Electronic Supplementary Material (ESI) for CrystEngComm.

ELECTRONIC SUPPLEMENTARY DATA

for

Temperature-induced one-dimensional chiral Ag(I) linear chain and left-handed 2_1 helix: DFT studies, luminescence and SHG response

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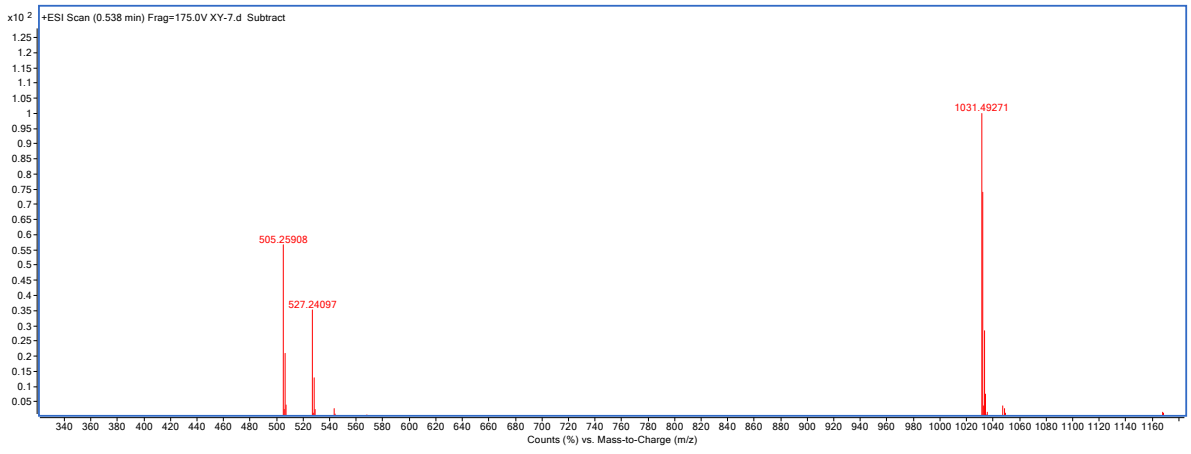
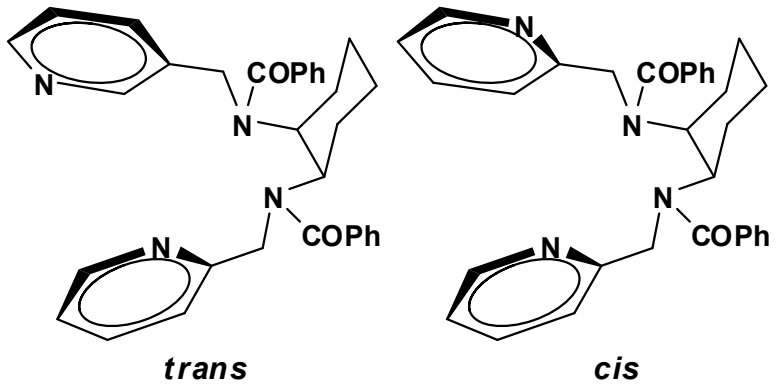
1. Procedure of the synthesis of (1*R*,2*R*)-3-bcpb

The mixture of (1*R*,2*R*)-2,3-pcd (1.48 g, 5 mmol), benzoyl chloride (1.69 g, 11 mmol), triethylamine (0.76 g, 7.5mmol) and toluene (50 mL) was refluxed for 15 hours. Then saturated NaCl solution (50 mL) was added to the cooled reaction. The layers were separated and the organic layer was dried over anhydrous $MgSO_4$, filtered and evaporated to give yellow oils. Water (80 mL) and ether (20 mL) were added to the oils and the mixture was refluxed for 3 hours, then cooled and white solids were precipitated. After washed by water and ether, the white products were collected and dried. Yiled: 54% (1.36 g). Anal. Calcd. (%) for $C_{32}H_{32}N_4O_2$: C 76.16, H 6.39, N 11.10; found: C 76.14, H 6.42, N 11.12. ESI MS: m/z: 505.26 $[M+H]^+$, 527.24 $[M+Na]^+$, 1031.49 $[2M+Na]^+$. ESI-MS spectrum of (1*R*,2*R*)-3-bcpb was shown as the following:





Scheme S1 The *trans*- and *cis*- isomers of (1*R*,2*R*)-3-bcpb.

