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Polymeric structure of (ethylenediamine)silver(I) 3-nitrobenzoate monohydrate

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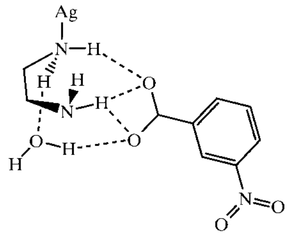
In the ternary title compound, *catena*-poly[[silver(I)-μ-ethylenediamine-κ^2N:N'] 3-nitrobenzoate monohydrate], $\{[\mathrm{Ag}(\mathrm{C_2H_8N_2})](\mathrm{C_7H_4NO_4})\cdot\mathrm{H_2O}\}_n$, the Ag atom is bicoordinated in a linear configuration by two different N atoms from two symmetry-related ethylenediamine ligands, thus giving linear polymeric chains with an $[-\mathrm{Ag}-\mathrm{N}-\mathrm{C}-\mathrm{C}-\mathrm{N}-]_n$ backbone running parallel to the *a* axis. In the crystal packing, these linear chains are interconnected by N—H···O and O—H···O hydrogen bonds to form layers parallel to the *ab* plane.

Comment

The synthesis or construction of polymeric supramolecular coordination architecture is currently receiving considerable attention. Ethylenediamine and its analogues are a family of organic ligands with this type of architecture. These analogues can also interact with almost all transition metal ions, thus giving a wide variety of supramolecular coordination possibilities. Furthermore, the coinage metals, especially silver, have been the subject of investigation for the construction of supramolecular complexes for decades. Interest in this area grew out of the diverse structural motifs displayed by these superficially similar monovalent cations. Some interesting ethylenediamine complexes with $\mathrm{Ag^I}$ atoms have been reported, such as silver ethylenediamine perchlorate (Bang, 1978) and the silver ethylenediamine thiocyanates (Ren *et al.*, 2001). Our interest in silver complexes has led us to the title complex, (I), a hydrate of (ethylenediamine)silver(I) 3-nitrobenzoate, whose structure is reported here.

The bond lengths in (I) (Table 1) are within the normal ranges (Allen *et al.*, 1987). The Ag—N bond lengths are slightly shorter than those in silver ethylenediamine perchlorate [2.17 (1) Å] or silver ethylenediamine thiocyanates [2.172 (2)–2.313 (3) Å]. The C—O bond distances of the 3-nitrobenzoate anion are intermediate between C—O single and double bonds, implying that the negative charge located on the anion is delocalized over the two C—O bonds. This assumption is supported by the geometry of the anion and by the unambiguous location of H atoms attached to the N and O atoms. Within the 3-nitrobenzoate anion, the carboxylate (O1/O2/C7) and the nitro groups (N3/O3/O4) are twisted out of the plane of the aromatic ring by 8.9 (1)° about the C1—C7 bond and by 13.1 (2)° about the N3—C3 bond.



(I)

Atom Ag1 is bicoordinated in an essentially linear configuration by two different N atoms (N1 and N2) from two symmetry-related ethylenediamine ligands belonging to different asymmetric units, the angle N1—Ag1—N2($x + 1$, y, z) being 177.1 (1)°. This configuration gives rise to a linear polymeric chain of (I) running parallel to the x axis, with an $[-\mathrm{Ag1}-\mathrm{N1}-\mathrm{C8}-\mathrm{C9}-\mathrm{N2}-]_n$ backbone.

In one asymmetric unit, the three components, *viz*. the ethylenediamine-coordinated silver cation, the 3-nitrobenzoate anion and the water molecule, are linked together by N—H···O and O—H···O hydrogen bonds (Fig. 1), namely N1—H11···O1, N2—H12···O1, N2—H12···O2, N1—H21···O1*W* and O1W—H2*W*···O2 (Table 2). The ethylenediamine ligand acts as a multiple hydrogen-bond donor *via* its amino groups, whereas the water molecule acts as both a donor and an acceptor. The donor function N2—H12 is involved in a three-centre hydrogen bond to the carboxylate O atoms, with an O1···H21···O2 angle of 52.1 (1)°. Within the

