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Supporting information

Absolute helicity induction: chiral information transfer from metal centre to ligand

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1. Experimental procedures

1.1 Materials and Instrumentations

All starting materials used in these synthetic reactions are purchased commercially and were used as obtained from the supplier. IR (KBr pellets) spectra were recorded on powdered samples with PerkinElmer Spectrum One instrument. Fluorescence spectra for the solid samples were performed on an Edinburgh Analytical instrument FLS920. The CD (KCl) spectra were recorded on a MOS 450 spectropolarimeter (Bio Logic). Thermogravimetric analysis was recorded using a NETZSCH STA 449C unit at a heating rate of 10 °C min^{-1} under nitrogen atmosphere. Elemental analyses of C, H and N were performed on a Vario EL III CHNO analyzer. Powder X-ray diffraction (PXRD) patterns were recorded by a RIGAKU DMAX2500 diffractometer with Cu Kα radiation (λ = 1.5406 Å). The NLO properties of compound **1** was tested on the powder samples by the Kurtz and Perry method using an Nd:YAG laser (1064 nm) with an input pulse of 350 mV.

1.2 Synthesis of compound 1

A mixture of 0.5 mmol $Cd(NO_3)_2 \cdot 4H_2O$, 1.0 mmol H_2OBA, and 0.5 mmol $BaNO_3$ were placed in a 20 mL of Teflon-lined stainless steel vessel with 6 mL of mixed solvent of DMF (*N*,*N*-dimethylformamide) and methanol (v/v = 1:1). The mixture was heated to 145 ºC in 4 h and kept at this temperature for three days. The reaction system was cooled slowly to room temperature during another two days. Colorless strip shaped crystals of **1** were collected, washed thoroughly with DMF and CH_3OH, and dried in air at room temperature (yield: 56% based on $Cd(NO_3)_2 \cdot 4H_2O$). Elemental analysis (%): calcd. for $C_{32}H_{30}BaCdNO_{14}$ (902.31): C 42.60, H 3.35, N 1.55; found: C 42.78, H 3.40, N 1.61. IR (KBr, cm^{-1}): 3434 s, 3061 s, 1668 s, 1533 vw, 1384 vs, 1299 vs, 1162 w, 1105 w, 856 vw, 783 w, 769 w, 697 vw, 619 vw, 530 vw.

1.3 X-Ray crystallography

Diffraction data for **Δ-1** and Λ-**1** were collected on a Mercury CCD area detector (Mo-Kα; λ = 0.71073 Å) at 273 K**.** Empirical absorption corrections were applied to the data using the *CrystalClear* program. The structures were solved by the direct method and refined by the full-matrix least squares on F^2 using the *SHELXTL*-97 program. All the non-hydrogen atoms were refined anisotropically. Hydrogen atoms bound to carbon atoms were placed in calculated positions and refined isotropically with a riding model.

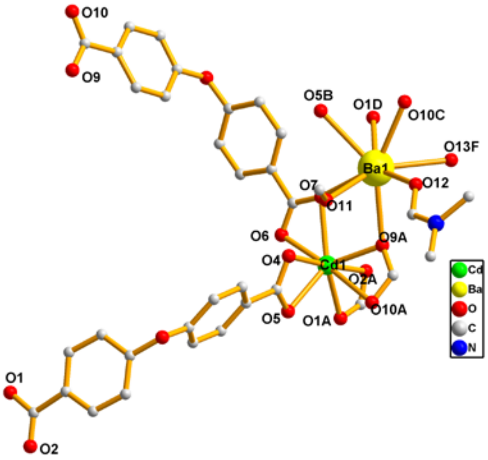

Fig. S1 Representation of the Cd(II)/Ba(II) coordination environments for Δ-**1**.

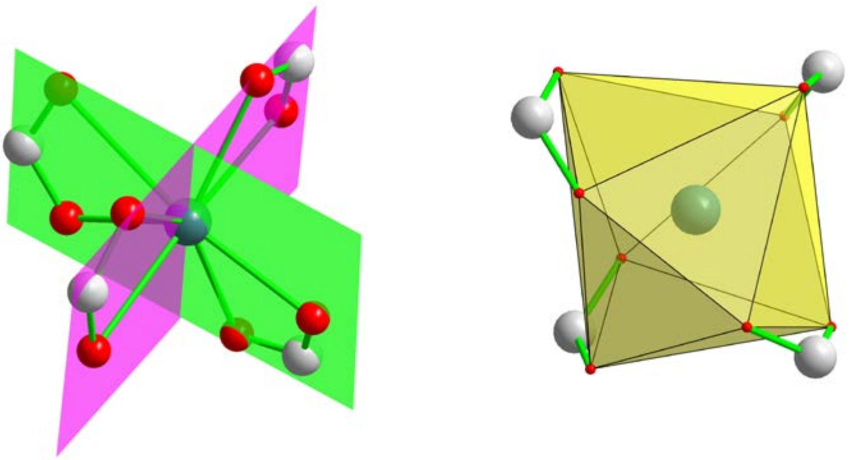

Fig. S2 Two sets of four oxygen atoms form two mutually orthogonal trapezoids constructing a distorted dodecahedron (DD) configuration for the pseudo-achiral metal centre.

