Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

catena-Poly[[(benzoato-κ*O*)silver(I)]-μ-2-aminopyrimidine-κ^2*N*^{1}:*N*^{3}]

Zhong-Lu You[a,b] and Hai-Liang Zhu[a]*

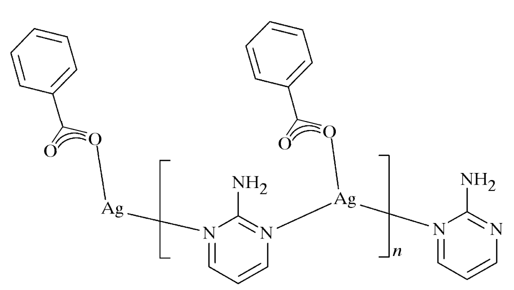
[a]Department of Chemistry, Fuyang Normal College, Fuyang, Anhui 236041, People's Republic of China, and [b]Department of Chemistry, Lanzhou University, Lanzhou 730000, People's Republic of China
Correspondence e-mail: hailiang_zhu@163.com

Received 26 August 2004
Accepted 29 September 2004
Online 11 November 2004

The title complex, $[Ag(C_7H_5O_2)(C_4H_5N_3)]_n$, is a polymer based on a mononuclear silver(I)-centered fragment. The Ag^I atom is trigonally coordinated by two N atoms from two 2-aminopyrimidine ligands and one O atom from one benzoate anion, giving zigzag polymeric chains with an $[-Ag-N-C-N-]_n$ backbone running along the *a* axis. It is proposed that intermolecular hydrogen bonding drives the formation of the chain polymer.

Comment

Inorganic supramolecular chemistry, and in particular the construction of polymeric silver(I) coordination networks, is an active area of research (Xu *et al.*, 2001; Yaghi & Li, 1996; Khlobystov *et al.*, 2001). The primary reason for interest in silver(I) compounds is their ability to afford functional solid materials with potentially controllable properties and novel molecular structures. Recent developments in supramolecular chemistry have made it possible to select building units for assembly into structures with specific network topologies (Blake *et al.*, 2000; Melcer *et al.*, 2001). Crystal engineering of coordination polymeric networks based on multidentate ligands is a growing area of coordination and supramolecular chemistry. Recently, we have focused our attention on the assembly of silver(I) ions with flexible ligands, since they can adopt diverse coordination modes according to the geometric needs of the silver(I) ions (You, Yang *et al.*, 2004; You, Zhu & Liu, 2004). As reported previously, we have used 2-aminopyridine as a bidentate ligand and the benzoate anion as the counter-ion to obtain a mononuclear silver(I) complex, namely bis(2-aminopyridine-κ*N*^{1})(benzoato-κ*O*)silver(I), (II) (Zhu *et al.*, 2003). In order to investigate the relationship between the starting materials and the resulting structures, we used the tridentate ligand 2-aminopyrimidine instead of the bidentate ligand 2-aminopyridine to obtain the title compound, (I). As expected, the structure of (I) consists of one-dimensional chains and is thus entirely different from that of (II).



(I)

Complex (I) is a polymeric 2-aminopyrimidine–Ag^I compound (Fig. 1). The smallest repeat unit for the complex contains a 2-aminopyrimidine–Ag^I cation and a benzoate anion. The Ag^I atom is in a distorted trigonal coordination environment and is three-coordinated by two N atoms of two different but symmetry-related 2-aminopyrimidine ligands and by one O atom of one benzoate anion. The angles subtended at atom Ag1 [136.15 (15), 125.40 (16) and 98.38 (15)°, respectively; Table 1] are comparable to the corresponding values observed in (II). In (I), the smallest of these angles is O1—Ag1—N2, which forms part of a six-atom ring (including an H atom) closed by the N1—H1*A*···O1 hydrogen bond.

