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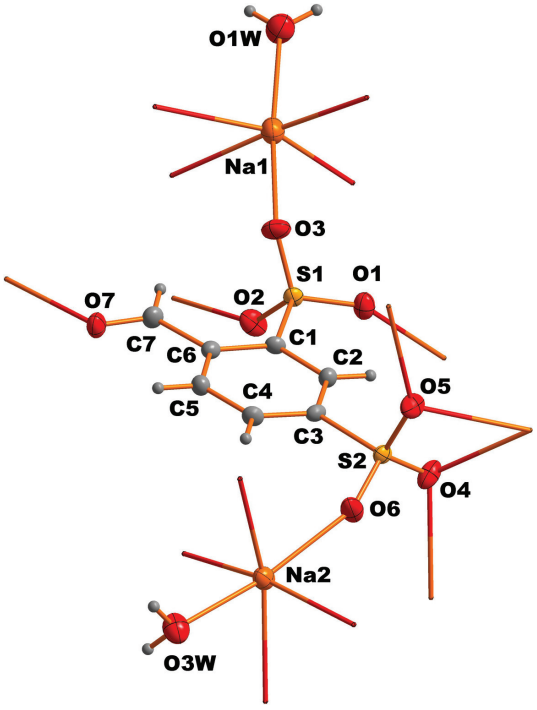
The crystal structure of poly[m_2-aqua-tetraaqua-bis(m_9-4-formylbenzene-1,3-disulfonato) tetrasodium(I) hydrate, $C_{14}H_{18}O_{19}S_4Na_4$



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Abstract

$C_{14}H_{18}O_{19}S_4Na_4$, triclinic, $P\bar{1}$ (no. 2), $a = 7.0769(14)$ Å, $b = 9.5622(19)$ Å, $c = 10.952(2))$ Å, $\alpha = 115.14(3)°$, $\beta = 90.46(3)°$, $\gamma = 106.53(3)°$, $V = 636.1(2)$ Å^3, $Z = 1$, $R_{gt}(F) = 0.0448$, $wR_{ref}(F^2) = 0.1191$, $T = 293(2)$ K.

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The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list

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Table 1: Data collection and handling.

Crystal:	Yellow block
Size:	0.21 × 0.20 × 0.19 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	0.53 mm^{-1}
Diffractometer, scan mode:	Bruker, φ and ω
θ_{max}, completeness:	25.0°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	4997, 2246, 0.040
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2128
$N(param)_{refined}$:	185
Programs:	Bruker [1], SHELX [2, 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}
S1	−0.07669(8)	−0.68903(6)	0.29435(5)	0.0184(2)
S2	−0.24073(8)	−1.33612(6)	0.16300(6)	0.0183(2)
Na1	−0.25680(16)	−0.35031(14)	0.43253(11)	0.0348(3)
Na2	−0.22474(15)	−1.62759(12)	−0.19927(10)	0.0272(3)
C1	−0.1633(3)	−0.8975(3)	0.1675(2)	0.0177(5)
C2	−0.1629(3)	−1.0170(3)	0.2079(2)	0.0189(5)
H2A	−0.1132	−0.9882	0.2971	0.023*
C3	−0.2380(3)	−1.1805(3)	0.1132(2)	0.0176(5)
C4	−0.3142(3)	−1.2257(3)	−0.0199(2)	0.0205(5)
H4A	−0.3679	−1.3352	−0.0814	0.025*
C5	−0.3094(3)	−1.1060(3)	−0.0602(2)	0.0204(5)
H5A	−0.3574	−1.1357	−0.1500	0.024*
C6	−0.2332(3)	−0.9409(3)	0.0321(2)	0.0182(5)
C7	−0.2353(4)	−0.8193(3)	−0.0177(2)	0.0237(5)
H7A	−0.2005	−0.7103	0.0457	0.028*
O1	−0.0144(3)	−0.6955(2)	0.41816(17)	0.0285(4)
O1W	−0.2952(3)	−0.0887(3)	0.5752(2)	0.0432(5)
H1WB	−0.2919	−0.0486	0.6619	0.065*
H1WA	−0.2786	−0.0083	0.5559	0.065*
O2	0.0871(3)	−0.6030(2)	0.24795(19)	0.0320(5)
O2W[a]	−0.5558(8)	−0.5381(7)	0.4310(5)	0.0584(13)*
H2WA	−0.5690	−0.4527	0.4879	0.088*
O3	−0.2486(3)	−0.6335(2)	0.30245(19)	0.0319(5)
O3W	−0.3076(3)	−1.8041(3)	−0.4411(2)	0.0393(5)
H3WA	−0.2192	−1.7738	−0.4860	0.059*
H3WB	−0.4228	−1.8298	−0.4858	0.059*
O4	−0.0710(3)	−1.2698(2)	0.2689(2)	0.0321(4)
O5	−0.4261(3)	−1.3706(2)	0.21709(19)	0.0291(4)
O6	−0.2264(4)	−1.4712(2)	0.0404(2)	0.0401(5)
O7	−0.2797(3)	−0.8543(2)	−0.13607(17)	0.0288(4)

[a]Occupancy: 0.5.

of the atoms including atomic coordinates and displacement parameters.

Source of material

Disodium 4-formylbenzene-1,3-disulfonate (0.1551 g; 0.5 mmol) was dissolved in 3 mL H_2O at room temperature. An amount of 10 mL CH_3CH_2OH containing 0.0685 g 3-pyridinecarboxylic hydrazide (0.5 mmol) was added with stirring. The mixture was stirred for 6.5 h at 75 °C. The crystals of the title compound were obtained by slow evaporating the filtrate at room temperature after 15 days.

Experimental details

The hydrogen atoms were positioned geometrically (C—H = 0.93 Å and O—H = 0.82–0.86 Å). Their U_{iso} values were set to $1.2U_{eq}$ or $1.5U_{eq}$ of the parent atoms. One water molecule is only half occupied.

Comment

Studies on coordination polymers with various structures are of current interest, because they have shown potential applications in many fields such as catalysis, luminecence, antitumor and antibacterial activities [5–7]. In order to explore the synthesis, structure and property of coordination polymers a new coordination polymer was synthesized and structurally characterized.

In the title compound, each Na(I) atom is six-coordinated with four O atoms of four different SO_3^- groups from four different benzaldehyde disulfonate ligands, one O atom of aldehyde group and one O atom from coordinated water molecule, which forms a distorted octahedral geometry. The title compound forms a three-dimensional network structure by the bridging effect of the organic disulfonato ligand. As shown in the figure each disulfonato ligand coordinates to nine crystallographically related, neighboring sodium cations.

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