

Electronic Supplementary Information

An unprecedented bridging $[\text{Ag}_2(\text{NO}_3)_6]^{4-}$ anion as a component of an infinite silver(I) molecular ladder incorporating a dinuclear cationic silver complex of a bis-dipyridylamine ligand

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DFT Calculations

Additional detail: Pseudopotentials were used for the silver ions in order to reduce the electronic basis functions and hence the amount of computational effort required. With unconstrained coordinates, a geometric optimization led to an increasing silver-silver distance and a more “in-plane” bonding of the silver ions; this is not comparable with the X-ray structural data and hence the atomic coordinates were fixed and the electronic structure was optimized using single-point calculations.

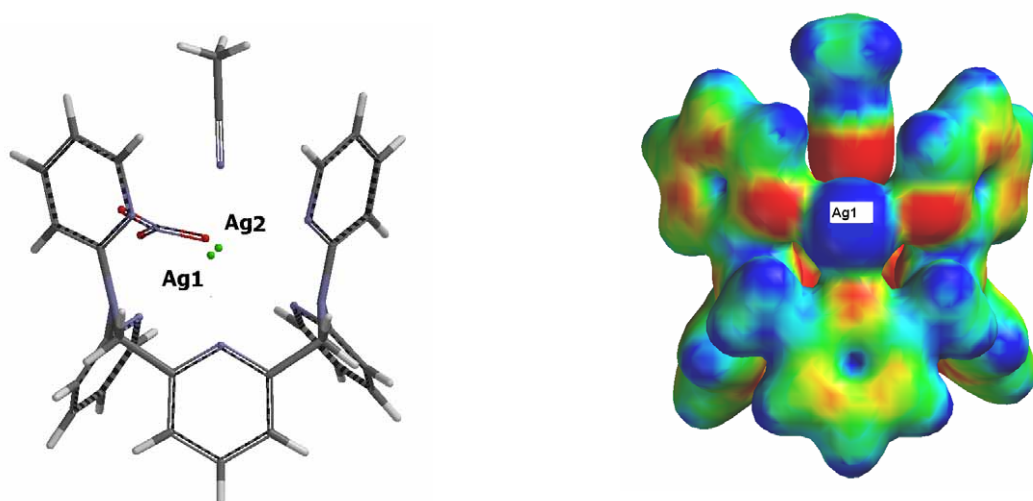


Fig. 1S. Isosurface for 98% of the electronic density of the cationic part of the structure orientated along the Ag(1)-Ag(2) axis. Colours indicate the positive electrostatic potential (red: 80 – blue: 140 kcal/mol). The oxygen of the bridging nitrate bound to Ag(1) is not shown.

The Ag(1) atom in Fig. 1S is shown as three coordinate, but this is an artefact caused by the separation of the structure into two parts. Even so, the mapping the potential of the

electronic density for the structure revealed a high positive value for the vacant tetrahedral position of Ag(1) and is hence consistent with the X-ray structure, where this silver ion is coordinated at this point with the oxygen of a bridging nitrate molecule.