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The crystal structure of poly[(μ_{10} -5-carboxyisophthalato- $\kappa^{10}O$)disodium], $C_9H_4Na_2O_6$

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.23 × 0.18 × 0.17 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.23 mm ⁻¹
Diffractometer, scan mode:	Bruker D8 quest, φ and ω
$\theta_{\max}$, completeness:	25.2°, 98%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	2184, 823, 0.036
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 632
$N(\text{param})_{\text{refined}}$:	82
Programs:	Bruker [1], SHELX [2], Olex2 [3]

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

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.000000	0.2994(3)	0.250000	0.0104(7)
C2	0.08153(14)	0.3710(2)	0.3226(3)	0.0111(5)
H2	0.137457	0.322938	0.374165	0.013*
C3	0.08230(13)	0.5117(2)	0.3209(3)	0.0107(5)
C4	0.000000	0.5828(3)	0.250000	0.0104(6)
H4	−0.000001	0.679143	0.250002	0.013*
C5	0.000000	0.1460(3)	0.250000	0.0122(7)
C6	0.17246(14)	0.5822(2)	0.4035(3)	0.0112(5)
Na1	0.14630(6)	0.92863(9)	0.20364(13)	0.0175(3)
O1	0.06809(10)	0.08735(16)	0.3630(2)	0.0160(4)
O2	0.17361(10)	0.71312(15)	0.3928(2)	0.0176(4)
H2A ^a	0.229(3)	0.742(6)	0.458(8)	0.021*
O3	0.24162(9)	0.51524(16)	0.4837(2)	0.0156(4)

^aOccupancy: 0.5.<https://doi.org/10.1515/ncrs-2020-0143>

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Abstract

$C_9H_4Na_2O_6$, monoclinic, $C2/c$ (no. 15), $a = 14.6828(15)$ Å, $b = 9.8602(10)$ Å, $c = 6.5024(7)$ Å, $\beta = 101.360(4)^\circ$, $V = 922.94(17)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0337$, $wR_{\text{ref}}(F^2) = 0.0775$, $T = 173(2)$ 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.

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Source of material

A mixture of 1,3,5-benzenetricarboxylic acid (0.21 g, 1 mmol), NaOH (0.08 g, 2 mmol) and N,N' -dimethylacetamide (10 mL) was sealed in a 25 mL Teflon-lined stainless steel vessel and heated at 120 °C for 4320 min. Yield: 60% based on Na.

Experimental details

The structure was solved by direct methods with the SHELXS-2018 program. All H-atoms from C atoms were positioned with idealized geometry and refined isotropically ($U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$), using a riding model $\text{C}—\text{H} = 0.95$ Å).

Comment

Remarkable attention has been devoted to coordination polymers (CPs, including metal-organic frameworks) because

of their enormous compositional diversity and structural tailorability leading to wide applications, such as gas absorption and separation [4], proton conductivity [5], environmental pollution control [6, 7] and energy conversion [8–12]. The CPs are constructed from inorganic vertices (metal ions/clusters) and organic linkers *via* coordination bonds and usually feature uniform infinite crystalline networks.

Single crystal diffraction study reveals that the asymmetric unit of the title compound is composed of one Na ion, one half of a 5-carboxyisophthalate monoanion (*cf.* the figure; located on a twofold axis; H2A disordered over two positions). The 5-carboxyisophthalate ligand (CI) is coordinated with ten Na ion to form a three-dimensional network. It is noteworthy that the incompletely deprotonated CI ligand connects ten sodium ions as a linker, which is very rare in such a high coordination number. To the best of our knowledge, although some hybrid metals based on transition metals and alkali metals Na as nodes had been connected by CI with different protonation states [13–16], and a corresponding isomeric ligand [17]. To the best of our knowledge, the title compound is the first coordination polymer based on single sodium ion and the CI ligand.

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