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(1,2-Diaminocyclohexane)silver(I) trifluoromethanesulfonate

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In the title compound, $[Ag(C_6H_{14}N_2)](CF_3SO_3)$, the Ag atom is coordinated by two N atoms from the two symmetry-related 1,2-diaminocyclohexane ligands, giving linear polymeric chains with a [-silver-ligand-]$_n$ backbone running parallel to the *a* direction. In the crystal packing, the polymeric chains are interconnected by Ag$\cdots$Ag short contacts, forming a two-dimensional crosslinked polymer perpendicular to the *b* direction. The Ag atom and the C, S, two O and two F atoms of the trifluoromethanesulfonate anion lie on the same glide plane.

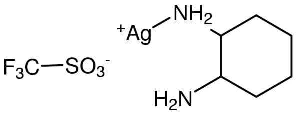
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.009 Å
Disorder in solvent or counterion
R factor = 0.065
wR factor = 0.163
Data-to-parameter ratio = 14.8

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

Comment

The usefulness of silver compounds as antimicrobial agents has been known for a long time. They are effective agents with low toxicity, which is especially important in the topical anti-bacterial treatment of burn wounds. Silver sulfonamides, particularly silver sulfadiazine (AgSD; Fuller *et al.*, 1994) have been used as the standard treatment for burns over the past two decades. Reported in this paper is the structure analysis of a silver sulfonate complex with 1,2-diaminocyclohexane, (I), which was isolated during our systematic study of silver complexes with ethylenediamine analogs. This complex and its other related complexes show strong cytotoxicity *in vitro*, which will be reported elsewhere along with their other properties.



(I)

In the crystal structure of (I), the asymmetric unit contains only one half of the molecule, the other half being generated by a glide plane (Fig. 1). The trifluoromethanesulfonate anion shows rotational disorder about the the S1—C4 bond. This disorder was approximated by a model with split positions for atoms O1 and F2. The occupancies of atoms O1, O1*A*, F2 and F2*A* were fixed at 0.5. In the partial occupancy, the trifluoromethanesulfonate anion is linked to the (1,2-diaminocyclohexane)silver cation *via* the Ag1$\cdots$O1^{i} [symmetry code: (i) $1 - x, y, z$] short contact [2.53 (1) Å]. This contact distance is longer than that of the sum of the covalent radii for Ag and O, *viz.* 2.27 Å (Shannon, 1976). Another short contact in the crystal is Ag$\cdots$Ag^{ii} [symmetry code: (ii) $1 - x, -y, -z$; 3.315 (1) Å], which is also slightly longer than the sum of the covalent radii for two Ag atoms (3.18 Å). Though the Ag^{I}

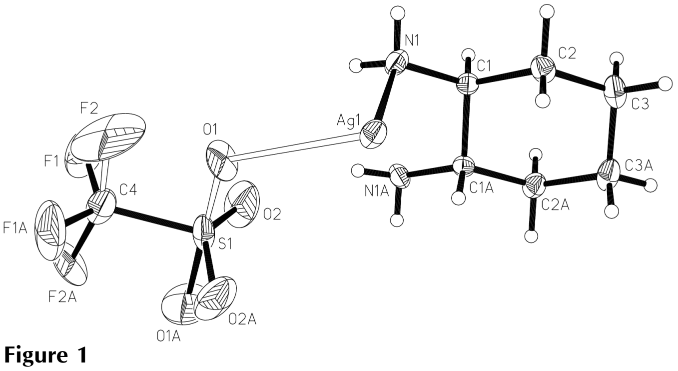


Figure 1
A section of the structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme. Atoms O1A and F2A are the minor conformers of atoms O1 and F2, respectively, whereas other atoms with the suffix A are symmetrically related ($\frac{5}{2} - x$, $1 - y$, $z + \frac{1}{2}$) to the corresponding atoms.

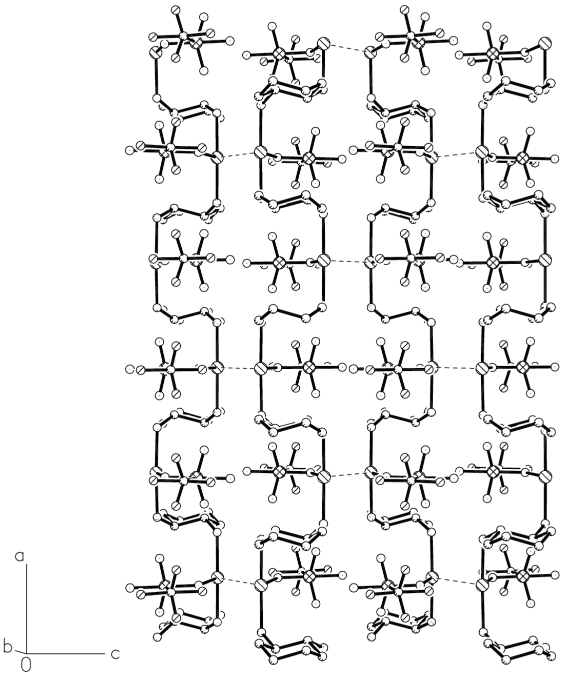


Figure 2
The packing of the title compound, viewed down the *b* axis, showing a two-dimensional crosslinked polymer. H atoms have been omitted for clarity. The dashed lines denote intermolecular Ag···Ag short contacts.