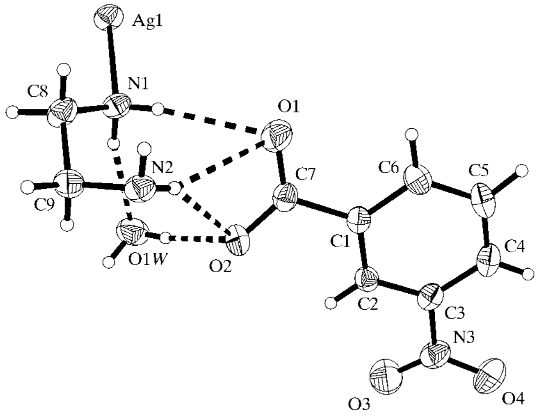


Figure 1
The structure of one monomeric unit of the polymeric title complex, showing displacement ellipsoids at the 50% probability level and the atom-numbering scheme.

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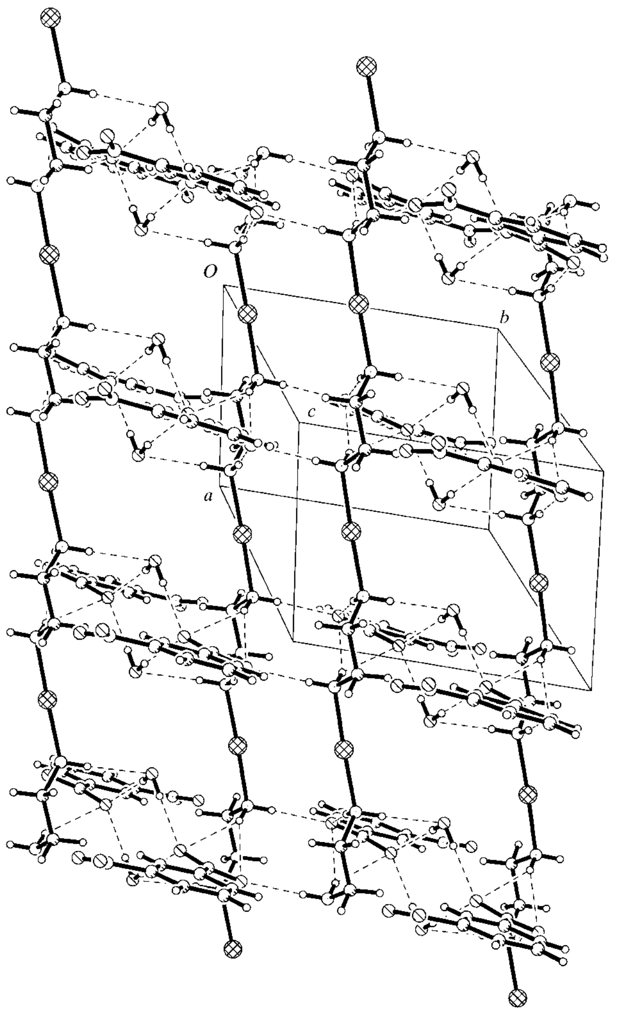

Figure 2
Part of the packing structure of (I), showing the layers parallel to the *ab* plane. Hydrogen bonds are indicated by dashed lines.

cation, atoms Ag1, N1, C8 and C9 are coplanar, and N2 is displaced by 1.226 (2) Å because C9 is sp^3 hybridized.

The packing structure comprises layers parallel to the *ab* plane (Fig. 2) in which the polymeric chains are interconnected symmetrically by O1*W*—H1*W*···O2^{ii} and N2—H22···O1^{iii} hydrogen bonds (see Table 2 for symmetry codes). The layers are further linked by C4—H4···O1*W*^{iv} contacts (Table 2) and four short Ag···O contacts (Table 3) into a three-dimensional network.

