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Key indicators

Single-crystal X-ray study
 $T = 298\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$
Disorder in solvent or counterion
 R factor = 0.030
 wR factor = 0.084
Data-to-parameter ratio = 15.6For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.catena-Poly[[bromatosilver(I)- μ -4,4'-bipyridine]
2.5-hydrate]

In the crystal structure of $\{[\text{Ag}(\text{BrO}_3)(\text{C}_{10}\text{H}_8\text{N}_2)] \cdot 2.5\text{H}_2\text{O}\}_n$, the Ag atom is coordinated by the N atoms of two different spacer donor ligands [$\text{Ag}-\text{N} = 2.147(2)$ and $2.152(2)\text{ \AA}$, and $\text{N}-\text{Ag}-\text{N} = 172.0(1)^\circ$], but is connected only weakly to the O atoms of two different bromate counter-ions [$\text{Ag}-\text{O} = 2.877(3)$ and $2.972(3)\text{ \AA}$, and $\text{O}-\text{Ag}-\text{O} = 162.3(1)^\circ$]; the coordination geometry of the Ag atom is approximately planar. The $(\text{C}_{10}\text{H}_8\text{N}_2)\text{Ag}$ chains, which propagate along $[10\bar{1}]$, are cross-linked in the b direction by bromate anions and $\text{Ag} \cdots \text{Ag}$ [$3.3197(6)\text{ \AA}$] interactions, thus forming sheets.

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Comment

The 4,4'-bipyridine spacer ligand forms a large number of complexes with the silver(I) cation; in some of these complexes, the $(\text{C}_{10}\text{H}_8\text{N}_2)\text{Ag}$ units are assembled into linear chains, and the inorganic counter-ions interact, although somewhat weakly, with the metal atoms, e.g. $(\text{C}_{10}\text{H}_8\text{N}_2)\text{Ag}(\text{NO}_3)$, which crystallizes in *Pmma* (Bi *et al.*, 2002) and *Fdd2* (Yaghi & Li, 1996) modifications. For the *Pmma* structure, if two other $\text{Ag} \cdots \text{O}$ contacts [$2.835(6)$ and $2.747(6)\text{ \AA}$] are considered as bonding interactions, the geometry approximates to that of a rectangular plane. The nitrite salt, which is also water-free, (Blake *et al.*, 1999), exhibits shorter and stronger $\text{Ag} \cdots \text{O}$ interactions [$\text{Ag} \cdots \text{O} = 2.487(6)\text{ \AA}$]. The present study of the bromate salt continues studies on these complexes with other inorganic anions; an earlier study of the dihydrogen orthophosphate reveals the existence of a phosphoric acid molecule in the formula unit (Tong *et al.*, 2000).

In the title compound, $(\text{C}_{10}\text{H}_8\text{N}_2)\text{Ag}(\text{BrO}_3) \cdot 2.5\text{H}_2\text{O}$, (I) (Fig. 1), the Ag atom is coordinated by the N atoms of two donor ligands [$\text{Ag}-\text{N} = 2.147(2)$ and $2.152(2)\text{ \AA}$, and $\text{N}-\text{Ag}-\text{N} = 172.0(1)^\circ$] in a nearly linear geometry. The rings are twisted by $30.9(1)^\circ$ with respect to each other. The Ag atom is linked to the O atoms of two bromate counter-ions so that the geometry approximates to that of a rectangular plane. The

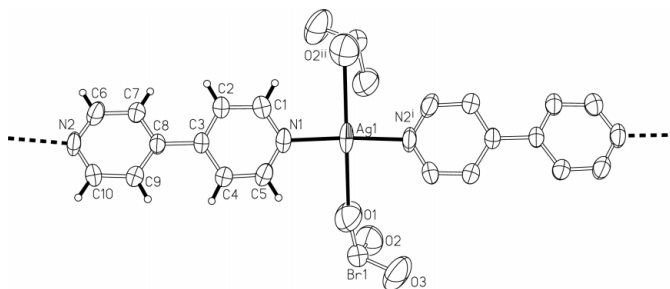
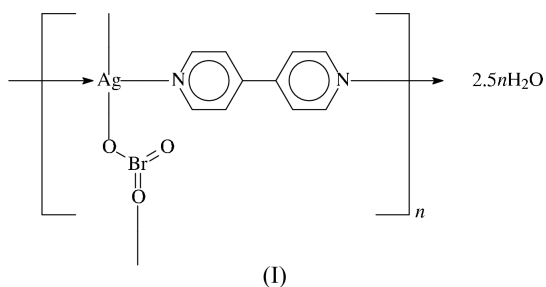


