Acta Cryst E CRYSTALLOGRAPHIC COMMUNICATIONS

ISSN 2056-9890

Synthesis, crystal structure and Hirshfeld surface analysis of sodium bis(malonato)borate monohydrate

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Received 28 November 2023
Accepted 14 January 2024

Edited by W. T. A. Harrison, University of Aberdeen, United Kingdom

Keywords: synthesis; crystal structure; bis(malonato)borate anion; sodium; Hirshfeld surface analysis..

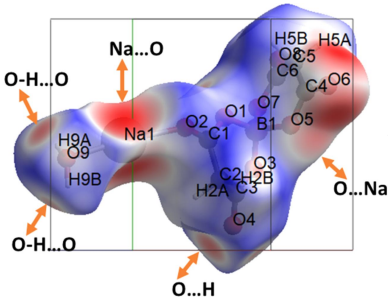
CCDC reference: 2325391

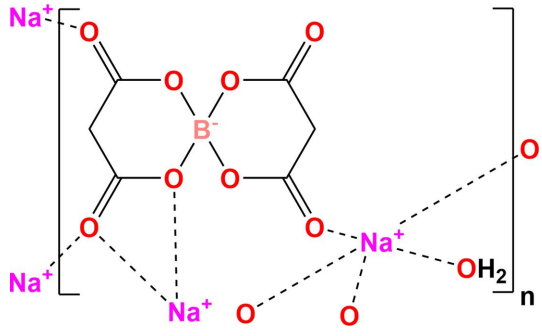
Supporting information: this article has supporting information at journals.iucr.org/e

In the title salt, poly[aqua[μ_4-bis(malonato)borato]sodium], {[Na($C_6H_4BO_8$)]·H_2O}$_n$ or Na^+·[$B(C_3H_2O_4)_2$]$^-$·H_2O, the sodium cation exhibits fivefold coordination by four carbonyl O atoms of the bis(malonato)borate anions and a water O atom. The tetrahedral B atom at the centre of the anion leads to the formation of a polymeric three-dimensional framework, which is consolidated by C—H···O and O—H···O hydrogen bonds. A Hirshfeld surface analysis indicates that the most significant contacts in the crystal packing are H···O/O···H (49.7%), Na···O/O···Na (16.1%), O···O (12.6%), H···H (10.7%) and C···O/O···C (7.3%).

1. Chemical context

The review by Vaalma *et al.* (2018) provides a comprehensive overview of the cost and resource implications of sodium-ion batteries, which are a promising alternative to lithium-ion batteries for energy storage applications. The authors conclude that sodium-ion batteries have the potential to be significantly less expensive than lithium-ion batteries, due to the abundance of sodium and the lower cost of sodium-based materials. Allen *et al.* (2012) described the structure of lithium bis(2-methyllactato)borate monohydrate and there is a growing interest, as highlighted in various recent studies (Vaalma *et al.*, 2018; Abraham, 2020; Li *et al.*, 2019; Wang *et al.*, 2018), in lithium bis(malonato)borate polymers as robust electrolytes.





The present study explores the substitution of 2-methyllactic acid and lithium carbonate with malonic acid and sodium carbonate, respectively, and presents the synthesis, crystal structure and Hirshfeld surface analysis of the title compound, Na^+·[$B(C_3H_2O_4)_2$]$^-$·H_2O, (I).

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Table 1
Selected geometric parameters (Å, °).

Na1—O9	2.3264 (12)	B1—O3	1.4508 (15)
Na1—O2	2.3402 (11)	B1—O7	1.4581 (16)
Na1—O6^{i}	2.4032 (10)	B1—O1	1.4697 (15)
Na1—O8^{ii}	2.4213 (12)	B1—O5	1.4779 (15)
Na1—O6^{iii}	2.4455 (11)		
O9—Na1—O2	171.38 (5)	O6^{i}—Na1—O8^{ii}	80.15 (4)
O9—Na1—O6^{i}	102.48 (4)	O9—Na1—O6^{iii}	84.03 (4)
O2—Na1—O6^{i}	85.61 (4)	O2—Na1—O6^{iii}	88.60 (4)
O9—Na1—O8^{ii}	88.27 (5)	O6^{i}—Na1—O6^{iii}	167.40 (3)
O2—Na1—O8^{ii}	90.22 (5)	O8^{ii}—Na1—O6^{iii}	111.10 (5)

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

2. Structural commentary

The asymmetric unit of (I) comprises a sodium cation, a bis(malonato)borate anion and a coordinated water molecule (Fig. 1). The tetrahedral B atom is bonded to two malonate ($C_3H_2O_4$) ligands coordinated in an *O*,*O*′-bidentate mode.