Experimental

Ethylenediamine and 3-nitrobenzoic acid were available commercially and were used without further purification. Ag_2O (0.5 mmol, 116 mg) and 3-nitrobenzoic acid (1 mmol, 167 mg) were dissolved in ammonium solution (10 ml). The mixture was stirred for *ca* 10 min to obtain a clear solution. To this solution was added ethylenediamine (2 mmol, 120 mg) in ammonium solution (2 ml). After keeping the resulting solution in air for 2 d, with ammonium gas escaping, large colourless single crystals formed. These were isolated, washed with water three times and dried in a vacuum desiccator using $CaCl_2$ (yield = 42%).

Crystal data

$[Ag(C_2H_8N_2)](C_7H_4NO_4)\cdot H_2O$
$M_r = 352.10$
Triclinic, $P\overline{1}$
$a = 7.1816$ (4) Å
$b = 9.6857$ (5) Å
$c = 10.1259$ (5) Å
$\alpha = 67.825$ (1)°
$\beta = 72.047$ (1)°
$\gamma = 83.078$ (1)°
$V = 620.48$ (6) Å^3

$Z = 2$
$D_x = 1.885$ Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 3342 reflections
$\theta = 2.6$–28.3°
$\mu = 1.64$ mm^{-1}
$T = 293$ (2) K
Block, colourless
0.40 × 0.24 × 0.12 mm

Data collection

Siemens SMART CCD area-detector diffractometer
ω scans
Absorption correction: empirical (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.560$, $T_{\max} = 0.827$
3951 measured reflections

2920 independent reflections
2776 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.013$
$\theta_{\max} = 28.3°$
$h = -9 \rightarrow 9$
$k = -7 \rightarrow 12$
$l = -12 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.023$
$wR(F^2) = 0.055$
$S = 1.13$
2920 reflections
187 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0162P)^2 + 0.384P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.002$
$\Delta\rho_{\max} = 0.61$ e Å^{-3}
$\Delta\rho_{\min} = -0.51$ e Å^{-3}

Table 1
Selected bond lengths (Å).

O1—C7	1.240 (3)	Ag1—N1	2.1409 (18)
O2—C7	1.250 (3)	N1—C8	1.470 (3)
O3—N3	1.214 (3)	N2—C9	1.470 (3)
O4—N3	1.220 (3)	C8—C9	1.522 (3)
Ag1—N2^{i}	2.1403 (19)		

Symmetry code: (i) $1 + x, y, z$.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*···O2^{ii}	0.84 (4)	1.93 (4)	2.754 (3)	171 (4)
O1*W*—H2*W*···O2	0.78 (4)	2.03 (4)	2.789 (3)	162 (3)
N1—H11···O1	0.82 (3)	2.34 (3)	3.156 (3)	171 (3)
N2—H12···O1	0.79 (3)	2.49 (3)	3.233 (3)	157 (3)
N2—H12···O2	0.79 (3)	2.54 (3)	3.253 (3)	151 (3)
N1—H21···O1*W*	0.87 (4)	2.21 (4)	3.061 (3)	165 (3)
N2—H22···O1^{iii}	0.82 (3)	2.10 (3)	2.916 (3)	175 (3)
C4—H4···O1*W*^{iv}	0.93	2.56	3.332 (3)	140

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

Table 3
Ag···O short-contact geometry (Å).

Ag1···O3^{v}	3.272 (3)	Ag1···O1*W*^{vi}	2.995 (2)
Ag1···O4^{v}	3.105 (3)	Ag1···O4^{vii}	2.976 (2)

Symmetry codes: (v) $x + 1, y + 1, z - 1$; (vi) $3 - x, 1 - y, -z$; (vii) $2 - x, 1 - y, 1 - z$.

H atoms attached to N and O atoms were located from Fourier maps and were refined isotropically, giving water O—H distances of 0.78 (4) and 0.84 (4) Å, and N—H distances in the range 0.79 (3)–0.87 (3) Å. H atoms attached to C atoms were fixed geometrically and treated as riding atoms, with C—H distances of 0.93–0.97 Å and $U_{\rm iso}$(H) values equal to 1.2$U_{\rm eq}$(C).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: JZ1543). Services for accessing these data are described at the back of the journal.

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