Figure 1

A view of (I), showing 75% probability displacement ellipsoids. H atoms are drawn as spheres of arbitrary radii. [Symmetry codes: (i) $\frac{1}{2} + x, \frac{5}{2} - y, z - \frac{1}{2}$; (ii) $-x, 2 - y, 1 - z$.]

chains propagate along $[10\bar{1}]$; they are cross-linked by the bromate anions and by $\text{Ag}\cdots\text{Ag}(-x, 2-y, 1-z)$ $[3.3197(6)\text{ \AA}]$ interactions, thus forming layers (Fig. 2). The metal–metal interaction in (I) is longer than that $[2.78(1)\text{ \AA}]$ found in the *Fdd2* modification of the nitrate (Yaghi & Li, 1996) but similar to that $[3.286(2)\text{ \AA}]$ found in the dihydrogen orthophosphate (Tong *et al.*, 2000). The latter study lists the $\text{Ag}\cdots\text{Ag}$ distances in several related systems. The present structure is consolidated by hydrogen bonds (Table 2); the water molecules can be envisaged as occupying the spaces between the layers. One of the water molecules lies on a special position with $\bar{1}$ site symmetry, and thus its H atoms are necessarily disordered.



Experimental

Silver bromate (0.24 g, 1 mmol), 4,4'-bipyridine (0.16 g, 1 mmol) and water (10 ml) were placed in a 23 ml Teflon-lined, stainless-steel bomb, which was heated at 413 K for 6 d. The bomb was then cooled at 5 K h⁻¹. Needle-shaped crystals were isolated in about 70% yield. A needle was cut into a block to provide the crystal for measurement. Analysis calculated for C₁₀H₁₂N₂O_{5.5}: C 27.55, H 2.77, N 6.45%; found: C 27.54, H 3.02, N 6.37%.

Crystal data

$[\text{Ag}(\text{BrO}_3)(\text{C}_{10}\text{H}_8\text{N}_2)]\cdot 2.5\text{H}_2\text{O}$
 $M_r = 437.00$
 Monoclinic, $P2_1/n$
 $a = 13.1128(8)\text{ \AA}$
 $b = 6.9843(4)\text{ \AA}$
 $c = 15.3908(9)\text{ \AA}$
 $\beta = 104.647(1)^\circ$
 $V = 1363.74(14)\text{ \AA}^3$
 $Z = 4$

$D_x = 2.128\text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation
 Cell parameters from 4053 reflections
 $\theta = 2.4\text{--}28.2^\circ$
 $\mu = 4.43\text{ mm}^{-1}$
 $T = 298(2)\text{ K}$
 Block, colorless
 $0.37 \times 0.25 \times 0.24\text{ mm}$

Data collection

Bruker APEX area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Bruker, 2001)
 $T_{\min} = 0.201$, $T_{\max} = 0.416$
 7759 measured reflections

3066 independent reflections
 2650 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.023$
 $\theta_{\max} = 27.5^\circ$
 $h = -14 \rightarrow 16$
 $k = -7 \rightarrow 9$
 $l = -19 \rightarrow 19$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.030$
 $wR(F^2) = 0.084$
 $S = 1.05$
 3066 reflections
 196 parameters
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0534P)^2 + 0.025P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.67\text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.77\text{ e \AA}^{-3}$

