

Electronic Supplementary Information (ESI)

**Structural diversity and fluorescent properties of Cd^{II} coordination
polymers with 5-halonicotines regulated by solvent and ligand
halogen-substituting effect**

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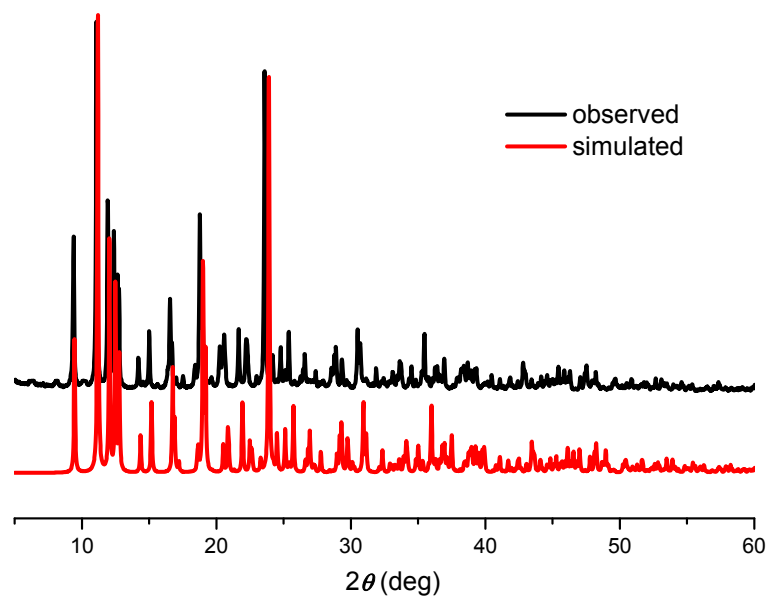
College of Chemistry, Tianjin Key Laboratory of Structure and Performance for Functional Molecules,

MOE Key Laboratory of Inorganic-Organic Hybrid Functional Material Chemistry, Tianjin Normal

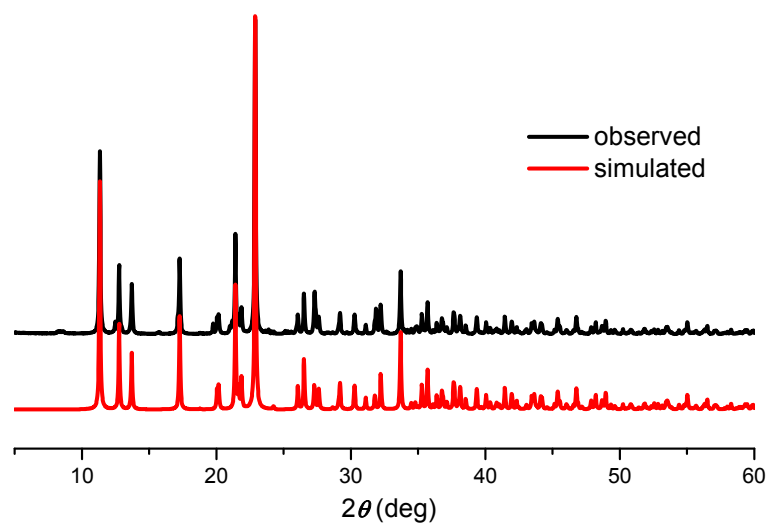
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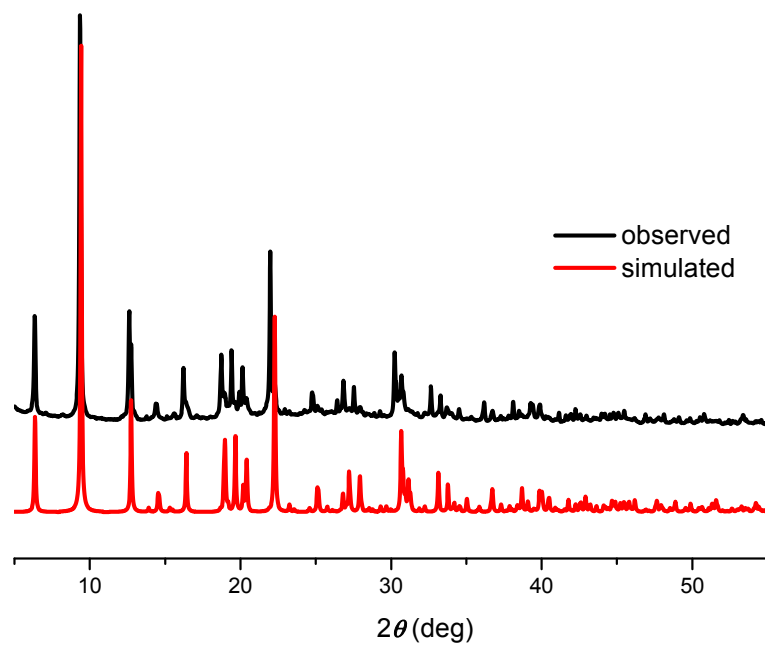
CrystEngComm



