Supporting Information for

1D zigzag chain *vs* 1D helical chain: the role of the supramolecular interactions in the formation of chiral architecture

Fangna Dai,^a Haiyan He,^a Xiaoliang Zhao,^a Yanxiong Ke,^{*b} Guoqing Zhang,^a Daofeng Sun^{*a}

Key Lab for Colloid and Interface Chemistry of Education Ministry, Department of Chemistry, Shandong University, Jinan 250100 (P. R. China), Engineering Research Center of Pharmaceutical Process Chemistry, Ministry of Education, School of Pharmacy, East China University of Science and Technology, 130 Meilong Road, Shanghai 200237, (P. R. China); E-mail:dfsun@sdu.edu.cn; <u>key@ecust.edu.cn</u>.

*To whom correspondence should be addressed

General Information. Commercially available reagents were used as received without further purification. Elemental analyses (C,H,N) were performed with a PerkinElmer 240 elemental analyzer. Thermal gravimetric analysis (TGA) was performed under N_2 on a PerkinElmer TGA 7 instrument. Photoluminescence spectra were performed on a Perkin Elmer LS 50B luminescence spectrometer.

Synthesis of 2 with bulk homochiral crystallization: $H_2atiip (0.02 \text{ g}, 0.04 \text{ mmol})$, $Cd(NO_3)_2 \cdot 4H_2O (0.02 \text{ g}, 0.08 \text{ mmol})$ and (S)-N-(1,2,3,4-tetrahydronaphthalen-1-yl)acetamide (0.01g,0.053mmol) were dissolved in 16 mL mixture of dmf, ethonal and $H_2O (v/v = 5:2:1)$, to which one drop of pyridine was added. The clear solution was allowed to evaporate at 90 ° for two days to give colorless block crystals of **2**.

Crystal structure determination of compound 1 and 2: Single-crystal X-ray diffraction was performed using a Bruker Apex II CCD diffractometer equipped with a fine-focus sealed-tube X-ray source ($Mo_{K\alpha}$ radiation, graphite monochromated). Structures were solved

by direct methods using SHELXTL and were refined by full-matrix least-squares on F^2 using SHELX-97. Non-hydrogen atoms were refined with anisotropic displacement parameters during the final cycles. Hydrogen atoms were placed in calculated positions with isotropic displacement parameters set to $1.2 \times U_{eq}$ of the attached atom.

	-	
	Compound 1	Compound 2
empirical formula	$C_{14}H_8CdI_3N_5O_4$	$C_{14}H_{12}CdI_3N_3O_5$
formula weight	803.35	795.37
temp (K)	298(2)	298(2)
crystal system	Monoclinic	Tetragonal
space group	$P2_{1}/c$	$P4_{3}2_{1}2$
<i>a</i> (Å)	9.701(2)	11.3689(3)
<i>b</i> (Å)	24.227(5)	11.3689(3)
<i>c</i> (Å)	9.861(2)	16.5658(11)
$\alpha(\text{deg})$	90	90
$\beta(\text{deg})$	111.821(4)	90
γ(deg)	90	90
$V(Å^3)$	2151.6(8)	2141.16(16)
Ζ	4	4
ρ calc (g/cm ³)	2.486	2.467
F(000)	1472	1512
data/restraints/params	4889 / 0 / 244	2194/0/125
GOF on F2	1.072	1.053
final R indices $[I \ge 2\phi(I)]$	R1 = 0.1077,	R1 = 0.0383,
	wR2 = 0.2923	wR2 = 0.0986

Table S1. Crystal Data Collection and Structure Refinement for compound 1 and 2

Table S2. A summary of the 10 structure determinations of complex **2** ($P4_32_12$) with the *R* factors and Flack absolute structure parameters for each refinement, after being added chiral (R)-N-(1,2,3,4-tetrahydronaphthalen-1-yl)acetamide as the cosolute.

	а	b	С	<i>R</i> 1	<i>wR</i> 1	Flack
						parameter
2	11.3689(3)	11.3689(3)	16.5658(11)	0.0395	0.1043	0.00(8)
#1	11.3702(10)	11.3702(10)	16.5651(4)	0.0413	0.1137	0.03(8)
#2	11.3687(4)	11.3687(4)	16.5721(15)	0.0492	0.1642	0.07(12)
#3	11.3632(2)	11.3632(2)	16.5725(4)	0.0403	0.1015	0.02(8)
#4	11.3736(10)	11.3736(10)	16.5547(3)	0.0426	0.1082	0.04(8)
#5	11.3672(10)	11.3672(10)	16.5682(4)	0.0386	0.1098	0.04(7)
#6	11.3591(2)	11.3591(2)	16.5835(5)	0.0415	0.1105	0.07(8)
#7	11.3682(10)	11.3682(10)	16.5606(4)	0.0406	0.1118	-0.02(8)
#8	11.3685(10)	11.3685(10)	16.5636(3)	0.0434	0.1105	0.05(8)
#9	11.3702(2)	11.3702(2)	16.5670(5)	0.0497	0.1114	0.04(10)



(R)-N-(1,2,3,4-tetrahydronaphthalen-1-yl)acetamide

Figure S1. (*R*)-N-(1,2,3,4-tetrahydronaphthalen-1-yl)acetamide.



Figure S2. TGA for complexes 1 and 2.



Figure S3. Photoluminescence emission spectra for compound 1 and 2 in the solid state at room temperature.