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	$5(C_{46}H_{44}N_4)\cdot 5Ag\cdot 5(BF_4)\cdot 1.5(CH_3NO_2)$ n[solvent]
M_r	4329.21
Crystal system, space group	Monoclinic, $P2_1$
Temperature (K)	153
a, *b*, *c* (Å)	17.2792 (10), 32.478 (3), 22.9158 (15)
β (°)	91.748 (8)
V (Å^3)	12854.2 (16)
Z	2
Radiation type	Mo *K*α
μ (mm^{-1})	0.45
Crystal size (mm)	0.45 × 0.30 × 0.25
Data collection	
Diffractometer	STOE *IPDS*
Absorption correction	–
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	98336, 49056, 7570
R_{int}	0.169
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	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 Å^{-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**

	L2
Crystal data	
CCDC 1559363	
Chemical formula	$C_{48}H_{46}N_4$
M_r	678.89
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	223
a, *b*, *c* (Å)	10.6918 (6), 12.5012 (7), 29.144 (2)
V (Å^3)	3895.3 (4)
Z	4
Radiation type	Mo *K*α
μ (mm^{-1})	0.07
Crystal size (mm)	0.60 × 0.20 × 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_{int}	0.063
$(\sin \theta/\lambda)_{max}$ (Å^{-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
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.12, −0.13
Absolute structure	The absolute structure of **L2** 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 [Ag (**L1**)] $_{\infty}^{+}$.