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

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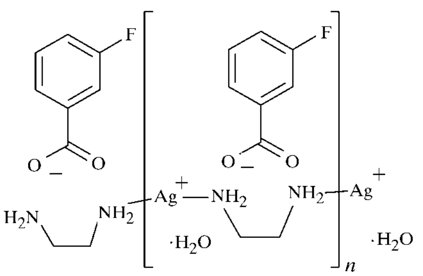
The title compound, $\{[Ag(C_2H_8N_2)](C_7H_4FO_2)\cdot H_2O\}_n$, has been synthesized and characterized by elemental analysis and single-crystal X-ray diffraction. The Ag atom is bicoordinated in a linear configuration by two N atoms from two symmetry-related ethylenediamine ligands, giving linear 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$\cdots$O*W* 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 these silver(I) carboxylates, the title novel complex, (I), is reported here.



(I)

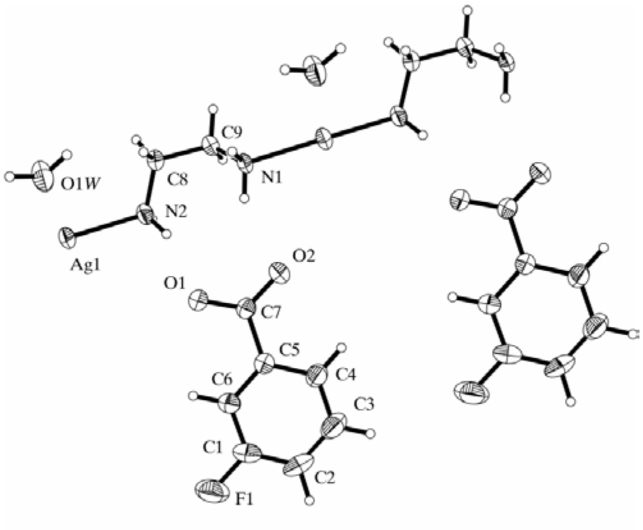


Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

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

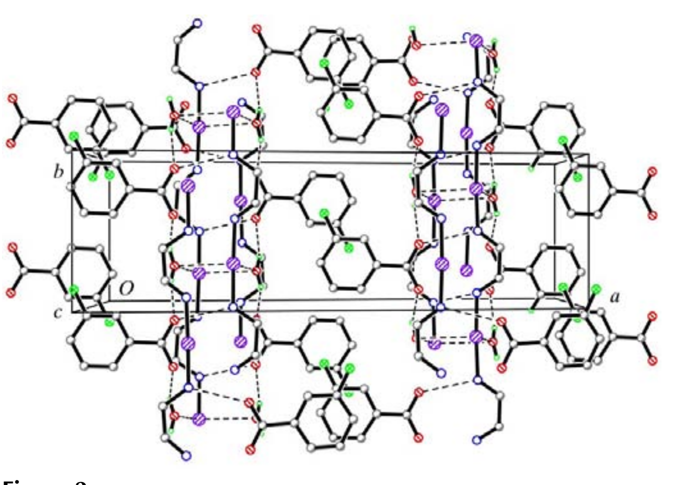


Figure 2
The crystal packing of (I), viewed along the *c* axis. H atoms have been omitted for clarity.

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(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 O1*W* at a distance of 2.611 (4) Å, leading to a T-shaped configuration at Ag1. If the longer Ag1···O1*W*($\frac{1}{2} - x, \frac{1}{2} - y, 1 - z$) contact of 2.993 (4) Å is also considered, coordination is further increased to four, giving Ag_2O_2 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—H1*A*···$O1^{i}$ and N1—H1*B*···$O2^{ii}$ hydrogen bonds. In addition, there are O1*W*—H1*WA*···$O1^{i}$ and O1*W*—H1*WB*···$O2^{i}$ 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 $CaCl_2$ (yield 85.2%). Analysis found: C 33.21, H 4.39, N 8.55%; calculated for $C_9H_{14}AgFN_2O_3$: 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 *Kα* radiation
Cell parameters from 4521 reflections
$\theta = 2.6$–$25.8°$
$\mu = 1.73$ mm^{-1}
$T = 293\ (2)$ K
Prism, colourless
0.40 × 0.31 × 0.16 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 $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 26.5°$
$h = -20 \rightarrow 29$
$k = -8 \rightarrow 8$
$l = -17 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.091$
$S = 1.07$
2372 reflections
145 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0446P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.54$ e Å^{-3}
$\Delta\rho_{min} = -0.56$ e Å^{-3}

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WA*···$O2^{i}$	0.85	1.95	2.739 (4)	154
O1*W*—H1*WB*···$O1^{ii}$	0.85	1.96	2.731 (4)	150
N1—N1*B*···$O1^{i}$	0.90	2.25	3.126 (4)	165
N2—H2*A*···$O2^{iii}$	0.90	2.15	2.958 (4)	149
N1—H1*A*···O2	0.90	2.13	2.964 (4)	154
N2—H2*C*···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_{iso}(H) values fixed at 0.08 Å^2. The U_{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.

References

Graham, S., Daniel, E. L. & Colin, H. L. K. (1996). *Inorg. Chem.* **35**, 2711–2712.
Kristiansson, O. (2001). *Inorg. Chem.* **40**, 5058–5059.
Nomiya, K., Takahashi, S., Noguchi, R., Nemoto, S., Takayama, T. & Oda, M. (2000). *Inorg. Chem.* **39**, 3301–3311.
Pingrong, W., Thomas, C. W. M. & David, A. A. (1998). *Inorg. Chem.* **37**, 2605–2607.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Usman, A., Fun, H.-K., Chantrapromma, S., Zhu, H.-L. & Wang, X.-J. (2003). *Acta Cryst.* C**59**, m97–m99.
Zheng, S.-L., Tong, M.-L., Zhu, H.-L. & Chen, X.-M. (2001). *New J. Chem.* **25**, 1425–1429.
Zheng, S.-L., Tong, M.-L., Zhu, H.-L., Fang, Y. & Chen, X.-M. (2001). *J. Chem. Soc. Dalton Trans.* pp. 2049–2053.
Zhu, H.-L., Liu, X.-Y., Wang, X.-J., Yang, F., Usman, A. & Fun, H.-K. (2003). *Z. Anorg. Allg. Chem.* **629**, 1986–1990.
Zhu, H.-L., Tong, Y.-X. & Chen, X.-M. (2000). *J. Chem. Soc. Dalton Trans.* pp. 4182–4186.
Zhu, H.-L., Tong, Y.-X., Long, L.-S., Tong, M.-L. & Chen, X.-M. (1999). *Supramol. Chem.* **11**, 119–133.
Zhu, H.-L., Usman, A., Fun, H.-K. & Wang, X.-J. (2003). *Acta Cryst.* C**59**, m218–m220.
Zhu, H.-L., Zhang, X.-M., Liu, G.-F. & Wang, D.-Q. (2003). *Z. Anorg. Allg. Chem.* **629**, 1059–1062.

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