Supplementary Information for

An Elastic Single Crystal Composed of One-dimensional Chiral Coordination Polymers

Yan Zhang [a], Yu-Xia Li [a], Kai-Ge Gao [b] Jia-Hui Zhang [a], Jie-Sheng Hu [a], Jun Tao [a], Zi-Shuo Yao *[a]

[a] Key Laboratory of Cluster Science of Ministry of Education, School of Chemistry and Chemical Engineering, Liangxiang Campus, Beijing Institute of Technology, Beijing 102488, People's Republic of China.

[b] College of Physical Science and Technology, Yangzhou University, Yangzhou, Jiangsu 225009, People's Republic of China.

E-mail: zishuoyao@bit.edu.cn, taojun@bit.edu.cn

Experimental section

Crystal Synthesis: **1** was made under a midtemperature hydrothermal condition. $CdCl_2 \cdot H_2O$ (0.078 g, 1.0 mmol), 1-Methyl-2-pyridone (0.312 g, 2.0 mmol), were added in a 20 mL Teflon-sealed autoclave. Then, 10.0 mL of ethanol was added to this reaction system as the only solvent. After mixing for 1 h at room temperature, the sealed autoclave is transformed and heated up to 100 °C for 2 days. Colorless needle-like crystals of the required quality for testing mechanical properties were harvested after cooling to room temperature. All the analytical grade reagents and solvents were purchased from Bei Jing TongGuang Fine Chemicals Company and used without further purification. The yield was *ca*. 65%. Anal. $C_6H_7CdCl_2NO$ (292.44); calcd C 24.62%, H 2.39%, N 4.79%; found C 24.63%, H 2.44%, N 4.79%.

Single-crystal X-ray diffraction (SC-XRD): The variable-temperature single-crystal X-ray diffraction data were collected using a Rigaku Oxford XtaLAB PRO diffractometer equipped with a Mo-Kα radiation source. The diffraction data were collected at 293 K. The structures were solved using direct methods and refined by full matrix least-squares techniques on F^2 with the SHELX program implemented in the Olex2 program. Non-hydrogen atoms are refined by anisotropy, and hydrogen atoms were generated geometrically and refined isotropically.

Thermogravimetric analyses (TGA): The thermogravimetric analyses were carried out from 300 K to 1000 K on a TG-DTA 6200 instrument under N_2 atmosphere with a heating rate of 10 K min^{-1}.

CrystalExplorer-Based Calculations: The fingerprint plots based on the Hirshfeld surface, which are 3D isosurfaces of the given molecular crystal, were generated using the program CrystalExplorer 17.5.

Circular Dichroism Measurements (CD): CD measurements were performed on a JASCO-1500 under a constant flow of nitrogen with light passing through the pellet sample of KBr and **1** powder.

Atomic force microscopy measurements (AFM): The mechanical measurements by AFM were carried out at room temperature using a commercially available Cypher ES (Oxford Instruments). The probe used was the AC240TS-R3 silicon probe. (Olympus, resonance frequency 300 kHz, spring constant 26 N m^{-1}).