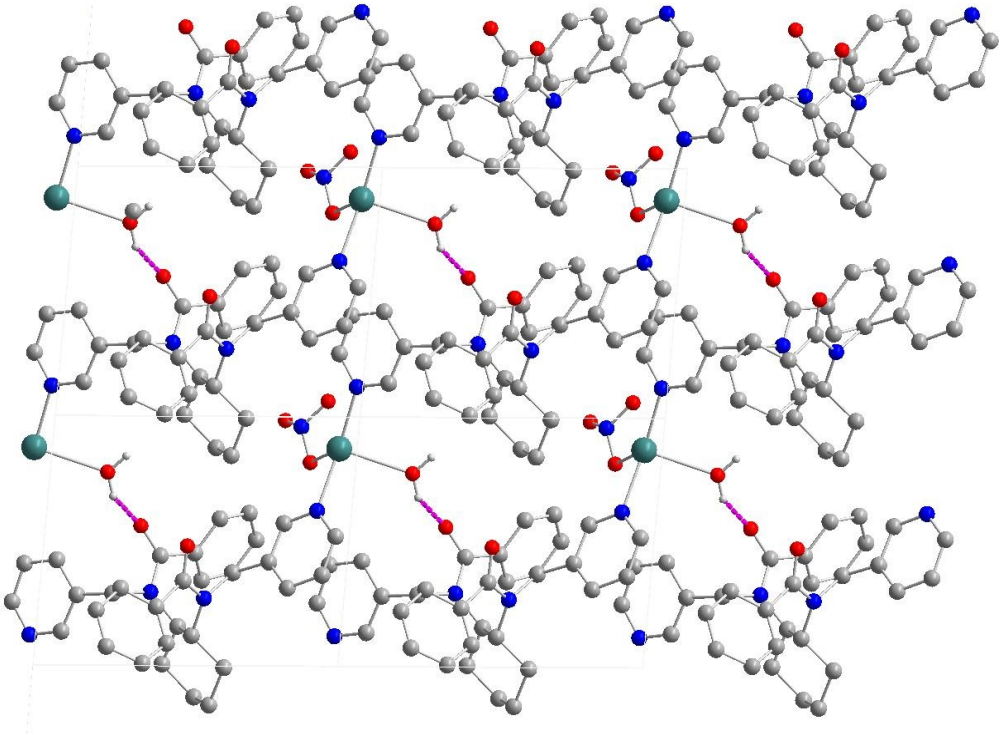


Fig. S1 The 2D hydrogen bonding network along the *ac* plane *via* interchain O-H···O hydrogen bonds in**1a**.

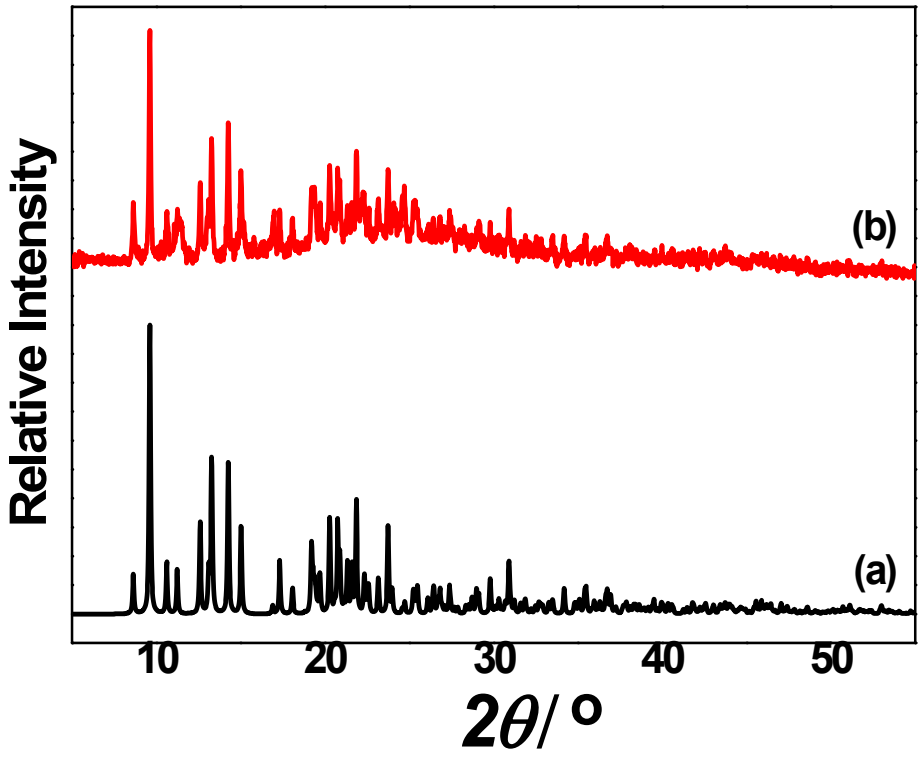


Fig. S2 The XRD patterns of **1a**, simulated from X-ray single crystal data (a) and polycrystalline as newly synthesized (b).

