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Sodium 2-nitrocinnamate dihydrate: a one-dimensional hydrogen-bonded coordination polymer

Graham Smith* and Urs D. Wermuth

School of Physical and Chemical Sciences, Queensland University of Technology,
GPO Box 2434, Brisbane, Qld 4001, Australia
Correspondence e-mail: g.smith@qut.edu.au

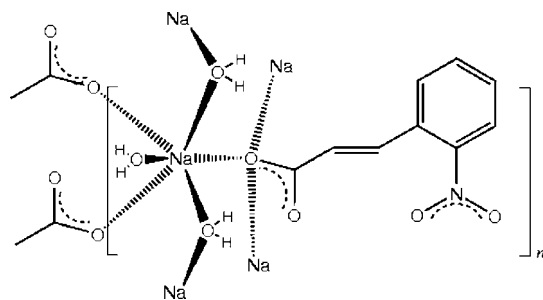
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Key indicators: single-crystal X-ray study; $T = 297$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å;
 R factor = 0.038; wR factor = 0.113; data-to-parameter ratio = 12.4.

The title compound *catena*-poly[aquasodium- μ_2 -aqua- μ_3 -2-nitrocinnamato], $[\text{Na}(\text{C}_9\text{H}_6\text{NO}_4)(\text{H}_2\text{O})_2]_n$, the sodium salt of *trans*-2-nitrocinnamic acid, is a one-dimensional coordination polymer based on six-coordinate octahedral NaO_6 centres, comprising three facially related monodentate carboxylate O-atom donors from separate ligands (all bridging) $[\text{Na}-\text{O} = 2.4370(13)-2.5046(13)$ Å], and three water molecules (two bridging and one monodentate) $[\text{Na}-\text{O} = 2.3782(13)-2.4404(17)$ Å]. The structure is also stabilized by intra-chain water-carboxylate and water-nitro $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds.

Related literature

For literature on similar compounds, see: Crowther *et al.* (2008); Kariuki *et al.* (1995); Kula *et al.* (2007); Schmidt (1964); Smith *et al.* (2006); Trividi *et al.* (2005).



Experimental

Crystal data

$[\text{Na}(\text{C}_9\text{H}_6\text{NO}_4)(\text{H}_2\text{O})_2]$
 $M_r = 251.17$

Monoclinic, $P2_1/c$
 $a = 19.4179(7)$ Å

$b = 3.6899(2)$ Å
 $c = 14.8738(7)$ Å
 $\beta = 92.239(4)^\circ$
 $V = 1064.90(9)$ Å³
 $Z = 4$

Mo $K\alpha$ radiation
 $\mu = 0.17$ mm⁻¹
 $T = 297$ K
 $0.40 \times 0.30 \times 0.13$ mm

Data collection

Oxford Diffraction Gemini-S CCD-
detector diffractometer
Absorption correction: multi-scan
(*SADABS*; Sheldrick, 1996)
 $T_{\min} = 0.93$, $T_{\max} = 0.98$

6531 measured reflections
2100 independent reflections
1626 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.019$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.038$
 $wR(F^2) = 0.113$
 $S = 1.09$
2100 reflections
170 parameters

H atoms treated by a mixture of
independent and constrained
refinement
 $\Delta\rho_{\max} = 0.30$ e Å⁻³
 $\Delta\rho_{\min} = -0.19$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H11W \cdots O32 ⁱ	0.78 (3)	2.14 (3)	2.8871 (17)	162 (2)
O1W—H12W \cdots O32 ⁱⁱ	0.89 (2)	1.90 (2)	2.7852 (17)	171 (2)
O2W—H21W \cdots O21 ⁱⁱⁱ	0.77 (3)	2.49 (3)	3.050 (2)	131 (3)
O2W—H22W \cdots O32 ⁱ	0.91 (4)	2.04 (5)	2.882 (2)	153 (4)

Symmetry codes: (i) $x, -y + \frac{1}{2}, z - \frac{1}{2}$; (ii) $-x, -y, -z$; (iii) $x, -y + \frac{3}{2}, z - \frac{1}{2}$.

