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catena-Poly[[[aqua(2-carboxy-6-nitrobenzoato-κ*O*)-sodium]-di-μ-aqua] monohydrate]

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.048
wR factor = 0.132
Data-to-parameter ratio = 13.6

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $\{[Na(C_8H_4NO_6)(H_2O)_3].H_2O\}_n$, forms polymeric chains by way of edge-sharing *via* pairs of water molecules between $NaO(H_2O)_5$ octahedra. The chains are crosslinked by O—H···O hydrogen bonds, resulting in a three-dimensional network.

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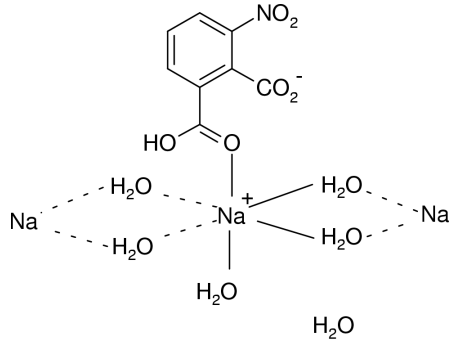
Comment

The crystal structure of the title sodium complex, (I), is reported here. The Na^+ cation is surrounded by five water molecules and one carboxyl O atom, in an approximately octahedral geometry (Table 1). Adjacent octahedra are linked into a polymeric chain by way of edge-sharing *via* pairs of water molecule O atoms. This results in Na1···Na1^{i} and Na1···Na1^{ii} (see Table 1 for symmetry codes) separations of 3.4642 (19) and 3.4876 (19) Å, respectively, and an Na1^{i}···Na1···Na1^{ii} angle of 170.09 (7)°.



(I)

The crystal structure of (I) is stabilized by a number of intra- and interchain O—H···O hydrogen bonds (Table 2 and Fig. 2).

Experimental

Crystals of (I) were obtained from a 1:1 aqueous solution of 3-nitrophathalic acid and sodium hydroxide by slow concentration for 6 d.

Crystal data

$[Na(C_8H_4NO_6)(H_2O)_3]\cdot H_2O$
M_r = 305.18
Triclinic, $P\overline{1}$
a = 6.9258 (19) Å
b = 7.513 (2) Å
c = 12.907 (4) Å
α = 77.622 (8)°
β = 83.212 (9)°
γ = 74.103 (8)°
V = 629.6 (3) Å^3
Z = 2
D_x = 1.610 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 766 reflections
θ = 3.0–26.2°
μ = 0.18 mm^{-1}
T = 293 (2) K
Block, colorless
0.26 × 0.22 × 0.16 mm

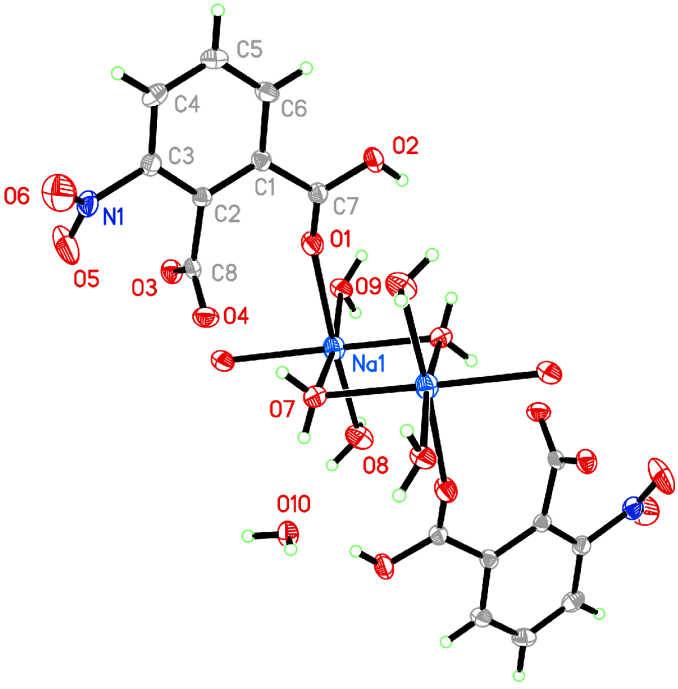


Figure 1
View of (I), showing 30% probability displacement ellipsoids. The unlabeled atoms are generated from labeled atoms by the symmetry operation $(1-x, 1-y, 1-z)$.