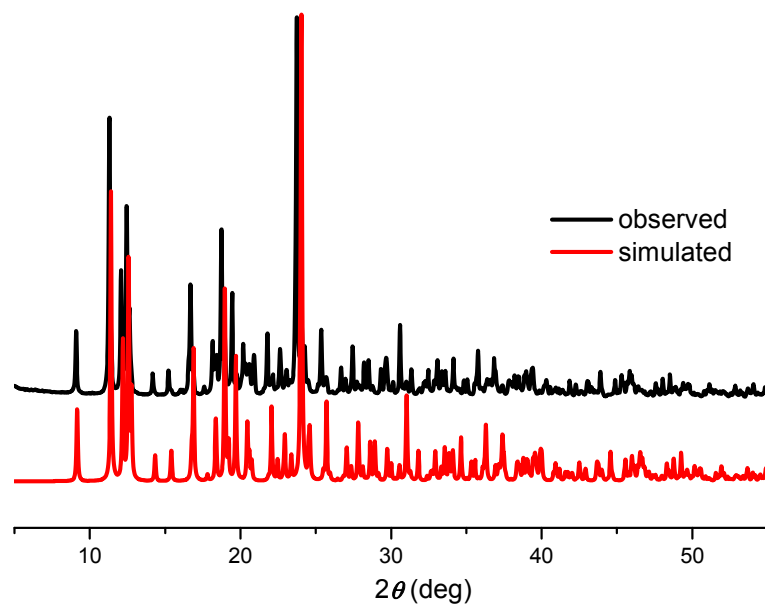
(a)



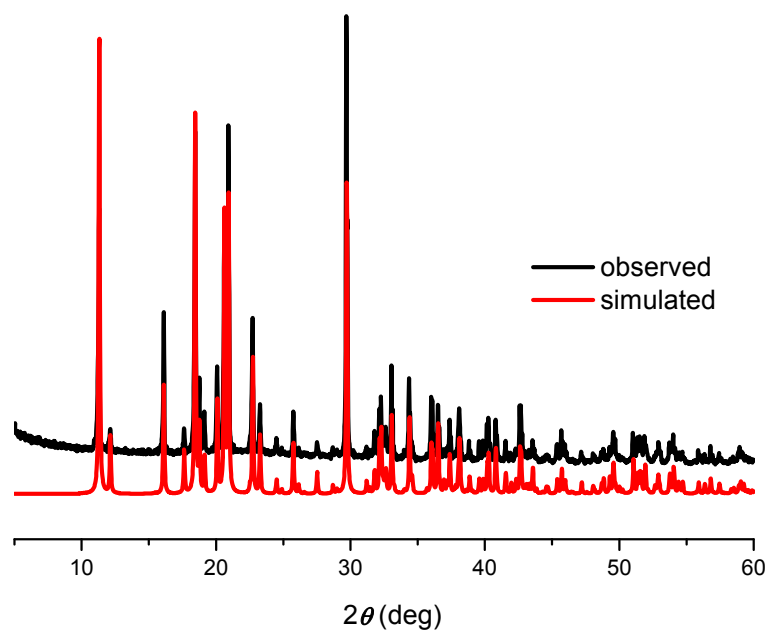
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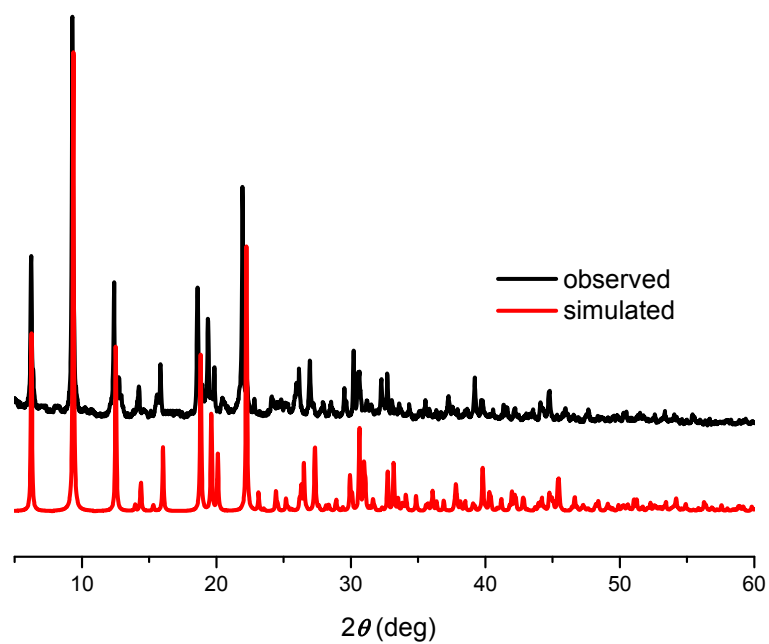
(c)