Data collection: *CrysAlis Pro* (Oxford Diffraction, 2009); cell refinement: *CrysAlis Pro*; data reduction: *CrysAlis Pro*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2131).

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supporting information

Acta Cryst. (2009). E65, m1048 [doi:10.1107/S1600536809030402]

Sodium 2-nitrocinnamate dihydrate: a one-dimensional hydrogen-bonded coordination polymer

Graham Smith and Urs D. Wermuth

S1. Comment

Although the structures of two polymorphs of *trans*-cinnamic acid have been determined (Schmidt, 1964; Smith *et al.*, 2006), the structures of neither *trans*-2-nitrocinnamic acid [(*E*)-3-(2-nitrophenyl)propenoic acid] nor any of its alkali metal salts are known, although the dicyclohexylammonium salt has been reported (Trividi *et al.*, 2005). The only structures of alkali metal compounds of analogous ring-substituted *trans*-cinnamic acids are the sodium complexes with 2-chlorocinnamic acid (Kariuki *et al.*, 1995), 3-chlorocinnamic acid (Crowther *et al.*, 2008), and 4-hydroxy-2-methoxycinnamic acid (Kula *et al.*, 2007). We have now prepared the sodium salt of *trans*-2-nitrocinnamic acid, a dihydrate [Na(C₉H₆NO₄)(H₂O)₂]_n and its structure is reported here.

The molecular structure of the title compound is illustrated in Fig. 1. The polymeric structure is based on octahedral six-coordinate NaO₆ centres comprising three facially related monodentate carboxylate O-donors from separate ligands (all bridging) [Na–O, 2.4370 (13)–2.5046 (13) Å] and three water molecules (two bridging, one monodentate) [Na–O, 2.3782 (13)–2.4404 (17) Å]. These units are linked into one-dimensional coordination polymer chains which extend along direction [010] (Fig. 1). The structure is similar to that of the sodium 2-chlorocinnamate complex (Kariuki *et al.*, 1995). The polymer chains are stabilized by intra-chain water *O*–*H*⋯*O*_{carboxylate} and *O*–*H*⋯*O*_{nitro} hydrogen bonds (Table 1).

In the substituted cinnamate ligand molecule, the nitro group is rotated out of the plane of the benzene ring [torsion angle C1–C2–N21–O22, 144.65 (17)°], while the carboxylate group is similarly non-coplanar [C11–C21–C31–O31, -169.51 (17)°].

S2. Experimental

The title compound was synthesized by heating together for 10 minutes under reflux 1 mmol quantities of *trans*-cinnamic acid [(*E*)-3-(2-nitrophenyl)propenoic acid] and sodium carbonate in 50 ml of 50% ethanol-water. After concentration to ca 30 ml, partial rt evaporation of the hot-filtered solution gave thin colourless plate-like crystals, suitable for X-ray analysis.

S3. Refinement

The H-atoms of the water molecules were located in difference electron-density maps and were freely refined: O–H = 0.77 (3)–0.91 (4) Å. The C-bound H-atoms were included in calculated positions and treated as riding atoms: C–H = 0.93 Å with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