The mean Ag—N bond length is 2.291 (4) Å in (I) and 2.218 (4) Å in (II). The Ag—O bond length in (I) [2.313 (4) Å] is comparable to the value of 2.344 (4) Å in (II). The coordination geometry around the Ag atom in (II) is approximately trigonal and is thus qualitatively the same pattern as that found in (I).

In the extended structure of (I), the 2-aminopyrimidine–Ag^I cation propagates as a zigzag chain along the *a* axis (Fig. 2), with the anionic benzoate ligands extending laterally, attached not only by the Ag—O bonds but also through intramolecular N—H···O hydrogen bonds (Table 2).

In (II), the layered structure is mediated by the formation of intermolecular hydrogen bonds. In contrast, in (I), the

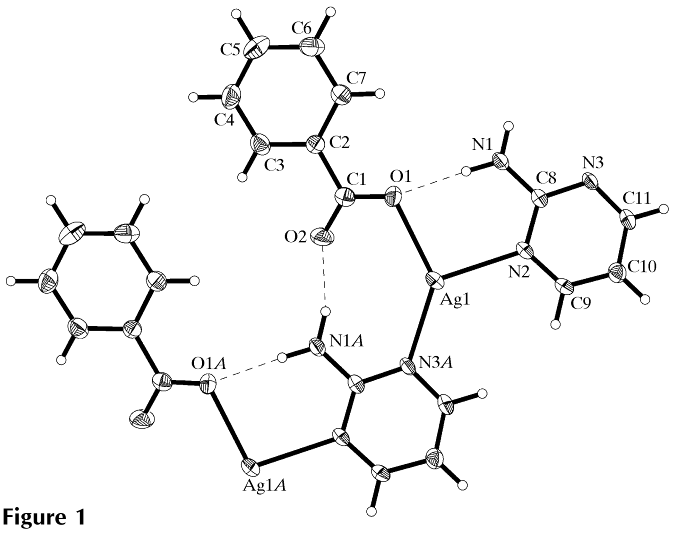


Figure 1
The structure and atom-numbering scheme of (I). Displacement ellipsoids are drawn at the 30% probability level. Atoms labeled with the suffix *A* are at the symmetry position (1 + *x*, *y*, *z*). Dashed lines indicate intramolecular interactions.

DOI: 10.1107/S0108270104024424

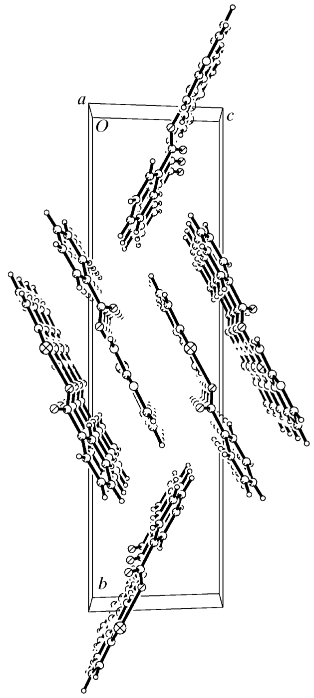


Figure 2
The crystal packing of (I), viewed along the *a* axis.

hydrogen bonds are located within each of the chains. The H atoms of the amine groups are disposed in such a way as to obviate a link to the O atoms of another chain. We propose that it is this fundamental difference in the arrangement of the non-covalent interactions in (I) that gives rise to a chain structure rather than to discrete molecules in layers or another arrangement mediated by non-covalent interactions.

Experimental

Ag_2O (0.1 mmol, 23.2 mg) and benzoic acid (0.2 mmol, 24.4 mg) were dissolved in a 30% aqueous ammonia solution (10 ml), and the resulting solution was stirred for *ca* 15 min to give a clear colorless solution. To this solution was added an acetonitrile solution (5 ml) of 2-aminopyrimidine (0.1 mmol, 9.5 mg) with stirring. The mixture was stirred for 1 h, and the resulting colorless solution was kept in the dark at room temperature for 8 d. Colorless block-shaped crystals formed on slow evaporation of the solvent.

