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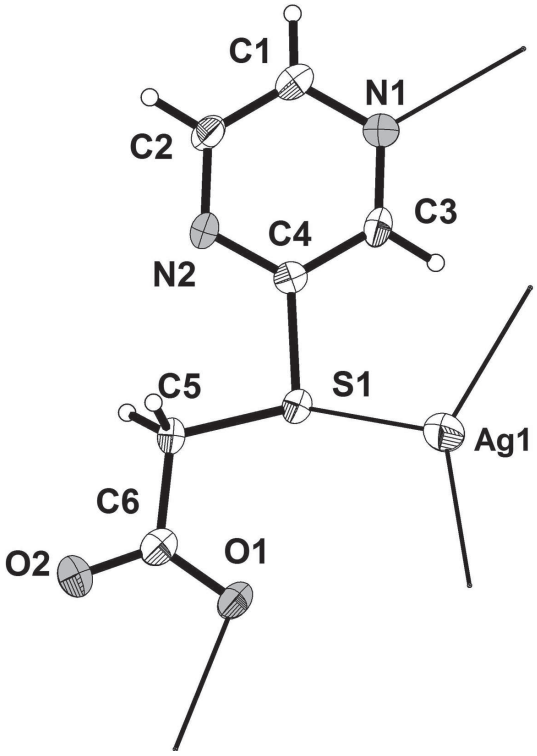
Crystal structure of poly[(μ_3-2-(pyrazin-2-ylthio)acetato-κ^3*N*:*O*:*S*)silver(I)], $C_6H_5AgN_2O_2S$



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Abstract

$C_6H_5AgN_2O_2S$, monoclinic, $P2_1/c$ (no. 14), $a = 10.0546(4)$ Å, $b = 10.7329(5)$ Å, $c = 6.9044(7)$ Å, $\beta = 99.255(6)°$, $V = 735.39(9)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0422$, $wR_{ref}(F^2) = 0.0967$, $T = 293(2)$ K.

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Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.20 × 0.18 × 0.16 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	29.7 cm^{-1}
Diffractometer, scan mode:	Xcalibur Eos, ω scans
$2\theta_{max}$, completeness:	50°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	2661, 1290, 0.036
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 1067
$N(param)_{refined}$:	109
Programs:	SHELX [1], CrysAlis^{PRO} [2]

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Ag1	1.07998(5)	0.02959(4)	0.82878(9)	0.0419(2)
S1	0.84968(14)	−0.00186(14)	0.6007(2)	0.0260(4)
O1	0.8937(3)	−0.2611(4)	0.6126(6)	0.0326(11)
O2	0.6941(4)	−0.3273(4)	0.6726(7)	0.0377(11)
N1	0.7864(4)	0.3621(4)	0.6046(7)	0.0236(11)
N2	0.6381(4)	0.1448(4)	0.6435(7)	0.0260(12)
C3	0.8381(5)	0.2502(5)	0.5909(8)	0.0244(14)
H3	0.9259	0.2436	0.5653	0.029*
C2	0.6566(5)	0.3665(6)	0.6347(9)	0.0309(15)
H2	0.6150	0.4433	0.6431	0.037*
C5	0.7238(5)	−0.1110(5)	0.6557(9)	0.0251(14)
H5A	0.7039	−0.0947	0.7862	0.030*
H5B	0.6414	−0.0999	0.5629	0.030*
C4	0.7665(5)	0.1414(5)	0.6134(9)	0.0240(13)
C6	0.7733(5)	−0.2448(5)	0.6447(9)	0.0268(14)
C1	0.5854(5)	0.2583(5)	0.6531(9)	0.0273(14)
H1	0.4963	0.2648	0.6731	0.033*

The asymmetric unit of the title crystal structure is shown in the figure. Tables 1 and 2 contain details of the measurement method and a list of the atoms including atomic coordinates and displacement parameters.

Source of materials

An excess of an aqueous NH_3 solution was added dropwise to a suspension of Ag_2O (0.023 g, 0.1 mmol) in MeOH/H_2O (8 mL, 1:1 *v*/*v*), and the mixture was stirred for 15 min. 2-(Pyrazin-2-ylthio)acetic acid (0.018 g, 0.1 mmol) was then

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slowly added, and stirring was continued for another 30 min. The resultant colorless solution was allowed to stand in the dark at room temperature for a week. Colorless prism crystals of the title complex were obtained.

Experimental details

Absorption corrections were applied by using the multi-scan method [2]. Hydrogen atoms were located in difference electron density maps, and treated as riding atoms. The U_{iso} values of the hydrogen atoms were set to $1.2U_{eq}$(C).

Comment

In the past few decades, the syntheses of silver(I) complexes attracted great interest because silver(I) principally is known for short Ag$\cdots$Ag contacts. Furthermore Ag(I) has a high affinity for hard donor atoms such as nitrogen, oxygen or sulfur atoms, being a favorable and fashionable building block for MOFs [3–7]. With the aim of constructing unusual coordination architectures, we have engaged in the synthesis of coordination polymer based on 2-(pyrazin-2-ylthio)acetic acid (HL) with silver HL which comprise a pyrazinyl moiety and a carboxylic groups, may show a rich variety of coordination modes with nitrogen, oxygen and sulfur atoms and help to construct novel coordination polymers. On the other hand, it is a flexible ligand because the carboxylic groups can rotate aroud the C—S single bond.

Single crystal structure analysis reveals that the title structure consists of one crystallographically unique Ag(I) atom, and one L^- ligand. All geomtric parameters within the L^- ligand are in the expected ranges. The central Ag1 cation adopts Y-shaped coordination with one nitrogen atom [Ag1—N1 = 2.247(4) Å], one oxygen atom [Ag1—O1 = 2.291(4) Å] and one sulfur atom [Ag1—S1 = 2.604(1) Å] (*cf*. the figure). Both Ag—O and Ag—N bonds are within normal ranges [8]. Each L^- ligand links adjacent Ag(I) centers to form infinite double chains along the *b* axis. Such chains are further interconnected through the weak Ag$\cdots$Ag contact (Ag1$\cdots$Ag1 = 3.131(9) Å) to give rise to a sheet structure.

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