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Possible strong symmetric hydrogen bonding in disodium trihydrogen bis(2,2'-oxydiacetate) nitrate

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Key indicators

Single-crystal X-ray study
$T = 293$ K
Mean σ(C–C) = 0.003 Å
R factor = 0.033
wR factor = 0.103
Data-to-parameter ratio = 9.8

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

In the title compound, $2Na^+ \cdot C_8H_{11}O_{10}^- \cdot NO_3^-$, the Na^I atom is heptacoordinate with an approximately pentagonal–bipyramidal geometry. A possible strong symmetric hydrogen bond, with the H atom located at an inversion centre and an O···O distance of 2.450 (2) Å, is observed in the crystal structure.

Comment

The nature of short hydrogen-bonding interactions is still a subject of much interest and debate (Meot-Ner, 2005). It appears that, for O—H—O interactions where O···O is less than about 2.50 Å, examples can be found of truly symmetric hydrogen bonds (Catti & Ferraris, 1976), most of which have crystallographic equivalence between donor–acceptor atoms. The title sodium compound, (I), displays just such a short and possibly symmetric hydrogen-bonding interaction.

(I)
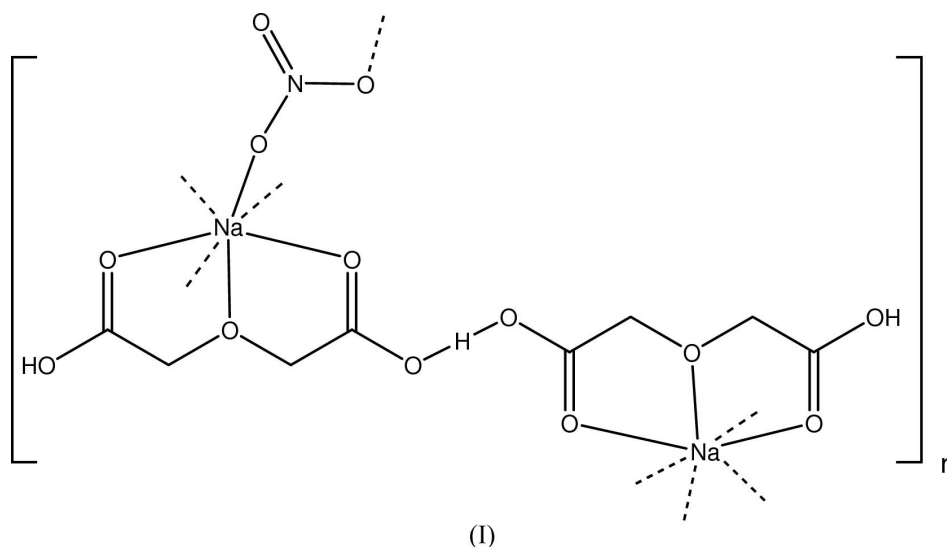
The compound can be viewed as a mixed sodium salt containing two monoanionic components, *viz.* nitrate and trihydrogen bis(2,2'-oxydiacetate) (a hydrogen-bonded adduct formed by the loss of a single H atom from two of the dicarboxylic acid molecules). These 2,2'-oxydiacetate molecules adopt the fairly common planar all-*trans* configuration (Albertsson & Grenthe, 1973; Albertsson *et al.*, 1973*a,b*; Hatfield *et al.*, 1987). The Na^I cation in (I) is heptacoordinate with an approximately pentagonal–bipyramidal geometry (Fig. 1); Na—O distances range from 2.4075 (17) to 2.5861 (18) Å. A tridentate chelating 2,2'-oxydiacetate molecule occupies three of the equatorial sites bonding through the two carboxyl and one ether O atoms. Symmetry-equivalent carboxyl atoms O2^{iii}, O5^{iv} and O1^v [symmetry codes: (iii)
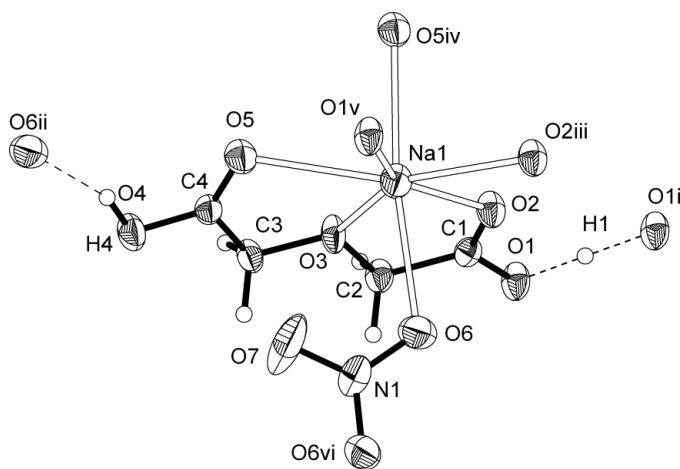
Figure 1
The molecular structure and sodium environment, with 50% probability displacement ellipsoids and the atom-labelling scheme. Dashed lines indicate hydrogen bonds. [Symmetry codes: (i) $\frac{3}{2} - x$, $\frac{3}{2} - y$, $1 - z$; (ii) x, $y - 1$, z; (iii) $1 - x$, $1 - y$, $1 - z$; (iv) $1 - x$, $-y$, $1 - z$; (v) $x - \frac{1}{2}$, $y - \frac{1}{2}$, z; (vi) $1 - x$, y, $\frac{3}{2} - z$].

