.5+z; #5: 0.5–x, 0.5+y, 1.5–z.

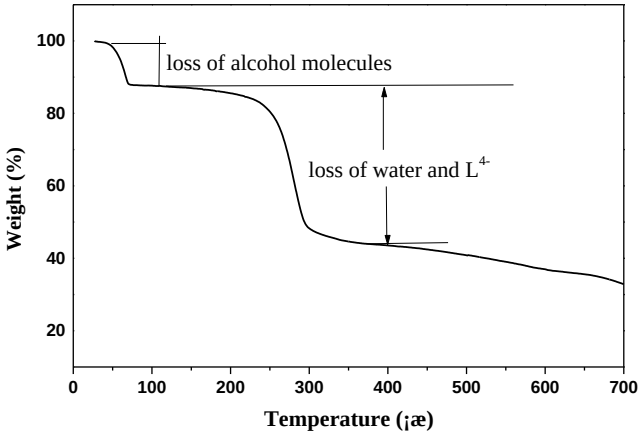
Table S3. The fundamental information of the seven coordination polymers[a]

No.	Formula	Dimension	Controlled evaporation	Two layers diffusion	Solvothermal at 80°C
1	**$\{[Cd(L)_{0.5}(2,2'\text{-bpy})(H_2O)_2]\cdot 3H_2O\}_n$**	1-D		☻	
2	**$\{[Cd(L)_{0.5}(2,2'\text{-bpy})(C_2H_5OH)(H_2O)]\cdot H_2O\cdot CH_3OH\}_n$**	1-D	☻		
3	**$\{[Cd(L)_{0.5}(phen)(H_2O)_2]\cdot H_2O\cdot CH_3OH\}_n$**	1-D	☻		
4	**$\{[Co(L)_{0.5}(phen)(H_2O)_2]\cdot CH_3OH\cdot 2H_2O\}_n$**	1-D	☻		
5	**$[Co(L)_{0.5}(phen)(H_2O)_2]_n\cdot nH_2O$**	2-D			☻
6	**$[Co(L)_{0.5}(4,4'\text{-bpy})(MeOH)]_n$**	3-D			☻
7	**$n[Co(4,4'\text{-bpy})_2(H_2O)_4]\cdot [Co(L)(H_2O)_2]_n$**	1-D		☻	

a: All the reactants are in 1:1:1 mole ratio (M:L:phen/bpy), and in methanol-water media.



(a)



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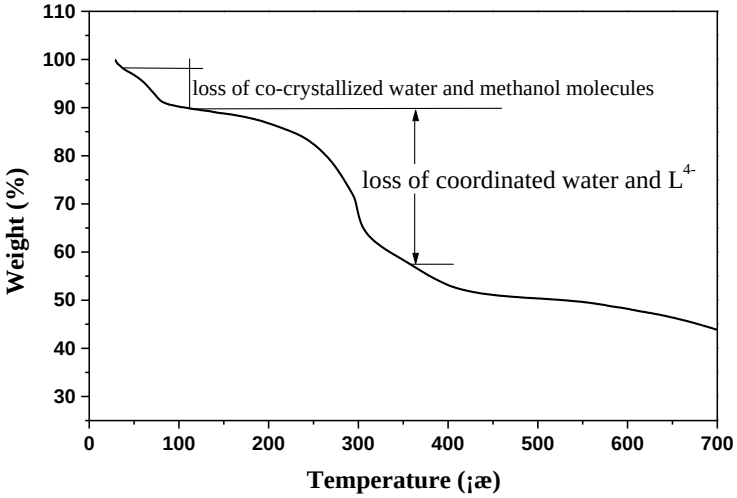