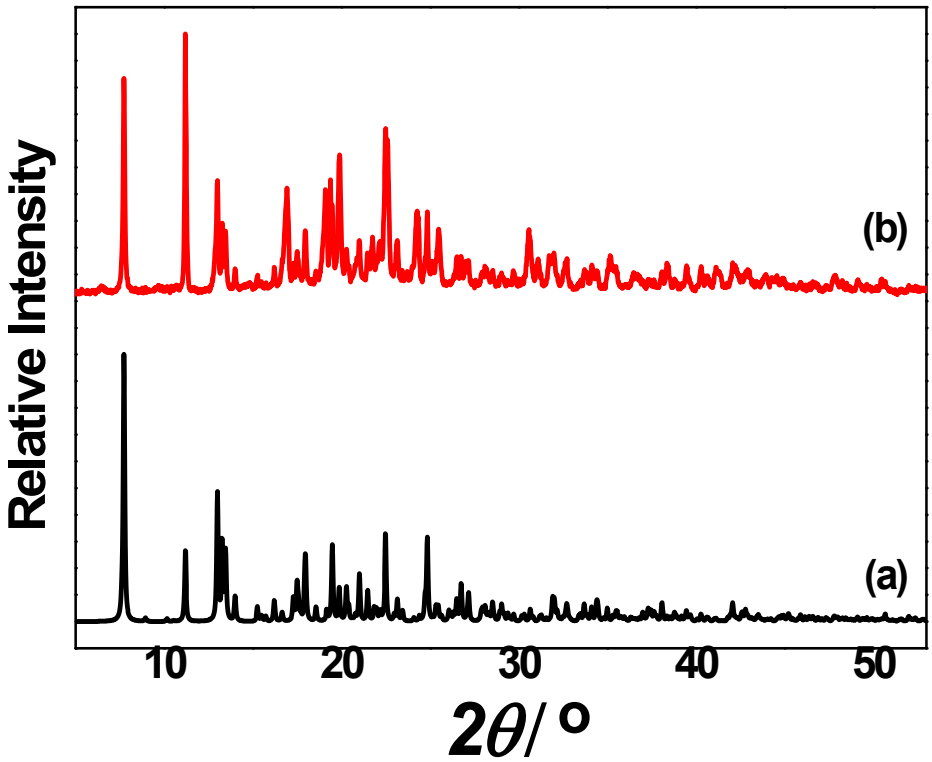


Fig. S3 The XRD patterns of **2a**, simulated from X-ray single crystal data (a) and polycrystalline as newly synthesized (b).

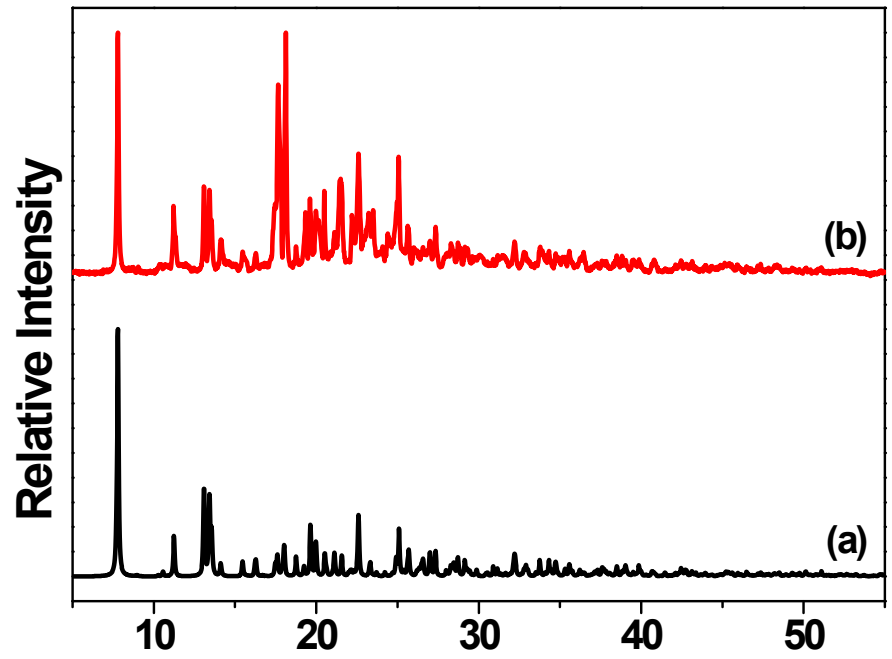


Fig. S4 The XRD patterns of **1b**, simulated from X-ray single crystal data (a) and polycrystalline as newly synthesized (b).