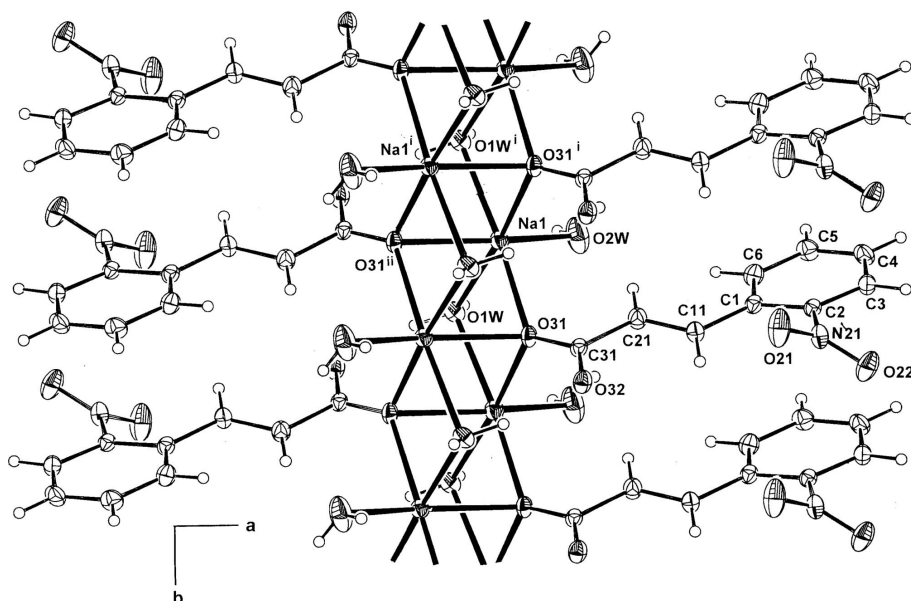


Figure 1

Molecular configuration and atom naming scheme for the title compound, showing the one-dimensional chain polymer structure extending along direction [010]. Displacement ellipsoids are drawn at the 50% probability level [Symmetry codes: (i) $x, y + 1, z$; (ii) $-x, -y + 1, -z$].

catena-poly[aquasodium- μ_2 -aqua- μ_3 -2-nitrocinnamato]

Crystal data

[Na(C₉H₆NO₄)(H₂O)₂]

$M_r = 251.17$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 19.4179$ (7) Å

$b = 3.6899$ (2) Å

$c = 14.8738$ (7) Å

$\beta = 92.239$ (4) $^\circ$

$V = 1064.90$ (9) Å³

$Z = 4$

$F(000) = 520$

$D_x = 1.567$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 2943 reflections

$\theta = 3.0$ – 28.7°

$\mu = 0.17$ mm⁻¹

$T = 297$ K

Plate, colourless

$0.40 \times 0.30 \times 0.13$ mm

Data collection

Oxford Diffraction Gemini-S CCD-detector
diffractometer

Radiation source: Enhance (Mo) X-ray source

Graphite monochromator

ω scans

Absorption correction: multi-scan

(*SADABS*; Sheldrick, 1996)

$T_{\min} = 0.93$, $T_{\max} = 0.98$

6531 measured reflections

2100 independent reflections

1626 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.019$

$\theta_{\max} = 26.0^\circ$, $\theta_{\min} = 3.0^\circ$

$h = -23 \rightarrow 21$

$k = -4 \rightarrow 4$

$l = -18 \rightarrow 17$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.038$
 $wR(F^2) = 0.113$
 $S = 1.09$
 2100 reflections
 170 parameters
 0 restraints
 Primary atom site location: structure-invariant
 direct methods

Secondary atom site location: difference Fourier
 map
 Hydrogen site location: inferred from
 neighbouring sites
 H atoms treated by a mixture of independent
 and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0708P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.30 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.19 \text{ e } \text{\AA}^{-3}$

Special details

Geometry. Bond distances, angles *etc.* have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Na1	0.05494 (3)	0.73072 (17)	-0.06704 (4)	0.0272 (2)
O1W	0.02635 (6)	0.2374 (3)	-0.16440 (8)	0.0319 (4)
O2W	0.16105 (8)	0.6812 (5)	-0.14886 (12)	0.0691 (7)
O21	0.29871 (7)	0.4625 (6)	0.31366 (9)	0.0637 (6)
O22	0.39979 (7)	0.2280 (5)	0.32066 (10)	0.0541 (6)
O31	0.06940 (6)	0.2430 (3)	0.04255 (8)	0.0282 (4)
O32	0.10417 (6)	0.0743 (4)	0.18086 (8)	0.0336 (4)
N21	0.35246 (7)	0.3769 (4)	0.27927 (10)	0.0339 (5)
C1	0.30837 (8)	0.4562 (5)	0.12070 (11)	0.0267 (5)
C2	0.36252 (8)	0.4742 (4)	0.18535 (11)	0.0261 (5)
C3	0.42813 (9)	0.5880 (5)	0.16617 (12)	0.0327 (6)
C4	0.44154 (10)	0.6987 (5)	0.08063 (14)	0.0384 (6)
C5	0.38972 (10)	0.6860 (5)	0.01494 (13)	0.0368 (6)
C6	0.32514 (9)	0.5634 (5)	0.03431 (12)	0.0346 (6)
C11	0.23935 (9)	0.3141 (5)	0.13955 (12)	0.0297 (5)
C21	0.18383 (9)	0.3638 (5)	0.08772 (13)	0.0345 (6)
C31	0.11421 (8)	0.2155 (4)	0.10637 (11)	0.0256 (5)
H3	0.46290	0.58950	0.21090	0.0390*
H4	0.48520	0.78150	0.06720	0.0460*
H5	0.39850	0.76120	-0.04320	0.0440*
H6	0.29140	0.55150	-0.01180	0.0420*
H11	0.23490	0.17970	0.19190	0.0360*
H11W	0.0460 (11)	0.241 (6)	-0.209 (2)	0.055 (8)*
H12W	-0.0168 (12)	0.157 (7)	-0.1733 (17)	0.044 (8)*
H21	0.18810	0.50100	0.03580	0.0410*

