Electronic Supplementary Information

Rational ligand design for metal ion recognition. Synthesis of a N-benzylated N$_2$S$_3$-donor macrocycle for enhanced silver(I) discrimination

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X-ray structure determination

The structure shows some edge to face π-π stacking present in the lattice between the C(27)-containing ring and the C(5)-containing ring in adjacent molecules; exemplified by a H(27) – C(6) distance of 2.75 Å.

Data for [Ag(2)]PF$_6$·MeCN were collected at 150(2) K ω scans to approximately 56° 2θ using a Bruker SMART 1000 diffractometer employing graphite-monochromated Mo-Kα radiation generated from a sealed tube (0.71073 Å). Data integration and reduction were undertaken with SAINT and XPREP$^1$ and subsequent computations were carried out using the WinGX-32 graphical user interface.$^2$ The structure was solved by direct methods using SIR97$^3$ Multi-scan
empirical absorption corrections were applied to data set using the program SADABS. Data were refined and extended with SHELXL-97. Non-hydrogen atoms were refined anisotropically. Carbon-bound hydrogen atoms were included in idealised positions and refined using a riding model. An ORTEP depiction of the crystal structures are provided below.

References


