Supplementary Material (ESI) for Chemical Communications

Supplementary Information

A luminescent homochiral 3D Cd(II) framework with a threefold interpenetrating uniform net 8^6†

Rui Feng,[ab] Fei-Long Jiang,[a] Lian Chen,[a] Chun-Feng Yan,[ab] Ming-Yan Wu,[a] and Mao-Chun Hong*[a]

[a]State Key Laboratory of Structure Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, 350002, China.

[b] Graduate School of the Chinese Academy of Sciences, Beijing, 100049, China.

- Corresponding author:

E-mail: *hmc@fjirsm.ac.cn.*
Tel: +86-591-83792460; Fax: +86-591-83794946

Synthesis of the Complex 1

Hydrothermal reaction of H_2dtba (115 mg, 0.375 mmol), bpp (74 mg, 0.375 mmol) and $Cd(CH_3CO_2)_2{\cdot}2H_2O$ (100 mg, 0.375 mmol) in H_2O (10 ml) solution was performed in a Teflon-lined stainless steel bomb at 120 °C for 6 days, and the mixture was then cooled to room temperature at a rate of *ca.* 10 °C/h. Brown crystals were obtained (yield: 77% based on $Cd(CH_3CO_2)_2{\cdot}2H_2O$). Anal. for $C_{27}H_{22}Cd_1N_2O_4S_2$ (%): Calcd.: C, 52.73; H, 3.60; N, 4.55. Found: C, 53.51; H, 3.51; N, 4.13. IR (KBr pellet, cm^{-1}): 3435 (s), 1614 (m), 1574 (m), 1537 (s), 1400 (vs), 859 (m), 746 (m).

Crystallographic Analyses

The intensity data were collected on a Saturn 70 CCD diffractometer for **1**, with graphite-monochromated MoKα radiation (λ = 0.71073 Å) at room temperature. All absorption corrections were performed by using the multiscan program. The structure were solved by direct methods and refined by full-matrix least squares on F^2 with the SHELXTL-97 program.[S1]

Thermal Gravimetric Analysis (TGA)

To examine the thermal stability of the compound **1**, the thermal gravimetric analysis (TGA) of **1** has been performed (Fig. S4). There is no significant mass loss up to 305 °C. Subsequent there follows a rapid mass loss between 305 and 420 °C, corresponding to the decomposition of **1**. This suggests that the framework of **1** possesses high thermal stability.

X-ray Diffractometer Analysis (XRD)

The positions of diffraction peaks of the experimental are consistent with the simulated XRD patterns well, indicating the phase purity of the as-synthesized simple (Fig. S5).

(S1) Sheldrick, G. M. SHELXTL-97, Program for the Solution of Crystal Stuctures; University of Göttingen: Germany 1997.

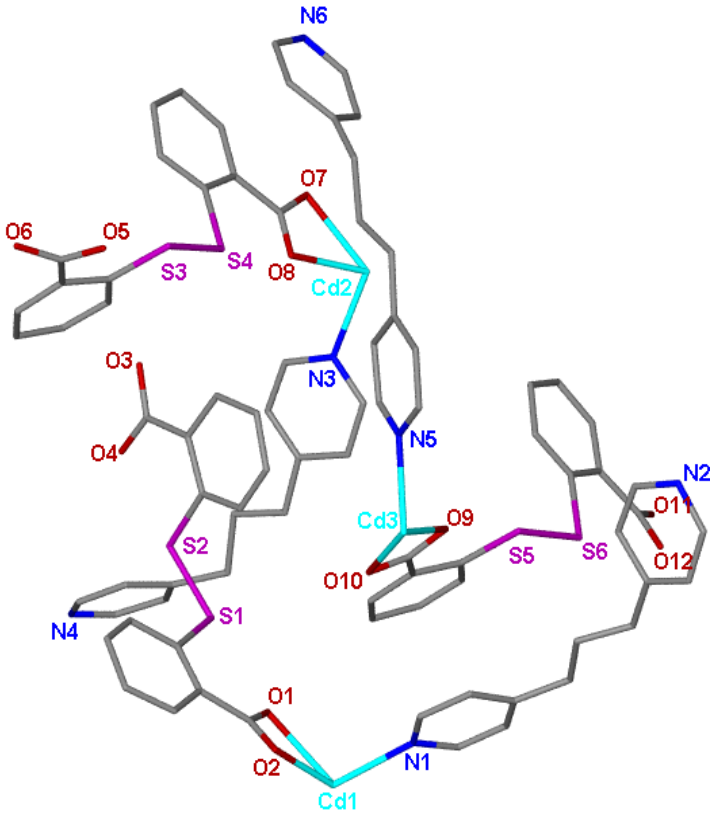


Fig. S1 The asymmetric unit of the compound **1**.

