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The crystal structure of poly[(μ_5 -2-((5-bromo-3-formyl-2-hydroxybenzylidene)amino)benzenesulfonato- κ^6 O:O:O,O':O':O'') sodium(I)], $C_{13}H_9O_4NSBrNa$

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.13 × 0.12 × 0.11 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	3.25 mm ⁻¹
Diffractometer, scan mode:	SuperNova, ω -scans
$\theta_{\max}$, completeness:	29.6°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	6341, 3192, 0.033
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2560
$N(\text{param})_{\text{refined}}$:	191
Programs:	CrysAlis ^{PRO} [1], OLEX2 [2], SHELX [3], DIAMOND [4]

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Abstract

$C_{13}H_9O_4NSBrNa$, monoclinic, $P2_1/c$ (no. 14), $a = 26.1300(15)$ Å, $b = 6.1547(4)$ Å, $c = 8.3908(5)$ Å, $\beta = 91.760(5)^\circ$, $V = 1348.79(14)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0402$, $wR_{\text{ref}}(F^2) = 0.0866$, $T = 100$ K.

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The crystal structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of materials

The title Na(I) complex has synthesized by one-pot method as following: at room temperature, 0.1732 g 3-aminobenzene sulfonic acid (1.0 mmol), 0.2010 g 5-bromosalicylaldehyde (1.0 mmol) and 0.040 g sodium hydrate (1.0 mmol) were dissolved into 20 mL water-ethanol (v:v = 2:3) solution with stirring. Then the mixture was heated to 75 °C and kept this temperature with stirring for 3 h. After cooled, the reactant

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

Atom	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	0.95834(2)	0.75948(5)	1.18744(4)	0.02245(11)
S1	0.56498(3)	0.63391(11)	0.55205(8)	0.00742(16)
Na1	0.51919(4)	0.36014(17)	0.19535(12)	0.0102(2)
O2	0.56013(7)	0.4782(3)	0.6817(2)	0.0110(4)
O4	0.52533(8)	0.8021(3)	0.5577(2)	0.0104(4)
O3	0.56692(8)	0.5338(3)	0.3962(2)	0.0132(4)
O1	0.80837(9)	0.2943(3)	0.7500(3)	0.0242(5)
H1	0.784166	0.373528	0.725445	0.036*
N1	0.75357(9)	0.6446(4)	0.7420(3)	0.0125(5)
C5	0.90891(11)	0.6100(5)	1.0589(3)	0.0153(6)
C6	0.86583(12)	0.7173(5)	1.0055(3)	0.0136(6)
H6	0.859710	0.858379	1.039770	0.016*
C9	0.66484(11)	0.6611(4)	0.6549(3)	0.0089(6)
H9	0.660807	0.518975	0.689894	0.011*
C11	0.62950(11)	0.9825(4)	0.5282(3)	0.0114(6)
H11	0.601943	1.054603	0.479496	0.014*
C12	0.67647(12)	1.0841(5)	0.5471(3)	0.0118(6)
H12	0.680476	1.225636	0.510771	0.014*
C1	0.83083(11)	0.6158(5)	0.8994(3)	0.0120(6)
C4	0.91852(12)	0.3971(5)	1.0112(3)	0.0160(7)
H4	0.947672	0.324846	1.049232	0.019*
C10	0.62404(11)	0.7704(4)	0.5833(3)	0.0082(6)
C7	0.78669(11)	0.7342(5)	0.8368(3)	0.0122(6)
H7	0.782297	0.878535	0.866077	0.015*
C3	0.88468(12)	0.2950(5)	0.9076(4)	0.0169(7)
H3	0.891176	0.153582	0.874773	0.020*
C8	0.71204(11)	0.7647(4)	0.6744(3)	0.0114(6)
C13	0.71769(11)	0.9770(5)	0.6196(3)	0.0132(6)
H13	0.749130	1.046900	0.631732	0.016*
C2	0.84086(12)	0.4010(5)	0.8516(4)	0.0152(6)

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was filtered. The colorless crystals of the title compound were obtained by slow evaporation in 18 days.

Experimental details

The hydrogen atoms were positioned geometrically (C—H = 0.93 Å, O—H = 0.82 Å). Their U_{iso} values were set to $1.2U_{\text{eq}}$ (C—H) or $1.5U_{\text{eq}}$ (O—H) of the parent atoms.

Comment

Coordination polymers as an extensive group of materials have been received attention, because they exhibit structural diversities (one-dimensional, two-dimensional and three-dimensional) and potential applications in many fields such as magnetism, catalysis, antitumor activity, and fluorescence [5–9]. However, in contrast with transition metal complexes, light-weight metals such as sodium or magnesium coordination polymers are relatively unexplored. In order to enrich the content of coordination chemistry, we have been devoted to the synthesis and properties of light-weight metal complexes [10, 11].

In the title complex, all O atoms of SO₃[−] group of the sulfonate ligand are coordinated to Na(I) ion. All three O atoms adopt different coordination modes: monodentate (O3), bidentate (O2) and tridentate (O4) (*cf.* the figure). The Na—O bond distances are 2.326(2), 2.606(2), 2.546(2), 2.345(2), 2.416(2) and 2.386(2) Å, respectively. The title compound forms a two-dimensional layered structure by the bridging of SO₃[−] groups [12].

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