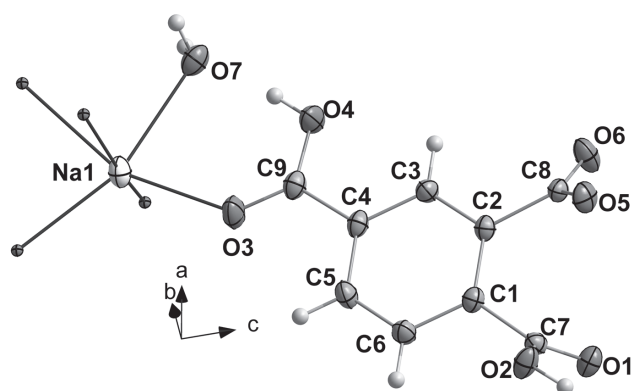


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Crystal structure of poly[aqua-(μ_5 -2,5-dicarboxybenzoato- $\kappa^5 O:O:O':O'':O'''$)sodium(I)], $C_9H_7NaO_7$



<https://doi.org/10.1515/ncrs-2017-0191>

Received September 22, 2017; accepted November 25, 2017;
available online December 16, 2017

Abstract

$C_9H_7NaO_7$, triclinic, $P\bar{1}$ (no. 2), $a = 7.0533(7)$ Å, $b = 7.1238(7)$ Å, $c = 10.5664(10)$ Å, $\alpha = 87.466(1)^\circ$, $\beta = 83.003(1)^\circ$, $\gamma = 66.690(1)^\circ$, $V = 483.95(8)$ Å³, $Z = 2$, $R_{gt}(F) = 0.0361$, $wR_{ref}(F^2) = 0.0936$, $T = 296(2)$ K.

CCDC no.: 1560000

The asymmetric unit of the title crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

The title compound was prepared by the following procedure: a mixture of Na_2CO_3 (0.10 g) and 1,2,4-Tricarboxybenzene (0.30 g) was dissolved in 5 mL deionized water, which was then placed in a 30 mL Teflon-lined stainless steel autoclave. The autoclave was sealed and heated at 165 °C under auto-genously pressure for seven days. After being slowly cooled to room temperature at a rate of 5 °C/h, some colorless prism

Table 1: Data collection and handling.

Crystal:	Prism, colorless
Size:	0.20 × 0.05 × 0.05 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	0.19 cm ⁻¹
Diffractometer, scan mode:	Bruker SMART APEX-II, ω -scans
θ_{max} , completeness:	28.3°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int} :	6182, 2386, 0.026
Criterion for I_{obs} , $N(hkl)_{gt}$:	$I_{obs} > 2 \sigma(I_{obs})$, 1840
$N(param)_{refined}$:	155
Programs:	Bruker programs [1], SHELX [2, 3]

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

Atom	x	y	z	U_{iso}^*/U_{eq}
Na1	0.77734(10)	0.18226(10)	0.08591(6)	0.02528(19)
C1	0.1876(2)	0.3076(2)	0.72296(14)	0.0179(3)
C2	0.3887(2)	0.2866(2)	0.74057(14)	0.0183(3)
C3	0.5357(2)	0.2566(2)	0.63487(14)	0.0199(3)
H3	0.6702	0.2402	0.6457	0.024*
C4	0.4824(2)	0.2510(2)	0.51276(14)	0.0196(3)
C5	0.2830(3)	0.2730(3)	0.49619(15)	0.0239(4)
H5	0.2479	0.2690	0.4146	0.029*
C6	0.1357(3)	0.3011(3)	0.60092(15)	0.0225(3)
H6	0.0019	0.3155	0.5896	0.027*
C7	0.0304(2)	0.3248(2)	0.83580(14)	0.0183(3)
C8	0.4412(2)	0.3097(2)	0.87183(14)	0.0185(3)
C9	0.6376(3)	0.2184(2)	0.39754(15)	0.0223(3)
O1	0.05394(18)	0.18875(17)	0.91401(10)	0.0246(3)
O2	−0.13675(18)	0.49567(18)	0.83874(11)	0.0262(3)
H2	−0.2316	0.5136	0.9098	0.031*
O3	0.59436(19)	0.2156(2)	0.29020(11)	0.0327(3)
O4	0.82419(19)	0.1925(2)	0.42435(11)	0.0320(3)
H4	0.9211	0.1682	0.3553	0.038*
O5	0.30587(18)	0.45865(17)	0.93593(10)	0.0250(3)
O6	0.60837(18)	0.18840(19)	0.90681(11)	0.0301(3)
O7	1.07454(19)	0.13720(18)	0.21125(11)	0.0288(3)
H7B	1.1907	0.0307	0.1810	0.035*
H7A	1.1082	0.2439	0.1907	0.035*

shaped crystals were collected by filtration, and washed by distilled water.

Experimental details

The H atoms of C atoms were positioned geometrically and refined with a riding model, with C–H = 0.93 Å and

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$U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The H atoms of water and carboxyl were located in difference Fourier maps, and then refined with a riding model, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$.

Discussion

During past twenty years, research interest in coordination polymers (CPs) is rapidly increasing not only owing to their versatile intriguing architectures and topologies but also for their potential applications in a variety of areas. Design and construction of CPs with specific architecture and useful properties still remain a significant challenge, because the construction of CPs will be influenced by many experimental and structural factors, such as the coordinating propensities of the ligands, the geometric preference of metal ions, relative stoichiometry of raw materials, reaction temperature and solvent systems. Moreover, weak non-covalent interactions such as hydrogen bonds, π - π and anion- π interactions also play an important role to determine the shape of the molecules and the crystal structures. The selection of suitable organic ligands is crucial for constructing extended coordination frameworks. 1,2,4-Tricarboxybenzene has been used extensively to construct a number of CPs, which usually display interesting electronic, optical and magnetic properties [4–7].

Structure solution revealed that the title compound features a 3D framework with one Na⁺ cation, one 2,5-dicarboxybenzoato ligand and one coordinated aqua in each asymmetric unit. Each Na⁺ cation is 6-coordinated by five oxygen atoms of organic ligands and one aqua ligand into a NaO₆ polyhedron with the Na–O distances ranging from 2.3462(13) to 2.5214(14) Å. The calculated total bond valence for Na(1) is 1.136, proving that the Na atom is in the reasonable value of +1 oxidation state [8]. The 2,5-dicarboxybenzoato

ligand adopts a μ_5 coordination mode connecting five Na⁺ cations (*cf.* the figure), to form the 3D framework.

Acknowledgements: I acknowledge support for the publication fee by the Science and Technology Research Project of Henan Province (No. 172102310678) and Key research project of Henan Province Office of Education (No. 17A150013).

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