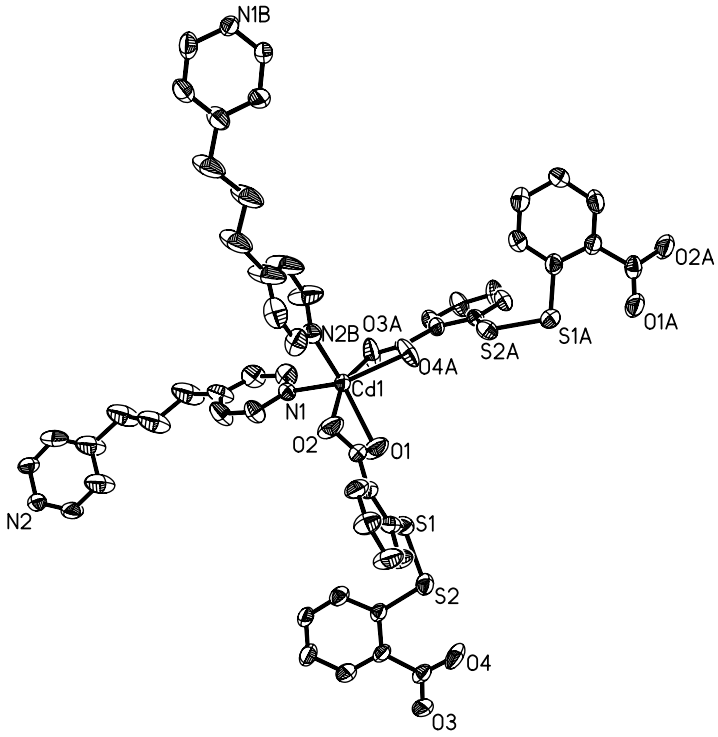


Fig. S2 The coordination environment of Cd(II) ion in **1** with the thermal ellipsoid at the 30% probability level. Symmetry codes: A: 1-y, 1+x-y, z-1/3, B: 1-x+y, 2-x, z-2/3.

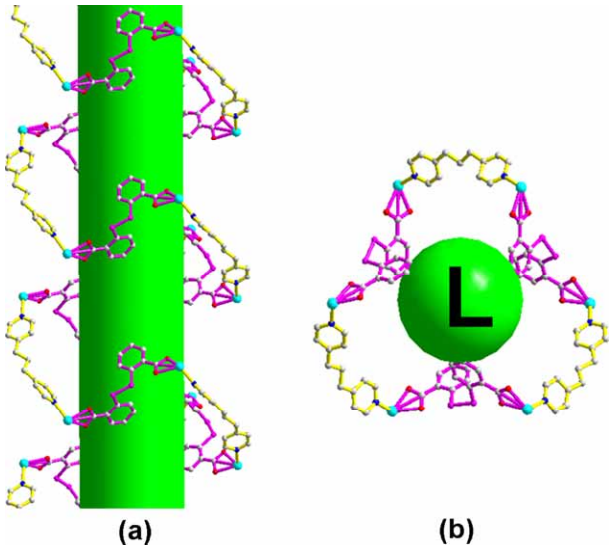


Fig. S3 The threefold left-handed $[Cd_2(dtba)(bpp)]_n$ single helix viewed perpendicular to the c axis (a) and viewed from the c axis (b). (dtba ligands, bpp ligands and screw axes are shown as pink line, yellow line and green rods, respectively)

