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catena-Poly[[silver(I)-μ-propane-1,3-diamine-$\kappa^2N:N'$]bis(4-nitrobenzoato-κO)argentate(I)]

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.007 Å
R factor = 0.044
wR factor = 0.118
Data-to-parameter ratio = 12.3

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

In the title compound, $\{[Ag(C_3H_{10}N_2)][Ag(C_7H_4NO_4)_2]\}_n$, one of three independent Ag^I atoms forms a mononuclear complex with a nearly linear environment, coordinated by two O atoms from two 4-nitrobenzoate anions. The other two Ag atoms lie on inversion centers and are coordinated in a linear configuration by two N atoms from two propane-1,3-diamine ligands, giving zigzag polymeric chains with an $[-Ag-N-C-C-C-N-]_n$ backbone running along the [011] direction.

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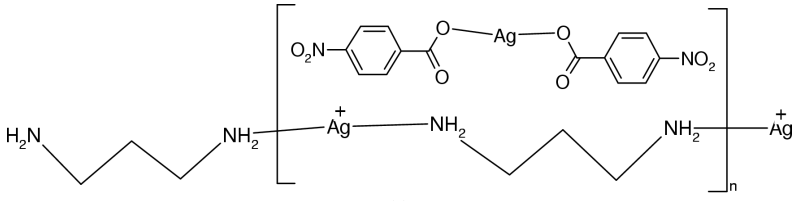
Comment

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 many years (Nomiya *et al.*, 2000; Kristiansson, 2001). Recently, we have reported a few silver(I)–carboxylate complexes with various amines and imines, all of which were structurally characterized (Zhu *et al.*, 1999, 2000; Zheng *et al.*, 2001; Usman *et al.*, 2003). As an extension of our work on the characterization of silver compounds, the structure of the title compound, (I), is reported here.



(I)

The title compound, (I), is a polymeric silver(I) complex (Fig. 1). The smallest repeat unit for the complex contains a propane-1,3-diamine–silver(I) cation segment and a bis(4-nitrobenzoato)silver(I) anion. Atom Ag1 in the anion is in a nearly linear coordination environment and is coordinated by two O atoms from two 4-nitrobenzoate anions. Each 4-nitrobenzoate anion coordinates to the Ag atom through one O

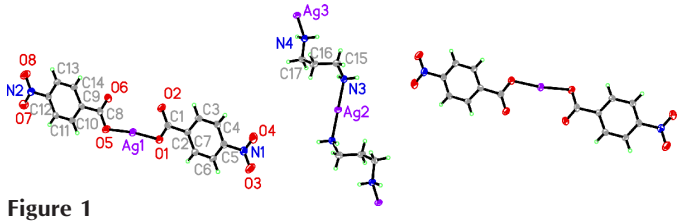


Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Unlabelled atoms are at the symmetry position $-x, 2-y, 2-z$.

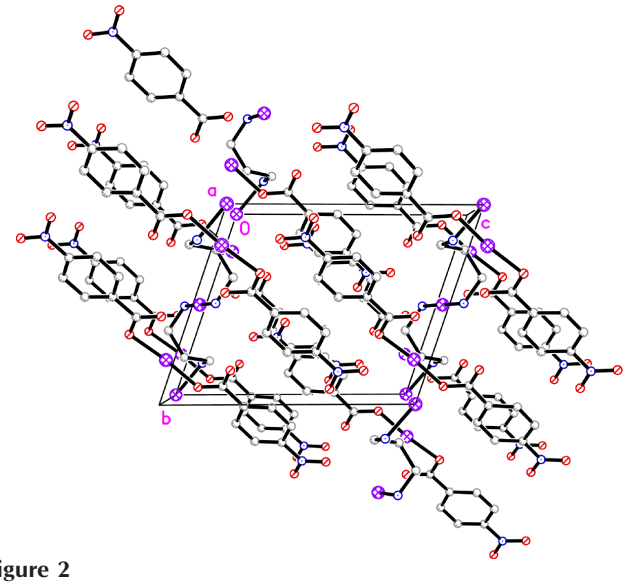


Figure 2
The crystal packing of (I), viewed along the *a* axis. H atoms have been omitted.

