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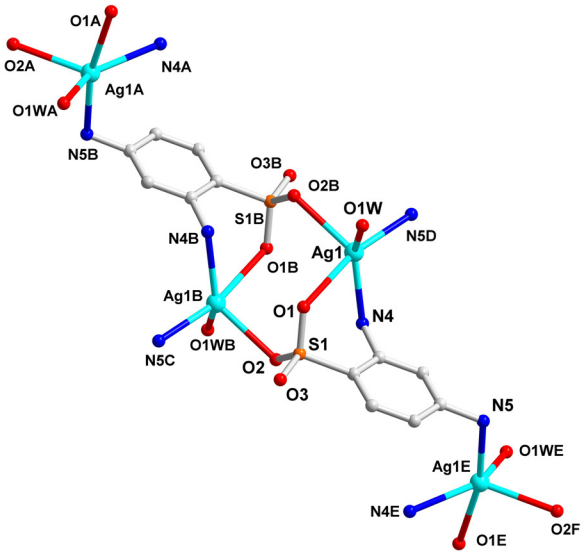
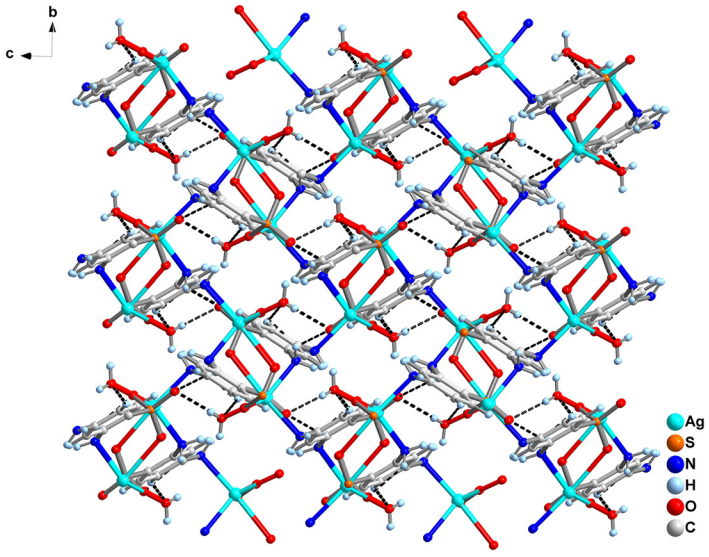
Crystal structure of poly[aqua(μ_3-2,4-diamino-benzenesulfonato-κ^4*N*:*N*′,*O*:*O*′)silver(I)], $C_{12}H_{18}O_8N_4S_2Ag_2$





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Abstract: $C_{12}H_{18}O_8N_4S_2Ag_2$, monoclinic, $P2_1/c$ (no. 14), a = 10.7841(10) Å, b = 8.0140(5) Å, c = 11.7220(11) Å, β = 117.278(11)°, V = 900.40(16) Å^3, Z = 2, $R_{gt}(F)$ = 0.0279, $wR_{ref}(F^2)$ = 0.0627, T = 293(2) K.

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Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.12 × 0.10 × 0.09 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	2.46 mm^{-1}
Diffractometer, scan mode:	Xcalibur, ω
θ_{max}, completeness:	25.0°, 98%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	3156, 1547, 0.027
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 1338
$N(param)_{refined}$:	144
Programs:	CrysAlis^{PRO} [1], SHELX [2, 4], WinGX/ORTEP [3], Diamond [5]

Source of material

The $AgNO_3$ (0.0850 g, 0.5 mmol) and 2,4-diamino-benzenesulfonic acid (0.0940 g, 0.5 mmol) were added to the 20 mL H_2O/CH_3OH (*v*/*v*, 1/3), it was stirred for 15 min in the air. The filtrate was kept at 293 K to obtain block crystals.

Experimental details

Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms.

Ze-Rong He and Han-Lin Zhao contributed equally to this work.

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Ag1	0.85713 (3)	0.28320 (4)	0.43692 (3)	0.03854 (17)
C1	0.6175 (4)	0.5703 (4)	0.3396 (3)	0.0221 (8)
C2	0.6603 (4)	0.6618 (4)	0.4535 (3)	0.0219 (7)
C3	0.5607 (4)	0.7173 (4)	0.4886 (3)	0.0237 (8)
H3	0.589172	0.777680	0.564279	0.028*
C4	0.4221 (4)	0.6855 (4)	0.4148 (3)	0.0267 (8)
H4	0.357038	0.725076	0.439759	0.032*
C5	0.3782 (4)	0.5933 (4)	0.3017 (3)	0.0247 (8)
C6	0.4761 (4)	0.5374 (4)	0.2657 (3)	0.0267 (8)
H6	0.446982	0.476250	0.190355	0.032*
H1WA	0.961 (3)	0.192 (6)	0.680 (4)	0.057 (17)*
H1WB	0.882 (5)	0.054 (3)	0.637 (5)	0.064 (16)*
H5A	0.185 (5)	0.570 (5)	0.258 (4)	0.039 (13)*
H5B	0.219 (5)	0.480 (6)	0.180 (5)	0.066 (17)*
N4	0.7168 (3)	0.5045 (4)	0.3049 (3)	0.0297 (7)
H4A	0.772889	0.586922	0.306352	0.036*
H4B	0.672109	0.467722	0.224399	0.036*
N5	0.2358 (4)	0.5648 (4)	0.2233 (3)	0.0321 (8)
O1	0.9047 (3)	0.5395 (3)	0.6006 (2)	0.0386 (7)
O1W	0.8818 (4)	0.1574 (4)	0.6307 (3)	0.0411 (7)
O2	0.8897 (3)	0.7784 (3)	0.4699 (3)	0.0356 (6)
O3	0.8491 (3)	0.8083 (3)	0.6552 (3)	0.0392 (7)
S1	0.83822 (10)	0.69982 (10)	0.55231 (8)	0.0256 (2)

Comment

As is shown in the left part of the picture, the Ag1 is five-coordinated by two nitrogen atoms and three oxygen atoms. The two nitrogen atoms come from different 2,4-diamino-benzenesulfonato (aneS) ligands, three oxygen atoms come from two aneS ligands and one water molecule desperately. Among them, the N4 and O1 atoms belong to the one aneS ligand. Thus, there is a $Ag_2O_4S_2$ polygon. The bond distances of Ag–N range from 2.384(3) to 2.432(3) Å and the distances of Ag–O range from 2.386(3) to 2.482(3) Å. The coordination mode leads to a three-dimensional structure [6–8] (*cf*. the right of picture) (symmetry codes: A = 1 + *x*, 1/2 – *y*, 1/2 + *z*; B = 2 – *x*, 1 – *y*, 1 – *z*; C = 1 + *x*, 3/2 – *y*, 1/2 + *z*; D = 1 – *x*, –1/2 + *y*, 1/2 – *z*; E = 1 – *x*, 1/2 + *y*, 1/2 – *z*; F = –1 + *x*, 3/2 – *y*, –1/2 + *z*).

Author contribution: Ze-Rong He and Han-Lin Zhao contributed equally to this work. All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.

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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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