Figure 3
Graph showing the distribution of C—O···O—C torsion angles as a function of O···O interatomic separations for short hydrogen-bonded interactions between two carboxylic acid groups. Data taken from 78 structures in the CSD (Version 5.25; Allen, 2002).
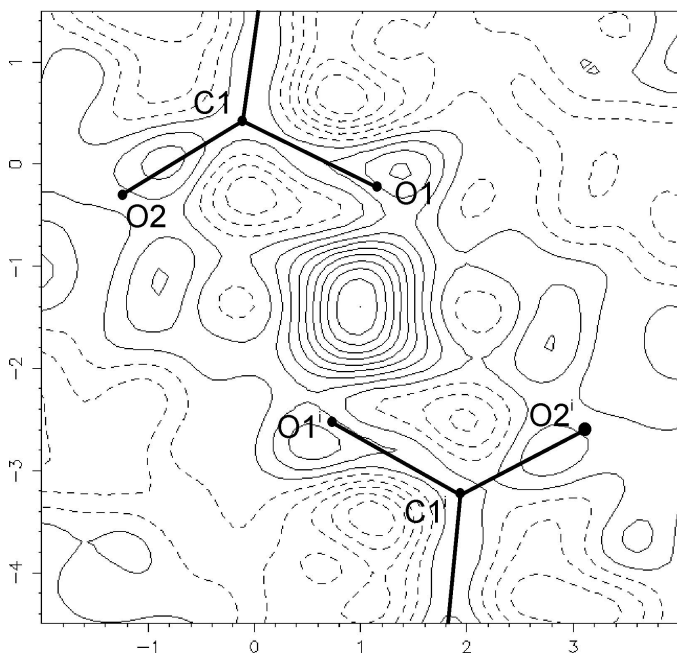

Figure 2
Difference Fourier map from a refined model where atom H1 is absent. The O1/C1/O2 plane is shown with the crystallographic inversion in the centre of the plot.

$1 - x$, $1 - y$, $1 - z$; (iv) $1 - x$, $-y$, $1 - z$; (v) $x - \frac{1}{2}$, $y - \frac{1}{2}$, z] from neighbouring 2,2′-oxydiacetate molecules and atom O6 of a bridging nitrate make up the rest of the coordination sphere.

The nitrate anion lies on the crystallographic twofold axis and links pairs of Na^{I} ions in an *anti–anti*-1,3-bridging coordination mode. The carboxyl O atoms act in a bis-μ-bridging capacity between Na^{I} ions, forming the polymeric structure.

