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Poly[(μ_4-5-bromopyridine-3-sulfonato)-silver(I)]

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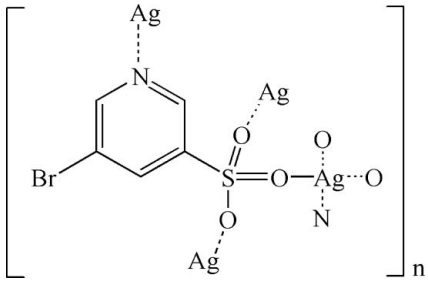
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.005 Å; R factor = 0.038; wR factor = 0.152; data-to-parameter ratio = 12.0.

The silver(I) complex, $[Ag(C_5H_3BrNO_3S)]_n$, was obtained by reaction of $AgNO_3$ and 5-bromopyridine-3-sulfonic acid. The Ag^I ion is coordinated by an O_3N donor set in a slightly distorted tetrahedral geometry. The Ag^I ions are linked by μ_4-5-bromopyridine-3-sulfonate ligands, forming a layer parallel to (100). The layers are further connected *via* C—H···Br hydrogen-bonding interactions into a three-dimensional supramolecular network. The Ag···Ag separation is 3.0159 (6) Å, indicating the presence of argentophilic interactions.

Related literature

For background information on pyridinesulfonato ligands, see: Chandler *et al.* (2002); Makinen *et al.* (2001); May & Shimizu (2005). For similar C—H···Br hydrogen bonding, see: Lu *et al.* (2011).



Experimental

Crystal data

$[Ag(C_5H_3BrNO_3S)]$
M_r = 344.92
Monoclinic, $C2/c$
a = 20.103 (3) Å
b = 5.0634 (9) Å
c = 16.036 (3) Å
β = 110.142 (2)°
V = 1532.5 (5) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 8.08 mm^{-1}
T = 296 K
0.20 × 0.18 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2008*a*)
T_{min} = 0.512, T_{max} = 0.746
4188 measured reflections
1310 independent reflections
1204 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.152
S = 1.01
1310 reflections
109 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.88 e Å^{-3}
$\Delta\rho_{min}$ = −1.72 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3A···Br1^{i}	0.93	2.92	3.832 (3)	168

Symmetry code: (i) $-x+1, y, -z+\frac{1}{2}$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008*b*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008*b*); molecular graphics: *SHELXTL* (Sheldrick, 2008*b*); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZJ2045).

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supporting information

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Poly[(μ_4-5-bromopyridine-3-sulfonato)silver(I)]

Ying-Bing Lu and Fang-Mei Jian

S1. Comment

As bridging ligands, sulfonate ligands and their derivatives have drawn much attention owing to their diverse coordination modes, forming numerous coordination complexes. In this paper, we report the new title compound **1**, which displays a two-dimensional layer structure.

X-ray diffraction analyses reveal that the title compound crystallizes in the *C2/c* group space. In the asymmetrical unit of **1** (Fig. 1), there is one crystallographically independent Ag^+ ion and one 5-Bromopyridine-3-sulfonato ligand. The Ag1 atom is in a distorted tetrahedral coordination environment and coordinated by one O1 atom, one O2 atom, one O3 atom and N1 atom from four different 5-Bromopyridine-3-sulfonato ligands. As shown in Figure 2, the Ag1 ions are linked by three oxygen atoms from sulfonate groups to form 1-D chain. Interestingly, the Ag···Ag separation in the [Ag1]2 dimers is 3.0159 (6) Å, which is much shorter than the sum of van der Waals radii for silver (3.4 Å), suggesting significant silver-silver interactions. These chains are further connected through N1 atoms from μ_4-5-Bromopyridine-3-sulfonato ligands to generate a two-dimensional layer. The layers are connected *via* C3—H3A···Br1 hydrogen bonding interactions (Lu *et al.*, 2011) into a three-dimensional supramolecular architecture (Fig. 3 and Table 1).

