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catena-Poly[[silver(I)-μ-1,2-diaminoethane] hexafluoroarsenate]

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.009 Å
R factor = 0.048
wR factor = 0.135
Data-to-parameter ratio = 15.3

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

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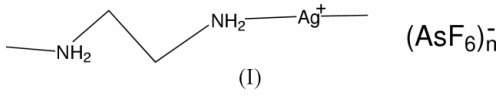
The title compound, $\{[Ag(C_2H_8N_2)](AsF_6)\}_n$, is a polymeric silver(I) complex. The Ag^I atom is coordinated by two N atoms from different ethylenediamine ligands, in a nearly linear geometry. The crystal structure consists of one-dimensional chains, which are stabilized by N—H···F hydrogen bonds and weak Ag···F interactions.

Comment

Recently we reported several Ag^I complexes with 1,2-diaminoethane (Zhu *et al.*, 2000; Zhu, Wang, Meng & Liu, 2003; Zhu, Wang, Sun & Wang, 2003; Usman *et al.*, 2003; Xia *et al.*, 2003). In this paper we report the crystal structure of a new silver complex with ethylenediamine, (I). The title complex crystallizes in the orthorhombic space group *Pnma*. It is a polymeric silver(I) complex. The smallest repeated unit consists of one-half of an ethylenediaminesilver(I) cation and one-half of a hexafluoroarsenate anion. The silver(I) atom in the complex is in a linear coordination environment and is two-coordinated by two N atoms from different ethylenediamine ligands, with an Ag–N bond length of 2.158 (6) Å. The angle at the Ag1 atom is 176.8 (3)°, indicating a slightly distorted linear geometry for the AgN_2 motif.



(I)

N—H···F hydrogen bonds (Fig. 2, Table 1) and weak Ag···F interactions (Fig. 2), with distances lying in the range 2.95–3.56 Å, extend the complex into a three-dimensional network.

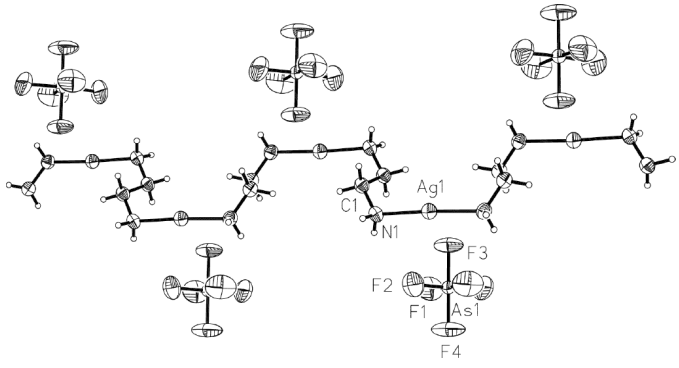


Figure 1
The structure of the title compound (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

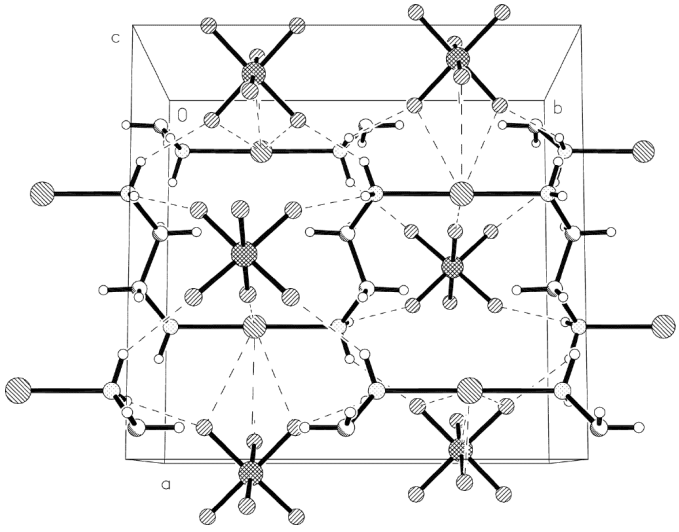


Figure 2
Crystal packing of (I), showing weak interactions as dashed lines.

Experimental

All reagents and solvents were used as obtained without further purification. C, H and N elemental analyses were performed on a Perkin–Elmer elemental analyser. $AgAsF_6$ (0.5 mmol, 148 mg) and 1,2-diaminoethane (0.5 mmol, 30 mg) were dissolved in ammonia solution (10 ml), stirring for *ca* 10 min. to obtain a clear solution. After keeping the mixture in air for three days with the ammonia gas escaping, large colorless crystals were formed. The crystals were isolated and washed three times with water, and dried in a vacuum desiccator using $CaCl_2$ (Yield 69%). Elemental analysis found: C, 35.45; H, 3.05; N, 13.55%; calculated for $C_{12}H_{12}AgF_3N_4O_2$: C, 35.23; H, 2.96; N, 13.69%.

Crystal data

$[Ag(C_2H_8N_2)]AsF_6$
M_r = 356.89
Orthorhombic, *Pnma*
a = 10.098 (2) Å
b = 10.477 (2) Å
c = 8.220 (2) Å
V = 869.6 (3) Å^3
Z = 4
D_x = 2.726 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2200 reflections
θ = 2.8–26.0°
μ = 6.14 mm^{-1}
T = 293 (2) K
Block, colorless
0.34 × 0.25 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.173, T_{max} = 0.374
3748 measured reflections
949 independent reflections
793 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 26.5°
$h = -12 \rightarrow 12$
$k = -13 \rightarrow 10$
$l = -9 \rightarrow 10$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.135
S = 1.05
949 reflections
62 parameters
H-atoms constrained
$w = 1/[\sigma^2(F_o^2) + (0.095P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.043
$\Delta\rho_{max}$ = 0.96 e Å^{-3}
$\Delta\rho_{min}$ = −0.69 e Å^{-3}

Table 1
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1C···F2^{i}	0.90	2.27	3.047 (9)	144
N1—H1D···F1^{ii}	0.90	2.33	3.126 (9)	148
N1—H1D···F2	0.90	2.60	3.270 (12)	132

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

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with N—H and C—H distances of 0.90 and 0.96 Å, respectively, and with U_{iso}(H) fixed at 0.080. The U_{eq} values for the fluorine atoms are quite large, but we did not attempt a disorder model.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1996); 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*); software used to prepare material for publication: *SHELXTL*.

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