In addition to these ionic interactions, the crystal structure is also held together by a network of two types of hydrogen
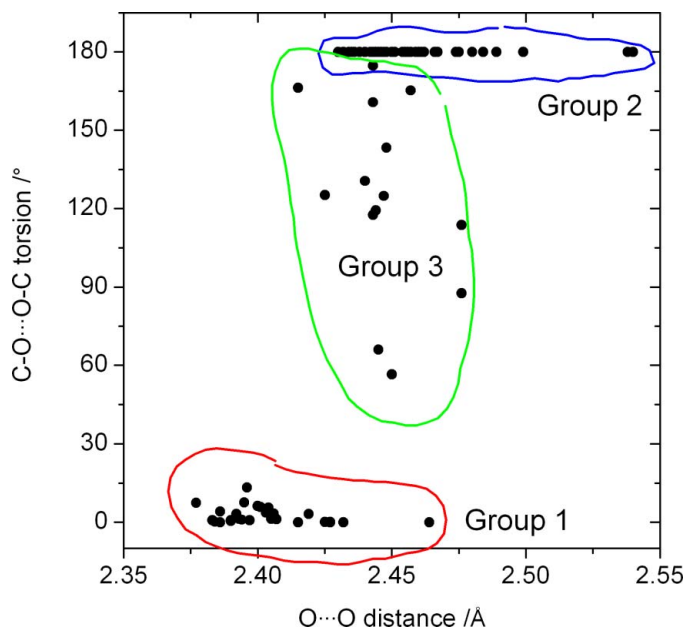
bonds. The first is formed between the O4-carboxyl group and the nitrate anion (Table 1). This hydrogen bond is asymmetric and non-linear. The nature of the second type of hydrogen bond is ambiguous. Certainly there exists a short hydrogen-bond interaction between the O1-carboxyl group and its crystallographically equivalent group; the O1···O1^{i} distance of 2.450 (2) Å [symmetry code:(i) $\frac{3}{2} - x$, $\frac{3}{2} - y$, $1 - z$] falls within the normal range for symmetric hydrogen bonds (Catti & Ferraris, 1976). A Fourier map section in the O1/C1/O2 plane (*MAPVIEW*; Farrugia, 1999) clearly indicates a peak of electron density centred on the crystallographic inversion (Fig. 2). Two alternative structural models have been studied. Placing atom H1 on the inversion centre gives a symmetric structure. Full-matrix least-squares refinement converged to a stable solution which is reported here. The residual difference Fourier map has a largest peak and hole of 0.16 and -0.23 e Å^{-3}, respectively. The crystallographic symmetry constrains the hydrogen-bond angle to 180° and the O1—H1 distance to 1.23 Å. A second structural model is one with the H1-atom site half occupied and displaced from the inversion centre towards O1. Free refinement of the x, y, z and U_{iso} parameters for the H1 atom (118 parameters in total) converged to give a sensible asymmetric hydrogen-bonding interaction; the crystallographic residuals are insignificantly different and the difference map shows essentially the same features. The limited data quality and resolution mean that we cannot unambiguously determine the nature of this hydrogen-bonding interaction. The compound clearly merits further study, if only to resolve this issue. Despite this uncertainty in the H-atom position, such a linear hydrogen-bonding interaction linking two 2,2′-oxydiacetate molecules in a *trans*
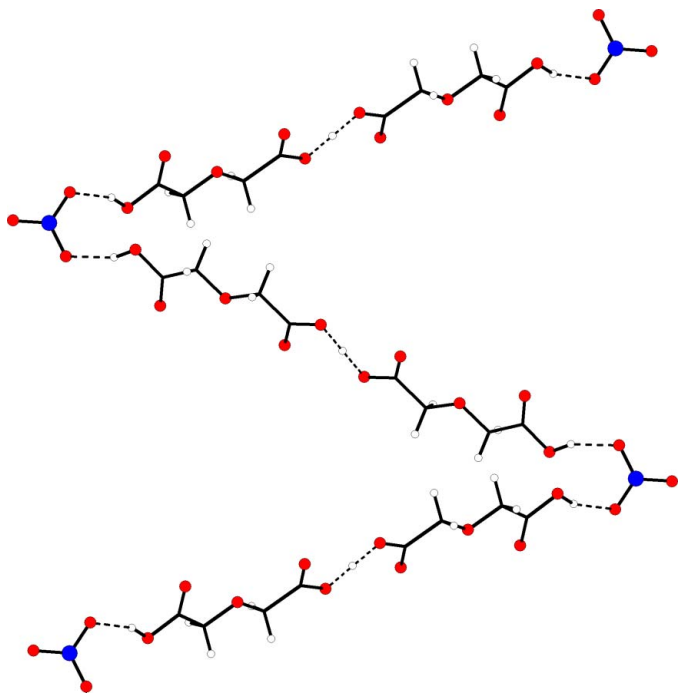
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Figure 4
The hydrogen-bonded network formed by both types of hydrogen-bonding interaction (dashed lines).

