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Key indicators

Single-crystal X-ray study T = 293 K Mean σ (C–C) = 0.005 Å R factor = 0.031 wR factor = 0.070 Data-to-parameter ratio = 15.3

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

Bis[µ-2-(2-pyridylsulfanylmethyl)pyridine]disilver(I) dinitrate

The title complex, $[Ag_2(C_{11}H_{10}N_2S)_2](NO_3)_2$, has a centrosymmetric dinuclear structure, in which the Ag^I centre adopts a tricoordinated geometry formed by two N atoms from two distinct ligands and an S atom of the ligand. In addition, there is weak Ag-O(nitrate) coordination from two different nitrate groups $[Ag \cdots O = 3.127 (3), 2.827 (3) \text{ and} 2.783 (3) \text{ Å}]$. Thus, the Ag^I centre can be considered as being hexacoordinated.

Comment

The generation of coordination architectures depends mainly on the combination of two factors, the coordination geometry of the metal ions and the nature of the ligands (Sun *et al.*, 2002; Goodgame *et al.*, 2002; Hamblin *et al.*, 2002). Therefore, the use of well designed ligands to control the assembly of supramolecular architectures has become a popular and rapidly growing discipline (Bu *et al.*, 2001). In previous studies, much attention has been paid to the use of flexible bridging ligands in the construction of supramolecular architectures (Bu *et al.*, 2002; Cai *et al.*, 2001). As part of our investigation of flexible ligands and their complexes, the crystal structure of a silver(I) complex, (I), with a flexible monothioether ligand, namely 2-(2-pyridylsulfanylmethyl)pyridine (L), is reported here.



The structure of the title complex consists of a dinuclear $[Ag_2(L)_2]^{2+}$ cation and two uncoordinated NO₃⁻ anions (Fig. 1). The $[Ag_2(L)_2]^{2+}$ cation is centrosymmetric, with the inversion centre midway between the two Ag^I atoms. The Ag^I atom is coordinated by two N atoms from two distinct ligands and an S atom of one ligand, giving a distorted T-shaped coordination geometry (Table 1). In the title complex, all three potential donors (two N and one S) of the ligand uses a pyridine N atom and an S atom to chelate an Ag^I centre, forming a five-

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membered ring, and uses another pyridine N atom to bridge to another Ag^I centre. The dihedral angle formed by the two terminal pyridine rings of the same ligand is 87.4 (4)°. In addition, there is weak coordination between Ag^I and NO₃⁻, as shown in Fig. 1. Each Ag^I is in contact with three O atoms of two NO₃⁻ groups, with Ag1-O2 = 3.127 (3), Ag1-O1B = 2.827 (3) and Ag1-O3B = 2.783 (3) Å [symmetry codes: (A) 1 - x, -y, 1 - z; (B) $-\frac{1}{2} + x, \frac{1}{2} - y, -\frac{1}{2} + z$]. Such weak interactions link the dinuclear entities, forming a threedimensional supramolecular framework (Fig. 2).

Experimental

The ligand 2-(2-pyridyl-sulfanylmethyl)pyridine (L) was prepared by a procedure described previously (Bu *et al.*, 2003). The title complex was synthesized by carefully layering a solution of AgNO₃ (17 mg, 0.1 mmol) in MeOH (10 ml) on top of a solution of L (20 mg, 0.1 mmol) in chloroform (10 ml) in a test-tube. After about 3 d at room temperature, colourless block-shaped single crystals suitable for X-ray investigation appeared at the boundary between MeOH and chloroform in a yield of 25%.

Z = 2

 $D_x = 1.931 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation

 $\mu = 1.74 \text{ mm}^{-1}$

T = 293 (2) K

 $\begin{aligned} R_{\rm int} &= 0.032\\ \theta_{\rm max} &= 26.5^\circ \end{aligned}$

Block colourless

 $0.30\,\times\,0.25\,\times\,0.20$ mm

7289 measured reflections

2631 independent reflections 1947 reflections with $I > 2\sigma(I)$

 $w = 1/[\sigma^{2}(F_{o}^{2}) + (0.0309P)^{2} + 0.2899P]$ where $P = (F_{o}^{2} + 2F_{c}^{2})/3$

 $(\Delta/\sigma)_{\text{max}} = 0.001$ $\Delta\rho_{\text{max}} = 0.44 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\text{min}} = -0.38 \text{ e } \text{\AA}^{-3}$

Crystal data

 $\begin{bmatrix} Ag_2(C_{11}H_{10}N_2S)_2 \\ M_r = 744.32 \\ Monoclinic, P2_1/n \\ a = 8.568 (3) Å \\ b = 14.919 (5) Å \\ c = 10.510 (4) Å \\ \beta = 107.688 (5)^{\circ} \\ V = 1280.0 (8) Å^{3} \end{bmatrix}$

Data collection

Bruker SMART 1000 CCD areadetector diffractometer φ and ω scans Absorption correction: multi-scan (*SADABS*; Bruker, 1998) $T_{\min} = 0.843, T_{\max} = 1.000$ (expected range = 0.595–0.706)

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.070$
S = 1.01
2631 reflections
172 parameters
H-atom parameters constrained

Tab	le 1		
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Ag1-N1	2.201 (3)	Ag1-N2	2.197 (3)
Ag1-S1 ⁱ	2.9588 (12)		
N1-Ag1-S1 ⁱ	73.71 (7)	N2-Ag1-S1 ⁱ	109.04 (7)
N2-Ag1-N1	171.06 (9)		

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

H atoms were included in calculated positions and treated in the subsequent refinement as riding atoms, with C-H = 0.93 or 0.97 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.



Figure 1

The structure of (I), showing the coordination entironment of Ag^I, with displacement ellipsoids at the 30% probability level. [Symmetry codes: (A) 1 - x, -y, 1 - z; (B) $-\frac{1}{2} + x, \frac{1}{2} - y, -\frac{1}{2} + z$.]



Figure 2

The three-dimensional supramolecular structure, including the weak coordination (dashed lines) between Ag^{I} and NO_{3}^{-} .

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97*; molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

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