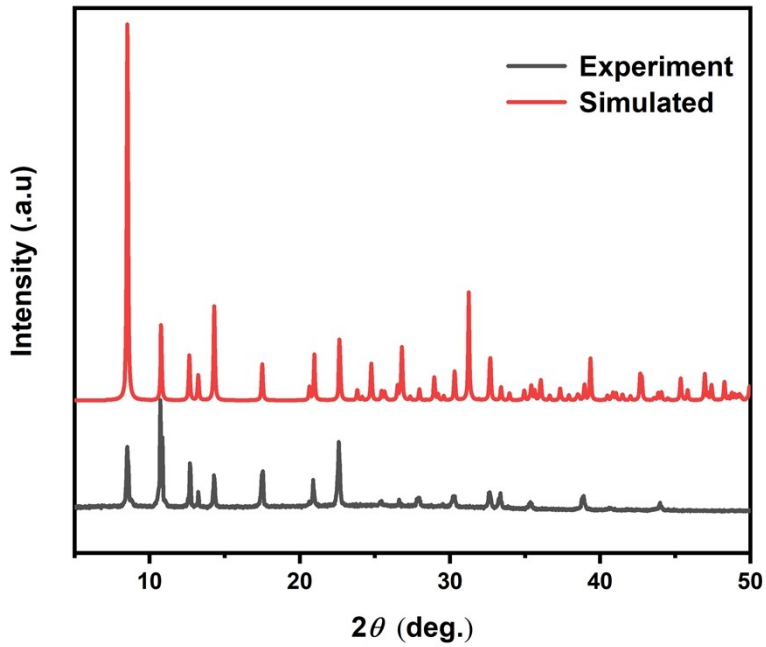

Fig. S1. The PXRD patterns of the powder at room temperature matched the simulated patterns, demonstrating the phase purity of the complexes.

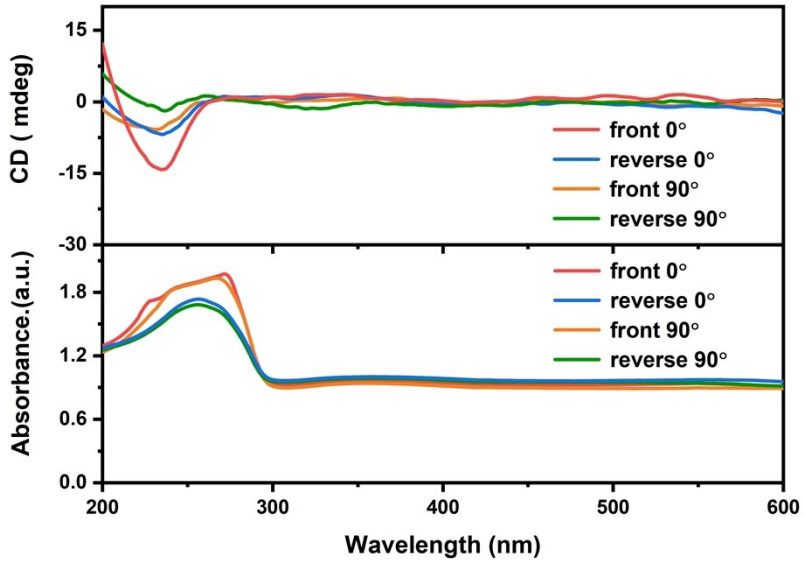

Fig. S2. CD spectra and absorption spectra upon sample flipping. The persistent CD signal upon sample flipping suggests that the signal stems mainly from genuine chiroptical activity of the sample.