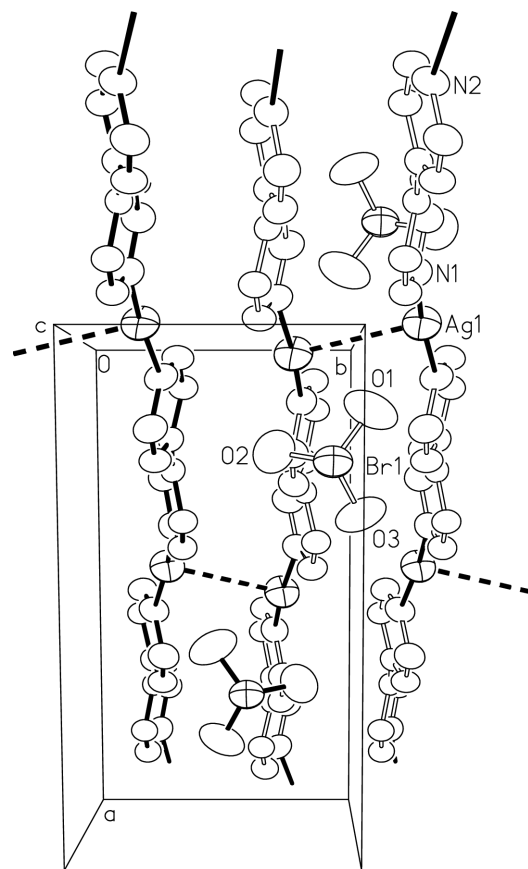


Figure 2

A view of (I), showing the extended chain structure of the $(\text{C}_{10}\text{H}_8\text{N}_2)\text{Ag}$ units linked by $\text{Ag}\cdots\text{Ag}$ interactions (dashed lines) into a layer structure. Water molecules and C-bound H atoms are not shown.

Table 1

Selected geometric parameters (\AA , $^\circ$).

Ag1–N1	2.147 (2)	Ag1–O1	2.877 (3)
Ag1–N2 ⁱ	2.152 (2)	Ag1–O2 ⁱⁱ	2.972 (3)
N1–Ag1–N2 ⁱ	172.0 (1)	N2 ⁱ –Ag1–O1	90.3 (1)
N1–Ag1–O1	88.2 (1)	N2 ⁱ –Ag1–O2 ⁱⁱ	92.81 (9)
N1–Ag1–O2 ⁱⁱ	91.1 (1)	O1–Ag1–O2 ⁱⁱ	162.3 (1)

Symmetry codes: (i) $\frac{1}{2} + x, \frac{5}{2} - y, z - \frac{1}{2}$; (ii) $-x, 2 - y, 1 - z$.

Table 2

Hydrogen-bonding geometry (\AA , $^\circ$).

$D\text{--}H\cdots A$	$D\text{--}H$	$H\cdots A$	$D\cdots A$	$D\text{--}H\cdots A$
O1W–H1W2 \cdots O2	0.86 (1)	2.12 (3)	2.927 (5)	155 (6)
O1W–H1W1 \cdots O3W	0.86 (1)	2.46 (6)	2.894 (5)	112 (5)
O2W–H2W1 \cdots O2W ⁱⁱⁱ	0.87 (1)	2.18 (5)	2.76 (1)	124 (5)
O2W–H2W2 \cdots O3 ^{iv}	0.86 (1)	2.13 (4)	2.853 (5)	141 (5)

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

The aromatic H atoms were placed at calculated positions in the riding-model approximation [$\text{C--H} = 0.93\text{ \AA}$ and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$]. Water H atoms were located and refined with distance restraints [$\text{O--H} = 0.85(1)\text{ \AA}$ and $\text{H}\cdots\text{H} = 1.39(1)\text{ \AA}$], and their

displacement parameters were tied to the U_{eq} values of the O atoms by a factor of 1.2. The O3W water molecule lies on an inversion center, so it should be bonded to only one H atom; however, the inversion symmetry element constrains the H—O—H angle to be 180°. Two H atoms were refined, each with a site occupancy of 0.5 (H3W1 and H3W2). Hydrogen bonds involving these disordered atoms are not listed in Table 2.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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