H21W	0.1828 (16)	0.851 (9)	-0.138 (2)	0.093 (13)*
H22W	0.1500 (18)	0.666 (12)	-0.209 (2)	0.101 (14)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Na1	0.0279 (4)	0.0275 (4)	0.0260 (4)	-0.0019 (3)	-0.0005 (3)	0.0007 (3)
O1W	0.0363 (7)	0.0350 (7)	0.0244 (7)	-0.0082 (5)	0.0026 (5)	-0.0002 (5)
O2W	0.0399 (9)	0.1143 (15)	0.0532 (10)	-0.0214 (9)	0.0046 (7)	0.0098 (9)
O21	0.0357 (8)	0.1222 (15)	0.0337 (8)	0.0081 (9)	0.0067 (6)	-0.0065 (9)
O22	0.0475 (9)	0.0775 (12)	0.0364 (9)	0.0164 (7)	-0.0096 (7)	0.0112 (7)
O31	0.0220 (6)	0.0370 (7)	0.0253 (6)	-0.0013 (5)	-0.0039 (5)	0.0011 (5)
O32	0.0290 (7)	0.0461 (8)	0.0255 (7)	0.0007 (5)	0.0005 (5)	0.0056 (6)
N21	0.0266 (8)	0.0471 (9)	0.0276 (8)	-0.0020 (7)	-0.0027 (6)	-0.0022 (7)
C1	0.0235 (8)	0.0281 (9)	0.0283 (9)	0.0035 (7)	0.0004 (7)	-0.0017 (7)
C2	0.0264 (8)	0.0257 (8)	0.0260 (9)	0.0040 (7)	0.0003 (7)	-0.0020 (7)
C3	0.0255 (9)	0.0331 (10)	0.0393 (11)	-0.0010 (8)	-0.0021 (7)	-0.0033 (8)
C4	0.0299 (10)	0.0362 (10)	0.0499 (13)	-0.0071 (8)	0.0106 (9)	-0.0017 (9)
C5	0.0405 (11)	0.0374 (10)	0.0331 (11)	-0.0045 (8)	0.0097 (8)	0.0035 (8)
C6	0.0340 (10)	0.0415 (11)	0.0281 (9)	0.0024 (8)	-0.0026 (7)	0.0020 (8)
C11	0.0261 (9)	0.0353 (10)	0.0276 (9)	-0.0015 (7)	0.0001 (7)	-0.0008 (7)
C21	0.0266 (9)	0.0435 (11)	0.0334 (10)	-0.0035 (8)	-0.0004 (7)	0.0093 (8)
C31	0.0231 (8)	0.0288 (9)	0.0248 (9)	0.0039 (7)	0.0008 (7)	-0.0028 (7)

Geometric parameters (Å, °)