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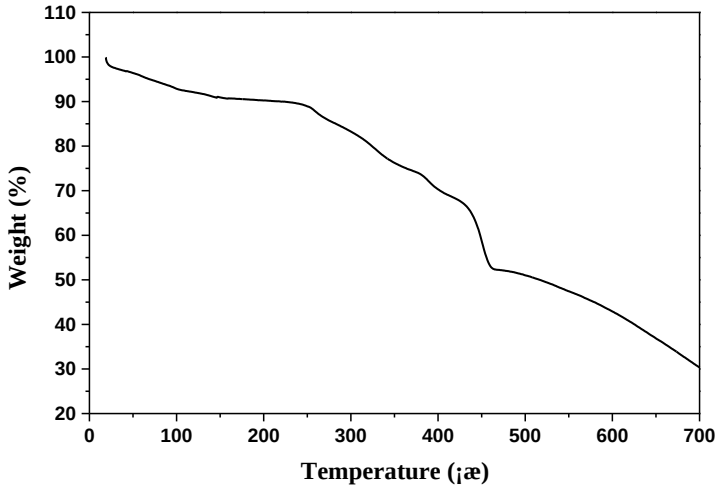

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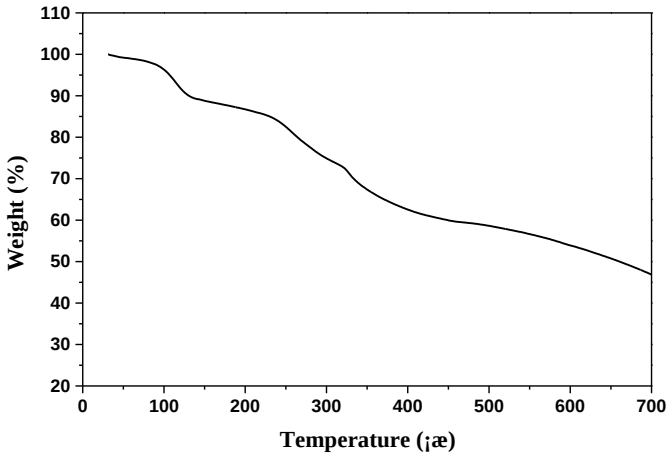
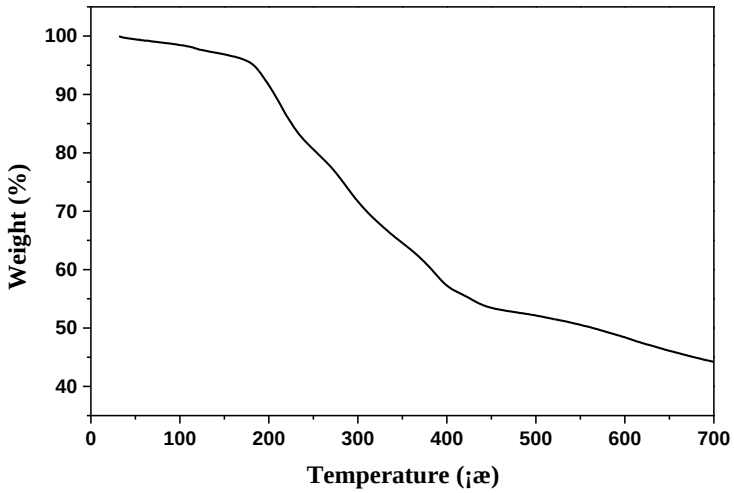
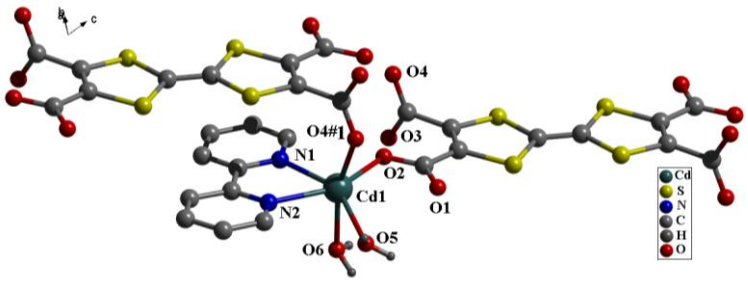