fashion is not an unusual motif when an H atom is shared between two carboxylic acid groups (Nahringbauer, 1969; Longo & Richardson, 1982; Misaki *et al.*, 1989).

An examination of the Cambridge Structural Database (CSD; Version 5.25; Allen, 2002) for short hydrogen bonds between two carboxylate groups reveals three distinct conformational/geometric groups (Fig. 3). Group 1 have a C—O⋯O—C torsion angles of about $0°$ and have O⋯O separations mostly in the range 2.38–2.43 Å. Group 2 have C—O⋯O—C torsion angles of $180°$ (invariably fixed by crystallographic symmetry) and O⋯O separations in the range 2.43–2.53 Å. Group 3 have intermediate torsion angles (unrestricted by symmetry) and have O⋯O distances all within the range 2.42–2.47 Å. The possibly symmetric hydrogen bond observed in (I) falls well within the known range for group 2 conformations, and this geometry is seen for many other dicarboxylate compounds (see, for example, Kalsbeek & Larsen, 1991; Leban & Rupnik, 1992; Flensburg *et al.*, 1995) and also in other 2,2′-oxydiacetate salts (Albertsson & Grenthe, 1973; Albertsson *et al.*, 1973*a*,*b*; Herbertsson & Hedman, 1982; Urbańczyk-Lipkowska, 2000).

We also note that the first hydrogen-bonding pattern (between the carboxylic acid and the nitrate anion), although asymmetric, seems to be a strong and important structural motif. In nine out of 14 reported structures that contain both a carboxylic acid and a nitrate anion, the acid is hydrogen bonded to the nitrate, and none of the structures displays the common $R_2^2(8)$ dimeric carboxylic acid motif (see, for example, Sridhar *et al.*, 2002).

Together, these two hydrogen-bonded motifs form a network. Using the nomenclature for graph theoretical analysis developed by Etter *et al.* (1990), we can describe this system as $N_1 = D_2^2(4)D$; $N_2 = C_3^3(20)$, where the second-order net consists of infinite chains that zigzag through the crystal structure (Fig. 4).

Experimental

Crystals of (I) were grown by slow evaporation from a methanolic solution which contained the bis(2,2′-oxydiacetic acid), sodium hydroxide and aluminium nitrate nonahydrate.

Crystal data

$2Na^+·C_8H_{11}O_{10}^-·NO_3^-$	$D_x = 1.808$ Mg m^{-3}
$M_r = 375.16$	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 101
$a = 12.010\ (2)$ Å	reflections
$b = 7.0290\ (14)$ Å	$\theta = 3.2$–$24.8°$
$c = 16.382\ (3)$ Å	$\mu = 0.22$ mm^{-1}
$\beta = 94.84\ (3)°$	$T = 293\ (2)$ K
$V = 1378.0\ (4)$ Å^3	Block, colourless
$Z = 4$	$0.16 \times 0.16 \times 0.06$ mm