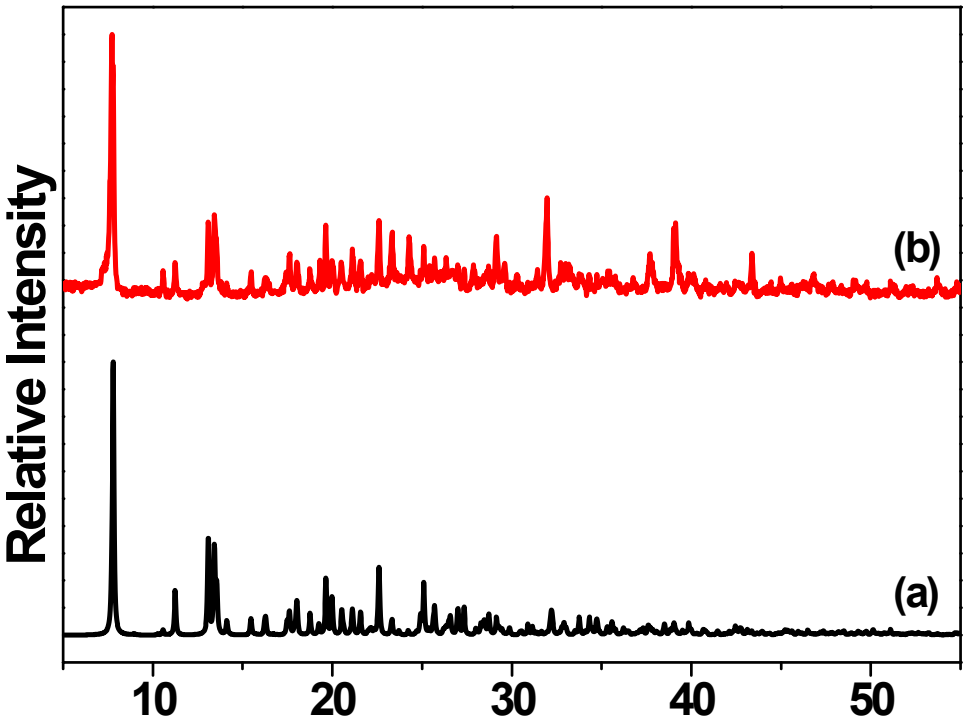


Fig. S5 The XRD patterns of **2b**, simulated from X-ray single crystal data (a) and polycrystalline as newly synthesized (b).