atom of the carboxylate group. The O1—Ag1—O5 angle [172.24 (13)°, Table 1] deviates slightly from the ideal value of 180°, which is probably due to the weak interactions involving atoms O2 and O6 of the 4-nitrobenzoate anion, with an average Ag···O distance of 2.972 (5) Å; these pull Ag^{I} in towards the direction of atoms O2 and O6. There are intermolecular N—H···O hydrogen bonds (Table 2). Ag2 and Ag3 both lie on inversion centers and are coordinated in a linear configuration by two N atoms from two propane-1,3-diamine ligands, giving zigzag polymeric cation chains with an $[-Ag-N-C-C-C-N-]_n$ backbone running along the [011] direction (Fig. 2). All the Ag—O and Ag—N bond lengths are comparable to the values observed in a similar silver(I) complex (Zhu *et al.*, 2003).

Experimental

Silver 4-nitrobenzoate (0.1 mmol, 27.4 mg) and propane-1,3-diamine (0.1 mmol, 7.4 mg) were dissolved in an aqueous ammonia solution (10 ml, 30%). The mixture was stirred for about 10 min at room temperature to obtain a clear colorless solution. The resulting solution was kept in the dark, and after slow evaporation of the solvent over a period of 8 d, crystals of (I) were isolated, washed three times with water and dried in a vacuum desiccator using anhydrous $CaCl_2$ (yield 73%). Elemental analysis calculated: C 32.8, H 2.9, N 9.0%; found: C 32.6, H 2.9, N 9.1%.

Crystal data

$[Ag(C_3H_{10}N_2)][Ag(C_7H_4NO_4)_2]$	$Z = 2$
$M_r = 622.09$	$D_x = 2.071$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 9.530$ (5) Å	Cell parameters from 3715 reflections
$b = 9.561$ (6) Å	$\theta = 2.3$–$26.5°$
$c = 11.609$ (5) Å	$\mu = 2.02$ mm^{-1}
$\alpha = 108.472$ (5)°	$T = 298$ (2) K
$\beta = 93.918$ (6)°	Block, colorless
$\gamma = 92.673$ (5)°	0.32 × 0.26 × 0.18 mm
$V = 998.3$ (9) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	3493 independent reflections
ω scans	2999 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$R_{int} = 0.021$
$T_{min} = 0.553$, $T_{max} = 0.699$	$\theta_{max} = 25.0°$
5306 measured reflections	$h = -11 \rightarrow 10$
	$k = -11 \rightarrow 11$
	$l = -13 \rightarrow 10$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.044$	$w = 1/[\sigma^2(F_o^2) + (0.0841P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.118$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.07$	$\Delta\rho_{max} = 3.45$ e Å^{-3}
3493 reflections	$\Delta\rho_{min} = -1.03$ e Å^{-3}
283 parameters	

Table 1
Selected geometric parameters (Å, °).

Ag1—O1	2.087 (5)	Ag2—N3	2.151 (5)
Ag1—O5	2.124 (5)	Ag3—N4	2.150 (6)
O1—Ag1—O5	172.24 (13)	$N4^{ii}$—Ag3—N4	180 (1)
$N3^{i}$—Ag2—N3	180 (1)		

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

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4B···$O6^{ii}$	0.90	2.13	3.008 (7)	167
N4—H4A···$O2^{ii}$	0.90	2.39	3.203 (9)	150
N3—H3B···$O6^{iii}$	0.90	2.14	3.025 (7)	167
N3—H3A···$O2^{iii}$	0.90	2.40	3.204 (8)	149

Symmetry codes: (ii) $1-x, 1-y, 2-z$; (iii) $x-1, y, z$.

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.93–0.97 Å and N—H distances of 0.90 Å, and with U_{iso}(H) = $1.2U_{eq}$(C/N). The maximum residual density is located 1.86 Å from atom Ag1, while the minimum residual density is 0.91 Å from Ag1.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; 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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