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Key indicators

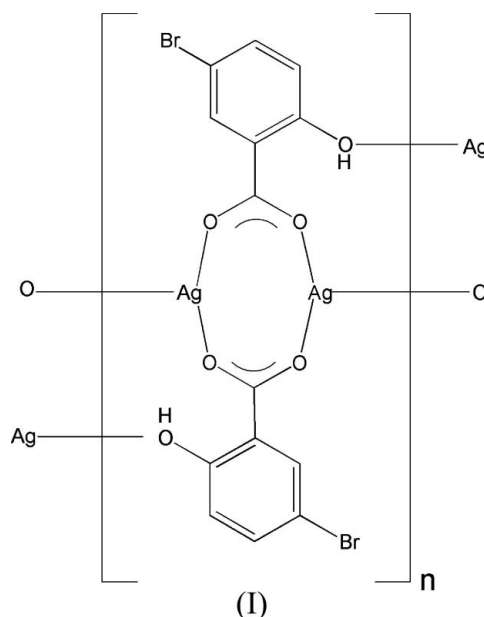
Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
 R factor = 0.021
 wR factor = 0.050
Data-to-parameter ratio = 12.7For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Poly[(μ_3 -5-bromosalicylato)silver(I)]

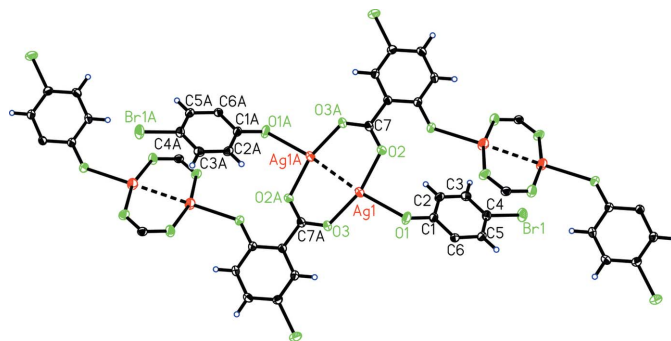
The title complex, $[\text{Ag}(\text{C}_7\text{H}_4\text{BrO}_3)]_n$, is a polymer based on a carboxylate double-bridged centrosymmetric binuclear Ag^{I} fragment, the $\text{Ag} \cdots \text{Ag}$ distance being 2.8666 (8) Å. The Ag atom is coordinated also by the hydroxy O atom of 5-bromosalicylate, showing a deformed trigonal coordination geometry. In the crystal structure, two-dimensional sheets are formed parallel to $(\bar{1}01)$.

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Comment

Inorganic supramolecular chemistry, and in particular the construction of polymeric Ag^{I} coordination networks, is an active area of research (Xu *et al.*, 2001; Khlobystov *et al.*, 2001). The primary reason for interest in Ag^{I} compounds is their ability to afford functional solid materials with potentially controllable properties and novel molecular structures. Recent developments in supramolecular chemistry have made it possible to select building units for assembly into structures with specific network topologies (Blake *et al.*, 2000). Crystal engineering of coordination polymeric networks based on multidentate ligands is a growing area of coordination and supramolecular chemistry. Recently, we have reported several silver(I)-carboxylate complexes, all of which have been structurally characterized (You & Zhu, 2004; Zhu *et al.*, 2004). As an extension of our work, the crystal structure analysis of the title complex, (I), is reported here.




Figure 1

Part of the polymeric structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. Dashed lines indicate hydrogen bonds. [Symmetry codes: (A) $1 - x, 1 - y, 2 - z$; (B) $\frac{1}{2} - x, y - \frac{1}{2}, \frac{3}{2} - z$; (C) $\frac{1}{2} + x, \frac{3}{2} - y, \frac{1}{2} + z$.]

atom is coordinated by three O atoms from the phenolic and two benzoate groups of 5-bromosalicylate ligands in a deformed trigonal configuration. Ag1 lies 0.036 (6) Å out of the plane defined by three donor atoms O1/O2ⁱⁱ/O3ⁱⁱⁱ [symmetry codes: (ii) $\frac{1}{2} - x, y - \frac{1}{2}, \frac{3}{2} - z$; (iii) $\frac{1}{2} + x, \frac{3}{2} - y, \frac{1}{2} + z$]. The Ag \cdots Ag distance of 2.8663 (8) Å is comparable to that observed in silver(I) 4-fluorobenzoate [2.850 (3) Å; Zhu, Zhang *et al.*, 2003]. The bond distances of Ag1–O2ⁱⁱ and Ag1–O3ⁱⁱⁱ (Table 1) are in the common range for Ag–O contacts in silver(I) carboxylates. The Ag–O(phenol) bond distance is similar to that observed in polymeric silver(I) 5-sulfosalicylate [2.533 (4) Å; Ma *et al.*, 2005]. There is an intramolecular O–H \cdots O hydrogen bond (Table 2) in the salicylate ligand.

