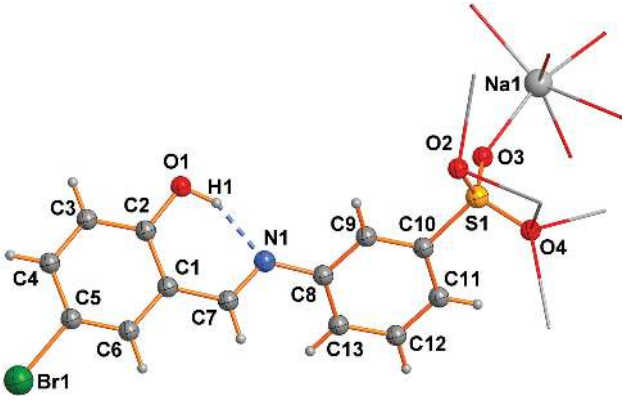
Xi-Shi Tai* and Li-Hua Wang

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



https://doi.org/10.1515/ncrs-2019-0114
Received February 14, 2019; accepted April 23, 2019; available online May 27, 2019

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, $\beta = 91.760(5)°$, $V = 1348.79(14)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0402$, $wR_{ref}(F^2) = 0.0866$, $T = 100$ K.

CCDC no.: 1910985

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

***Corresponding author: Xi-Shi Tai,** College of Chemistry and Chemical Engineering, Weifang University, Weifang, Shandong 261061, P.R. China, e-mail: taixs@wfu.edu.cn
Li-Hua Wang: College of Information and Engineering, Weifang University, Weifang, Shandong 261061, P.R. China

Table 1: Data collection and handling.

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

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{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)

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 $1.2U_{eq}$ (C—H) or $1.5U_{eq}$ (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 SO_3^- 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 SO_3^- groups [12].

Acknowledgements: This project was supported by the National Natural Science Foundation of China (no. 21171132), the Natural Science Foundation of Shandong (ZR2014BL003), the project of Shandong Province Higher Educational Science and Technology Program (J14LC01) and Science Foundation of Weifang.

References

1. Agilent Technologies: CrysAlis^{PRO} Software system, version 1.171.38.43f, Agilent Technologies UK Ltd, Oxford, UK (2011).
2. Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H.: OLEX2: a complete structure solution, refinement and analysis program. J. Appl. Cryst. **42** (2009) 339–341.
3. Sheldrick, G. M.: Crystal structure refinement with SHELXL. Acta Crystallogr. **C71** (2015) 3–8.
4. Brandenburg, K.: DIAMOND. Visual Crystal Structure Information System. Ver. 3.2. Crystal Impact, Bonn, Germany (2012).
5. Zhou, X.-J.; Liu, L.-L.; Tai, X.-S.; Zhang, H.: (3,3)-Connected three-dimentional supramolecular metal organic polyhedral based on nanometresized ligand with magnetism properties. Chem. Res. Chinese U. **34** (2018) 723–726.
6. Tai, X.-S.; Wang, X.: Synthesis, structural characterization and antitumor activity of a Ca(II) coordination polymer based on 4-formyl-1,3-benzenedisulfonate-2-furoic acid hydrazide ligands. Crystallogr. Rep. **62** (2017) 242–245.
7. Tai, X.-S.; Meng, Q.-G.; Liu, L.-L.: Synthesis, crystal structure and spectroscopic analysis of a new sodium coordination polymer. Open Chem. **14** (2016) 274–278.
8. Tai, X.-S.; Guo, Q.-Q.; Li, P.-F.; Liu, L.-L.: A Ca(II) coordination polymer of 2-carboxybenzaldehyde: Synthesis, crystal structure, and catalytic activity in oxidation of benzyl alcohol. Crystals **8** (2018) 150.
9. Song, T.-Q.; Dong, J.; Gao, H.-L.; Cui, J.-Z.: Three coordination polymers based on M2 (M = Co, Ni and Zn) clusters: structures, magnetic and fluorescent properties. Inorg. Chim. Acta **466** (2017) 393–397.
10. Tai, X.-S.; Yin, J.: Synthesis, crystal structure and antibacterial activity of Mg(II) complex $[Mg(H_2O)_6](4\text{-amino-3-methylbenzenesulfonate})_2$. Crystals **5** (2015) 294–301.
11. Tai, X.-S.; Zhang, Y.-P.; Zhao, W.-H.: Synthesis, crystal structure and antitumor activity of a dinuclear calcium complex based on 1,5-naphthalenedisulfonate and 2,2-bipyridine ligands. Res. Chem. Intermed. **41** (2015) 4339–4347.
12. Feng, Y. M.; Guo, H.-M.; Liu, Q. Y.; Tai, X.-S.: The crystal structure of poly[μ_2-aqua-(μ_2-2-naphthylamine-1-sulfonato-$\kappa^3O,O':O''$)sodium(I)], $C_{10}H_{10}NO_4SNa$. Z. Kristallogr. NCS **233** (2018) 603–604.