# metal-organic papers

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#### Key indicators

Single-crystal X-ray study T = 298 K Mean  $\sigma$ (C–C) = 0.007 Å Disorder in main residue R factor = 0.052 wR factor = 0.116 Data-to-parameter ratio = 13.4

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

# *catena*-Poly[[nitratosilver(I)]-*µ*-2,2'-dithiobis(5-nitropyridine)]

In the title compound,  $[Ag(NO_3)(C_{10}H_6N_4O_4S_2)]_n$ , the Ag<sup>+</sup> cation has a five-coordinate environment completed by two N and two S atoms of the 2,2'-dithiobis(5-nitropyridine) ligand and by one O atom from the nitrate group. The Ag coordination geometry is best described as distorted trigonal-bipyramidal. The material is composed of one-dimensional extended polymeric chains in which the 2,2'-dithiobis(5-nitropyridine) ligand bridges Ag atoms.

### Comment

The propensity for  $d^{10}$  Ag<sup>+</sup> cations to form coordination complexes with a variety of ligands, such as those containing N, O and S donors, has been widely studied (Buchholz et al., 1996; Amoroso et al., 1995; Michaelides et al., 1995). Many factors, such as the nature of the ligands, solvents and anions, appear to influence the stereochemistry and stoichiometry of Ag<sup>+</sup> compounds. We report here the crystal structure of the title compound, (I). It crystallizes as yellow needles, which were found to be stable to air and light. The molecular dimensions of the 2,2'-dithiobis(5-nitropyridine) ligand are within normal ranges (Allen et al., 1987). The Ag<sup>+</sup> cation is bonded to two N and two S atoms belonging to two different ligands (Table 1). The coordination geometry of the Ag<sup>+</sup> cation is best described as distorted trigonal-bipyramidal with N2, N3 and O7 in the equatorial plane and the Ag<sup>+</sup> cation displaced from it by 0.382 (3) Å. The trigonal bipyramid is completed by two long axial distances provided by the Ag-S bonds.



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The capacity of both sulfur non-bonded electron pairs in a thioether to bridge Ag<sup>+</sup> cations has been reported (Küppers *et al.*, 1987; Blake *et al.*, 1993; Clarkson *et al.*, 1987; Norén &

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### Figure 1

Part of the polymeric structure and the atom-numbering scheme of the title compound. Displacement ellipsoids are shown at the 30% probability level and H atoms have been omitted for clarity. [Symmetry codes: (i) x - 1, y, z; (ii) x + 1, y, z.]



#### Figure 2

Part of the structure of (I) showing the one-dimensional chain viewed along the *c* axis [symmetry code: (i) x - 1, y, z].



#### Figure 3

A different chain of silver (I) cations, in a zigzag fashion, viewed along the *a* axis [symmetry code: (iii)  $x, -y + \frac{3}{2}, z + \frac{1}{2}$ ].

Oskarsson, 1984). In our case, the disulfide S atoms coordinate with one electron pair each of the 2,2'-dithiobis(5-nitropyridine) unit, giving rise in the crystal structure to an infinite one-dimensional chain  $[Ag-ONO_2(C_{10}H_6N_4O_4S_2)]_n$ , along the [100] direction (Fig. 2). In this polymeric chain the Ag<sup>+</sup> cations are situated in an almost linear fashion, as shown by the torsion angle of  $Ag-S1-S2-Ag^i = -167.25$  (4)° [symmetry code: (i) -1 + x, y, z; Fig. 2]. In the same direction a different chain of nitrate-bridged  $Ag^+$  cations forms a zigzag arrangement (Fig. 3). In this case  $Ag^+$  cations are bridged by means of a weak  $O \cdots Ag^+$  intermolecular interaction between atom O5, belonging to a nitrate group coordinated *via* O7 to the original metal cation, and the corresponding glide-transformed  $Ag^+$  cation  $[O5\cdots Ag = 2.898$  (6) Å]. The crystal packing of (I) is governed by three  $C-H\cdots O$  interactions (Table 2). In addition, crystalline cohesion is ensured by numerous van der Waals contacts, the shortest being O6B- $N1^{iii}$  of 2.824 (2) Å [symmetry code: (iii)  $x, -y + \frac{3}{2}, z - \frac{1}{2}]$ .