Crystal data

$[Ag(C_7H_5O_2)(C_4H_5N_3)]$
$M_r = 324.09$
Monoclinic, $P2_1/n$
$a = 6.457\ (3)$ Å
$b = 25.594\ (7)$ Å
$c = 7.111\ (3)$ Å
$\beta = 106.488\ (3)^\circ$
$V = 1126.8\ (8)$ Å^3
$Z = 4$
$D_x = 1.910$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1213 reflections
$\theta = 2.2$–25.3°
$\mu = 1.78$ mm^{-1}
$T = 293\ (2)$ K
Block, colorless
$0.28 \times 0.25 \times 0.22$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.636$, $T_{max} = 0.695$
5115 measured reflections
2297 independent reflections
1870 reflections with $I > 2\sigma(I)$
$R_{int} = 0.041$
$\theta_{max} = 26.5^\circ$
$h = -7 \rightarrow 8$
$k = -23 \rightarrow 32$
$l = -6 \rightarrow 8$

Table 1
Selected geometric parameters (Å, °).

Ag1—N3^{i}	2.237 (4)	Ag1—N2	2.345 (4)
Ag1—O1	2.313 (4)		
N3^{i}—Ag1—O1	136.15 (15)	O1—Ag1—N2	98.38 (15)
N3^{i}—Ag1—N2	125.40 (16)		

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

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N1—H1$B\cdots$O2^{ii}	0.90	1.99	2.843 (7)	157
N1—H1$A\cdots$O1	0.90	1.93	2.825 (6)	177

Symmetry code: (ii) $x - 1, y, z$.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.057$
$wR(F^2) = 0.125$
$S = 1.18$
2297 reflections
154 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0468P)^2 + 0.8969P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.80$ e Å^{-3}
$\Delta\rho_{min} = -0.74$ e Å^{-3}

All H atoms were placed in idealized positions and allowed to ride on their parent atoms (N—H = 0.90 Å and C—H = 0.96 Å), with U_{iso}(H) values fixed at 0.08 Å^2.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*).

The authors thank the Education Office of Anhui Province, People's Republic of China, for research grant No. 2004kj300zd.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: FA1091). Services for accessing these data are described at the back of the journal.

References

Blake, A. J., Champness, N. R., Cooke, P. A., Nicolson, J. E. B. & Wilson, C. (2000). *J. Chem. Soc. Dalton Trans.* pp. 3811–3819.
Bruker (1998). *SMART* (Version 5.628) and *SAINT* (Version 6.02). Bruker AXS Inc., Madison, Wisconsin, USA.
Khlobystov, A. N., Blake, A. J., Champness, N. R., Lemenovskii, D. A., Majouga, A. G., Zyk, N. V. & Schröder, M. (2001). *Coord. Chem. Rev.* **222**, 155–192.
Melcer, N. J., Enright, G. D., Ripmeester, J. A. & Shimizu, G. K. H. (2001). *Inorg. Chem.* **40**, 4641–4648.
Sheldrick, G. M. (1996). *SADABS.* University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXL*97 and *SHELXS*97. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL.* Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Xu, A.-W., Su, C.-Y., Zhang, Z.-F., Cai, Y.-P. & Chen, C.-L. (2001). *New J. Chem.* **25**, 479–482.
Yaghi, O. M. & Li, H. (1996). *J. Am. Chem. Soc.* **118**, 295–296.
You, Z.-L., Yang, L., Zou, Y., Zeng, W.-J., Liu, W.-S. & Zhu, H.-L. (2004). *Acta Cryst.* C**60**, m117–m118.
You, Z.-L., Zhu, H.-L. & Liu, W.-S. (2004). *Acta Cryst.* C**60**, m231–m232.
Zhu, H.-L., Usman, A., Fun, H.-K. & Wang, X.-J. (2003). *Acta Cryst.* C**59**, m218–m220.