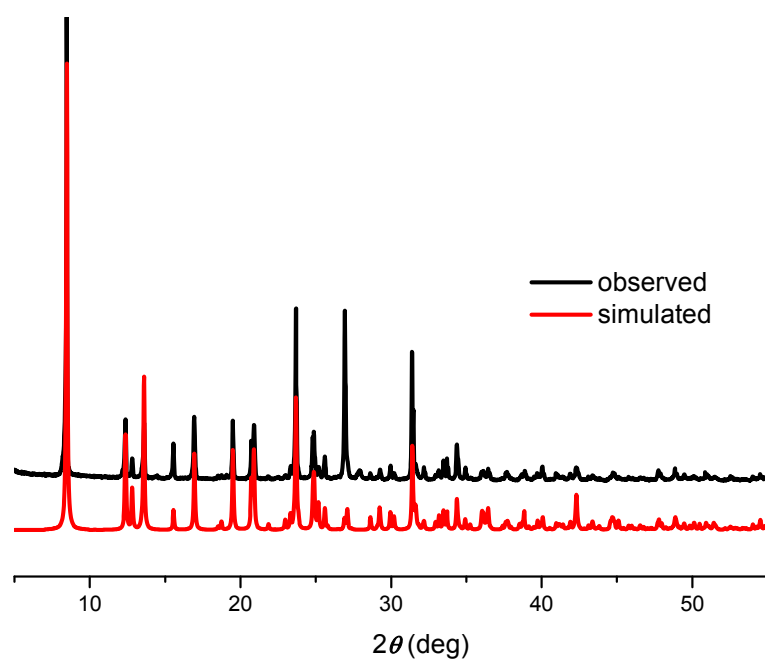
(d)



(e)



(f)



(g)

Fig. S1 Powder X-ray diffraction (PXRD) patterns for complexes 1–7 (a–g).

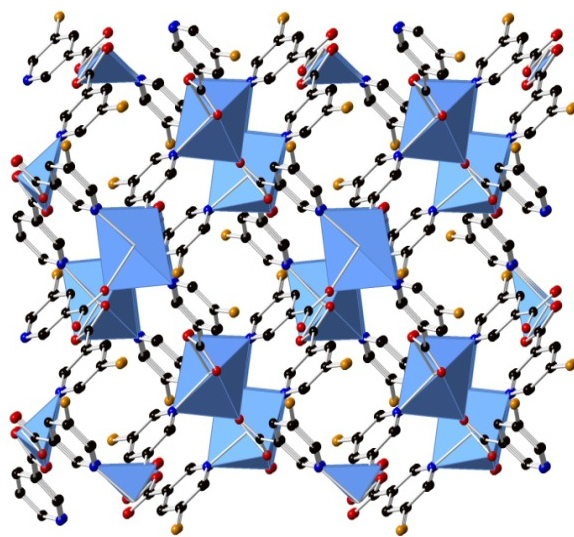


Fig. S2 3-D coordination framework of **1** with Cd^{II} ions shown in polyhedral model.