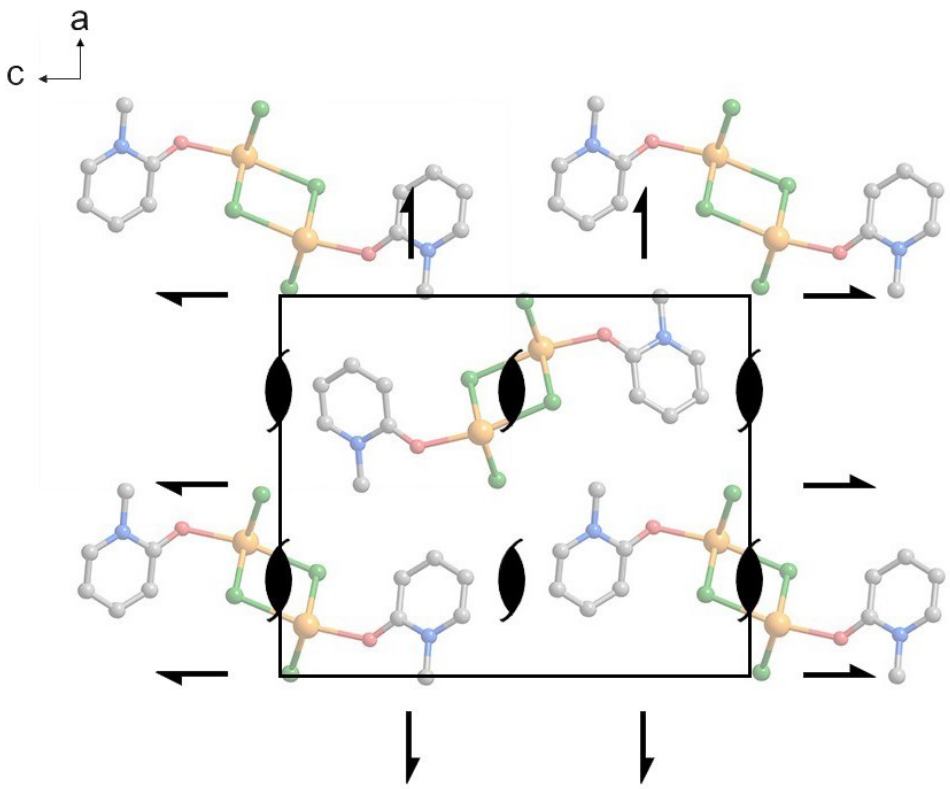

Fig. S3. Symmetry operations of compound **1**.

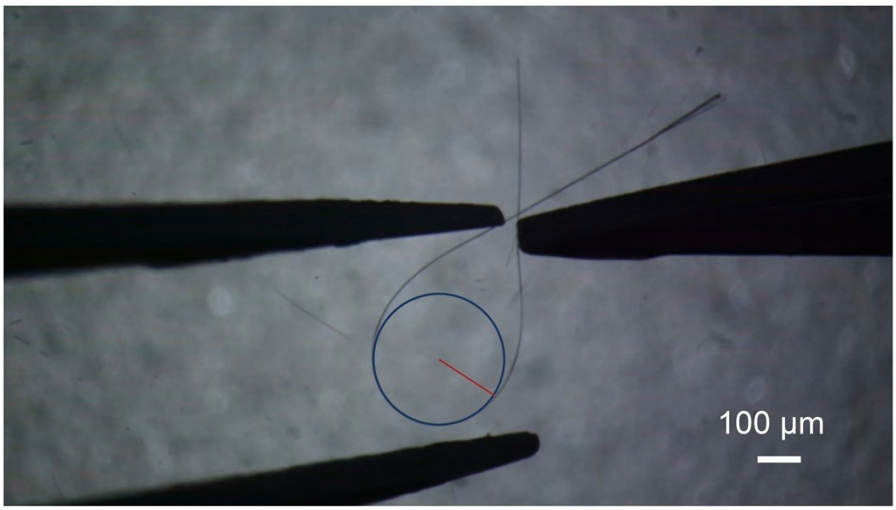

Fig. S4. The bending strain (ε) calculated from ε = h/2R (h is the thickness of single crystal, R is the radius of curvature of the bent crystal) is ca. 2.24%.

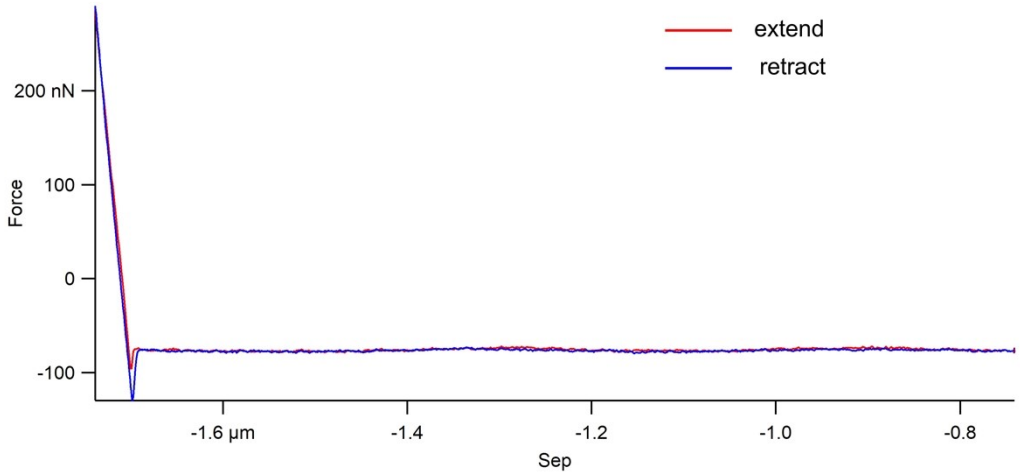

Fig. S5. Force distance curves of **1**. The Young's modulus of compound **1** was determined to be approximately 312 ± 63 MPa, which is close to those of reported elastic single crystals[1, 2].