(e)

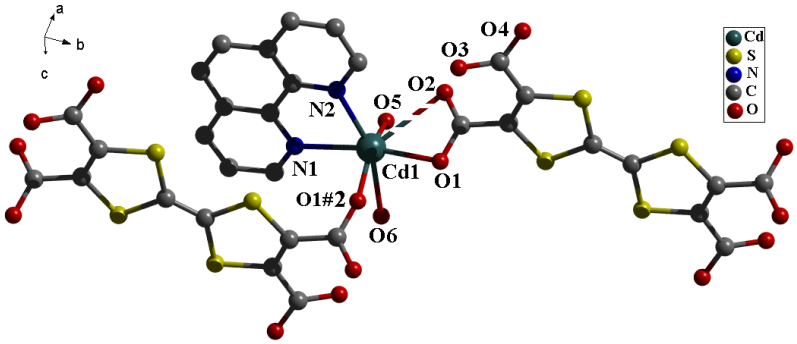


(f)

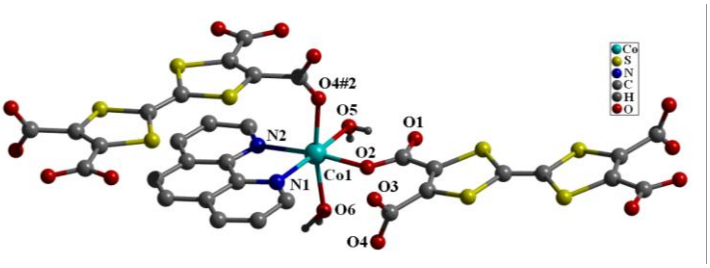
Figure S1. Thermal gravimetric measurements of (a) **1**, (b) **2**, (c) **3**, (d) **4**, (e) **5**, and (e) **6**.



(a) (#1: 1-x, 1-y, -z)

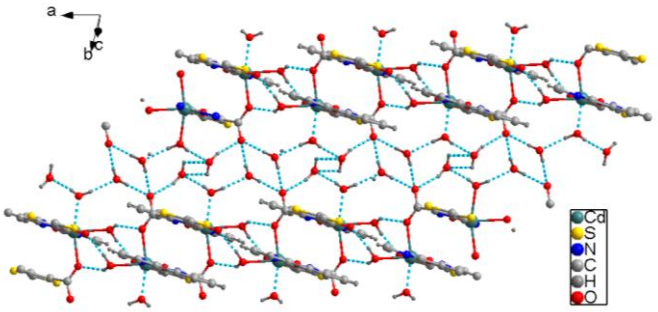


(b) (#2: 1-x, 1-y, 1-z)

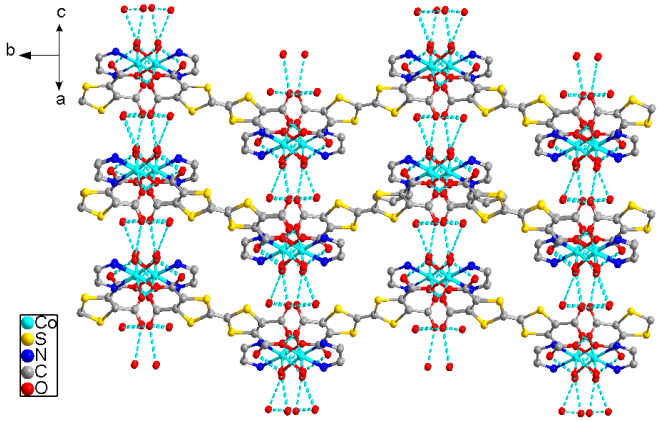


(c) (#2: 0.5+x, -0.5-y, 0.5+z)

Figure S2. Coordination environment of Cd(II) in **1** (a), **3** (b), and Co(II) in **5** (c).