S2. Experimental

$AgNO_3$ (85 mg, 0.5 mmol) and bromopyridinesulfonato ligands (103 mg, 0.5 mmol) were dissolved in 20 ml water, stirring for 2 h. The resulting solution was filtrated and allowed to evaporate slowly at room temperature. Colorless block crystals appeared after 1 week. Yield based on Ag: 15%.

S3. Refinement

H atoms were placed in calculated positions with C—H = 0.93 Å (aromatic), and refined in riding mode with U_{iso}(H) = 1.2U_{eq}(C). The abnormal reflections (-7 1 2), (-4 2 3), (8 0 0), (1 1 6) (-4 0 2), (-2 06) and (-5 1 3) have been omitted during the refinement. The "delu 0.005 C1 N1 Ag1 O1" has been employed during the refinement to modify the small difference of anisotropic displacement parameters along chemical bonds.

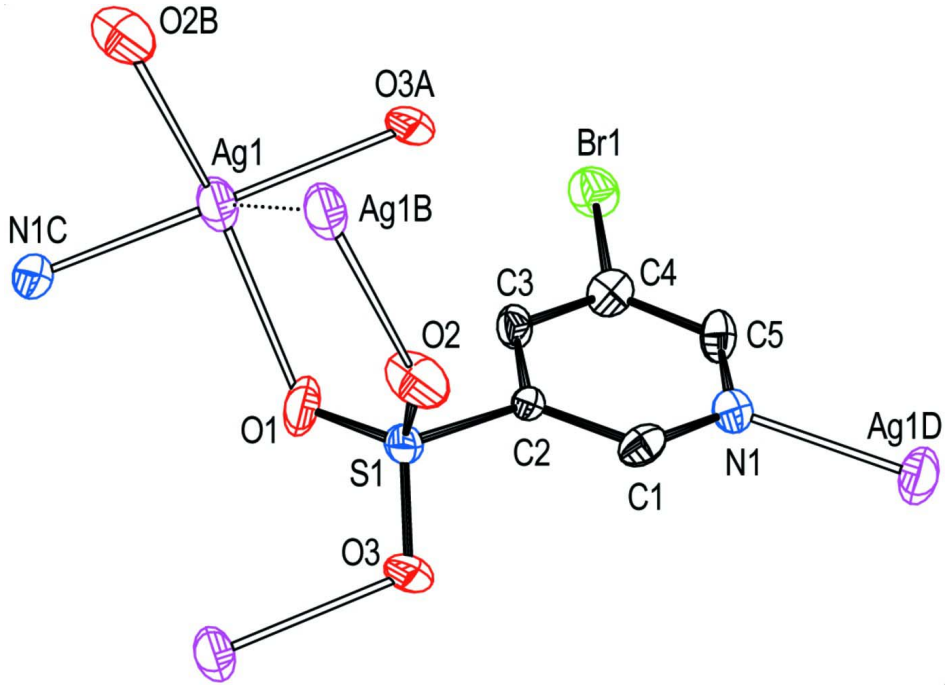

Figure 1

ORTEP drawing of **1** with 50% thermal ellipsoids with hydrogen atoms being omitted for clarity. (Symmetry codes: A: *x*, 1 + *y*, *z*; B: 1/2 - *x*, 3/2 - *y*, - *z*; C: *x*, 1 - *y*, -1/2 + *z*; D: *x*, 1 - *y*, 1/2 + *z*;).

