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catena-Poly[[silver(I)- μ -ethane-1,2diamine- $\kappa^2 N:N'$] 3-fluorobenzoate monohydrate]

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The title compound, $\{[Ag(C_2H_8N_2)](C_7H_4FO_2)\cdot H_2O\}_n$, has been synthesized and characterized by elemental analysis and single-crystal X-ray diffraction. The Ag atom is bicoordinated in a linear configuration by two N atoms from two symmetryrelated ethylenediamine ligands, giving linear polymeric chains with $[-Ag-N-C-C-N-]_n$ backbones running parallel to the *b* axis. In the crystal packing, these linear chains are interconnected by $N-H\cdots O$ and $O-H\cdots O$ hydrogen bonds, and by weak $Ag\cdots OW$ interactions, forming layers parallel to the *ab* plane.

Comment

Silver(I) complexes with carboxylate anions as counter-ions or ligands are a group of metal compounds which, due to their wide usage in many fields, have been structurally characterized for 30 years (Graham *et al.*, 1996; Kristiansson, 2001; Nomiya *et al.*, 2000; Pingrong *et al.*, 1998). Recently, we have reported a few dozen silver(I)-carboxylate complexes with various



amines and imines, all of which have been structurally characterized (Usman *et al.*, 2003; Zhu *et al.*, 1999, 2000; Zhu, Usman *et al.*, 2003; Zhu, Zhang *et al.*, 2003; Zheng, Tong, Zhu & Chen, 2001; Zheng, Tong, Zhu, Fang & Chen, 2001). As an extension of our work on the structural characterization of





The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

these silver(I) carboxylates, the title novel complex, (I), is reported here.

Complex (I) is a polymeric ethylenediamine–silver(I) complex. The smallest repeat unit for the complex contains an ethylenediamine–silver(I) cation, a 3-fluorobenzoate anion and a lattice water molecule (see scheme). In the cation, the Ag^{I} atom is in a linear coordination environment and is bicoordianted by two N atoms from different ethylenediamine ligands. The N1–Ag1–N2 angle is 170.50 (11)°, indicating a significantly distorted linear geometry for atom Ag1, which is comparable with the value of 172.37 (8)° observed in a similar silver complex (Zhu, Liu *et al.*, 2003). The average Ag–N bond length is 2.148 (3) Å, which is a little longer than the value of 2.138 (2) Å observed in the related complex described above. In the anion, the dihedral angle between the benzene ring and the plane formed by the carboxylate group



Figure 2

The crystal packing of (I), viewed along the c axis. H atoms have been omitted for clarity.

(O1/C7/O2) is 9.4 (5)°. The C6-C5-C7-O2 and C4-C5-C7-O1 torsion angles are -171.1 (4) and -170.2 (4)°, respectively. Atom F1 lies in the plane of the phenyl ring.

The Ag–N bonds link the amine molecules and the Ag^I atoms to form a chain along the *b* axis. Coordinatoin is increased to three by the water atom O1W at a distance of 2.611 (4) Å, leading to a T-shaped configuration at Ag1. If the longer Ag1···O1W($\frac{1}{2} - x, \frac{1}{2} - y, 1 - z$) contact of 2.993 (4) Å is also considered, coordination is further increased to four, giving Ag₂O₂ tetragons, as shown in Fig. 2. The tetragons link the chains to form layers along the *ab* direction.

The 3-fluorobenzoate anions in (I) are located among the chains, their carboxylate-group ends linking to the chains through $N1-H1A\cdotsO1^{i}$ and $N1-H1B\cdotsO2^{ii}$ hydrogen bonds. In addition, there are $O1W-H1WA\cdotsO1^{i}$ and $O1W-H1WB\cdotsO2^{i}$ hydrogen bonds between the water molecules and the carboxylate groups.