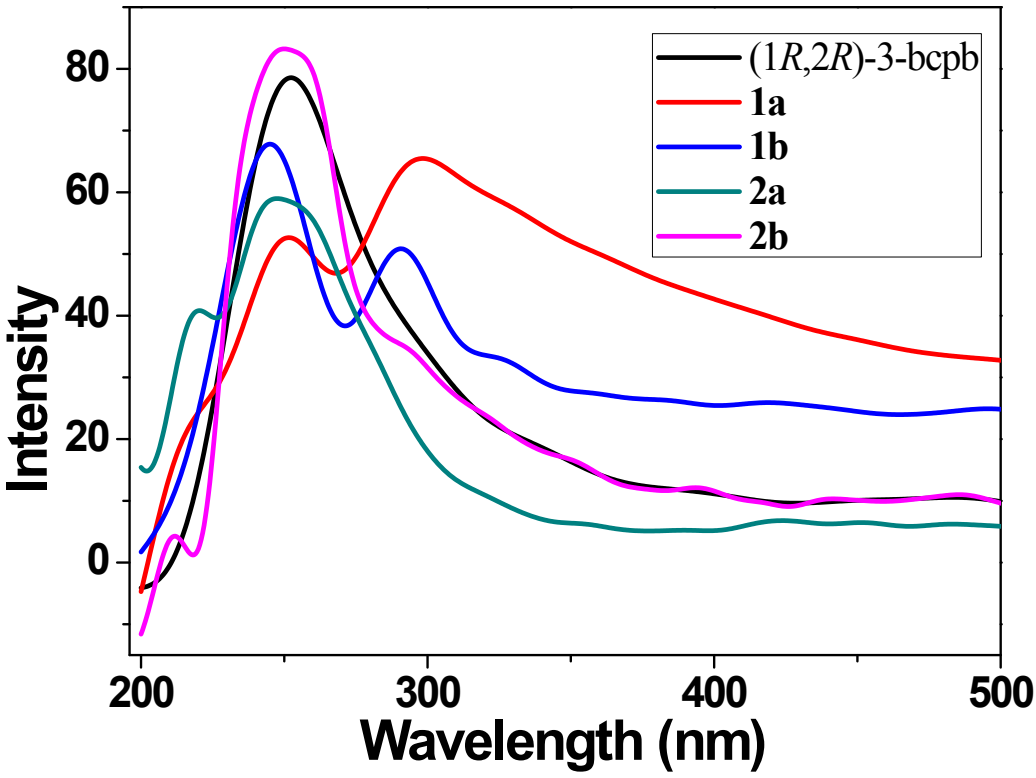


Fig. S6 CD spectra of (1*R*,2*R*)-3-bcpb and the four CCPs in the solid state at room temperature.

Table S1. Selected bond lengths (Å) and angles (°) for **1a**, **2a**, **1b** and **2b**.

		1a	
Ag1-O1W	2.613(8)	Ag1-N1	2.233(11)
Ag1-O5	2.632(13)	Ag1-N4a	2.258(12)
O1W-Ag1-O5	107.1(4)	O5-Ag1-N1	120.8(4)
O1W-Ag1-N1	92.5(4)	O5-Ag1-N4a	84.0(4)
O1W-Ag1-N4a	91.1(3)	N1-Ag1-N4a	152.4(4)
		2a	
Ag1-N1	2.165(5)	Ag1-N4b	2.147(5)
N1-Ag1-N4b	167.55(19)		
		1b	
Ag1-O1W	2.648(9)	Ag1-N4b	2.171(11)
Ag1-N1	2.193(12)	O1W-Ag1-N1	93.3(4)
O1W-Ag1-N4b	94.7(4)	N1-Ag1-N4b	160.5(4)
		2b	
Ag1-N1	2.181(10)	Ag1-N4a	2.147(9)
N1-Ag1-N4a	168.6(4)		

Symmetry code for **1a**: a, -1+x, y, -1+z; for **2a**: b, 5/2-x, 1-y, 1/2+z; for **1b**: b, 1+x, y, 1+z; for **2b**: a, -3/2-x, -1-y, -1/2+z.

Table S2. Selected Hydrogen Bond Lengths (Å) and Bond Angles (º) of **1a**, **2a**, **1b** and **2b**. (D, donor atom; A, acceptor atom).

D-H···A	D-H [Å]	H···A [Å]	D···A [Å]	D-H···A [º]]
		1a		
O1W-H1WB···O1d	0.85	2.16	2.822(13)	135
		2a		
O1W-H1WB···O2W	0.85	1.88	2.73(3)	174
O2W-H2WA···O3r	0.80	2.45	3.25(2)	176
O2W-H2WB···O3Ws	0.80	1.96	2.75(4)	167
O3W-H3WA···O1	0.80	1.98	2.77(3)	171
O3W-H3WB···O1W	0.70	2.45	2.86(4)	120
		1b		
O1W-H1WA···O2d	0.85	1.98	2.835(14)	179
O7-H7B···O1W	0.90	2.28	2.752(14)	113
		2b		
O1W-H1WA···O2	0.85	2.20	3.049(18)	179
O1W-H1WB···O2Ws	0.85	2.08	2.93(3)	177
O2W-H2WA···O3W	0.85	2.29	3.11(3)	161
O2W-H2WB···O4c	0.85	2.28	3.13(3)	178
O2W-H2WB···O6c	0.85	2.51	3.10(2)	128
O3W-H3WB···O1W	0.85	2.33	3.18(3)	179

Symmetry code for **1a**: d, -1+x, y, z. for **2a**: r, 7/2-x, 2-y, -1/2+; s, 1/2+x, 3/2-y, 1-z. for **1b**: d, x, y, 1+z. for **2b**:c, -1/2+x, -1/2-y, -z; s, -1/2+x, -3/2-y, -z.