

## Supporting Information

### **Solvent-dependent assemblies, structure diversities and magnetic properties of two homochiral Co(II)/Na(I) coordination polymers**

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**Table S1** Selected bond lengths (Å) and angles (°) for **S-1** and **S-2**

<b>S-1</b>			
Co1—O4	2.069 (2)	Na1—O1	2.659 (3)
Co1—O7	2.065 (2)	Na1—O7 <sup>i</sup>	2.697 (4)
Co1—O1	2.089 (2)	Na1—O2 <sup>ii</sup>	2.828 (4)
Co1—O6	2.087 (2)	O2—Na1 <sup>iii</sup>	2.828 (4)
Co1—O5	2.114 (2)	O7—Na1 <sup>iv</sup>	2.697 (4)
Co1—N1	2.165 (3)		
O4—Co1—O7	179.04 (11)	C2—O1—Co1	116.2 (2)
O4—Co1—O1	91.79 (11)	C2—O1—Na1	126.1 (2)
O7—Co1—O1	87.81 (10)	Co1—O1—Na1	116.38 (13)
O4—Co1—O6	89.98 (10)	C2—O2—Na1 <sup>iii</sup>	110.0 (2)
O7—Co1—O6	89.33 (11)	C4—O4—Co1	116.7 (2)
O1—Co1—O6	109.42 (10)	C6—O5—Co1	113.6 (2)
O4—Co1—O5	92.88 (11)	Co1—O7—Na1 <sup>iv</sup>	122.49 (12)
O7—Co1—O5	87.81 (10)	O5—Co1—N1	79.83 (10)
O1—Co1—O5	157.16 (10)	O1—Na1—O7 <sup>i</sup>	122.76 (13)
O6—Co1—O5	92.93 (10)	O1—Na1—O2 <sup>ii</sup>	101.00 (12)
O4—Co1—N1	81.29 (9)	O7 <sup>i</sup> —Na1—O2 <sup>ii</sup>	114.90 (14)
O7—Co1—N1	99.49 (11)	C3—N1—Co1	108.06 (19)
O1—Co1—N1	78.82 (10)	C1—N1—Co1	106.05 (19)
O6—Co1—N1	168.29 (10)	C5—N1—Co1	103.8 (2)

Symmetry codes: (i)  $x-1, y, z$ ; (ii)  $-x, y+1/2, -z+3/2$ ; (iii)  $-x, y-1/2, -z+3/2$ ; (iv)  $x+1, y, z$ .

<b>S-2</b>			
Co1—O1	2.050 (2)	Na1—O3	2.625 (4)

Co1—O4 <sup>i</sup>	2.075 (2)	Na1—O5 <sup>ii</sup>	2.722 (4)
Co1—O2	2.090 (2)	Na1—O4 <sup>iii</sup>	2.901 (4)
Co1—O3	2.095 (2)	O4—Co1 <sup>iv</sup>	2.075 (2)
Co1—O6	2.151 (2)	O4—Na1 <sup>v</sup>	2.901 (4)
Co1—N1	2.169 (3)	O5—Na1 <sup>vi</sup>	2.722 (4)
O1—Co1—O4 <sup>i</sup>	93.82 (9)	C1—N1—Co1	107.0 (2)
O1—Co1—O2	95.28 (10)	C6—N1—Co1	105.06 (19)
O4 <sup>i</sup> —Co1—O2	96.63 (9)	C3—N1—Co1	105.75 (19)
O1—Co1—O3	89.63 (10)	C2—O1—Co1	116.1 (2)
O4 <sup>i</sup> —Co1—O3	104.17 (9)	C9—O2—Co1	115.7 (2)
O2—Co1—O3	158.26 (9)	C4—O3—Co1	111.9 (2)
O1—Co1—O6	176.52 (11)	C4—O3—Na1	103.9 (2)
O4 <sup>i</sup> —Co1—O6	86.07 (10)	Co1—O3—Na1	120.75 (12)
O2—Co1—O6	88.19 (10)	C9—O4—Co1 <sup>iv</sup>	124.7 (2)
O3—Co1—O6	87.02 (10)	C9—O4—Na1 <sup>v</sup>	115.4 (2)
O1—Co1—N1	81.57 (9)	Co1 <sup>iv</sup> —O4—Na1 <sup>v</sup>	102.87 (11)
O4 <sup>i</sup> —Co1—N1	172.88 (10)	C2—O5—Na1 <sup>vi</sup>	113.1 (2)
O2—Co1—N1	78.49 (9)	O3—Na1—O5 <sup>ii</sup>	116.90 (13)
O3—Co1—N1	81.32 (10)	O3—Na1—O4 <sup>iii</sup>	130.17 (13)
O6—Co1—N1	98.87 (10)	O5 <sup>ii</sup> —Na1—O4 <sup>iii</sup>	105.46 (12)