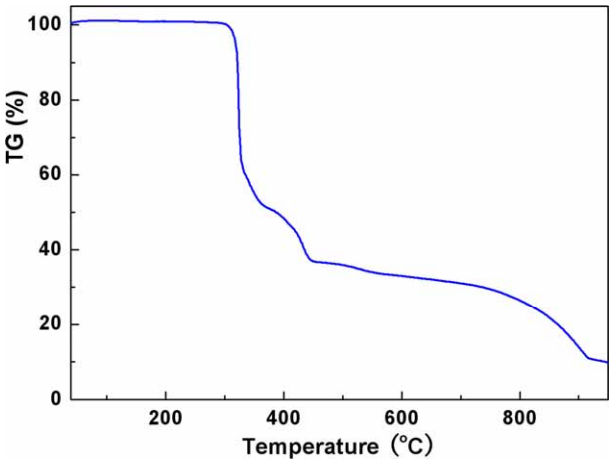


Fig. S4 TGA curve of compound **1.**

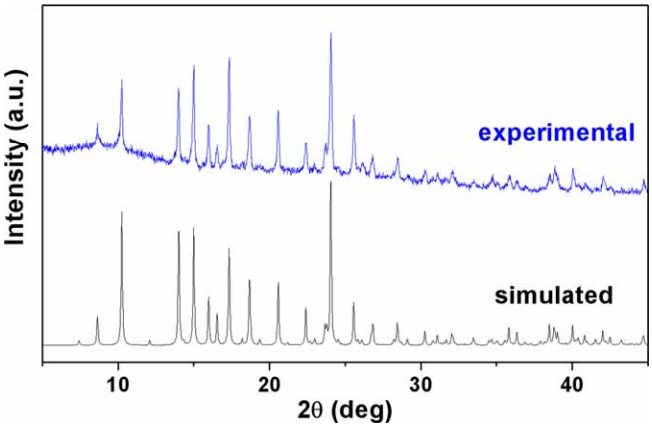
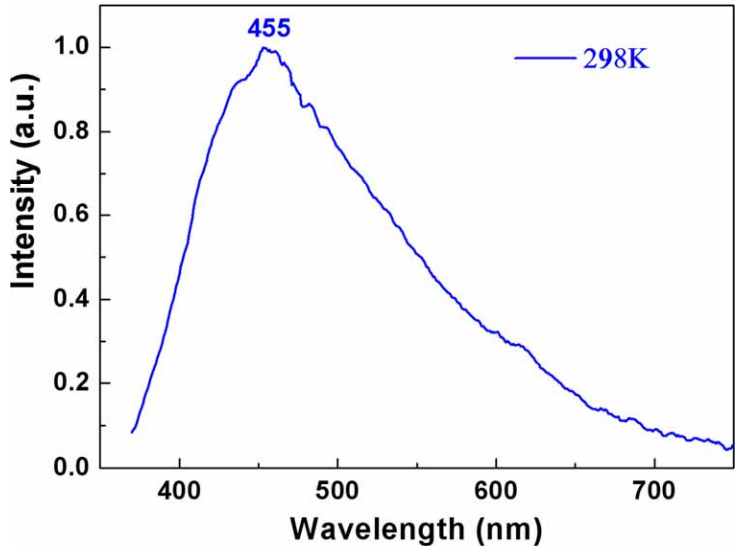
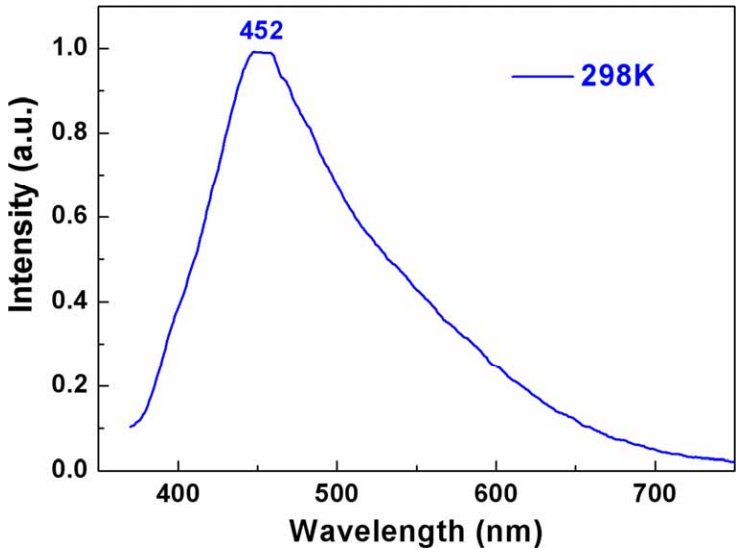


Fig. S5 Powder XRD patterns of experimental (up) and of simulated from single-crystal data (bottom) for compound **1.**



(a)