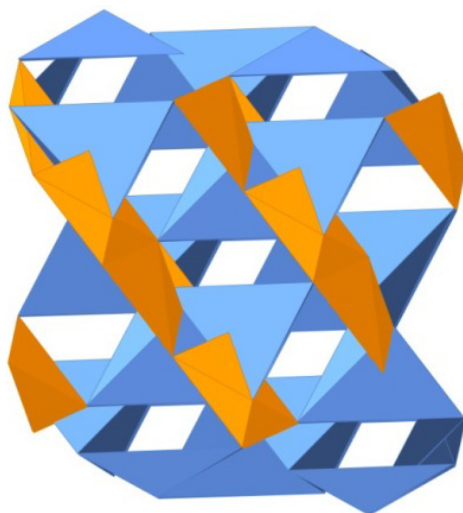


Fig. S3 Topological view of the 3-D network of **1** (orange and blue polyhedra for the 3-connected L-F⁻ ligands and 5-connected Cd^{II} ions, respectively).

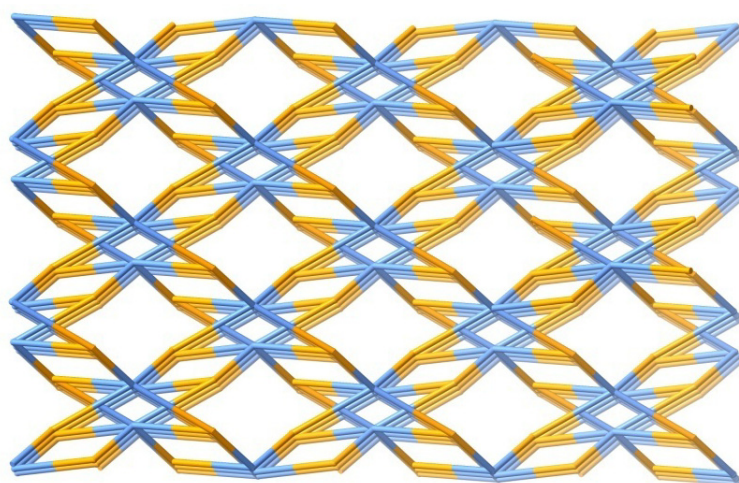


Fig. S4 Topological view of the 3-D network of **2** (orange and blue nodes for the 3-connected L-F^- ligands and 6-connected Cd^{II} ions, respectively).

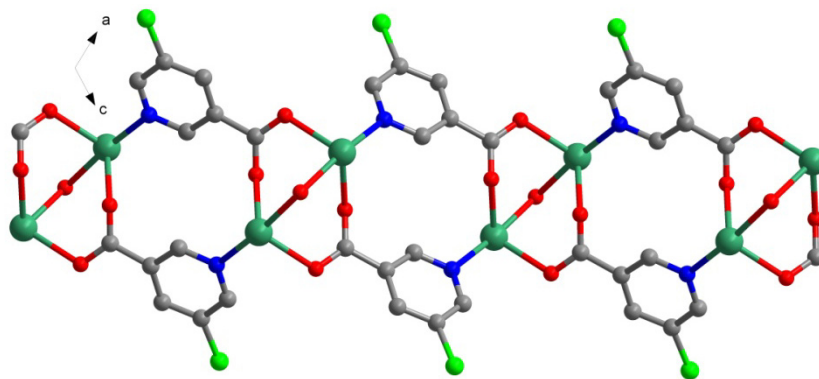


Fig. S5 A view of 1-D polymeric chain formed by μ_3 -L-Cl⁻ ligands and [Cd₂(H₂O)(COO)₂] bimetallic units in **7**.

