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Crystal structure of *catena*-poly[(μ_2 -3-amino-benzenedisulfonato- $\kappa^2 N:O$)-bis (3-methyl-isoquinoline- κN)silver(I)], $C_{26}H_{24}N_3O_3SAg$

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Abstract

$C_{26}H_{24}N_3O_3SAg$, monoclinic, $P2_1/c$ (no. 14), $a = 13.1936(9)$ Å, $b = 11.0544(7)$ Å, $c = 16.3653(9)$ Å, $\beta = 99.214(6)^\circ$, $V = 2356.0(3)$ Å³, $Z = 4$, $R_{gt}(F) = 0.0495$, $wR_{ref}(F^2) = 0.1080$, $T = 293(2)$ 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:	0.20 × 0.15 × 0.11 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.98 mm ⁻¹
Diffractometer, scan mode:	Xcalibur, φ and ω
θ_{max} , completeness:	29.3°, 99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int} :	10,272, 5475, 0.041
Criterion for I_{obs} , $N(hkl)_{gt}$:	$I_{obs} > 2 \sigma(I_{obs})$, 3263
$N(param)_{refined}$:	315
Programs:	CrysAlis ^{PRO} [1], SHELX [2, 4], WinGX/ORTEP [3], Diamond [5]

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

Atom	<i>x</i>	<i>y</i>	<i>z</i>	U_{iso}^*/U_{eq}
Ag1	0.78252 (3)	0.41021 (3)	0.47837 (2)	0.05579 (14)
S1	0.92810 (8)	0.15306 (8)	0.16332 (5)	0.0391 (3)
O1	0.8200 (2)	0.1533 (3)	0.12837 (15)	0.0603 (8)
N1	0.9456 (3)	0.3536 (3)	0.44953 (18)	0.0429 (9)
H1A	0.977 (3)	0.408 (3)	0.428 (2)	0.051*
H1B	0.976 (3)	0.340 (4)	0.4952 (12)	0.051*
O2	0.9788 (3)	0.2607 (3)	0.14550 (15)	0.0653 (9)
N2	0.6650 (3)	0.2701 (3)	0.4187 (2)	0.0456 (8)

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Table 2: (continued)

Atom	x	y	z	<i>U</i> _{iso} */ <i>U</i> _{eq}
O3	0.9766 (3)	0.0441 (3)	0.14198 (16)	0.0722 (10)
N3	0.7536 (3)	0.6072 (3)	0.4994 (2)	0.0478 (9)
C2	0.9405 (3)	0.2521 (3)	0.31745 (19)	0.0324 (8)
H2	0.9462	0.3262	0.2917	0.039*
C1	0.9306 (3)	0.1475 (3)	0.27163 (19)	0.0307 (8)
C3	0.9418 (3)	0.2468 (3)	0.40205 (19)	0.0342 (9)
C4	0.9326 (3)	0.1361 (3)	0.4390 (2)	0.0395 (9)
H4	0.9329	0.1317	0.4958	0.047*
C6	0.9222 (3)	0.0371 (3)	0.3087 (2)	0.0376 (9)
H6	0.9160	−0.0335	0.2773	0.045*
C7	0.6819 (3)	0.2071 (3)	0.3542 (2)	0.0440 (10)
H7	0.7375	0.2292	0.3290	0.053*
C8	0.6223 (3)	0.1093 (3)	0.3207 (2)	0.0450 (10)
C18	0.7805 (3)	0.7791 (3)	0.5895 (2)	0.0418 (10)
C5	0.9231 (3)	0.0323 (3)	0.3923 (2)	0.0414 (10)
H5	0.9172	−0.0420	0.4178	0.050*
C23	0.7494 (3)	0.8564 (3)	0.5223 (3)	0.0439 (10)
C17	0.7815 (3)	0.6560 (4)	0.5726 (2)	0.0467 (10)
H17	0.8036	0.6041	0.6166	0.056*
C13	0.5393 (3)	0.0763 (4)	0.3590 (3)	0.0504 (11)
C19	0.8120 (3)	0.8275 (4)	0.6679 (3)	0.0570 (12)
H19	0.8314	0.7763	0.7128	0.068*
C9	0.6449 (4)	0.0423 (4)	0.2520 (3)	0.0562 (12)
H9	0.6999	0.0643	0.2261	0.067*
C25	0.7201 (4)	0.6836 (4)	0.4343 (2)	0.0545 (11)
C22	0.7505 (4)	0.9823 (4)	0.5366 (3)	0.0588 (12)
H22	0.7282	1.0347	0.4930	0.071*
C15	0.5823 (4)	0.2392 (4)	0.4545 (3)	0.0547 (11)
C14	0.5205 (4)	0.1457 (4)	0.4258 (3)	0.0622 (12)
H14	0.4642	0.1275	0.4514	0.075*
C20	0.8146 (4)	0.9498 (5)	0.6791 (3)	0.0679 (14)
H20	0.8372	0.9820	0.7313	0.081*
C21	0.7832 (4)	1.0271 (4)	0.6120 (4)	0.0659 (14)
H21	0.7852	1.1104	0.6200	0.079*
C24	0.7189 (4)	0.8046 (4)	0.4450 (3)	0.0580 (12)
H24	0.6972	0.8542	0.3997	0.070*
C10	0.5864 (5)	−0.0531 (5)	0.2248 (3)	0.0755 (15)
H10	0.6002	−0.0964	0.1791	0.091*
C11	0.5057 (5)	−0.0875 (5)	0.2642 (4)	0.0817 (17)
H11	0.4674	−0.1555	0.2453	0.098*
C12	0.4810 (4)	−0.0257 (5)	0.3289 (3)	0.0732 (15)
H12	0.4258	−0.0502	0.3537	0.088*
C16	0.5663 (4)	0.3162 (5)	0.5276 (3)	0.0861 (17)
H16A	0.6246	0.3085	0.5706	0.129*
H16B	0.5057	0.2898	0.5480	0.129*
H16C	0.5584	0.3993	0.5107	0.129*
C26	0.6853 (6)	0.6236 (5)	0.3528 (3)	0.104 (2)
H26A	0.7419	0.5812	0.3358	0.155*
H26B	0.6603	0.6837	0.3122	0.155*
H26C	0.6313	0.5673	0.3581	0.155*

Source of material

The AgNO₃ (0.085 g, 0.5 mmol) and 3-amino-benzenesulfonic acid (0.866 g, 0.5 mmol) were added to the distilled

water (15 mL). Then 3-methyl-isoquinoline was added to the reaction system. It was stirred for 30 min in the air. The filtrate was maintained at room temperature in a dark room to produce block colorless crystals after several weeks.

Experimental details

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

Comment

As is depicted in the left part of the picture, the Ag1 is four-coordinated by three nitrogen atoms and one oxygen atom. The two nitrogen atoms coming from two 3-methyl-isoquinoline ligands and one nitrogen atom coming from a 3-amino-benzenesulfonic acid (abeS) ligand. One oxygen atom of another abeS ligand is coordinated (left part of the figure). The bond distances of Ag–N range from 2.247(3) to 2.360(4) Å [6]. Its structure is one-dimensional chain, well known in this class of structures [7] (*cf.* right part of the picture). (symmetry codes: A = x , $1/2 - y$, $1/2 + z$; B = x , $1/2 - y$, $-1/2 + z$; C = x , $1/2 - y$, $-1/2 + z$).

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