Experimental

All reagents and solvents were used as obtained without further purification. Silver 3-fluorobenzoate (0.5 mmol, 124 mg) and 1,2-diaminoethane (0.5 mmol, 30 mg) were dissolved in an ammonia solution (10 ml, 30%). The mixture was stirred for about 10 min at room temperature to give a clear colourless solution. The resulting solution was kept in air and, after slow evaporation of the solvent over a period of 2 d, large colourless crystals of (I) formed at the bottom of the vessel. The crystals were isolated, washed three times with water and dried in a vacuum desiccator using CaCl₂ (yield 85.2%). Analysis found: C 33.21, H 4.39, N 8.55%; calculated for C₉H₁₄AgFN₂O₃: C 33.25, H 4.34, N 8.62%.

Crystal data

$[Ag(C_2H_8N_2)](C_7H_4FO_2) \cdot H_2O$ $M_r = 325.09$ Monoclinic, C2/c a = 23.721 (5) Å b = 7.1800 (10) Å c = 13.961 (3) Å $\beta = 100.45$ (3)° V = 2338.4 (8) Å ³ Z = 8 $D_x = 1.847$ Mg m ⁻³	Mo K α radiation Cell parameters from 4521 reflections $\theta = 2.6-25.8^{\circ}$ $\mu = 1.73 \text{ mm}^{-1}$ T = 293 (2) K Prism, colourless $0.40 \times 0.31 \times 0.16 \text{ mm}$
Data collection	
Siemens SMART CCD area- detector diffractometer φ and ω scans Absorption correction: multi-scan $(SADABS;$ Sheldrick, 1996) $T_{min} = 0.530, T_{max} = 0.758$ 5175 measured reflections 2372 independent reflections	1973 reflections with $I > 2\sigma(I)$ $R_{int} = 0.023$ $\theta_{max} = 26.5^{\circ}$ $h = -20 \rightarrow 29$ $k = -8 \rightarrow 8$ $l = -17 \rightarrow 16$
Refinement	

Refinement on F^2 $R[F^2 > 2\sigma(F^2)] = 0.040$ $wR(F^2) = 0.091$ S = 1.072372 reflections 145 parameters H-atom parameters constrained $w = 1/[\sigma^{2}(F_{o}^{2}) + (0.0446P)^{2}]$ where $P = (F_{o}^{2} + 2F_{c}^{2})/3$ $(\Delta/\sigma)_{\text{max}} = 0.001$

 $\Delta \rho_{\text{max}} = 0.54 \text{ e } \text{\AA}^{-3}$ $\Delta \rho_{\text{min}} = -0.56 \text{ e } \text{\AA}^{-3}$

Table 1

Hydrogen-bonding geometry (Å, °).

$D - H \cdots A$	D-H	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - \mathbf{H} \cdots A$
$O1W-H1WA\cdots O2^{i}$	0.85	1.95	2.739 (4)	154
$O1W - H1WB \cdots O1^{ii}$	0.85	1.96	2.731 (4)	150
$N1 - N1B \cdots O1^{i}$	0.90	2.25	3.126 (4)	165
$N2-H2A\cdots O2^{iii}$	0.90	2.15	2.958 (4)	149
$N1 - H1A \cdots O2$	0.90	2.13	2.964 (4)	154
$N2-H2C\cdots O1$	0.90	2.08	2.941 (4)	160

Symmetry codes: (i) $\frac{1}{2} - x, \frac{3}{2} - y, 1 - z$; (ii) $\frac{1}{2} - x, \frac{1}{2} - y, 1 - z$; (iii) x, y - 1, z.

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with N-H = 0.90 Å, C-H = 0.96 Å and O-H = 0.85 Å, and with $U_{\rm iso}$ (H) values fixed at 0.08 Å². The $U_{\rm eq}$ value for the F atom is large, but no attempt was made to split it.

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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Supplementary data for this paper are available from the IUCr electronic archives (Reference: NA1632). Services for accessing these data are described at the back of the journal.

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