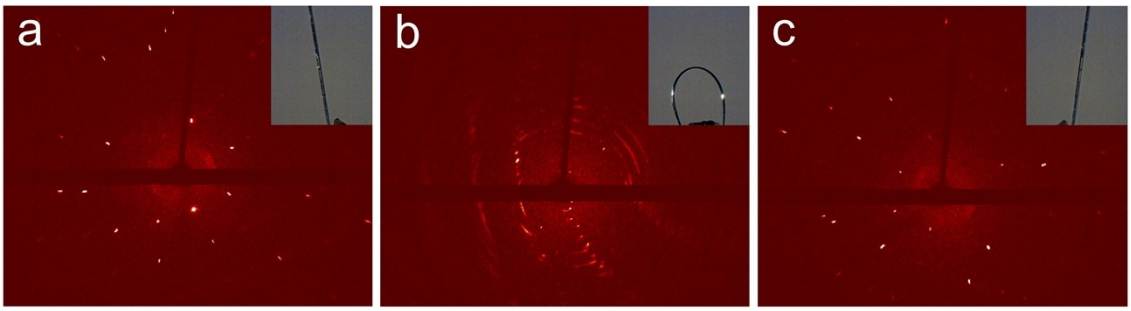

Fig. S6. X-ray diffraction analysis of an elastically bendable crystal of **1**. **a** Straight crystal **1** before bending and its diffraction image. **b** Curved crystal adhering to glass filament **1** and its diffraction image. **c** Recovering mechanically relaxed elongated crystal and its diffraction pattern.