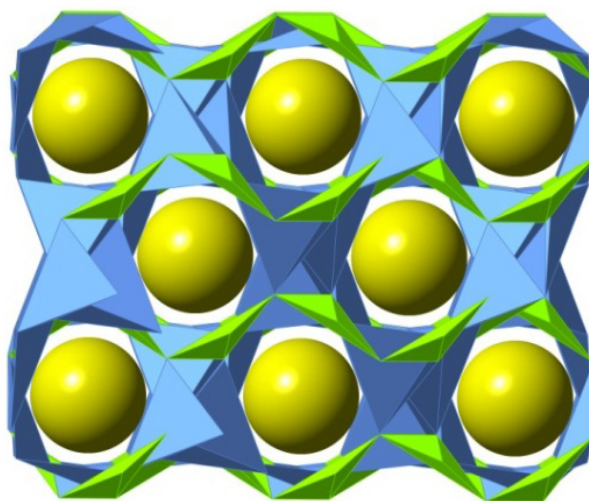
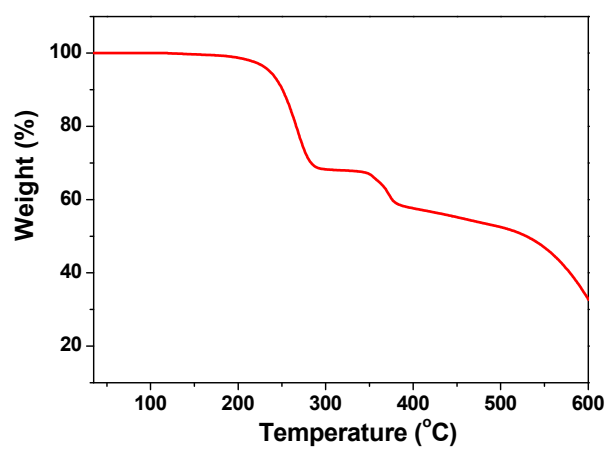
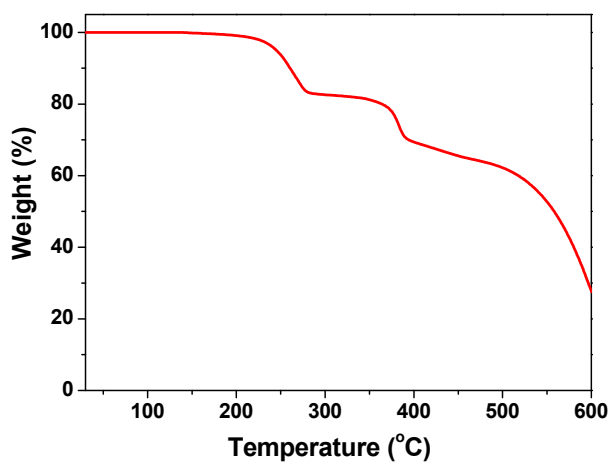


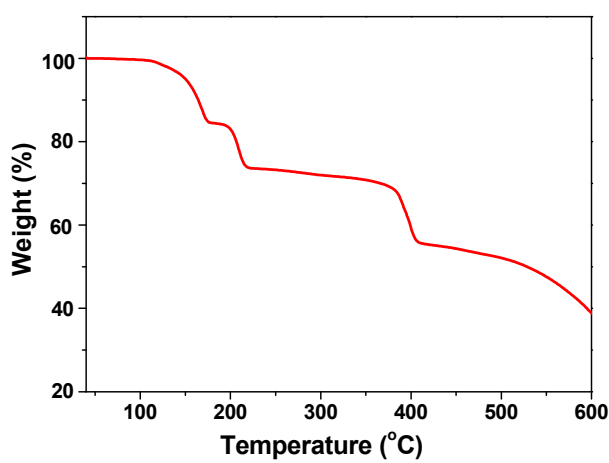
Fig. S6 Topological view of the 3-D network of **7** (green and blue polyhedra for the 3-connected L-Cl⁻ and 6-connected Cd^{II}, respectively; yellow balls for the void spaces).



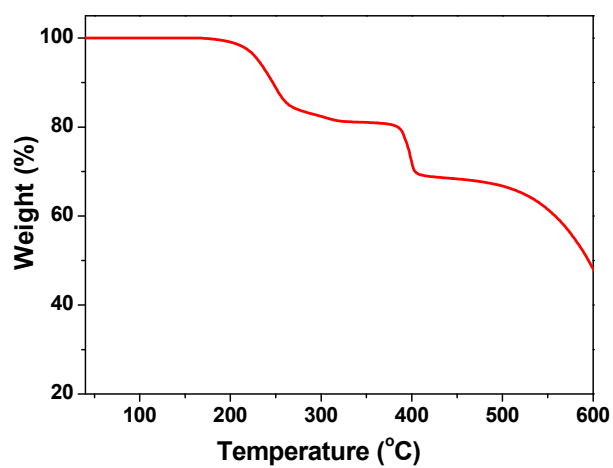
(a)