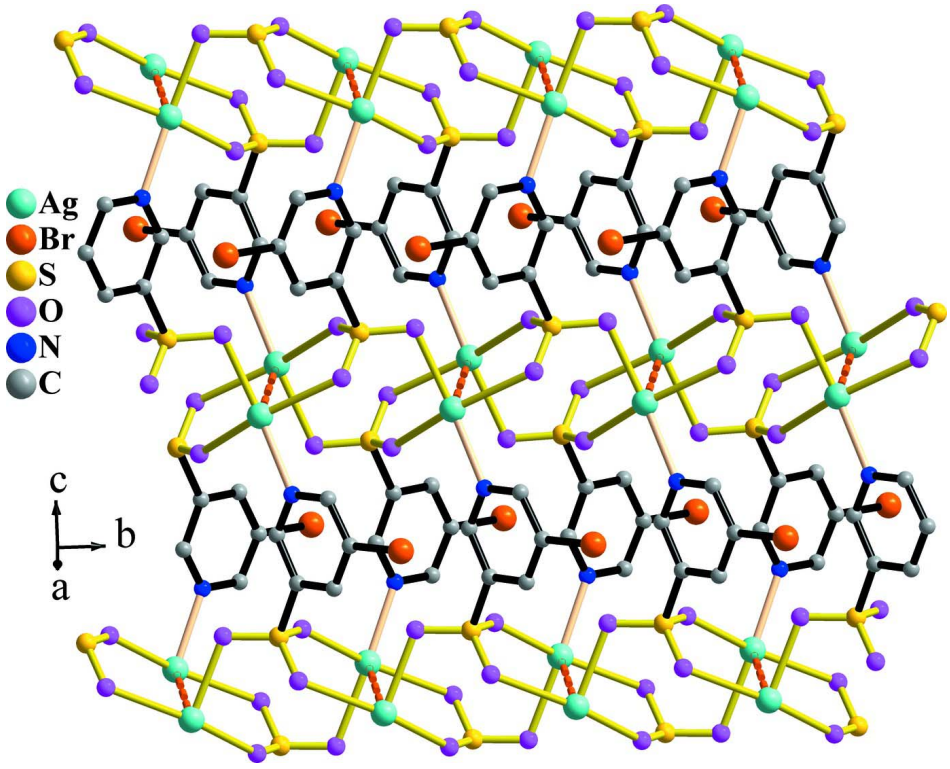

Figure 2

View of two-dimensional layer of **1** along the *a* axis. The yellow–green bonds represent the 1-D chain originating from Ag and SO_3 groups of 5-Bromopyridine-3-sulfonato ligands. The silver-silver interactions are represented as orange dashed lines (H atoms are omitted for clarity).

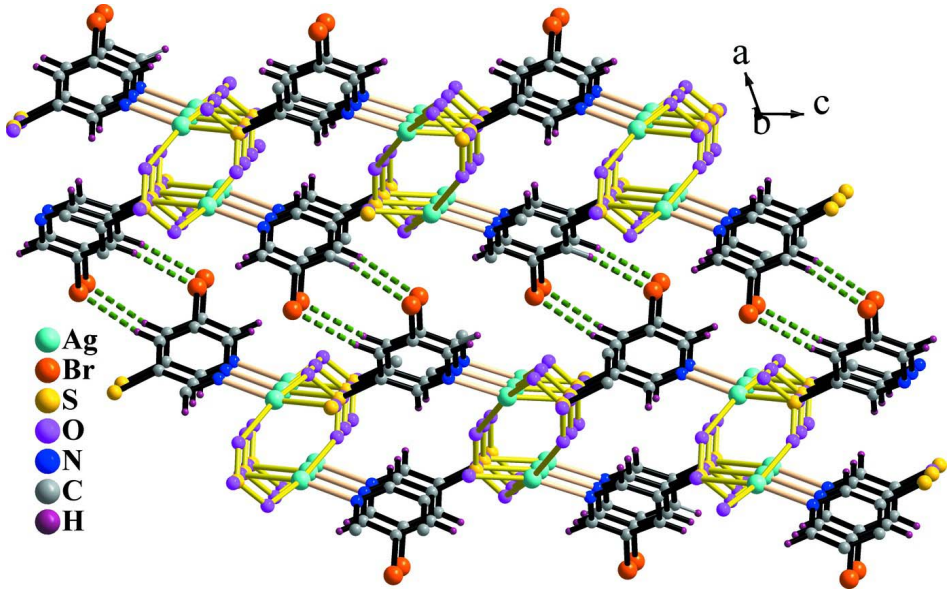

Figure 3

Three-dimensional supramolecular network of **1** showing C3—H3···Br hydrogen-bonding interactions (green dashed lines).