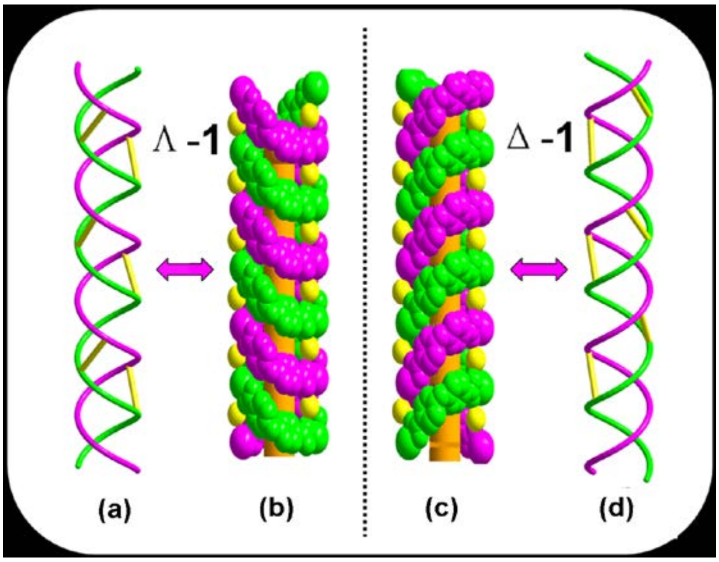

Fig. S3 The left- and right-handed double helices in Λ-**1** (a, b) and in Δ-**1** (c, d).

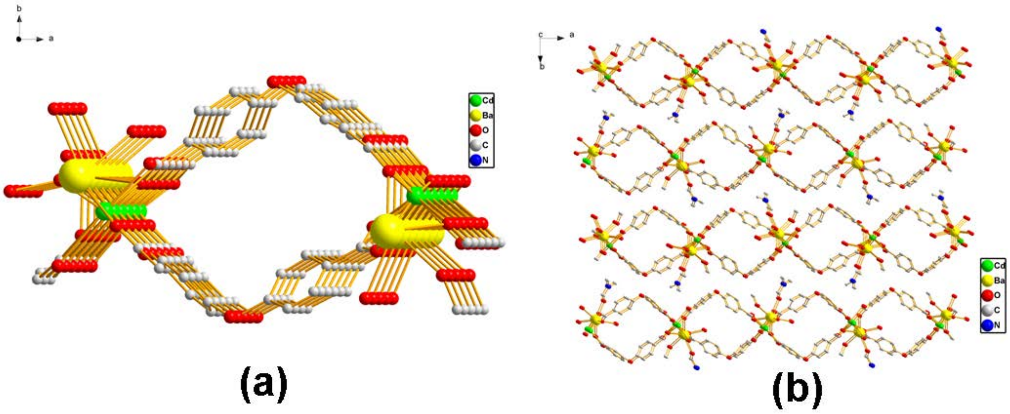

Fig. S4 Chiral channel (a) connected with neighboring channels and then stacked into a 3D supramolecular structure (b).

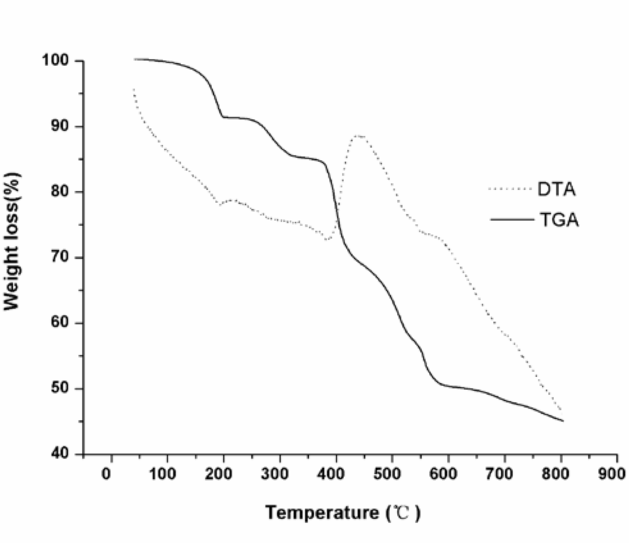

Fig. S5 TG and DTA curves for compound **1**.

As shown in Fig. S5, compound **1** underwent a 16.1% mass decrease between ~30 and ~280 ºC, corresponding to the elimination of its coordinated water, methanol, and DMF molecules in the channels of the framework (15.5% predicted), which are in agreement with the endothermic peaks observed at the differential thermal analysis (DTA) diagrams. And the residue composition of this complex is then decomposed in the temperature arrange of ~280 to ~800 ºC.