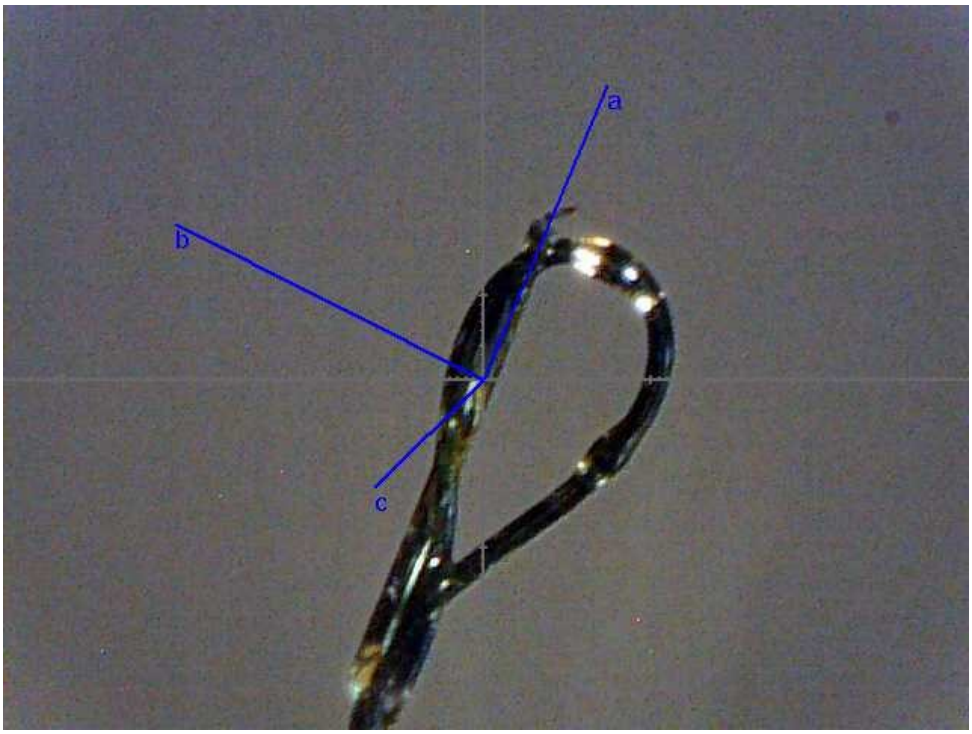

Fig. S7. Crystal morphology with the face indices of compound **1.**

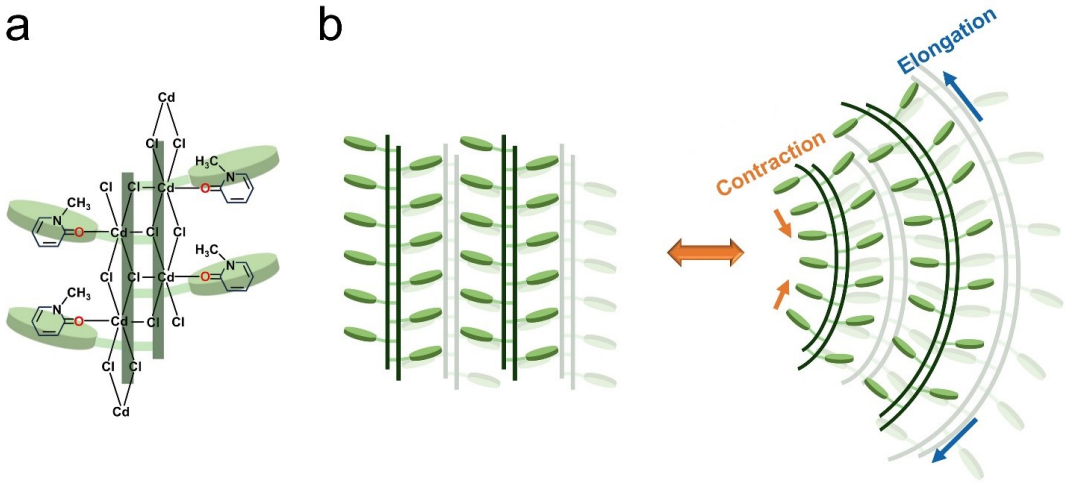

Fig. S8. Molecular mechanism of the elastic bending of **1**. **a** Structural skeleton consisting of a cadmium(II) halide polymer. **b** Structural model of the elastic bending.

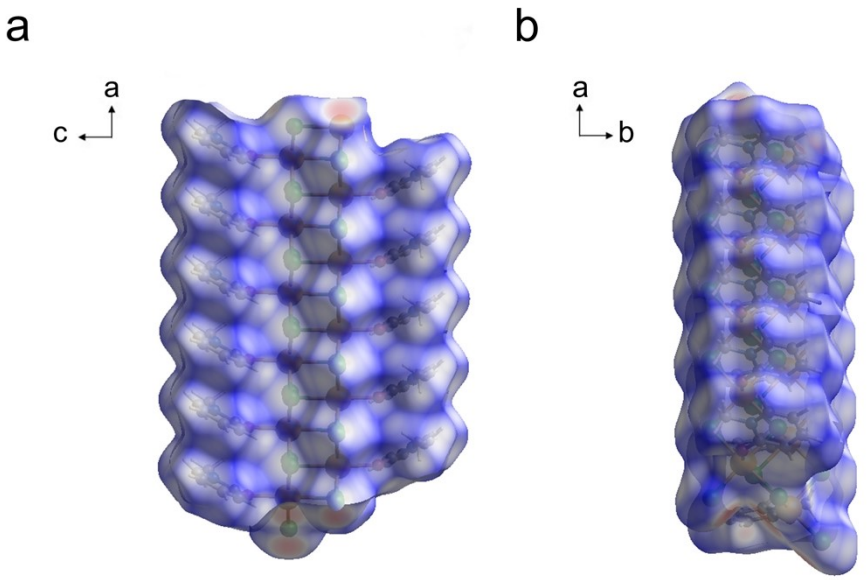

Fig. S9. Hirshfeld surface analyses of individual molecules viewed along the *b* axis (a) and *c* axis (b). Red and blue regions of the surface represent molecular contacts shorter and longer than the van der Waals distance, respectively. The diagram shows the intra-chain interactions in red, which occur along the chain extension direction, and should not be confused with intermolecular interactions.