Poly[(μ_4-5-bromopyridine-3-sulfonato)silver(I)]

Crystal data

$[Ag(C_5H_3BrNO_3S)]$
M_r = 344.92
Monoclinic, $C2/c$
a = 20.103 (3) Å
b = 5.0634 (9) Å
c = 16.036 (3) Å
β = 110.142 (2)°
V = 1532.5 (5) Å^3
Z = 8
$F(000)$ = 1296
D_x = 2.990 Mg m^{-3}
Melting point: not measured K
Mo $K\alpha$ radiation, λ = 0.71073 Å
θ = 2.2–25°
μ = 8.08 mm^{-1}
T = 296 K
Blcok, colorless
0.20 × 0.18 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2008*a*)
T_{min} = 0.512, T_{max} = 0.746
4188 measured reflections
1310 independent reflections
1204 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 25.0°, θ_{min} = 2.2°
h = −23→23
k = −6→6
l = −19→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.152
S = 1.01
1310 reflections
109 parameters
2 restraints
0 constraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.132P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.009
$\Delta\rho_{max}$ = 0.88 e Å^{-3}
$\Delta\rho_{min}$ = −1.72 e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Ag1	0.325354 (14)	0.79247 (6)	0.004298 (16)	0.03990 (8)
Br1	0.505370 (16)	0.92599 (7)	0.38247 (2)	0.03684 (10)
S1	0.31936 (4)	0.26125 (15)	0.13294 (5)	0.0237 (2)
N1	0.36109 (14)	0.3610 (6)	0.39356 (17)	0.0280 (7)

O1	0.36615 (13)	0.3588 (6)	0.08721 (15)	0.0417 (6)
O2	0.25004 (15)	0.3786 (6)	0.10181 (17)	0.0468 (8)
O3	0.31813 (13)	−0.0272 (5)	0.13609 (16)	0.0365 (7)
C1	0.33643 (16)	0.2719 (7)	0.3129 (2)	0.0252 (8)
H1A	0.3026	0.1385	0.2993	0.030*
C2	0.35925 (15)	0.3708 (6)	0.24497 (18)	0.0201 (7)
C3	0.40983 (15)	0.5648 (7)	0.26565 (19)	0.0237 (8)
H3A	0.4265	0.6324	0.2226	0.028*
C4	0.43547 (15)	0.6575 (7)	0.3514 (2)	0.0269 (8)
C5	0.41094 (16)	0.5505 (7)	0.4151 (2)	0.0285 (9)
H5A	0.4292	0.6107	0.4733	0.034*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.05584 (14)	0.04198 (16)	0.02679 (13)	0.01450 (12)	0.02051 (11)	0.00050 (10)
Br1	0.03597 (16)	0.0366 (2)	0.03715 (17)	−0.00643 (15)	0.01160 (13)	−0.00657 (15)
S1	0.0333 (3)	0.0199 (4)	0.0160 (3)	0.0027 (3)	0.0060 (3)	−0.0009 (3)
N1	0.0360 (12)	0.0253 (13)	0.0241 (11)	−0.0001 (12)	0.0120 (9)	−0.0010 (11)
O1	0.0639 (13)	0.0433 (10)	0.0244 (9)	−0.0083 (12)	0.0236 (9)	0.0060 (9)
O2	0.0498 (13)	0.0449 (14)	0.0294 (12)	0.0224 (13)	−0.0071 (11)	−0.0057 (12)
O3	0.0608 (13)	0.0185 (11)	0.0306 (10)	−0.0012 (11)	0.0164 (10)	−0.0084 (9)
C1	0.0207 (11)	0.0258 (16)	0.0285 (14)	−0.0027 (12)	0.0075 (11)	0.0065 (12)
C2	0.0308 (12)	0.0156 (13)	0.0149 (11)	0.0024 (12)	0.0091 (10)	0.0012 (11)
C3	0.0241 (11)	0.0291 (17)	0.0216 (12)	0.0056 (12)	0.0126 (10)	0.0014 (12)
C4	0.0160 (11)	0.0322 (17)	0.0297 (15)	0.0008 (14)	0.0044 (11)	0.0033 (14)
C5	0.0294 (13)	0.0385 (19)	0.0159 (13)	0.0021 (15)	0.0056 (11)	0.0012 (13)