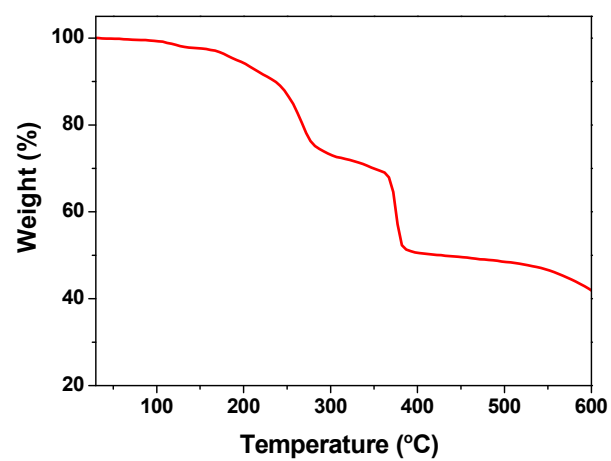
(b)



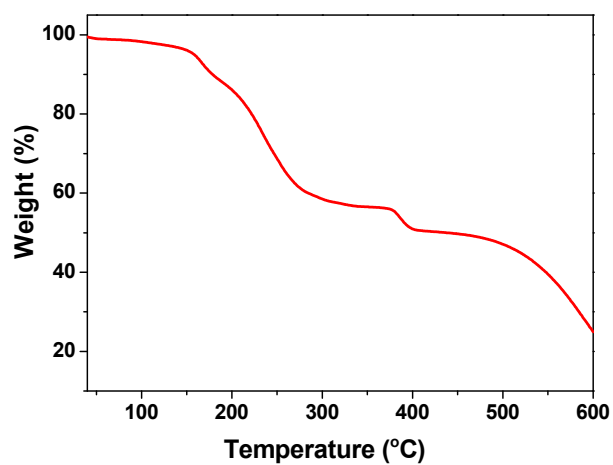
(c)



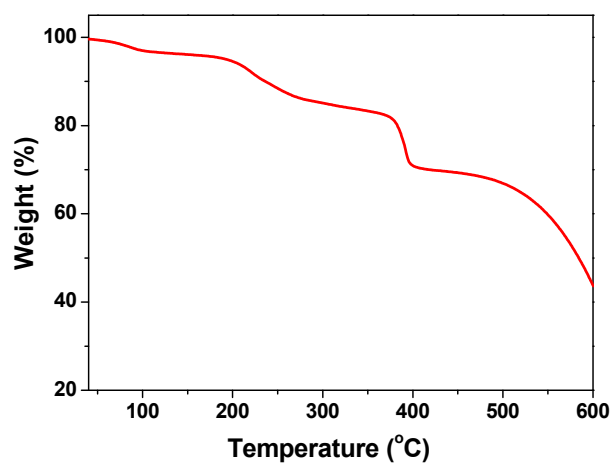
(d)



(e)

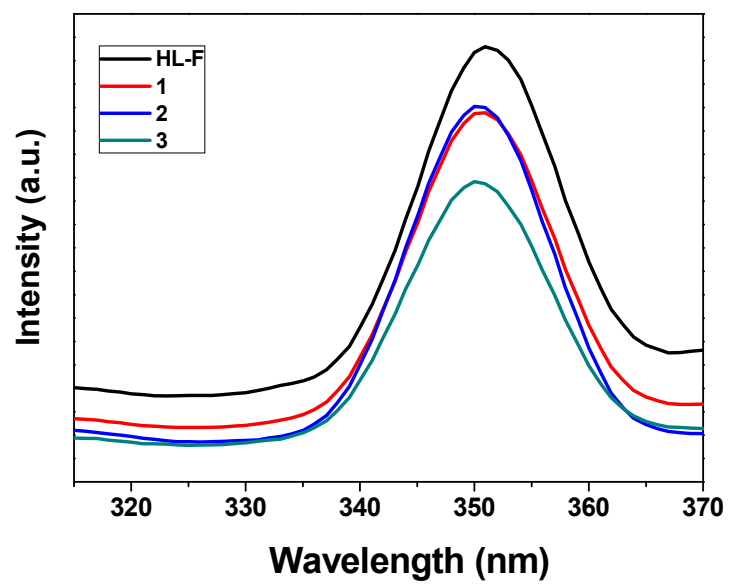


(f)

