Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

catena-Poly[silver(I)-μ_3-2-(pyrimidin-2-ylsulfanyl)acetate]: a one-dimensional chiral coordination polymer

Lei Han,* Yan Zhou and Shi-Jie Huang

Faculty of Materials Science and Chemical Engineering, Ningbo University, Ningbo, Zhejiang 315211, People's Republic of China

Correspondence e-mail: hanlei@nbu.edu.cn

Received 5 December 2006
Accepted 4 January 2007

Key indicators

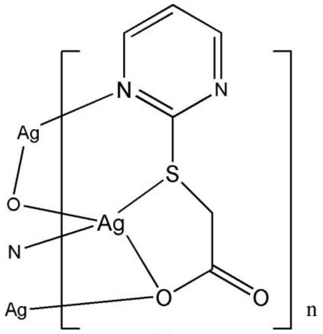
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.012 Å
R factor = 0.045
wR factor = 0.118
Data-to-parameter ratio = 11.6

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

The title chiral coordination polymer, $[Ag(C_6H_5N_2O_2S)]_n$, has a one-dimensional chain structure in which the Ag atom is four coordinated by S, O and N atoms from three different anions. Weak Ag···O and Ag···S interactions cross-link the chains, forming a two-dimensional layer network.

Comment

The construction of chiral coordination polymers has attracted much attention due to their potential applications in asymmetric catalysis, enantioselective separation and optical activity (Bradshaw *et al.*, 2005; Evans & Lin, 2002). Chiral coordination polymers may be obtained either by enantioselective synthesis using enantiopure chiral species, which yields enantiopure products, or by spontaneous resolution upon crystallization without any enantiopure chiral auxiliary, which yields a racemic conglomerate (Han & Hong, 2005).



(I)

With the goal of designing and synthesizing chiral coordination polymers, we are currently adopting an approach of self-assembly reactions between metal ions and asymmetric linking ligands by spontaneous resolution upon crystallization (Han *et al.*, 2003). We report here a new one-dimensional chiral coordination polymer constructed from silver(I) and 2-(pyrimidin-2-ylsulfanyl)acetic acid, (I).

The title compound crystallizes in the orthorhombic non-centrosymmetric space group $P2_12_12_1$ and the asymmetric unit contains one Ag(I) cation and one 2-(pyrimidin-2-ylsulfanyl)acetate anionic ligand. As shown in Fig. 1 and Table 1, atom Ag1 is bidentate coordinated by the S atom and one of the carboxylate O atoms from one ligand, by one N atom from a second ligand and by the same carboxylate O atom from a third ligand. One atom of the carboxylate group is, therefore, bridging two Ag atoms, while the other O atom is non-coordinating. As a consequence of the coordination modes, the Ag atoms and ligands are linked *via* the Ag—O—Ag—O— bridges into one-dimensional coordination polymer chains.

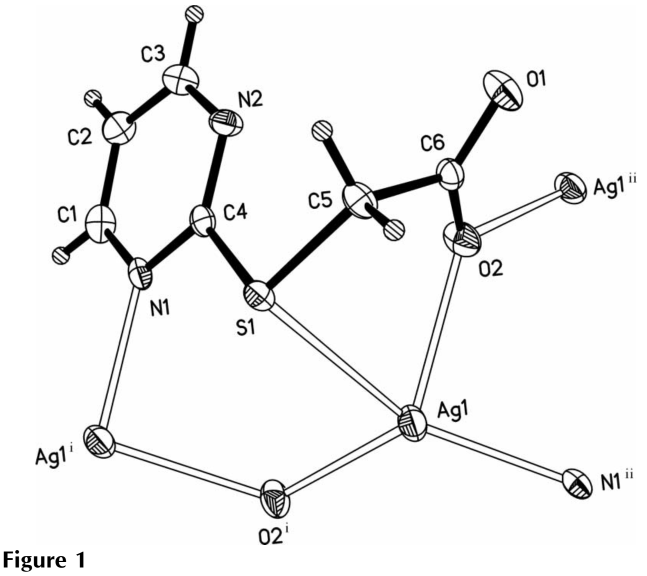


Figure 1
A perspective view of the title compound with the atom-labelling scheme, showing the coordination environment of the Ag atom and the coordination mode of the ligand. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii [symmetry codes: (i) $x - \frac{1}{2}, -y + \frac{1}{2}, -z$; (ii) $x + \frac{1}{2}, -y + \frac{1}{2}, -z$].

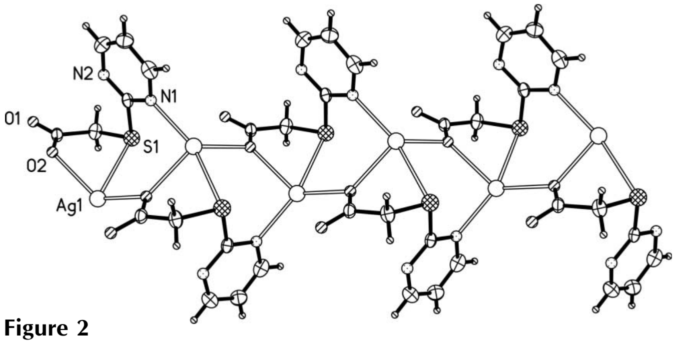


Figure 2
A view of the one-dimensional chain structure of the title compound.