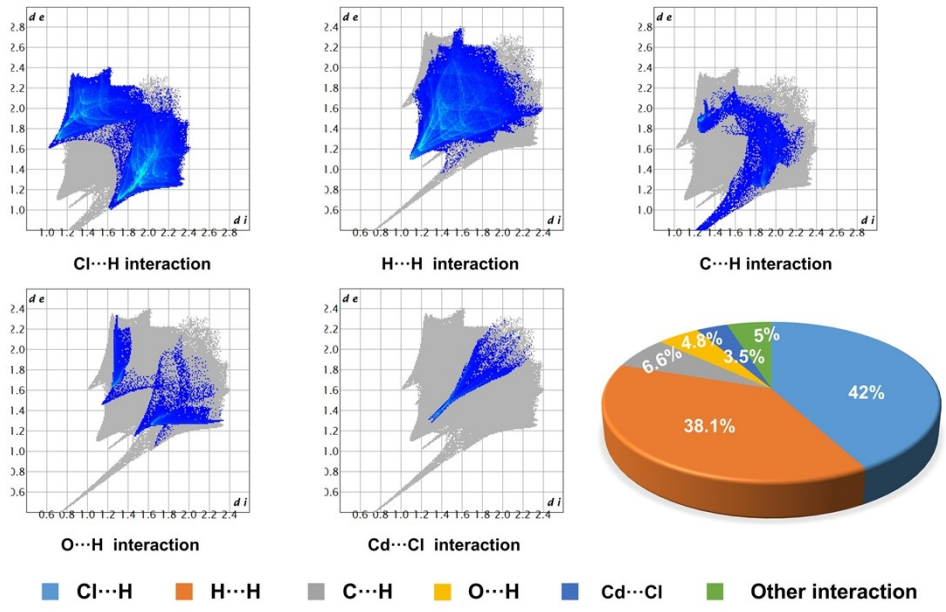

Fig. S10. The fingerprint plots and percentage contribution of intermolecular contacts in compound **1**.

Table S1. Crystal data and structure refinement for compound **1**.

Compound	**1** (*P*-helicity)	**1** (*M*-helicity)
Empirical formula	$C_6H_7CdCl_2NO$	
Formula weight	292.43	
Temperature/K	293	293
Crystal system	orthorhombic	
Space group	$P2_12_12_1$	
a / Å	3.8401(2)	3.8327(2)
b / Å	13.4023(8)	13.3752(6)
c / Å	16.4598(11)	16.4327(8)
α / °	90	90
β /°	90	90
γ / °	90	90
Volume/ Å^3	847.12(9)	842.39(7)
Z	4	4
Dcalc./ g·cm^{-3}	2.293	2.306
μ / mm^{-1}	3.145	3.163
F_{000}	560.0	560.0
2*θ* range /°	4.95 to 60.488	7.858 to 59.542
Index ranges	-4 ≤ h ≤ 4, -18 ≤ k ≤ 13, -21 ≤ l ≤ 20	-4 ≤ h ≤ 5, -18 ≤ k ≤ 17, -21 ≤ l ≤ 20
Reflections collected	7830	7279
Independent reflections	2066 [R_{int} = 0.0453, R_{sigma} = 0.0411]	2141 [R_{int} = 0.0368, R_{sigma} = 0.0357]
Data/restraints/parameters	2066/0/102	2141/0/102
Goodness-of-fit on F^2	1.030	1.039
Final *R* indexes [I>=2σ (I)]	R_1 = 0.0284, wR_2 = 0.0592	R_1 = 0.0243, wR_2 = 0.0481
Final *R* indexes [all data]	R_1 = 0.0396, wR_2 = 0.0627	R_1 = 0.0294, wR_2 = 0.0498
Largest diff. peak/hole / e Å^{-3}	0.61/-0.79	0.49/-0.66
Flack parameter	0.43(8)	0.49(6)
CCDC no.	2343813	2343814

References

1 H. Liu, K. Ye, Z. Zhang, H. Zhang, *Angew. Chem. Int. Ed.*, 2019, **58**, 19081-19086.

2 B. Liu, Z. Lu, B. Tang, H. Liu, H. Liu, Z. Zhang, K. Ye, H. Zhang, *Angew. Chem. Int. Ed.*, 2020, **59**, 23117-23121.