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Polymeric di-μ-azido-μ-1,2-diaminoethane-disilver(I)

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.011 Å
R factor = 0.049
wR factor = 0.152
Data-to-parameter ratio = 16.1

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

In the crystal structure of the title compound, $[Ag_2(N_3)_2(C_2H_8N_2)]$, the Ag atoms of adjacent polymeric AgN_3 chains are bridged by the 1,2-diaminoethane ligand to furnish a ribbon structure. The Ag atom shows trigonal planar coordination. The 1,2-diaminoethane ligand lies on an inversion center.

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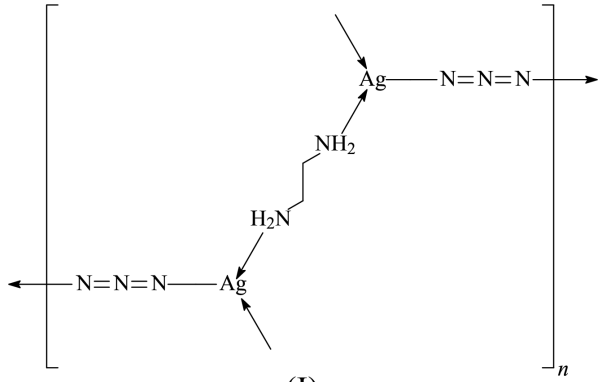
Comment

A number of silver salts have been structurally characterized as their complexes with 1,2-diaminoethane. In the hexafluoroarsenate (Zhu, Sun *et al.*, 2003), phenolate (Zhu, Wang *et al.*, 2003) and 3-fluorobenzoate (You *et al.*, 2004), the Ag atom shows trigonal-planar coordination and the counterion does not participate in bonding to the metal atom. An earlier study has investigated the thiocyanate adduct, which adopts a ribbon structure in which two $(AgSCN)_n$ chains are bridged by the ligand. The present azide analog, (I), is isostructural with the thiocyanate, whose structure has been described in detail (Ren *et al.*, 2001). The 1,2-diaminoethane ligand lies on an inversion center.



(I)

Experimental

To a solution of silver nitrate (0.17 g, 1 mmol) dissolved in a 1:1 acetonitrile–water mixture were added several drops of 1,2-diaminoethane (approximately 3 mmol) and sodium azide (0.65 g, 1 mol) dissolved in water. Crystals separated from the solution after a few days in about 40% yield. Elemental analysis, found: C 6.72, H 2.21, N 31.34%; calculated for CH_4AgN_4: C 6.68, H 2.24, N 31.14%. IR (cm^{-1}): 3355 (*m*), 3254 (*m*), 2929 (*s*), 2035 (*s*), 1583 (*m*), 1469 (*m*), 1383 (*m*), 1321 (*m*), 1136 (*w*), 1053 (*w*), 988 (*m*), 812 (*w*), 627 (*w*), 535 (*w*).

Crystal data

$[Ag_2(N_3)_2(C_2H_8N_2)]$	$Z = 1$
$M_r = 359.90$	$D_x = 2.892$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 5.782$ (5) Å	Cell parameters from 25 reflections
$b = 6.171$ (8) Å	$\theta = 7.5$–$15.0°$
$c = 6.588$ (7) Å	$\mu = 4.70$ mm^{-1}
$\alpha = 67.99$ (1)°	$T = 298$ (2) K
$\beta = 71.93$ (1)°	Block, colorless
$\gamma = 86.89$ (1)°	0.31 × 0.24 × 0.16 mm
$V = 206.7$ (4) Å^3	

Data collection

Siemens *R*3 four-circle diffractometer	$R_{int} = 0.065$
ω scans	$\theta_{max} = 27.0°$
Absorption correction: ψ scan (North *et al.*, 1968)	$h = 0 \rightarrow 7$
$T_{min} = 0.233$, $T_{max} = 0.472$	$k = -7 \rightarrow 7$
992 measured reflections	$l = -8 \rightarrow 8$
903 independent reflections	2 standard reflections every 120 reflections
858 reflections with $I > 2\sigma(I)$	intensity decay: none

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.1081P)^2 + 0.6251P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.050$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.152$	$\Delta\rho_{max} = 0.90$ e Å^{-3}
$S = 1.12$	$\Delta\rho_{min} = -1.64$ e Å^{-3}
903 reflections	Extinction correction: *SHELXL*97
56 parameters	Extinction coefficient: 0.74 (7)
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Ag1—N1	2.246 (7)	Ag1—N4	2.243 (7)
Ag1—N3^{i}	2.556 (7)		
N1—Ag1—N3^{i}	101.4 (3)	N3^{i}—Ag1—N4	103.8 (2)
N1—Ag1—N4	153.3 (2)		

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

The H atoms were placed in geometrically idealized positions and were allowed to ride on the parent N or C atoms [N—H = 0.90 Å, C—H = 0.97 Å and $U_{iso}(H) = 1.2U_{eq}(N,C)$]. The refinement led to a large value for the extinction coefficient; the *R* index exceeded 8% when this was not refined. The reason for the large value is not understood. The largest peak is about 1 Å from Ag1.

Data collection: *XSCANS* (Siemens, 1990); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

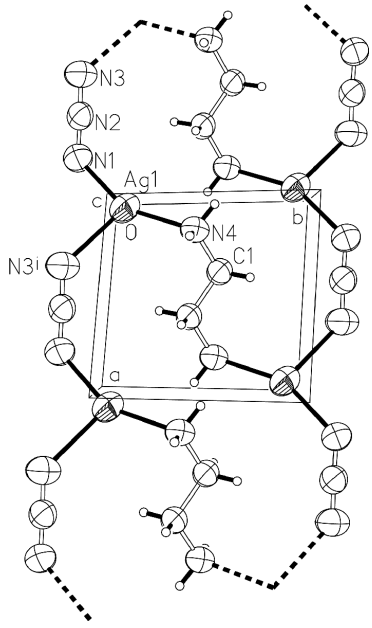


Figure 1
*ORTEP*II (Johnson, 1976) plot, with displacement ellipsoids drawn at the 75% probability level, illustrating the polymeric structure and the trigonal-planar geometry of the Ag atom. H atoms are drawn as spheres of arbitrary radii. [Symmetry code: (i) $1 + x, y, z$.]

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