Na1—O1W	2.3782 (13)	C1—C2	1.399 (2)
Na1—O2W	2.4404 (17)	C1—C6	1.395 (2)
Na1—O31	2.4370 (13)	C1—C11	1.476 (2)
Na1—O1W ⁱ	2.4162 (13)	C2—C3	1.382 (2)
Na1—O31 ⁱ	2.5046 (13)	C3—C4	1.371 (3)
Na1—O31 ⁱⁱ	2.4577 (13)	C4—C5	1.376 (3)
O21—N21	1.222 (2)	C5—C6	1.374 (3)
O22—N21	1.217 (2)	C11—C21	1.314 (3)
O31—C31	1.267 (2)	C21—C31	1.494 (2)
O32—C31	1.247 (2)	C3—H3	0.9300
O1W—H11W	0.78 (3)	C4—H4	0.9300
O1W—H12W	0.89 (2)	C5—H5	0.9300
O2W—H21W	0.77 (3)	C6—H6	0.9300
O2W—H22W	0.91 (4)	C11—H11	0.9300
N21—C2	1.463 (2)	C21—H21	0.9300
O1W—Na1—O2W	79.67 (5)	C2—C1—C6	115.06 (15)
O1W—Na1—O31	81.96 (4)	C2—C1—C11	123.37 (15)
O1W—Na1—O1W ⁱ	100.64 (4)	C6—C1—C11	121.46 (15)
O1W—Na1—O31 ⁱ	172.53 (5)	N21—C2—C1	121.34 (14)
O1W—Na1—O31 ⁱⁱ	85.02 (4)	N21—C2—C3	115.49 (14)
O2W—Na1—O31	101.58 (6)	C1—C2—C3	123.16 (15)

