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catena-Poly[[silver(I)-µ-hexane-1,6-diamine- $\kappa^2 N:N'$] cinnamate dihydrate]

Zhong-Lu You,^{a,b} Hai-Liang Zhu^{a,b*} and Wei-Sheng Liu^b

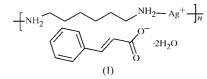
^aDepartment of Chemistry, Fuyang Normal College, Fuyang Anhui 236041, People's Republic of China, and ^bDepartment of Chemistry, Lanzhou University, Lanzhou 730000, People's Republic of China Correspondence e-mail: hailiang_zhu@163.com

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The title compound, $\{[Ag(C_6H_{16}N_2)](C_9H_7O_2)\cdot 2H_2O\}_n$, has been synthesized and characterized by elemental analysis and single-crystal X-ray diffraction. The Ag atom is coordinated in a linear configuration by two N atoms from two hexane-1,6-diamine ligands, giving a zigzag polymeric chain with an $[-Ag-N-C-C-C-C-C-N-]_n$ backbone running parallel to the c axis. In the crystal packing, adjacent chains interact with the anions via the lattice water molecules, thus forming layers parallel to the bc plane.

Comment

The structural characterization of silver(I) complexes with carboxylate anions as counter-ions or ligands has attracted much interest over the past 30 years because of the use of these compounds in a wide range of fields (Graham et al., 1996; Pingrong et al., 1998; Nomiya et al., 2000; Kristiansson, 2001). Recently, we have reported a few dozen silver(I)-carboxylate complexes with various amines and imines, all of which have been structurally characterized (Zhu et al., 1999, 2000; Zheng, Tong, Zhu & Chen, 2001; Zheng, Tong, Zhu, Fang & Chen, 2001; Usman et al., 2003; Zhu, Usman et al., 2003; Zhu, Zhang et al., 2003; You et al., 2004). As an extension of our work on the structural characterization of these silver(I) carboxylates, the title complex, (I), is reported here.



Complex (I) is a polymeric (1,6-diaminohexane)silver(I) complex. Each of the smallest repeat units in the complex contains a (1,6-diaminohexane)silver(I) cation, a cinnamate anion and two lattice water molecules, as shown in Fig. 1. In the cation, the Ag atom has a linear coordination environment and is coordinated by two N atoms from two 1,6-diaminohexane ligands. The Ag1-N1 and Ag1-N2 bond lengths [2.133 (4) and 2.155 (4) Å, respectively] are slightly longer than the mean Ag–N bond lengths [2.126 (4) Å] reported for a similar silver complex with 1,6-diaminohexane (Zhu, Wang et al., 2003). The N1-Ag1-N2 angle [174.47 (15)°], indicating a slightly distorted linear geometry for atom Ag1, is comparable to the value observed in another similar silver complex [172.37 (8)°; Zhu, Liu et al., 2003]. In the anion, the

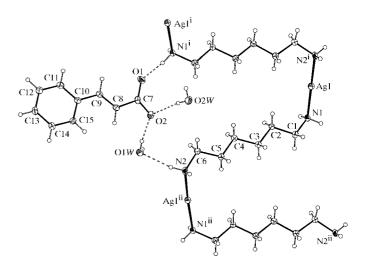


Figure 1

Part of the extended structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry codes: (i) $x - \frac{1}{2}, \frac{1}{2} - y, z - \frac{1}{2}$; (ii) $\frac{1}{2} + x, \frac{1}{2} - y, \frac{1}{2} + z$.]

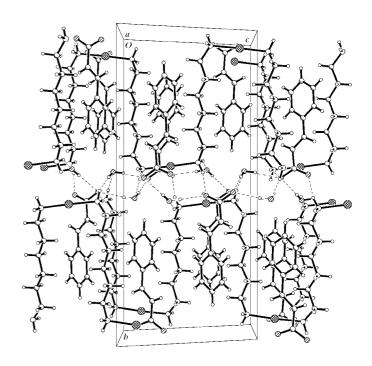


Figure 2

The crystal packing of (I), viewed along the a axis. Ag, water O and N atoms are represented by large cross-hatched, medium hatched and medium unfilled spheres, respectively.

metal-organic compounds

dihedral angle between the plane of the benzene ring and the plane of the carboxy group (O1/C7/O2) is 25.1 (4)°. The O2-C7-C8-C9 and C7-C8-C9-C10 torsion angles are -168.9 (4) and 176.8 (4)°, respectively. Atom C9 lies in the plane of the phenyl ring. The aminohexane chain is almost planar, the largest displacement from the least-squares plane being only 0.17 Å. This plane makes a dihedral angle of 4.2 (2)° with the plane of the phenyl ring.