Data collection

Rigaku R-AXIS-IIc diffractometer	$R_{int} = 0.016$
φ scans	$\theta_{max} = 24.8°$
Absorption correction: none	$h = 0 \to 14$
1999 measured reflections	$k = -8 \to 8$
1124 independent reflections	$l = -19 \to 19$
996 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0446P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.033$	$+ 1.8079P]$
$wR(F^2) = 0.103$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.17$	$(\Delta/\sigma)_{max} < 0.001$
1124 reflections	$\Delta\rho_{max} = 0.16$ e Å^{-3}
115 parameters	$\Delta\rho_{min} = -0.23$ e Å^{-3}
H atoms treated by a mixture of independent and constrained refinement	

Table 1
Hydrogen-bonding geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1⋯O1^i	1.225	1.225	2.450 (2)	180
O4—H4⋯O6^{ii}	0.92 (4)	1.82 (4)	2.703 (3)	160 (3)

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

All methylene H atoms were located in idealized positions and refined in riding mode. C—H distances were set at 0.97Å and U_{iso}(H) values were constained to be $1.5U_{eq}$ of the parent C atom. Both H atoms involved in hydrogen bonding were found in a Fourier difference map and were refined, subject only to the inversion centre constraint.

Data collection: *MSC R-AXIS-II Control Software*; cell refinement: *DENZO* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS86* (Robinson & Sheldrick, 1988); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997) in *WinGX* (Farrugia, 1999); molecular graphics: *DIAMOND* (Brandenburg, 1999).

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supporting information

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disodium trihydrogen bis(2,2′-oxydiacetate) nitrate

Crystal data

$2Na^+ \cdot C_8H_{11}O_{10}^- \cdot NO_3^-$	$F(000) = 768$
$M_r = 375.16$	$D_x = 1.808$ Mg m^{-3}
Monoclinic, $C2/c$	Melting point: not measured K
Hall symbol: -C 2yc	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 12.010$ (2) Å	Cell parameters from 101 reflections
$b = 7.0290$ (14) Å	$\theta = 3.2$–24.8°
$c = 16.382$ (3) Å	$\mu = 0.22$ mm^{-1}
$\beta = 94.84$ (3)°	$T = 293$ K
$V = 1378.0$ (4) Å^3	Block, colourless
$Z = 4$	$0.16 \times 0.16 \times 0.06$ mm