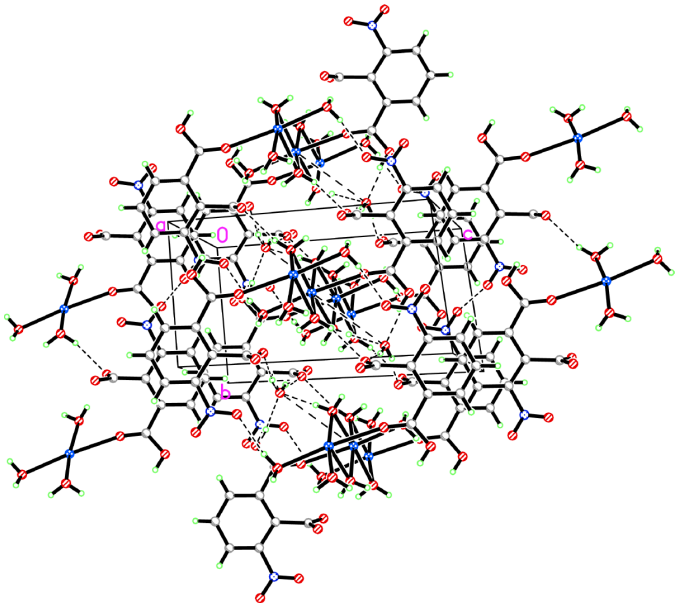


Figure 2
Packing diagram of (I), showing hydrogen bonds as dashed lines.

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.916$, $T_{max} = 0.972$
3650 measured reflections
2536 independent reflections
1968 reflections with $I > 2\sigma(I)$
$R_{int} = 0.019$
$\theta_{max} = 26.4°$
$h = -8 \rightarrow 8$
$k = -9 \rightarrow 8$
$l = -16 \rightarrow 10$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.132$
$S = 1.11$
2536 reflections
186 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0497P)^2 + 0.4847P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.38$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ e Å^{-3}
Extinction correction: *SHELXTL*
Extinction coefficient: 0.093 (8)

Table 1
Selected geometric parameters (Å, °).

Na1—O7	2.373 (2)	Na1—O7^{i}	2.333 (3)
Na1—O9	2.386 (2)	Na1—O9^{ii}	2.435 (3)
Na1—O8	2.437 (2)	O7—Na1^{i}	2.333 (2)
Na1—O1	2.538 (2)	O9—Na1^{ii}	2.435 (2)
O7^{i}—Na1—O7	85.18 (8)	O7—Na1—O8	102.85 (8)
O7^{i}—Na1—O9	98.15 (8)	O9—Na1—O8	86.90 (7)
O7—Na1—O9	169.63 (8)	O9^{ii}—Na1—O8	90.81 (8)
O7^{i}—Na1—O9^{ii}	173.92 (8)	O7^{i}—Na1—O1	85.94 (7)
O7—Na1—O9^{ii}	88.98 (7)	Na1^{i}—O7—Na1	94.82 (8)
O9—Na1—O9^{ii}	87.33 (7)	Na1—O9—Na1^{ii}	92.67 (7)
O7^{i}—Na1—O8	92.13 (8)		

Symmetry codes: (i) $1-x, 1-y, 1-z$; (ii) $-x, 1-y, 1-z$.

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O10—H10B···O4^{iii}	0.85	1.89	2.722 (3)	166
O10—H10A···O3^{iv}	0.85	1.92	2.749 (3)	165
O9—H9B···O4^{v}	0.85	2.11	2.939 (3)	166
O9—H9A···O3^{ii}	0.85	1.89	2.740 (3)	173
O8—H8B···O3^{iv}	0.85	2.03	2.846 (3)	160
O8—H8A···O5^{iv}	0.85	2.12	2.962 (3)	171
O7—H7B···O4	0.85	1.99	2.834 (3)	176
O7—H7A···O10	0.85	1.96	2.809 (3)	173
O2—H2···O10^{i}	0.85 (1)	1.783 (12)	2.631 (3)	169 (3)

Symmetry codes: (i) $1-x, 1-y, 1-z$; (ii) $-x, 1-y, 1-z$; (iii) $1-x, 2-y, 1-z$; (iv) $-x, 2-y, 1-z$; (v) $x, y-1, z$.

Atom H2 was refined with an O—H distance restraint of 0.859 (10) Å. All other H atoms attached to oxygen were found in difference Fourier maps. During refinement, they were treated as riding, with O—H = 0.85 Å and U_{iso}(H) = 1.2U_{eq}(O). The H atoms attached to carbon were placed in idealized positions and refined as riding, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

References

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