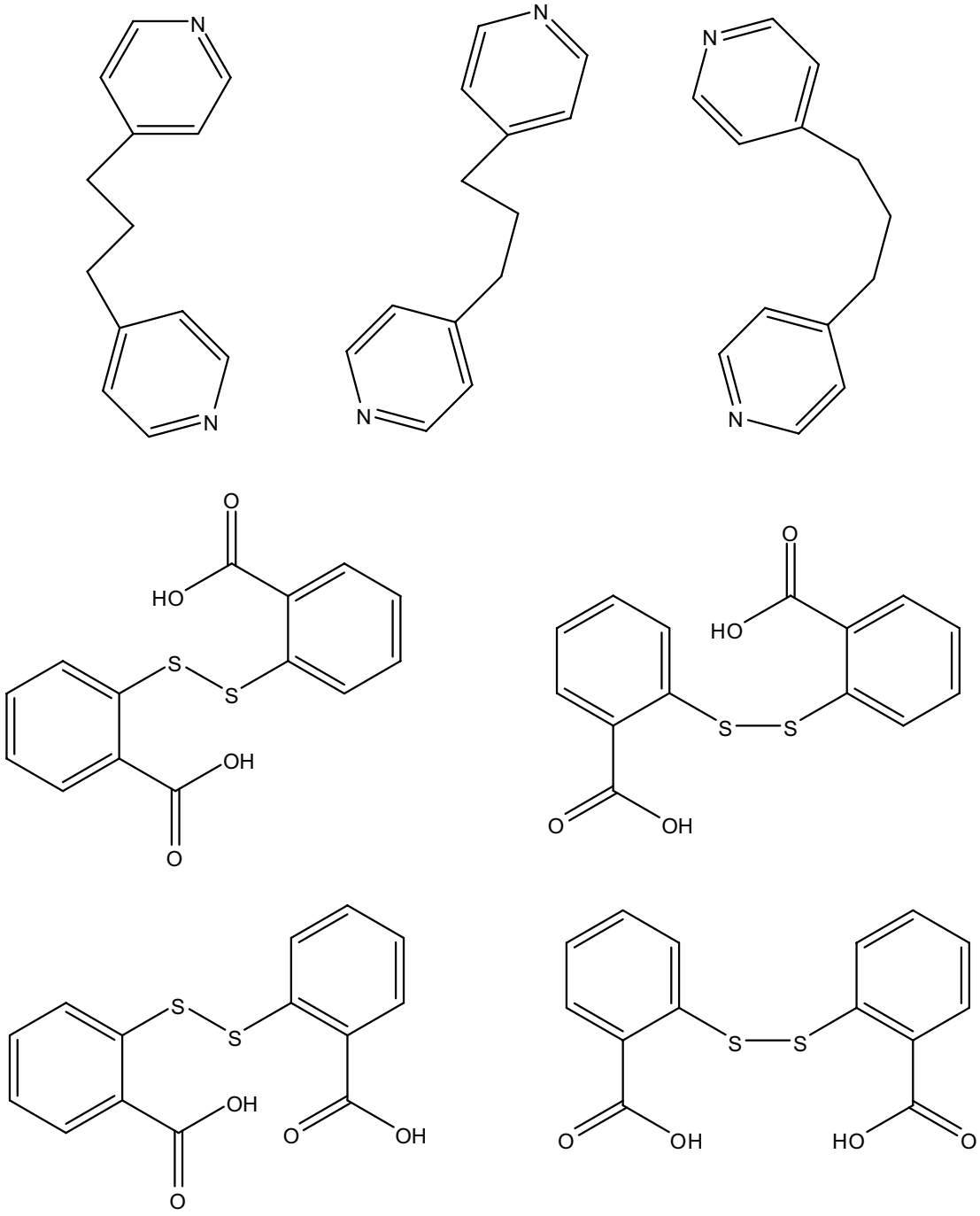
(b)

Fig. S6 (a) Emission spectrum of free H_2dtba ligand (λ_{ex} = 360 nm). (b) Emission spectrum of free bpp ligand (λ_{ex} = 360 nm).

Table S1. Photoluminescent lifetime data for compound **1** at room temperature

compound	Lifetime (ns)	
	τ_1	τ_2
1	1.128 (73.29%)	4.255 (26.81%)

Scheme S1. Conformational isomers of the H_2dtba and bpp ligands



CIF:

Although PLATON ADDSYM Detects Additional (Pseudo) Symm.Elem...S, We can not add symmetry any more by the platon software. It may be due to the disorder of some atoms.