Data collection

Rigaku R-AXIS-IIc diffractometer	996 reflections with $I > 2\sigma(I)$
Radiation source: Mo rotating anode	$R_{int} = 0.016$
Graphite monochromator	$\theta_{max} = 24.8°$, $\theta_{min} = 3.4°$
φ scans	$h = 0 \rightarrow 14$
1999 measured reflections	$k = -8 \rightarrow 8$
1124 independent reflections	$l = -19 \rightarrow 19$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.033$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.103$	
$S = 1.17$	H atoms treated by a mixture of independent and constrained refinement
1124 reflections	
115 parameters	$w = 1/[\sigma^2(F_o^2) + (0.0446P)^2 + 1.8079P]$ where $P = (F_o^2 + 2F_c^2)/3$
0 restraints	
Primary atom site location: structure-invariant direct methods	$(\Delta/\sigma)_{max} < 0.001$
	$\Delta\rho_{max} = 0.16$ e Å^{-3}
	$\Delta\rho_{min} = -0.23$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Na1	0.48509 (7)	0.24986 (12)	0.55036 (5)	0.0308 (3)
O3	0.67561 (12)	0.1858 (2)	0.60051 (9)	0.0301 (4)
O2	0.62402 (12)	0.4925 (2)	0.51549 (9)	0.0296 (4)
O6	0.48709 (15)	0.4402 (3)	0.68343 (9)	0.0407 (5)
N1	0.5000	0.3494 (4)	0.7500	0.0348 (7)
C1	0.71748 (17)	0.4937 (3)	0.55231 (11)	0.0228 (5)
C2	0.75705 (17)	0.3318 (3)	0.60802 (13)	0.0269 (5)
H2A	0.8281	0.2839	0.5926	0.040*
H2B	0.7671	0.3756	0.6643	0.040*
C3	0.70115 (18)	0.0316 (3)	0.65405 (12)	0.0276 (5)
H3A	0.7083	0.0754	0.7104	0.041*
H3B	0.7713	−0.0263	0.6421	0.041*
O7	0.5000	0.1751 (4)	0.7500	0.0792 (11)
O5	0.53165 (13)	−0.0997 (2)	0.58891 (9)	0.0317 (4)
O4	0.62185 (14)	−0.2512 (2)	0.69492 (10)	0.0364 (4)
C4	0.60827 (17)	−0.1102 (3)	0.64181 (12)	0.0241 (5)
O1	0.78860 (12)	0.6300 (2)	0.54870 (9)	0.0310 (4)
H4	0.568 (3)	−0.341 (5)	0.6805 (17)	0.058 (9)*
H1	0.7500	0.7500	0.5000	0.071 (14)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Na1	0.0263 (5)	0.0288 (5)	0.0361 (5)	−0.0002 (4)	−0.0038 (4)	0.0014 (3)
O3	0.0254 (8)	0.0217 (8)	0.0416 (9)	−0.0057 (7)	−0.0069 (6)	0.0124 (7)
O2	0.0235 (8)	0.0269 (8)	0.0374 (8)	−0.0024 (7)	−0.0043 (6)	0.0074 (6)
O6	0.0509 (11)	0.0411 (10)	0.0298 (8)	−0.0082 (9)	0.0018 (7)	−0.0005 (7)
N1	0.0335 (15)	0.0254 (15)	0.0480 (17)	0.000	0.0173 (12)	0.000
C1	0.0228 (10)	0.0199 (11)	0.0260 (10)	−0.0012 (9)	0.0040 (8)	−0.0001 (8)
C2	0.0240 (11)	0.0228 (11)	0.0331 (11)	−0.0050 (9)	−0.0031 (8)	0.0043 (9)
C3	0.0273 (11)	0.0250 (11)	0.0291 (10)	−0.0020 (9)	−0.0051 (8)	0.0084 (9)
O7	0.120 (3)	0.0227 (15)	0.104 (3)	0.000	0.064 (2)	0.000
O5	0.0286 (8)	0.0313 (9)	0.0340 (8)	−0.0041 (7)	−0.0051 (6)	0.0038 (6)
O4	0.0427 (10)	0.0282 (9)	0.0365 (9)	−0.0095 (8)	−0.0073 (7)	0.0121 (7)
C4	0.0270 (11)	0.0217 (11)	0.0237 (10)	0.0004 (9)	0.0032 (8)	0.0019 (8)
O1	0.0258 (8)	0.0243 (8)	0.0420 (9)	−0.0068 (7)	−0.0027 (6)	0.0080 (7)

Geometric parameters (Å, º)