## **Experimental**

A mixture of 2,2'-dithiobis(5-nitropyridine) (1 mmol, 0.310 g) and silver nitrate (1 mmol, 0.170 g) in acetonitrile (80 ml) was refluxed for 8 h. After slow cooling of the reaction system to room temperature, yellow needle-shaped crystals of (I) were formed that were filtered off and washed with cold ethanol.

#### Crystal data

N a b

$D_x = 480.21$ Monoclinic, $P2_1/c$ $D_x = 2.187 \text{ Mg m}^{-3}$ Mo $K\alpha$ radiation	
Aonoclinic, $P2_1/c$ Mo K $\alpha$ radiation	
±'	
$= 5.9734 (8) \text{ Å} \qquad \mu = 1.72 \text{ mm}^{-1}$	
= 24.911 (3)  Å $T = 298 (2)  K$	
= 9.8107 (13) Å Block cut from a needle, yello	эw
$B = 92.709 \ (2)^{\circ}$ $0.45 \times 0.25 \times 0.19 \ \text{mm}$	
$V = 1458.2 (3) \text{ Å}^3$	

#### Data collection

Bruker SMART CCD area-detector<br/>diffractometer10449 measured reflections<br/>3154 independent reflections<br/>982 reflections with  $I > 2\sigma(I)$ <br/> $R_{int} = 0.070$ <br/> $\theta_{max} = 27^{\circ}$ <br/>Bruker, 2000)<br/> $T_{min} = 0.590, T_{max} = 0.721$ 

## Refinement

Refinement on  $F^2$ H-atom parameters constrained $R[F^2 > 2\sigma(F^2)] = 0.052$  $w = 1/[\sigma^2(F_o^2) + (0.0483P)^2]$  $wR(F^2) = 0.116$ where  $P = (F_o^2 + 2F_c^2)/3$ S = 1.00 $(\Delta/\sigma)_{max} = 0.007$ 3154 reflections $\Delta\rho_{max} = 0.66$  e Å<sup>-3</sup>236 parameters $\Delta\rho_{min} = -0.62$  e Å<sup>-3</sup>

# Table 1

Selected geometric parameters (Å, °).

Ag-N3	2.327 (4)	Ag-S1	2.7123 (15)
Ag-O7	2.344 (4)	Ag-S2 <sup>i</sup>	2.9567 (15)
Ag-N2	2.404 (4)		
N3-Ag-O7	131.50 (15)	N3-Ag-S2 <sup>i</sup>	71.71 (11)
N3-Ag-N2	101.13 (14)	O7-Ag-S2 <sup>i</sup>	71.86 (11)
O7-Ag-N2	119.25 (15)	S1-Ag-S2 <sup>i</sup>	164.73 (4)
N2-Ag-S1	74.75 (10)		

Symmetry code: (i) x + 1, y, z.

Table 2	
Hydrogen-bond geometry (Å, °).	

$D - H \cdots A$	D-H	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - H \cdot \cdot \cdot A$
C7–H7···O3 <sup>iv</sup>	0.93	2.58	3.466 (7)	159
$C9-H9\cdots O1^{v}$	0.93	2.55	3.210 (7)	128
$C10-H10\cdots O6B^{vi}$	0.93	2.48	3.40 (4)	172

Symmetry codes: (iv) -x, -y + 1, -z; (v) x + 1, y, z - 1; (vi) x + 1,  $-y + \frac{3}{2}$ ,  $z - \frac{1}{2}$ .

Atom O6 is disordered and was refined with a split model over two positions, with an occupancy of 0.31 (7) for O6A and 0.69 (7) for O6B. H atoms were positioned geometrically. In the final cycles of the refinement, all H atoms were constrained to ride on their parent atoms, with C-H distances of 0.93 Å and with  $U_{iso}(H) = 1.2U_{eq}(C)$ .

Data collection: *SMART-NT* (Bruker, 2001); cell refinement: *SMART-NT*; data reduction: *SAINT-NT* (Bruker, 2000); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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