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Crystal structure of poly[aqua(μ_2 -2-amino-1,4-benzenedisulfonato- $\kappa^2 O:O'$)bis(μ_2 -pyrazin- $\kappa^2 N:N'$)silver(I)], $C_{14}H_{16}Ag_2N_5O_8S_2$

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Abstract

$C_{14}H_{16}Ag_2N_5O_8S_2$, triclinic, $P\bar{1}$ (no. 2), $a = 7.1305(7)$ Å, $b = 7.3558(6)$ Å, $c = 9.8517(10)$ Å, $\alpha = 73.816(9)^\circ$, $\beta = 82.648(8)^\circ$, $\gamma = 88.080(7)^\circ$, $V = 492.17(8)$ Å³, $Z = 1$, $R_{gt}(F) = 0.0491$, $wR_{ref}(F^2) = 0.1515$, $T = 293(2)$ K.

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A part of the molecular structure is shown in the left part of the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

A mixture of $AgNO_3$ (0.170 g, 1 mmol) and 2-amino-1,4-benzenedisulfonic acid (0.126 g, 0.5 mmol) in 10 mL H_2O /methanol (1:1, v/v) reacted for 25 min. The ammonia

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Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	$0.16 \times 0.14 \times 0.11$ mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	2.26 mm^{-1}
Diffractometer, scan mode:	XtaLAB Pro, ω
$\theta_{\max}$, completeness:	29.7° , 99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	6251, 2409, 0.038
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2040
$N(\text{param})_{\text{refined}}$:	151
Programs:	CrysAlis ^{PRO} [1], SHELX [2, 3], WinGX/ORTEP [4]

solution was dropwise added into reaction system to make it clear. The pyrazine (0.040 g, 0.5 mmol) was put into solution. The colourless single crystals were obtained by evaporating after three weeks.

Experimental details

The data of single crystal were collected using the CrysAlis^{PRO} software [1], and the structure was solved by SHELXT [2] using WinGX [3], and refined by SHELXL [4]. All hydrogen atoms were include with $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C)$, $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(N)$ and $U_{\text{iso}}(H) = 1.5U_{\text{eq}}(O)$. The graphics were finished by Diamond [5]. Last but not least, the amino group (N1) is disordered.

Comment

With the rapid development of inorganic chemistry, the coordination polymers including silver have given rise to extensive

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	0.73938(6)	0.64445(9)	0.79125(7)	0.0448(2)
C1	0.1254(8)	0.7057(10)	0.8924(7)	0.0320(13)
H1	0.049888	0.749298	0.960981	0.038*
C2	0.3199(9)	0.7089(10)	0.8880(8)	0.0364(14)
H2	0.372319	0.755419	0.953399	0.044*
C3	0.3525(8)	0.5829(9)	0.7003(7)	0.0311(13)
H3	0.428404	0.538806	0.632145	0.037*
C4	0.1566(8)	0.5805(9)	0.7034(7)	0.0299(12)
H4	0.104272	0.535797	0.637053	0.036*
C5	0.8916(8)	0.0803(8)	0.5942(6)	0.0273(11)
C6	1.0884(9)	0.0964(9)	0.5803(7)	0.0297(12)
C7	1.1956(8)	0.0134(9)	0.4863(7)	0.0290(12)
H7	1.326789	0.020076	0.476666	0.035*
N1 ^a	1.1735(15)	0.1777(17)	0.6581(13)	0.036(3)
H1A ^a	1.294994	0.179235	0.650531	0.044*
H1B ^a	1.108004	0.229562	0.716704	0.044*
N2	0.4337(6)	0.6471(7)	0.7926(6)	0.0283(10)
N3	0.0433(6)	0.6410(7)	0.7997(6)	0.0272(10)
S1	0.7479(2)	0.1977(2)	0.70530(18)	0.0331(4)
O1	0.8244(8)	0.1465(9)	0.8401(6)	0.0524(14)
O2	0.7656(8)	0.3985(7)	0.6339(6)	0.0450(12)
O3	0.5573(7)	0.1268(9)	0.7185(7)	0.0524(15)
O1W	0.3053(9)	0.1974(10)	0.9601(7)	0.0517(14)
H1WA	0.268(17)	0.066(17)	1.035(13)	0.078*
H1WB	0.354(18)	0.193(17)	0.886(13)	0.078*

^aOccupancy: 0.5.

attention of plenty of chemists because of their comprehensive applications such as luminescence [6] and so on.

As is shown in the left part of figure, the silver(I) atom is four-coordinated by two nitrogen atoms from two pyrazine ligands, two oxygen atoms from water and the oxygen of a sulfonate group desperately to form an irregular plane. Its bond lengths and angles are similar to other polymers [7] except the

distance of Ag1—O1WD is slightly longer than others (Ag1—O1WD = 2.9741(3) Å). In accord with the literature the N₂O₂-coordination is distorted from planarity [8]. At the same time, the existence of intramolecular interactions such as NH...O, CH...O make it become a three-dimensional structure (*cf.* right part of the figure).

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