Symmetry codes: (i)  $-x+2, y-1/2, -z+1/2$ ; (ii)  $x-1/2, -y+1/2, -z$ ; (iii)  $x, y-1, z$ ; (iv)  $-x+2, y+1/2, -z+1/2$ ; (v)  $x, y+1, z$ ; (vi)  $x+1/2, -y+1/2, -z$ .

**Table S2** Bond lengths (Å) and angles (°) of hydrogen bonds for **S-1**

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O6-H6C $\cdots$ O3 <sup>iii</sup>	0.90	2.25	2.7993	119
O6-H6D $\cdots$ O2 <sup>ii</sup>	0.90	2.16	2.7498	122
O7-H7D $\cdots$ O3 <sup>i</sup>	0.90	2.14	2.7148	121

Symmetry codes: (i)  $1/2-x, -y, 1/2+z$ ; (ii)  $-x, 1/2+y, 3/2-z$ ; (iii)  $1/2+x, 1/2-y, 1-z$ .

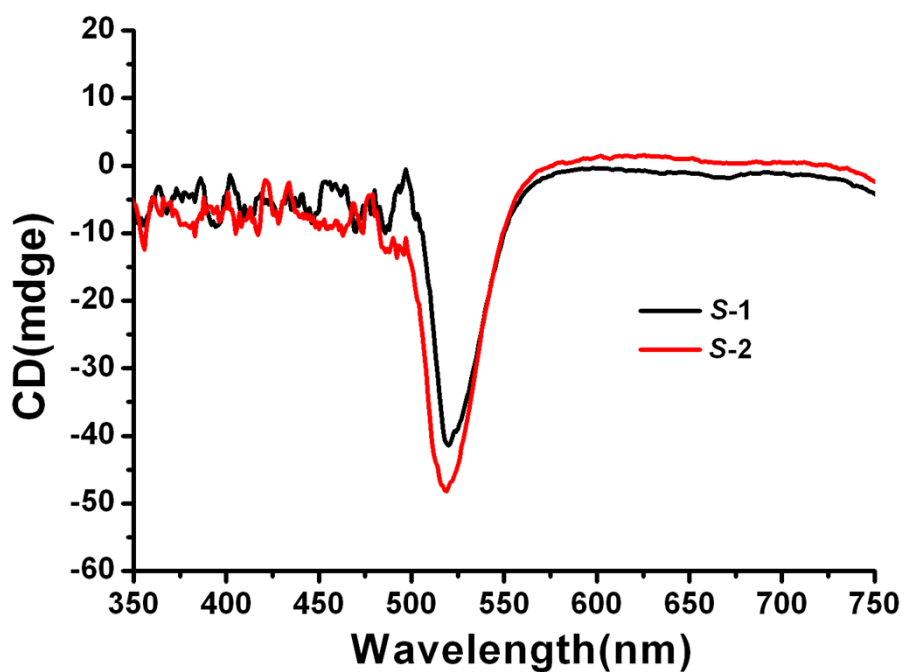


Fig. S1 The solid-state CD spectra of *S-1* and *S-2*.