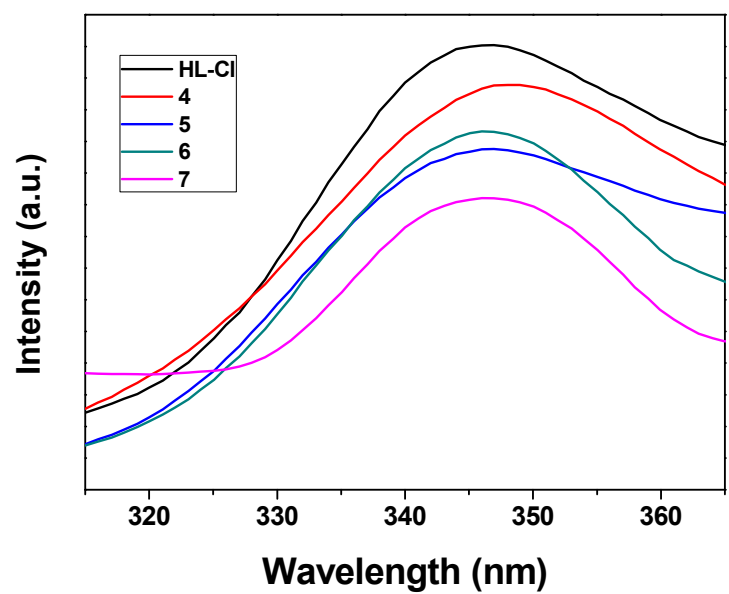


(g)

Fig. S7 Thermogravimetric analysis (TGA) curves of complexes **1–7 (a–g)**.



(a)



(b)

Fig. S8 Solid-state excitation spectra of (a) HL-F and 1–3 and (b) HL-Cl and 4–7.

Table S1 Selective bond lengths (Å) and angles (°) for complexes **1–7**

1			
Cd1–O3	2.274(3)	Cd1–O4	2.299(3)
Cd1–N2	2.333(3)	Cd1–O2A	2.334(3)
Cd1–N1	2.340(4)	Cd1–O1A	2.483(4)
O3–Cd1–O4	124.04(13)	O3–Cd1–N2	91.32(12)
O4–Cd1–N2	89.96(14)	O3–Cd1–O2A	93.78(12)
O4–Cd1–O2A	142.08(13)	N2–Cd1–O2A	91.99(13)
O3–Cd1–N1	88.56(12)	O4–Cd1–N1	85.15(14)
N2–Cd1–N1	174.01(13)	O2A–Cd1–N1	93.99(13)
O3–Cd1–O1A	147.85(11)	O4–Cd1–O1A	88.10(12)
N2–Cd1–O1A	87.49(12)	O2A–Cd1–O1A	54.19(11)
N1–Cd1–O1A	95.79(12)		
2			
Cd1–O2A	2.2723(18)	Cd1–O2B	2.2723(18)
Cd1–O1	2.3140(17)	Cd1–O1C	2.3140(17)
Cd1–N1D	2.376(2)	Cd1–N1E	2.376(2)
O2A–Cd1–O2B	81.27(10)	O2A–Cd1–O1	99.16(6)
O2B–Cd1–O1	89.35(7)	O2A–Cd1–O1C	89.35(7)
O2B–Cd1–O1C	99.16(6)	O1–Cd1–O1C	168.82(10)
O2A–Cd1–N1D	84.69(7)	O2B–Cd1–N1D	165.58(8)
O1–Cd1–N1D	89.64(7)	O1C–Cd1–N1D	83.91(6)
O2A–Cd1–N1E	165.58(7)	O2B–Cd1–N1E	84.69(7)
O1–Cd1–N1E	83.91(7)	O1C–Cd1–N1E	89.64(7)
N1D–Cd1–N1E	109.50(11)		

3

Cd1–O2A	2.2015(16)	Cd1–O3	2.3149(16)
Cd1–O1B	2.3329(17)	Cd1–N1	2.3898(19)
Cd1–Cl	2.6052(6)	Cd1–Cl1C	2.6270(6)
O2A–Cd1–O3	165.47(7)	O2A–Cd1–O1B	84.34(7)
O3–Cd1–O1B	84.73(6)	O2A–Cd1–N1	87.60(7)
O3–Cd1–N1	81.76(7)	O1B–Cd1–N1	84.02(6)
O2A–Cd1–Cl1	99.72(5)	O3–Cd1–Cl1	91.28(5)
O1B–Cd1–Cl1	98.13(4)	N1–Cd1–Cl1	172.52(5)
O2A–Cd1–Cl1C	98.58(5)	O3–Cd1–Cl1C	91.21(5)
O1B–Cd1–Cl1C	172.67(4)	N1–Cd1–Cl1C	89.37(5)
Cl1–Cd1–Cl1C	88.028(17)		

