

Bao-Hong Hou, Li-Na Zhou,
 Hong-Yuan Wei,* Jing-Kang
 Wang and Wei Chen

The State Research Centre of Industrialization for
 Crystallization Technology, Tianjin
 University, Tianjin 300072, People's Republic
 of China

Correspondence e-mail: chenweink@you.com

Key indicators

Single-crystal X-ray study
 T = 292 K
 Mean $\sigma(C-C)$ = 0.007 Å
 Disorder in solvent or counterion
 R factor = 0.043
 wR factor = 0.127
 Data-to-parameter ratio = 13.1

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

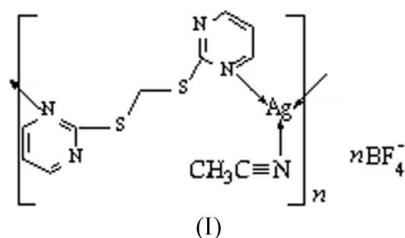
catena-Poly[[[(acetonitrile- κN)silver(I)]- μ -bis-(pyrimidin-2-ylsulfanyl)methane- $\kappa^2 N^1:N^1'$]
 tetrafluoroborate]

In the title complex, $\{[Ag(C_9H_8N_4S_2)(C_2H_3N)]BF_4\}_n$, the Ag^I atom shows trigonal-planar coordination, as it is coordinated by the N atoms from two bis(pyrimidin-2-ylsulfanyl)methane molecules and the N-atom donor of an acetonitrile molecule. The manner in which the donor molecules connect to the Ag atoms leads to a linear chain structure. Adjacent chains are connected into a layer *via* weak Ag...S interactions.

Received 7 June 2005
 Accepted 17 June 2005
 Online 30 July 2005

Comment

Following a report on silver (I) *N*-heterocyclic thioether complexes featuring unusual coordination motifs (Hong *et al.*, 2000), we report the silver tetrafluoroborate complex, (I), of bis(pyrimidin-2-ylsulfanyl)methane. The Ag^I atom exists in a distorted trigonal-planar geometry (Fig. 1) which comprises two pyrimidine N-atom donors from different donor molecules and the N-atom donor from an acetonitrile molecule.



The bond dimensions are within the range reported in similar complexes (Carlucci *et al.*, 1998; Constable *et al.*, 1998; Hou *et al.*, 2004). In the donor molecule, the two pyrimidine

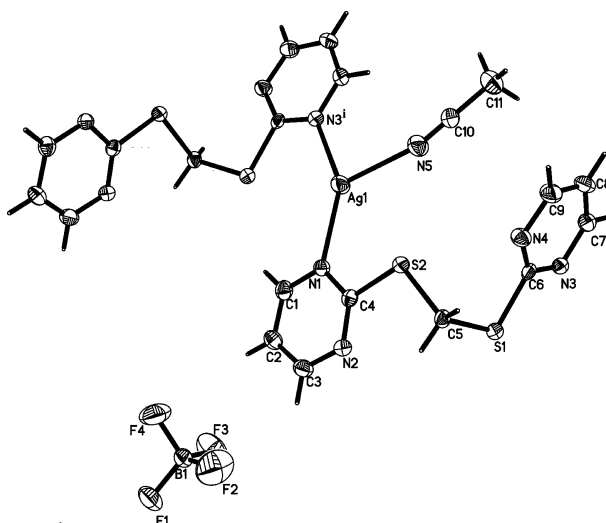


Figure 1
 ORTEP (Johnson, 1976) view of the title compound with 30% probability displacement ellipsoids. [Symmetry codes: (i) $\frac{3}{2} - x, \frac{1}{2} + y, z$].

rings are nearly perpendicular to each other [dihedral angle = $87.7(1)^\circ$], the twist being necessary for the pyrimidine rings to engage in coordination to give rise to a linear chain running along the b axis. As the Ag atom in one chain interacts weakly with the S atoms of adjacent chains [$\text{Ag} \cdots \text{S} = 3.050(2) \text{ \AA}$], the geometry is distorted towards trigonal bipyramidal; the weak interactions lead to a layer structure (Fig. 2). The anions are found between the layers. The analogous nitrate complex (Zheng *et al.*, 2003) adopts a paired-chain structure.

Experimental

Bis(pyrimidin-2-ylsulfanyl)methane (*L*) was prepared according to a reported procedure (Zheng *et al.*, 2003) and the product was characterized by NMR and IR spectroscopy. A solution containing a 1:1 molar ratio of AgBF_4 (0.2 mmol, 0.08 g) and the ligand (0.2 mmol, 0.04 g) in acetonitrile–chloroform (1:1) was stirred for 30 min. The mixture was filtered and the solvent allowed to evaporate to afford colourless crystals. CHN elemental analyses confirmed the formulation determined from the diffraction study. FT-IR data (KBr pellet, cm^{-1}): 3073 (*m*), 3011 (*w*), 2933 (*w*), 1560 (*s*), 1582 (*s*), 1057 (*s*), 752 (*m*), 693 (*m*), 494 (*w*).