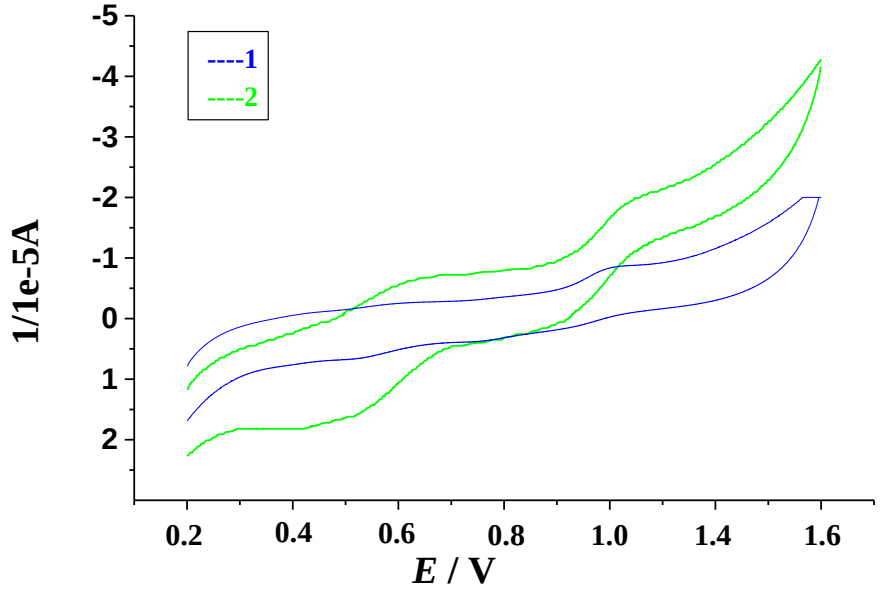


(a)

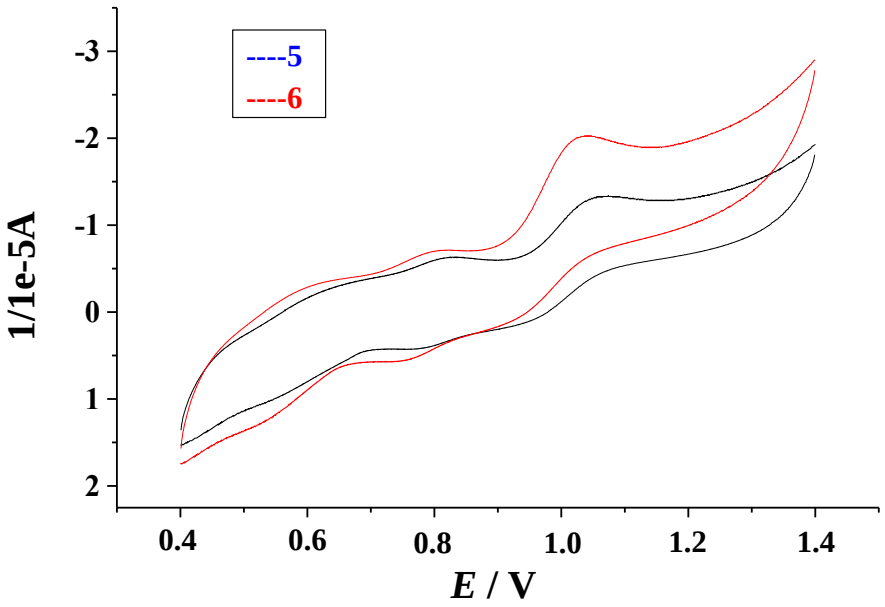


(b)

Figure S3. (a) The belt-like H-bonding structure of compound **1**. (b) The H-bonding connection within the layered structure in crystal of compound **5**.



(a)



(b)

Figure S4. Solid state cyclic voltammogram of complexes (a) **1** and **2**, (b) **5** and **6** (CH_3CN, 0.1 mol·L^{-1} Bu_4NClO_4, 100 mV s^{-1}).