4

Cd1–O3	2.2445(17)	Cd1–O4	2.2776(19)
Cd1–O1	2.2938(18)	Cd1–N2	2.332(2)
Cd1–N1A	2.347(2)	Cd1–O2	2.506(2)
O3–Cd1–O4	118.40(7)	O3–Cd1–O1	101.85(7)
O4–Cd1–O1	139.46(7)	O3–Cd1–N2	90.39(7)
O4–Cd1–N2	89.57(8)	O1–Cd1–N2	95.11(7)
O3–Cd1–N1A	87.19(7)	O4–Cd1–N1A	85.27(8)
O1–Cd1–N1A	92.42(7)	N2–Cd1–N1A	172.42(7)
O3–Cd1–O2	155.56(7)	O4–Cd1–O2	85.95(7)
O1–Cd1–O2	54.19(6)	N2–Cd1–O2	87.46(7)
N1A–Cd1–O2	97.69(7)		

5

Cd1–O3	2.2913(15)	Cd1–O1A	2.3003(13)
Cd1–N1	2.3680(16)		

O2–Cd1–O1A	89.04(5)	O3–Cd1–N1	87.11(6)
O1A–Cd1–N1	87.82(5)		

6

Cd1–O2A	2.2049(17)	Cd1–O3	2.3144(17)
Cd1–O1B	2.3439(17)	Cd1–N1	2.393(2)
Cd1–Cl2	2.6396(6)	Cd1–Cl2C	2.6145(6)
O2A–Cd1–O3	168.78(7)	O2A–Cd1–O1B	85.65(7)
O3–Cd1–O1B	86.34(7)	O2A–Cd1–N1	87.54(7)
O3–Cd1–N1	83.62(7)	O1B–Cd1–N1	82.40(7)
O2A–Cd1–Cl2C	97.61(6)	O3–Cd1–Cl2C	91.26(5)
O1B–Cd1–Cl2C	97.83(5)	N1–Cd1–Cl2C	174.85(5)
O2A–Cd1–Cl2	96.45(5)	O3–Cd1–Cl2	90.48(5)
O1B–Cd1–Cl2	172.09(5)	N1–Cd1–Cl2	90.05(5)
Cl2–Cd1–Cl2C	89.470(17)		

7

Cd1–O2A	2.275(3)	Cd1–N1	2.303(3)
Cd1–O5	2.305(2)	Cd1–O1B	2.313(3)
Cd1–O3C	2.335(3)	Cd1–N2	2.375(3)
O2A–Cd1–N1	92.32(11)	O2A–Cd1–O5	89.77(9)
N1–Cd1–O5	172.87(11)	O2A–Cd1–O1B	105.35(11)
N1–Cd1–O1B	86.31(12)	O5–Cd1–O1B	86.57(10)
O2A–Cd1–O3C	172.46(11)	N1–Cd1–O3C	91.41(11)
O5–Cd1–O3C	87.31(8)	O1B–Cd1–O3C	81.42(11)
O2A–Cd1–N2	85.33(11)	N1–Cd1–N2	91.02(12)
O5–Cd1–N2	95.94(11)	O1B–Cd1–N2	169.07(11)
O3C–Cd1–N2	88.05(11)		

Symmetry codes: A = $-x + 2, y + 1/2, -z + 3/2$ for **1**; A = $-x + 1, -y + 1, -z + 1$; B = $x, -y + 1, z + 1/2$; C = $-x + 1, y, -z + 3/2$; D = $x + 1/2, -y + 1/2, z + 1/2$; E = $-x + 1/2, -y + 1/2, -z + 1$ for **2**; A = $-x, y + 1/2, -z + 1/2$; B = $-x, -y + 2, -z$; C = $x, -y + 5/2, z + 1/2$ for **3**; A = $-x + 1, y + 1/2, -z + 3/2$ for **4**; A = $-x + 2, y - 1/2, -z + 3/2$ for **5**; A = $-x + 1, y - 1/2, -z + 1/2$; B = $-x + 1, -y, -z$; C = $x, -y - 1/2, z - 1/2$ for **6**; A = $x - 1/2, -y + 1/2, z - 1/2$; B = $-x + 1/2, -y + 1/2, -z + 2$; C = $x, -y, z + 1/2$ for **7**.