Geometric parameters (Å, º)

Ag1—N1^{i}	2.270 (3)	N1—C5	1.344 (4)
Ag1—O3^{ii}	2.352 (3)	N1—Ag1^{iv}	2.270 (3)
Ag1—O2^{iii}	2.488 (3)	O2—Ag1^{iii}	2.488 (3)
Ag1—O1	2.552 (3)	O3—Ag1^{v}	2.352 (3)
Ag1—Ag1^{iii}	3.0159 (8)	C1—C2	1.411 (5)
Br1—C4	1.894 (3)	C1—H1A	0.9300
S1—O2	1.437 (3)	C2—C3	1.370 (4)
S1—O3	1.462 (3)	C3—C4	1.374 (4)
S1—O1	1.463 (3)	C3—H3A	0.9300
S1—C2	1.785 (3)	C4—C5	1.388 (5)
N1—C1	1.297 (4)	C5—H5A	0.9300
N1^{i}—Ag1—O3^{ii}	165.92 (9)	S1—O1—Ag1	113.87 (15)
N1^{i}—Ag1—O2^{iii}	88.66 (10)	S1—O2—Ag1^{iii}	143.5 (2)
O3^{ii}—Ag1—O2^{iii}	98.22 (9)	S1—O3—Ag1^{v}	110.48 (15)
N1^{i}—Ag1—O1	88.93 (10)	N1—C1—C2	122.2 (3)
O3^{ii}—Ag1—O1	88.52 (8)	N1—C1—H1A	118.9
O2^{iii}—Ag1—O1	160.60 (9)	C2—C1—H1A	118.9

N1^{i}—Ag1—Ag1^{iii}	119.93 (7)	C3—C2—C1	118.6 (3)
O3^{ii}—Ag1—Ag1^{iii}	74.01 (6)	C3—C2—S1	120.3 (2)
O2^{iii}—Ag1—Ag1^{iii}	72.45 (7)	C1—C2—S1	120.9 (2)
O1—Ag1—Ag1^{iii}	92.22 (6)	C2—C3—C4	118.6 (3)
O2—S1—O3	113.53 (16)	C2—C3—H3A	120.7
O2—S1—O1	113.59 (17)	C4—C3—H3A	120.7
O3—S1—O1	112.07 (17)	C3—C4—C5	119.8 (3)
O2—S1—C2	105.49 (15)	C3—C4—Br1	119.8 (3)
O3—S1—C2	106.43 (14)	C5—C4—Br1	120.4 (2)
O1—S1—C2	104.83 (15)	N1—C5—C4	120.8 (3)
C1—N1—C5	120.0 (3)	N1—C5—H5A	119.6
C1—N1—Ag1^{iv}	123.1 (2)	C4—C5—H5A	119.6
C5—N1—Ag1^{iv}	116.9 (2)		

Symmetry codes: (i) x, $-y+1$, $z-1/2$; (ii) x, $y+1$, z; (iii) $-x+1/2$, $-y+3/2$, $-z$; (iv) x, $-y+1$, $z+1/2$; (v) x, $y-1$, z.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3*A*···Br1^{vi}	0.93	2.92	3.832 (3)	168

Symmetry code: (vi) $-x+1$, y, $-z+1/2$.