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Crystal structure of *catena*-poly[aqua(μ_4 -piperazine-1,4-bis(2-hydroxypropanesulfonato- $\kappa^8 O, O':O', N:N', O'':O'', O''')$)silver(I)], $C_{10}H_{24}Ag_2N_2O_{10}S_2$

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Abstract

$C_{10}H_{24}Ag_2N_2O_{10}S_2$, triclinic, $P\bar{1}$ (no. 2), $a = 6.9547(9)$ Å, $b = 8.4684(12)$ Å, $c = 8.9563(15)$ Å, $\alpha = 117.888(15)^\circ$, $\beta = 101.740(13)^\circ$, $\gamma = 93.026(11)^\circ$, $V = 449.75(13)$ Å³, $Z = 1$, $R_{gt}(F) = 0.0365$, $wR_{ref}(F^2) = 0.0858$, $T = 293(2)$ K.

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Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of materials

The Ag_2CO_3 (0.014 g, 0.05 mmol) and piperazine-1, 4-bis(2-hydroxypropanesulfonic acid) (0.040 g, 0.1 mmol) in 15 mL

Table 1: Data collection and handling.

Crystal:	Block, colorless
Size:	$0.15 \times 0.12 \times 0.12$ mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	2.46 mm^{-1}
Diffractometer, scan mode:	XtaLAB Pro, ω -scans
$\theta_{\max}$, completeness:	29.8° , 88% (up to 25.0° , >99%)
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	6174, 2258, 0.055
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1846
$N(\text{param})_{\text{refined}}$:	123
Programs:	CrysAlis ^{PRO} [1], SHELX [2, 4], WinGX and ORTEP [3]

H_2O/CH_3CN (2:1, v/v) reacted for 25 minutes. The filtrate was kept at room temperature to produce colourless block crystals after several days.

Experimental details

Data were collected via CrysAlis^{PRO} 1.171.39.7e [1], the structure of crystal was determined by SHELXT [2] within WinGX [3] and refined by SHELXL [4].

Comment

As illustrated in the left part of the figure, the structure of crystal comprises a unique Ag(I) center, one half of a piperazine-1, 4-bis(2-hydroxypropanesulfonato) ligand (pipS) and one water molecule. The Ag1 is five-coordinated by one nitrogen atom and three oxygen atoms from different pipS

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
Ag1	−0.00140(5)	0.65550(4)	0.76175(4)	0.04218(12)
N1	0.0416(4)	0.4230(4)	0.8290(3)	0.0231(5)
O1	0.4987(5)	−0.0031(4)	0.2480(4)	0.0476(8)
O2	0.3240(4)	0.2243(4)	0.2225(4)	0.0409(7)
O1W	0.1604(4)	0.9530(4)	0.8671(4)	0.0396(6)
H1A	0.270933	0.952296	0.834559	0.059*
H1B	0.201681	1.009151	0.981200	0.059*
O3	0.6039(4)	0.3107(4)	0.4697(4)	0.0443(7)
O4	0.1815(4)	0.4387(3)	0.5520(3)	0.0317(5)
S1	0.43913(13)	0.17156(11)	0.34130(11)	0.02623(18)
H10	0.297(12)	0.513(12)	0.579(11)	0.12(3)*
C1	0.2790(5)	0.1422(5)	0.4605(4)	0.0269(7)
H1	0.149678	0.077698	0.380436	0.032*
H2	0.332499	0.066785	0.507980	0.032*
C2	0.2504(5)	0.3184(4)	0.6103(4)	0.0239(6)
H3	0.375306	0.376693	0.702347	0.029*
C3	0.0892(5)	0.2688(4)	0.6814(4)	0.0259(7)
H4	−0.031559	0.208768	0.587169	0.031*
H5	0.131646	0.182514	0.718458	0.031*
C4	0.2008(5)	0.4916(5)	0.9915(4)	0.0272(7)
H6	0.322808	0.536993	0.977145	0.033*
H7	0.225409	0.393490	1.016294	0.033*
C5	0.1419(5)	0.6418(5)	1.1424(4)	0.0273(7)
H8	0.249497	0.687387	1.247776	0.033*
H9	0.120434	0.740797	1.118380	0.033*

ligands including two oxygen atoms from the same ligand and one oxygen atom from water to construct a chain structure [5]. At the same time, the structure contains OH⋯O interactions connecting adjacent chains [6] and the Ag₂O₂ moiety is

well known [7] (*cf.* right part of the figure). (symmetry codes: A = −*x*, 1 − *y*, 1 − *z*; B = −*x*, 1 − *y*, 2 − *z*; C = *x*, *y*, 1 + *z*).

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