Crystal data

$[\text{Ag}(\text{C}_9\text{H}_8\text{N}_4\text{S}_2)(\text{C}_2\text{H}_3\text{N})]\text{BF}_4$	Mo $K\alpha$ radiation
$M_r = 472.05$	Cell parameters from 1758 reflections
Orthorhombic, <i>Pbca</i>	$\theta = 2.9\text{--}26.4^\circ$
$a = 8.7063(12) \text{ \AA}$	$\mu = 1.57 \text{ mm}^{-1}$
$b = 14.7402(16) \text{ \AA}$	$T = 292(1) \text{ K}$
$c = 24.965(2) \text{ \AA}$	Block, colourless
$V = 3203.9(6) \text{ \AA}^3$	$0.20 \times 0.18 \times 0.14 \text{ mm}$
$Z = 8$	
$D_x = 1.957 \text{ Mg m}^{-3}$	

Data collection

Bruker SMART 1000 CCD diffractometer	3322 independent reflections
φ and ω scans	2441 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (<i>SADABS</i> ; Sheldrick, 1996)	$R_{\text{int}} = 0.041$
$T_{\text{min}} = 0.706$, $T_{\text{max}} = 0.804$	$\theta_{\text{max}} = 26.5^\circ$
17366 measured reflections	$h = -8 \rightarrow 10$
	$k = -17 \rightarrow 18$
	$l = -31 \rightarrow 23$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0613P)^2 + 2.423P]$
$R[F^2 > 2\sigma(F^2)] = 0.043$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.127$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.18$	$\Delta\rho_{\text{max}} = 0.79 \text{ e \AA}^{-3}$
3322 reflections	$\Delta\rho_{\text{min}} = -0.68 \text{ e \AA}^{-3}$
253 parameters	Extinction correction: <i>SHELXL97</i>
H-atom parameters constrained	Extinction coefficient: 0.0078 (5)

Table 1

Selected geometric parameters ($^\circ$).

$\text{N1} - \text{Ag1} - \text{N3}^i$	141.32 (13)	$\text{N3}^i - \text{Ag1} - \text{N5}$	92.35 (14)
$\text{N1} - \text{Ag1} - \text{N5}$	124.56 (15)		

Symmetry code: (i) $-x + \frac{1}{2}, y + \frac{1}{2}, z$.

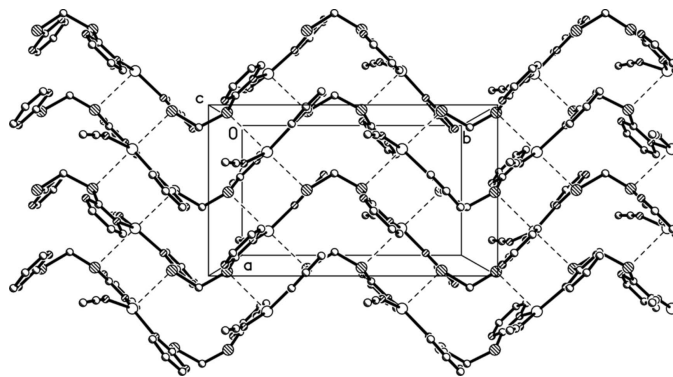


Figure 2

View of the zigzag chains linked through weak $\text{Ag} \cdots \text{S}$ interactions, shown as dashed lines. H atoms have been omitted.

All H atoms were positioned geometrically, with $C_{\text{sp}^2} - \text{H} = 0.93 \text{ \AA}$ and $C_{\text{sp}^3} - \text{H} = 0.97 \text{ \AA}$; they were constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The BF_4^- anion was disordered and was modelled as two components with site occupancies of 0.86 (1) and 0.14 (1). The B–F distances were restrained as $1.35(1) \text{ \AA}$.

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

We gratefully acknowledge financial support from the National Natural Science Foundation of China (No. 20206022) and the Tianjin Natural Science Foundation (05YFJZJC02000).

References

- Bruker (1998). *SMART, SAINT and SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Carlucci, L., Giani, G., Proserpio, D. M. & Sironi, A. (1998). *Inorg. Chem.* **37**, 5941–5943.
- Constable, E. C., Edwards, A. J., Haire, G. R., Hannon, M. J. & Raithby, P. R. (1998). *Polyhedron*, **17**, 243–253.
- Hou, L., Li, D., Yin, Y.-G., Wu, T. & Ng, S. W. (2004). *Acta Cryst.* **E60**, m1106–m1107.
- Hong, M.-C., Zhao, Y.-J., Su, W.-P., Cao, R., Fujita, M., Zhou, Z.-Y. & Chan, A. S. C. (2000). *Angew. Chem. Int. Ed.* **39**, 2468–2470.
- Johnson, C. K. (1976). *ORTEP II*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
- Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*, University of Göttingen, Germany.
- Zheng, Y., Du, M., Zhang, R.-H. & Bu, X.-H. (2003). *J. Chem. Soc. Dalton Trans.* pp. 1509–1514.