

## Supplementary information

### Self-assembly of Ag(I) helicates with new enantiopure 5,6-Chiragen type ligands

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**Table S1** Crystal data, data collection and structure refinement details of **[Ag(L1)]**

	[Ag(L1)]
Crystal data	
Chemical formula	5(C <sub>46</sub> H <sub>44</sub> N <sub>4</sub> )·5Ag·5(BF <sub>4</sub> )·1.5(CH <sub>3</sub> NO <sub>2</sub> ) n[solvent]
<i>M</i> <sub>r</sub>	4329.21
Crystal system, space group	Monoclinic, <i>P</i> 2 <sub>1</sub>
Temperature (K)	153
<i>a</i> , <i>b</i> , <i>c</i> (Å)	17.2792 (10), 32.478 (3), 22.9158 (15)
β (°)	91.748 (8)
<i>V</i> (Å <sup>3</sup> )	12854.2 (16)
<i>Z</i>	2
Radiation type	Mo <i>K</i> α
μ (mm <sup>-1</sup> )	0.45
Crystal size (mm)	0.45 × 0.30 × 0.25
Data collection	
Diffractometer	STOE <i>IPDS</i>
Absorption correction	–
No. of measured, independent and observed [ <i>I</i> > 2σ( <i>I</i> )] reflections	98336, 49056, 7570
<i>R</i> <sub>int</sub>	0.169
(sin θ/λ) <sub>max</sub> (Å <sup>-1</sup> )	0.619

Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.092, 0.258, 0.63
No. of reflections	49056
No. of parameters	1046
No. of restraints	4
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\max}, \Delta\rho_{\min}$ (e $\text{\AA}^{-3}$ )	0.56, -0.56
Absolute structure	Flack, H. D. (1983). Acta Cryst. A39, 876-881
Absolute structure parameter	0.13 (4)

**Table S2.** Crystal data, data collection and structure refinement details for ligand **L2**

<b>L2</b>	
Crystal data	
CCDC 1559363	
Chemical formula	$\text{C}_{48}\text{H}_{46}\text{N}_4$
$M_r$	678.89
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	223
$a, b, c$ ( $\text{\AA}$ )	10.6918 (6), 12.5012 (7), 29.144 (2)
$V$ ( $\text{\AA}^3$ )	3895.3 (4)
$Z$	4
Radiation type	Mo $K\alpha$
$\mu$ ( $\text{mm}^{-1}$ )	0.07
Crystal size (mm)	0.60 $\times$ 0.20 $\times$ 0.10
Data collection	
Diffractometer	STOE Image Plate Diffraction System
Absorption correction	–
No. of measured, independent	23287, 7516, 3536

and observed [ $I > 2\sigma(I)$ ] reflections	
$R_{\text{int}}$	0.063
$(\sin \theta/\lambda)_{\text{max}}$ ( $\text{\AA}^{-1}$ )	0.616
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.037, 0.080, 0.72
No. of reflections	7516
No. of parameters	474
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ ( $e \text{\AA}^{-3}$ )	0.12, -0.13
Absolute structure	The absolute structure of <b>L2</b> could not be determined by resonant scattering.

Computer programs: *EXPOSE* (Stoe IPDS Software, 2000), *CELL* (Stoe IPDS Software, 2000), *INTEGRATE* (Stoe IPDS Software, 2000), *SHELXS97* (Sheldrick, 2008), *Mercury* (Macrae *et al.*, 2008), *SHELXL97* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

#### References:

Stoe & Cie. (2000). *Stoe IPDS Software*. Stoe & Cie GmbH, Darmstadt, Germany.

G. M. Sheldrick, *Acta Cryst.*, 2008, A64, 112-122.

C. F. Macrae, I. J. Bruno, J. A. Chisholm, P. R. Edgington, P. McCabe, E. Pidcock, L. Rodriguez-Monge, R. Taylor, J. van de Streek & P. A. Wood, *J. Appl. Cryst.*, 2008, 41, 466-470.

A. L. Spek, *Acta Cryst.*, 2009, D65, 148-155.

**Figure S1.** Perspective view parallel to the C5 helical axis of the *P* polymeric mono-stranded helicate  $[\text{Ag}(\text{L1})]_{\infty}^{+}$ .