In the crystal, the cinnamate anions are located among the chains. The Ag—N bonds link the amine molecules and the Ag atoms into a zigzag chain along the c axis. Adjacent chains interact with the anions *via* the lattice water molecules, thus forming layers along the *bc* direction (Fig. 2). These layers are linked together by the hydrogen bonds listed in Table 1, thus forming a three-dimensional structure.

Experimental

All reagents and solvents were used as obtained without further purification. Silver cinnamate (1 mmol, 255 mg) and 1,6-diaminohexane (1 mmol, 116 mg) were dissolved in an ammonia solution (10 ml, 30%), and the mixture was stirred for about 20 min at room temperature. The resulting clear colorless solution was kept in air and, after slow evaporation of the solvent over a period of a week, large colorless 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 anhydrous CaCl₂ (yield 78.7%). Analysis found: C 44.19, H 6.72, N 6.82%; calculated for C₁₅H₂₇AgN₂O₄: C 44.24, H 6.68, N 6.88%.

Crystal data

$[Ag(C_6H_{16}N_2)](C_9H_7O_2)\cdot 2H_2O$	$D_x = 1.567 \text{ Mg m}^{-3}$
$M_r = 407.26$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 7511
a = 7.272 (1) Å	reflections
b = 23.070(5) Å	$\theta = 2.8 - 25.5^{\circ}$
c = 10.753 (2) Å	$\mu = 1.19 \text{ mm}^{-1}$
$\beta = 106.82 \ (3)^{\circ}$	T = 293 (2) K
$V = 1726.8 (5) \text{ Å}^3$	Block, colorless
Z = 4	$0.45 \times 0.32 \times 0.19 \text{ mm}$

Data collection

Bruker SMART CCD area-detector	r 3381 independent reflections		
diffractometer	2800 reflections with $I > 2\sigma(I)$		
φ and ω scans	$R_{\rm int} = 0.035$		
Absorption correction: multi-scan	$\theta_{\rm max} = 26.0^{\circ}$		
(SADABS; Sheldrick, 1996)	$h = -6 \rightarrow 8$		
$T_{\min} = 0.641, T_{\max} = 0.798$	$k = -28 \rightarrow 26$		
7641 measured reflections	$l = -13 \rightarrow 13$		

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.049$	$w = 1/[\sigma^2(F_o^2) + (0.0361P)^2]$
$wR(F^2) = 0.097$	where $P = (F_o^2 + 2F_c^2)/3$
S = 1.13	$(\Delta/\sigma)_{\rm max} < 0.001$
3381 reflections	$\Delta \rho_{\rm max} = 0.70 \ {\rm e} \ {\rm \AA}^{-3}$
199 parameters	$\Delta \rho_{\rm min} = -0.57 \ {\rm e} \ {\rm \AA}^{-3}$

All H atoms were placed in idealized positions and constrained to ride on their parent atoms, with N–H distances of 0.90 Å, C–H distances of 0.96 Å and O–H distances of 0.94–1.0 Å, and with $U_{\rm iso}({\rm H})$ values fixed at 0.08 Å². The coordinates of the water H atoms were localized using the *HYDROGEN* program (Nardelli, 1999).

Table 1

Hydrogen-bonding geometry (Å, °).

$D - H \cdots A$	$D-\mathrm{H}$	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - H \cdots A$
$N1-H1A\cdotsO1^{i}$	0.90	2.03	2.901 (4)	161
$N1 - H1B \cdot \cdot \cdot O2W^{ii}$	0.90	2.38	3.194 (5)	150
$N2-H2B\cdots O2^{iii}$	0.90	2.48	3.261 (5)	144
$O1W-H1WB\cdots O2^{iv}$	0.85	2.11	2.955 (5)	175
$O2W - H2WB \cdots O1^{v}$	0.84	1.97	2.798 (4)	172
$N2-H2A\cdots O1W$	0.90	2.11	2.977 (5)	162
$O1W-H1WA\cdots O2$	0.84	2.04	2.876 (4)	172
$O2W-H2WA\cdots O2$	0.86	2.24	3.091 (4)	171

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

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: NA1655). Services for accessing these data are described at the back of the journal.

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