These chains propagate with helical 2_1 symmetry along the crystallographic *a*-axis direction(Fig. 2). The chains are cross-linked by a weak Ag1$\cdots$O1($x - \frac{1}{2}, -y - \frac{1}{2}, -z$) interaction of 2.709 (2) Å and an Ag1$\cdots$S1($x + \frac{1}{2}, -y - \frac{1}{2}, -z$) interaction of 3.382 (2) Å, forming a two-dimensional layer network (Fig. 3).

Experimental

A mixture of equivalent amounts of $AgNO_3$ (85 mg, 0.5 mmol) and 2-(pyrimidin-2-ylsulfanyl)acetic acid (85 mg, 0.5 mmol) in 10 ml mixed solvents CH_3CN and H_2O (1:1) was stirred for 0.5 h, and then 1 ml $NH_3{\cdot}H_2O$ was added dropwise. A quantity of colorless, rod-like crystals of the title compound were obtained in *ca* 65% yield after allowing the solution to stand for two days at room temperature.

Crystal data

[Ag($C_6H_5N_2O_2S$)]
M_r = 277.05
Orthorhombic, $P2_12_12_1$
a = 7.2966 (12) Å
b = 5.0707 (9) Å
c = 20.238 (3) Å
V = 748.8 (2) Å^3
Z = 4
D_x = 2.458 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 2.92 mm^{-1}
T = 298 (2) K
Rod, colorless
0.30 × 0.20 × 0.18 mm

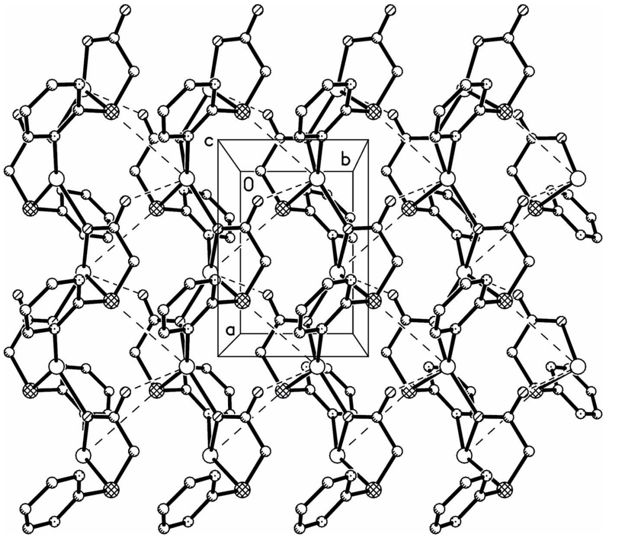


Figure 3
A view of a two-dimensional layer network constructed from one-dimensional chains through weak Ag$\cdots$O and Ag$\cdots$S interactions (dashed lines). H atoms have been omitted for clarity.

Data collection

Bruker SMART APEX-II CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min}$ = 0.652, $T_{\max}$ = 0.769 (expected range = 0.501–0.591)
1789 measured reflections
1271 independent reflections
1200 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.027
$\theta_{\max}$ = 25.1°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.118
S = 1.11
1271 reflections
110 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0827P)^2 + 0.7036P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max}$ = 0.001
$\Delta\rho_{\max}$ = 0.89 e Å^{-3}
$\Delta\rho_{\min}$ = −1.23 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.030 (3)
Absolute structure: Flack & Bernardinelli (2000), 470 Friedel pairs
Flack parameter: 0.05 (9)

Table 1
Selected geometric parameters (Å, °).

Ag1—O2^{i}	2.294 (6)	Ag1—O2	2.480 (6)
Ag1—N1^{ii}	2.299 (6)	Ag1—S1	2.826 (2)
O2^{i}—Ag1—N1^{ii}	122.8 (2)	N1^{ii}—Ag1—S1	151.27 (17)
O2^{i}—Ag1—O2	130.54 (9)	O2—Ag1—S1	68.18 (13)
N1^{ii}—Ag1—O2	95.0 (2)	Ag1^{ii}—O2—Ag1	121.0 (2)
O2^{i}—Ag1—S1	84.71 (15)		

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

All H atoms were positioned geometrically and allowed to ride on their respective parent atoms, with C—H = 0.93 or 0.97 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C). The deepest residual density hole is located 0.95 Å from atom Ag1.

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine

m456 Han *et al.* • [Ag($C_6H_5N_2O_2S$)] *Acta Cryst.* (2007). E**63**, m455–m457

structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

This work was supported by the Foundation of Ningbo University.

References

Bradshaw, D., Claridge, J. B., Cussen, E. J., Prior, T. J. & Rosseinsky, M. J. (2005). *Acc. Chem. Res.* **38**, 273–282.

Bruker (2003). *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.

Evans, O. R. & Lin, W. (2002). *Acc. Chem. Res.* **35**, 511–522.

Flack, H. D. & Bernardinelli, G. (2000). *J. Appl. Cryst.* **33**, 1143–1148.

Han, L. & Hong, M. (2005). *Inorg. Chem. Commun.* **8**, 406–419.

Han, L., Hong, M., Wang, R., Luo, J., Lin, Z. & Yuan, D. (2003). *Chem. Commun.* pp. 2580–2581.

Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.

Sheldrick, G. M. (1997*a*). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.10. Bruker AXS inc., Madison, Wisconsin, USA.

Acta Cryst. (2007). E**63**, m455–m457 Han *et al.* • [Ag($C_6H_5N_2O_2S$)] **m457**