In the crystal structure, 5-bromosalicylate serves as a tridentate ligand, and two-dimensional sheets are formed parallel to (101). Between the neighboring sheets, there is an Ag1 \cdots Br1($x + \frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}$) contact of 3.151 (1) Å, which is shorter than the sum of the van der Waals radii of Ag and Br (3.57 Å; Bondi, 1964).

Experimental

Ag₂O (0.1 mmol, 23.2 mg) and 5-bromosalicylic acid (0.1 mmol, 21.7 mg) were dissolved in an aqueous ammonia solution (10 ml, 30%), and stirred for *ca* 15 min, giving a clear colorless solution. To this solution was added acetonitrile (5 ml). The mixture was stirred for 1 h, and the resulting yellow solution was allowed to stand in the dark at room temperature for 11 d. Yellow block-shaped crystals formed by slow evaporation of the solvent. These were then dried in a vacuum desiccator over anhydrous CaCl₂ (yield 78%). Elemental analysis calculated for C₇H₄AgBrO₃: C 25.90, H 1.12%; found: C 25.95, H 1.24%.

Crystal data

[Ag(C₇H₄BrO₃)]
M_r = 323.87
 Monoclinic, *P*2₁/*n*
a = 7.3160 (15) Å
b = 8.1710 (16) Å
c = 13.051 (3) Å
 β = 95.14 (3)°
V = 777.0 (3) Å³

Z = 4
D_x = 2.769 Mg m^{−3}
 Mo *K*α radiation
 μ = 7.69 mm^{−1}
T = 293 (2) K
 Block, yellow
 0.30 × 0.20 × 0.10 mm

Data collection

Bruker APEX area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
T_{min} = 0.172, *T_{max}* = 0.463

7324 measured reflections
 1448 independent reflections
 1364 reflections with *I* > 2σ(*I*)
R_{int} = 0.026
 θ_{\max} = 25.5°

Refinement

Refinement on *F*²
R[*F*² > 2σ(*F*²)] = 0.021
wR(*F*²) = 0.050
S = 1.08
 1448 reflections
 114 parameters
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.018P)^2 + 1.1193P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.54 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\min} = -0.35 \text{ e } \text{Å}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Ag1 \cdots Ag1 ⁱ	2.8666 (8)	Ag1–O2 ⁱⁱ	2.210 (2)
Ag1–O1	2.519 (2)	Ag1–O3 ⁱⁱⁱ	2.179 (2)
O3 ⁱⁱⁱ –Ag1–O2 ⁱⁱ	163.42 (8)	O2 ⁱⁱ –Ag1–O1	90.80 (9)
O3 ⁱⁱⁱ –Ag1–O1	105.65 (9)		

Symmetry codes: (i) $-x + 1, -y + 1, -z + 2$; (ii) $-x + \frac{1}{2}, y - \frac{1}{2}, -z + \frac{3}{2}$; (iii) $x + \frac{1}{2}, -y + \frac{3}{2}, z + \frac{1}{2}$.

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> –H \cdots <i>A</i>	<i>D</i> –H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> –H \cdots <i>A</i>
O1–H1 \cdots O2	0.89 (3)	1.73 (3)	2.534 (3)	147 (5)

Symmetry codes: .

The hydroxy H atom was positioned assuming an intramolecular hydrogen bond, and restrained with O–H = 0.90 (8) Å and *U*_{iso}(H) = 0.08 Å². All other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C–H = 0.93 Å, and *U*_{iso}(H) = 1.2*U*_{eq}(C).

Data collection: SMART (Bruker, 2003); cell refinement: SAINT (Bruker, 2003); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997*a*); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997*a*); molecular graphics: SHELXTL (Sheldrick, 1997*b*); software used to prepare material for publication: SHELXTL.

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