The ‘Trinity’ helix: Synthesis and structural characterisation of a $C_3$-symmetric tris-bidentate ligand and its coordination to Ag(I).

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Figure ESI 1: Crystal structure of L. H-atoms and toluene molecule removed for clarity.

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The ligand forms an elaborate 3D H-bonded network involving at least three different modes of interaction as described below. Additional ‘weaker’ interactions (C-H⋯π type) are omitted here and will be described in a subsequent publication.

A H-bond interaction between a central aromatic ring hydrogen to an adjacent pyridyl nitrogen links two arms:
H6c⋯N3c 2.580 Å, < C6c–H6c⋯N3c 155°; symmetry code 1 - x, 1 - y, 1 - z).

H-bonding between an imino hydrogen and pyridyl nitrogen links these units together forming a 2D sheet:
H7b⋯N3b 2.678 Å, < C7b–H7b⋯N3b 163°; symmetry code 1 - x, 1 - y, 1 - z).
A H-bond interaction between a central aromatic ring hydrogen to an adjacent pyridyl nitrogen links the sheets into 3D: H3a⋯N3b 2.611 Å, < C3a–H3a⋯N3b 144°; symmetry code - x, - y, 2 -z).

Disordered toluene molecules (not shown) occupy channels.

Figures generated with Mercury 1.1.2, CCDC: www.ccdc.cam.ac.uk/mercury/
Figure ESI 3: Electrospray Mass Spectrum of [Ag₃L₂](PF₆)₃

(a) The ESMS of [Ag₃L₂](PF₆)₃ from MeCN/CHCl₃ solutions showing the parent ion, [Ag₃L₂]⁺⁺⁺ (iii), centred around m/z 479.762. Note the absence of peaks accounting for any other M:L stoichiometry. Peaks (i) and (ii) are fragmentation products.

Peak (i) at 383.08 m/z is assigned to fragmentation product resulting on loss of a pyridyl unit generating L', where L' = C₃₀H₂₄N₆, to give [Ag₂(MeCN)₂L']⁺⁺⁺. (Calc. m/z for [Ag₂C₃₄H₃₀N₈]^{2+} = 383.02)

Peak (ii) at 427.56 m/z is assigned to the fragmentation product that results on loss of L and Ag(I) to give [Ag₂(MeCN)₃L]⁺⁺⁺. (Calc. m/z for [Ag₂C₄₀H₃₃N₉]^{2+} = 427.75)

(b) The theoretical mass and isotopic peak pattern (top) compared with the experimentally found mass and isotopic peak pattern (bottom) for [Ag₃L₂]^{3+} i.e. [Ag₃C₇₂H₅₄N₁₄]^{3+}
Figure ESI 4: Molecular models of (a) rac-[Ag₃L₂]³⁺ and (b) meso-[Ag₃L₂]³⁺

(a) rac-[Ag₃L₂]³⁺ showing the helical nature of the complex. Note how each ligand ‘arm’ crosses over the Ag-Ag axis. The Λ-enantiomer is shown.

(b) meso-[Ag₃L₂]³⁺ showing both the helical nature of the complex as indicated by the arrow, and the non-helical nature as indicated by the crossed arrows. Note how only one ligand ‘arm’ (from each ligand) crosses over the Ag-Ag axis. Irrespectively, the ‘meso’- isomer must always retain a helical strand.

The models were generated using ISIS Draw version 2.1.1 (MDL Information Systems) and the geometries optimised using Hyperchem version 7.0 (Hypercube Inc.).