atom is coordinated in a linear geometry by two N atoms from two 1,2-diaminocyclohexane ligands of different asymmetric units, the two short contacts distort significantly the N1—Ag—N1^{i} angle from a linear geometry (180°) to 171.1 (3)°. The Ag1···O1^{i} short contact also affects the S—O bond distance of the trifluoromethanesulfonate anion, in which S1—O1 is about 0.20 Å longer than that of the S—O bond distances for sulfonates (Allen *et al.*, 1987).

In the crystal structure, the almost linear N1—Ag—N1^{i} formation gives rise to a linear polymer of the title complex, running parallel to the *a* direction (Fig. 2) and having a [-silver-(1,2-diaminocyclohexane-)]$_n$ backbone. This polymeric structure of a silver complex was observed in another related ethylenediamine–silver complex (Usman *et al.*, 2003). The Ag—N bond distance [2.140 (2) Å] is also comparable to that in the related structure. The polymeric chains are interconnected by Ag···Ag short contacts, forming a two-dimensional crosslinked polymer chain perpendicular to the *b* direction. These two-dimensional polymers are stacked one above the other along the *b* axis.

Experimental

All starting materials and solvents were obtained commercially. Equimolar amounts of 1,2-diaminocyclohexane and $AgSO_3CF_3$ were dissolved in acetonitrile. After slow diffusion of diethyl ether into this solution over a period of 2 d at 295 K, colorless crystals were precipitated, which were then isolated, washed with acetonitrile three times, and dried in a vacuum desiccator using $CaCl_2$ (yield 87%).

Crystal data

$[Ag(C_6H_{14}N_2)](CF_3SO_3)$
$M_r = 371.13$
Orthorhombic, *Cmca*
$a = 10.0830$ (7) Å
$b = 23.9960$ (16) Å
$c = 10.3082$ (7) Å
$V = 2494.1$ (3) Å^3
$Z = 8$
$D_x = 1.977$ Mg m^{-3}

Mo *Kα* radiation
Cell parameters from 4148 reflections
$\theta = 2.6$–28.3°
$\mu = 1.82$ mm^{-1}
$T = 293$ (2) K
Slab, colorless
0.40 × 0.26 × 0.10 mm

Data collection

Siemens SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.530$, $T_{max} = 0.839$
7471 measured reflections

1633 independent reflections
1384 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 28.3°$
$h = -13 \rightarrow 13$
$k = -28 \rightarrow 31$
$l = -13 \rightarrow 10$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.065$
$wR(F^2) = 0.163$
$S = 1.20$
1633 reflections
110 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0599P)^2 + 22.9337P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.34$ e Å^{-3}
$\Delta\rho_{min} = -0.91$ e Å^{-3}

Table 1
Selected geometric parameters (Å).

Ag1—N1	2.167 (6)	S1—O1*A*	1.65 (2)
S1—O2	1.354 (8)	S1—C4	1.748 (12)
S1—O1	1.553 (15)		

The H atoms attached to atoms N1 and C1 were located from Fourier maps and were refined isotropically [N—H = 0.83 (8)–0.84 (7) Å and C1—H1 = 0.95 (6) Å], whereas the H atoms attached to atoms C2 and C3 were fixed geometrically (C—H = 0.97 Å) and were treated as riding. The maximum and minimum electron-density peaks are located 0.76 and 0.74 Å from atoms Ag1 and O1 , respectively

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL, PARST* (Nardelli, 1995) and *PLATON* (Spek, 1990).

m132 Anwar Usman *et al.* • $[Ag(C_6H_{14}N_2)](CF_3SO_3)$ *Acta Cryst.* (2003). E**59**, m131–m133

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References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans.* 2, pp. S1–19.

Fuller, F. W., Parrish, M. & Nance, F. C. (1994). *J. Burn Care Rehabil.* **15**, 213–219.

Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.

Shannon, R. D. (1976). *Acta Cryst.* A**32**, 751–767.

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

Sheldrick, G. M. (1997). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.

Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

Spek, A. L. (1990). *Acta Cryst.* A**46**, C-34.

Usman, A., Fun, H.-K., Chantrapromma, S., Zhu, H.-L. & Wang, X.-J. (2003). *Acta Cryst.* C**59**, m97–m99.

Acta Cryst. (2003). E**59**, m131–m133 Anwar Usman *et al.* • $[Ag(C_6H_{14}N_2)](CF_3SO_3)$ **m133**