Na1—O3	2.4075 (17)	N1—O6iv	1.262 (2)
Na1—O2i	2.4333 (17)	C1—O1	1.288 (2)
Na1—O2	2.4860 (17)	C1—C2	1.511 (3)
Na1—O1ii	2.5038 (17)	C2—H2A	0.9700
Na1—O5iii	2.5065 (18)	C2—H2B	0.9700
Na1—O6	2.5562 (19)	C3—C4	1.496 (3)
Na1—O5	2.5861 (18)	C3—H3A	0.9700
Na1—Na1iii	3.9100 (18)	C3—H3B	0.9700
Na1—Na1i	3.9135 (18)	O5—C4	1.212 (2)
O3—C3	1.412 (2)	O5—Na1iii	2.5065 (18)
O3—C2	1.416 (3)	O4—C4	1.320 (3)
O2—C1	1.229 (2)	O4—H4	0.92 (3)
O2—Na1i	2.4333 (17)	O1—Na1v	2.5038 (17)
O6—N1	1.262 (2)	O1—H1	1.2250 (14)
N1—O7	1.225 (4)		
O3—Na1—O2i	138.69 (6)	C3—O3—C2	112.97 (15)
O3—Na1—O2	64.51 (5)	C3—O3—Na1	120.39 (12)
O2i—Na1—O2	74.59 (6)	C2—O3—Na1	121.61 (12)
O3—Na1—O1ii	143.96 (6)	C1—O2—Na1i	130.39 (14)
O2i—Na1—O1ii	76.93 (6)	C1—O2—Na1	119.67 (13)
O2—Na1—O1ii	151.48 (6)	Na1i—O2—Na1	105.41 (6)
O3—Na1—O5iii	103.47 (7)	N1—O6—Na1	117.66 (15)
O2i—Na1—O5iii	84.90 (6)	O7—N1—O6iv	120.38 (13)
O2—Na1—O5iii	94.80 (6)	O7—N1—O6	120.38 (13)
O1ii—Na1—O5iii	81.09 (6)	O6iv—N1—O6	119.2 (3)
O3—Na1—O6	82.33 (7)	O2—C1—O1	124.38 (18)
O2i—Na1—O6	87.40 (6)	O2—C1—C2	121.28 (18)
O2—Na1—O6	83.03 (6)	O1—C1—C2	114.34 (17)
O1ii—Na1—O6	97.27 (7)	O3—C2—C1	108.29 (16)
O5iii—Na1—O6	172.29 (7)	O3—C2—H2A	110.0
O3—Na1—O5	63.86 (5)	C1—C2—H2A	110.0
O2i—Na1—O5	155.85 (6)	O3—C2—H2B	110.0
O2—Na1—O5	124.92 (6)	C1—C2—H2B	110.0
O1ii—Na1—O5	82.36 (5)	H2A—C2—H2B	108.4
O5iii—Na1—O5	79.71 (6)	O3—C3—C4	107.92 (16)
O6—Na1—O5	107.62 (6)	O3—C3—H3A	110.1
O3—Na1—Na1iii	81.83 (5)	C4—C3—H3A	110.1
O2i—Na1—Na1iii	123.13 (5)	O3—C3—H3B	110.1
O2—Na1—Na1iii	115.62 (6)	C4—C3—H3B	110.1
O1ii—Na1—Na1iii	79.21 (5)	H3A—C3—H3B	108.4
O5iii—Na1—Na1iii	40.60 (4)	C4—O5—Na1iii	128.54 (14)
O6—Na1—Na1iii	146.66 (6)	C4—O5—Na1	111.59 (14)
O5—Na1—Na1iii	39.10 (4)	Na1iii—O5—Na1	100.29 (6)
O3—Na1—Na1i	101.17 (5)	C4—O4—H4	107.3 (18)
O2i—Na1—Na1i	37.76 (4)	O5—C4—O4	124.1 (2)

O2—Na1—Na1^{i}	36.83 (4)	O5—C4—C3	124.60 (18)
O1^{ii}—Na1—Na1^{i}	114.68 (5)	O4—C4—C3	111.24 (17)
O5^{iii}—Na1—Na1^{i}	89.88 (5)	C1—O1—Na1^{v}	151.39 (13)
O6—Na1—Na1^{i}	83.95 (5)	C1—O1—H1	109.02 (14)
O5—Na1—Na1^{i}	158.59 (6)	Na1^{v}—O1—H1	94.58 (8)
Na1^{iii}—Na1—Na1^{i}	127.91 (5)		

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) *x*−1/2, *y*−1/2, *z*; (iii) −*x*+1, −*y*, −*z*+1; (iv) −*x*+1, *y*, −*z*+3/2; (v) *x*+1/2, *y*+1/2, *z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O1^{vi}	1.23	1.23	2.450 (2)	180
O4—H4···O6^{vii}	0.92 (4)	1.82 (4)	2.703 (3)	160 (3)

Symmetry codes: (vi) −*x*+3/2, −*y*+3/2, −*z*+1; (vii) *x*, *y*−1, *z*.