O1W ⁱ —Na1—O2W	86.43 (5)	C2—C3—C4	119.49 (17)
O2W—Na1—O31 ⁱ	107.80 (5)	C3—C4—C5	119.26 (18)
O2W—Na1—O31 ⁱⁱ	158.48 (6)	C4—C5—C6	120.69 (18)
O1W ⁱ —Na1—O31	171.93 (5)	C1—C6—C5	122.29 (16)
O31—Na1—O31 ⁱ	96.60 (4)	C1—C11—C21	124.71 (17)
O31—Na1—O31 ⁱⁱ	91.04 (4)	C11—C21—C31	124.59 (17)
O1W ⁱ —Na1—O31 ⁱ	79.83 (4)	O31—C31—C21	115.57 (14)
O1W ⁱ —Na1—O31 ⁱⁱ	81.62 (4)	O32—C31—C21	119.48 (15)
O31 ⁱ —Na1—O31 ⁱⁱ	87.68 (4)	O31—C31—O32	124.96 (15)
Na1—O1W—Na1 ⁱⁱⁱ	100.64 (5)	C2—C3—H3	120.00
Na1—O31—C31	128.20 (10)	C4—C3—H3	120.00
Na1—O31—Na1 ⁱⁱⁱ	96.60 (5)	C3—C4—H4	120.00
Na1—O31—Na1 ⁱⁱ	88.96 (4)	C5—C4—H4	120.00
Na1 ⁱⁱⁱ —O31—C31	118.92 (10)	C4—C5—H5	120.00
Na1 ⁱⁱ —O31—C31	122.84 (10)	C6—C5—H5	120.00
Na1 ⁱⁱⁱ —O31—Na1 ⁱⁱ	92.32 (4)	C1—C6—H6	119.00
H11W—O1W—H12W	112 (2)	C5—C6—H6	119.00
H21W—O2W—H22W	111 (4)	C1—C11—H11	118.00
O21—N21—C2	118.98 (14)	C21—C11—H11	118.00
O22—N21—C2	117.87 (14)	C11—C21—H21	118.00
O21—N21—O22	123.06 (16)	C31—C21—H21	118.00
O2W—Na1—O1W—Na1 ⁱⁱⁱ	95.66 (6)	O31—Na1—O31 ⁱⁱ —C31 ⁱⁱ	-136.41 (11)
O31—Na1—O1W—Na1 ⁱⁱⁱ	-7.75 (5)	Na1—O31—C31—O32	145.52 (13)
O1W ⁱ —Na1—O1W—Na1 ⁱⁱⁱ	180.00 (6)	Na1—O31—C31—C21	-35.11 (19)
O31 ⁱⁱ —Na1—O1W—Na1 ⁱⁱⁱ	-99.51 (5)	Na1 ⁱⁱⁱ —O31—C31—O32	-87.48 (18)
O1W—Na1—O31—C31	142.67 (13)	Na1 ⁱⁱⁱ —O31—C31—C21	91.89 (14)
O1W—Na1—O31—Na1 ⁱⁱⁱ	7.39 (4)	Na1 ⁱⁱ —O31—C31—O32	26.8 (2)
O1W—Na1—O31—Na1 ⁱⁱ	-84.82 (4)	Na1 ⁱⁱ —O31—C31—C21	-153.81 (11)
O2W—Na1—O31—C31	65.02 (14)	O21—N21—C2—C1	-38.6 (2)
O2W—Na1—O31—Na1 ⁱⁱⁱ	-70.26 (6)	O21—N21—C2—C3	140.47 (18)
O2W—Na1—O31—Na1 ⁱⁱ	-162.47 (5)	O22—N21—C2—C1	144.65 (17)
O31 ⁱ —Na1—O31—C31	-44.72 (13)	O22—N21—C2—C3	-36.2 (2)
O31 ⁱ —Na1—O31—Na1 ⁱⁱⁱ	180.00 (4)	C6—C1—C2—N21	178.85 (15)
O31 ⁱ —Na1—O31—Na1 ⁱⁱ	87.79 (4)	C6—C1—C2—C3	-0.2 (3)
O31 ⁱⁱ —Na1—O31—C31	-132.51 (13)	C11—C1—C2—N21	-4.8 (3)
O31 ⁱⁱ —Na1—O31—Na1 ⁱⁱⁱ	92.21 (5)	C11—C1—C2—C3	176.18 (17)
O31 ⁱⁱ —Na1—O31—Na1 ⁱⁱ	0.00 (3)	C2—C1—C6—C5	-1.5 (3)
O1W—Na1—O1W ⁱ —Na1 ⁱ	-180.00 (6)	C11—C1—C6—C5	-177.99 (17)
O2W—Na1—O1W ⁱ —Na1 ⁱ	-101.22 (6)	C2—C1—C11—C21	164.51 (18)
O2W—Na1—O31 ⁱ —Na1 ⁱ	75.56 (6)	C6—C1—C11—C21	-19.4 (3)
O2W—Na1—O31 ⁱ —C31 ⁱ	-65.26 (12)	N21—C2—C3—C4	-177.36 (16)
O31—Na1—O31 ⁱ —Na1 ⁱ	180.00 (3)	C1—C2—C3—C4	1.7 (3)
O31—Na1—O31 ⁱ —C31 ⁱ	39.19 (12)	C2—C3—C4—C5	-1.6 (3)
O1W—Na1—O31 ⁱⁱ —Na1 ⁱⁱ	81.83 (4)	C3—C4—C5—C6	-0.1 (3)
O1W—Na1—O31 ⁱⁱ —C31 ⁱⁱ	-54.58 (11)	C4—C5—C6—C1	1.7 (3)
O2W—Na1—O31 ⁱⁱ —Na1 ⁱⁱ	126.42 (15)	C1—C11—C21—C31	179.16 (16)

O2W—Na1—O31 ⁱⁱ —C31 ⁱⁱ	-10.0 (2)	C11—C21—C31—O31	-169.51 (17)
O31—Na1—O31 ⁱⁱ —Na1 ⁱⁱ	0.00 (5)	C11—C21—C31—O32	9.9 (3)

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

Hydrogen-bond geometry (Å, °)

<i>D—H...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
O1W—H11W...O32 ^{iv}	0.78 (3)	2.14 (3)	2.8871 (17)	162 (2)
O1W—H12W...O32 ^v	0.89 (2)	1.90 (2)	2.7852 (17)	171 (2)
O2W—H21W...O21 ^{vi}	0.77 (3)	2.49 (3)	3.050 (2)	131 (3)
O2W—H22W...O32 ^{iv}	0.91 (4)	2.04 (5)	2.882 (2)	153 (4)
C11—H11...O21	0.93	2.39	2.846 (2)	110

Symmetry codes: (iv) $x, -y+1/2, z-1/2$; (v) $-x, -y, -z$; (vi) $x, -y+3/2, z-1/2$.