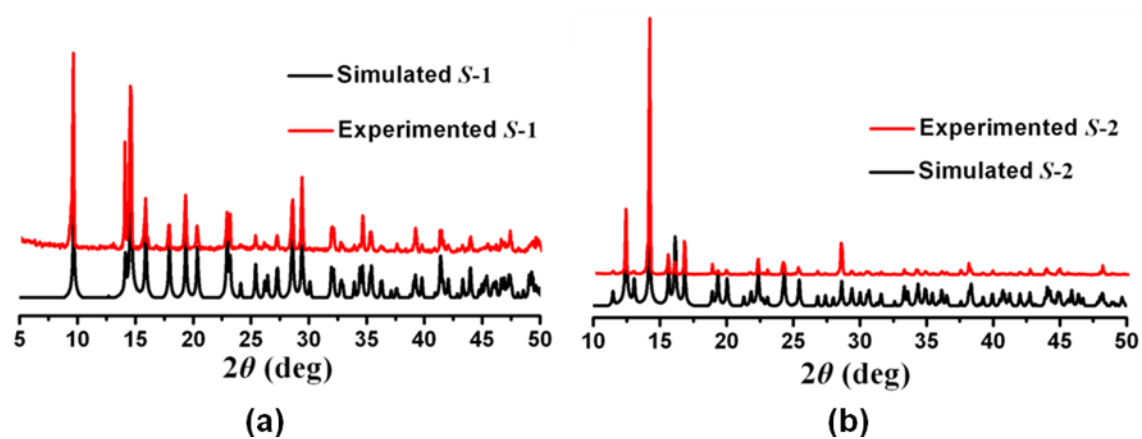


Fig. S2 X-ray powder diffraction (XRPD) patterns of *S-1* and *S-2*

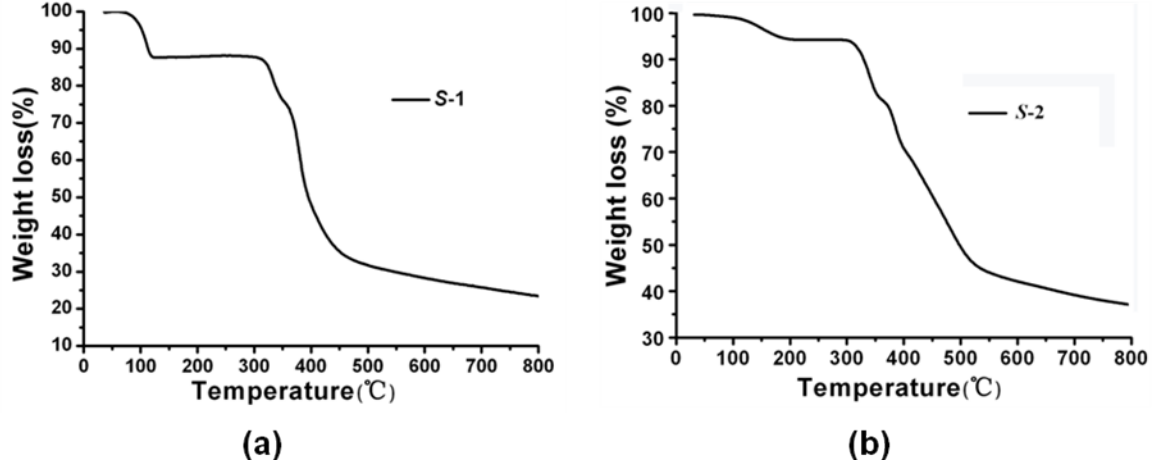


Fig. S3 View of the TGA curves of S-1 and S-2

For S-1:

$$\hat{H} = D \left[ \hat{S}_z^2 - \frac{1}{3} S(S+1) \right] + g_{\parallel} \beta H_z S_z + g_{\perp} \beta (H_x S_x + H_y S_y)$$

The expressions of the molar magnetic susceptibility ( $\chi_m$ ) can be derived from the above Hamiltonian, where N is Avogadro's number,  $\beta$  is the Bohr magneton,  $k$  is Boltzmann's constant,  $g$  is the Landé g-factor and  $D$  is the zero-field splitting.

$$\chi_{\parallel} = \frac{N g_{\parallel}^2 \beta^2}{kT} \times \frac{1 + 9e^{-2D/kT}}{4(1 + e^{-2D/kT})}$$

$$\chi_{\perp} = \frac{N g_{\perp}^2 \beta^2}{kT} \times \frac{4 + (3kT / D)(1 - e^{-2D/kT})}{4(1 + e^{-2D/kT})}$$

$$\chi_m = \frac{\chi_{\parallel} + 2\chi_{\perp}}{3}$$