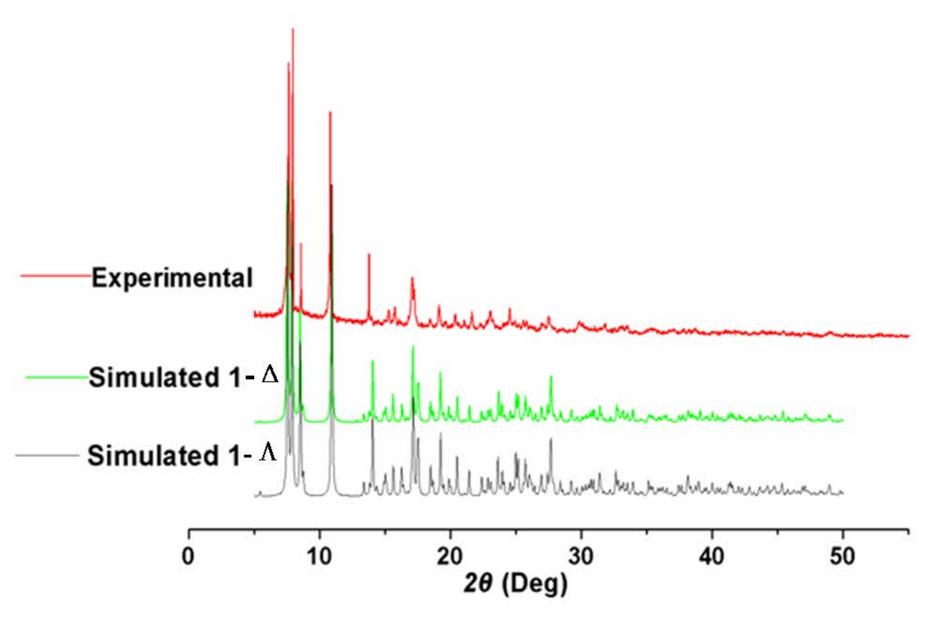

Fig. S6 The powder X-ray diffraction patterns of **1**.

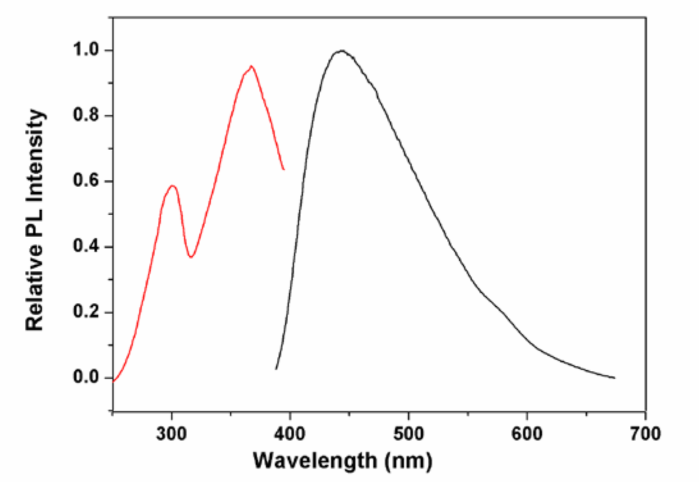

Fig. S7 (a) Normalized emission (black) and excitation (red) spectra of **1** collected in solid state at room temperature.

Table S1 Crystallographic data and structure refinement details for Δ-**1** and Λ-**1**.

Compound	Δ-**1**	Λ-**1**
Empirical formula	$C_{32}H_{30}NO_{14}Ba_1Cd_1$	$C_{32}H_{30}NO_{14}Ba_1Cd_1$
Formula weight	902.31	902.31
Crystal system	Orthorhombic	Orthorhombic
Space group	$P2_12_12_1$	$P2_12_12_1$
a [Å]	7.2339(4)	7.2243(6)
b [Å]	22.3320(14)	22.315(2)
c [Å]	23.4396(13)	23.376(2)
V [Å^3]	3786.6(4)	3768.5(6)
Z	4	4
Dc [g/cm^{-3}]	1.583	1.590
μ [mm^{-1}]	1.658	1.666
F(000)	1780	1780
Reflns. Collected	24084	29401
Reflns. Unique	6669	8546
Reflns. [$I > 2\sigma(I)$]	6460	7340
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0367$, $wR_2 = 0.1120$	$R_1 = 0.0585$, $wR_2 = 0.1708$
R indices (all data)	$R_1 = 0.0381$, $wR_2 = 0.1142$	$R_1 = 0.0693$, $wR_2 = 0.1822$
Goodness-of-fit	1.108	0.927
Flack parameter	–0.02(2)	0.00(3)