In the boron–oxygen tetrahedron, the mean B—O bond length of 1.4641 Å is in good agreement with the expected B(sp^3)—O bond length of 1.468 Å (Allen *et al.*, 1987). The largest O—B—O bond angles are the intracyclic angles: O1—B1—O3 = 112.92 (9)° and O5—B1—O7 = 112.21 (9)°. The six-membered boro–malonate rings O1/C1/C2/C3/O3/B1 and O5/C4/C5/C6/O7/B1 both adopt boat conformations [puckering parameters Q = 0.4082 (13) Å, θ = 87.85 (18)° and φ = 309.10 (18)° for the first ring, and Q = 0.4267 (13) Å, θ = 84.32 (16)° and φ = 317.00 (17)° for the second ring]. The 'prow and stern' atoms in the first ring, B1 and C2, are displaced by 0.3680 (18) and 0.330 (2) Å, respectively, from C1/C3/O1/O3 (r.m.s. deviation = 0.0323 Å). In the second ring, the equivalent data are a B1 displacement of 0.4048 (17), a C5 displacement of 0.298 (2) Å and an r.m.s. deviation of 0.0621 Å. The dihedral angle between the O1/C1/C3/O3 and O5/C4/C6/O7 least-squares planes is 73.34 (4)°.

Na1 is surrounded by five O atoms [carbonyl O2 and O6 at $(x-1, y, z)$, water O9, carbonyl O8 at $(x-\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2})$ and O6 at $(-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{3}{2})$], forming a square-based pyramidal coordination polyhedron (Table 1). A possible sixth bond [Na1—O5 at $(x-1, y, z)$], which would generate a distorted octahedron, is much longer at 3.0195 (10) Å and presumably only represents a marginal interaction in the structure.

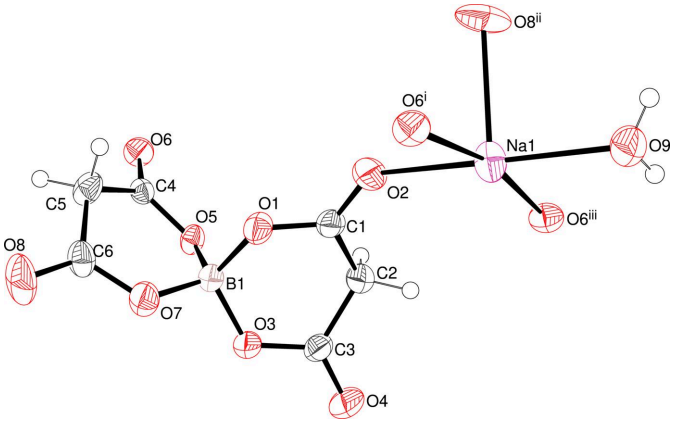

Figure 1
View of the molecular structure of (I), showing 50% probability displacement ellipsoids (arbitrary spheres for the H atoms).

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2B···O9^{iv}	0.97	2.54	3.4247 (18)	151
C5—H5B···O4^{v}	0.97	2.46	3.2830 (18)	143
O9—H9A···O4^{vi}	0.85 (1)	2.23 (2)	2.9932 (17)	151 (3)
O9—H9B···O1^{vii}	0.84 (1)	2.46 (2)	3.1520 (14)	140 (3)
O9—H9B···O2^{vii}	0.84 (1)	2.39 (2)	3.1166 (17)	146 (3)

Symmetry codes: (iv) $x+1, y, z$; (v) $x, y+1, z$; (vi) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$; (vii) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$.

3. Supramolecular features and Hirshfeld surface analysis

The crystal structure of (I) is consolidated by two C—H···O links with the acceptors being one water O9 atom and one carbonyl O4 atom, and three O—H···O links, one of which is bifurcated, with the acceptors being one borate O1 atom and carbonyl atoms O4 and O2 (Table 2). The packing of the structure is shown in Fig. 2.

The Hirshfeld surface analysis of (I) was performed with *CrystalExplorer* (Version 21.5; Spackman *et al.*, 2021). Fig. 3 shows the d_{norm} surface for the bis(malonato)borate anion plotted over the limits from −0.66 to +0.93 a.u. The intense red spots represent the shortest intermolecular contacts (attractive interactions like hydrogen bonds) and the blue

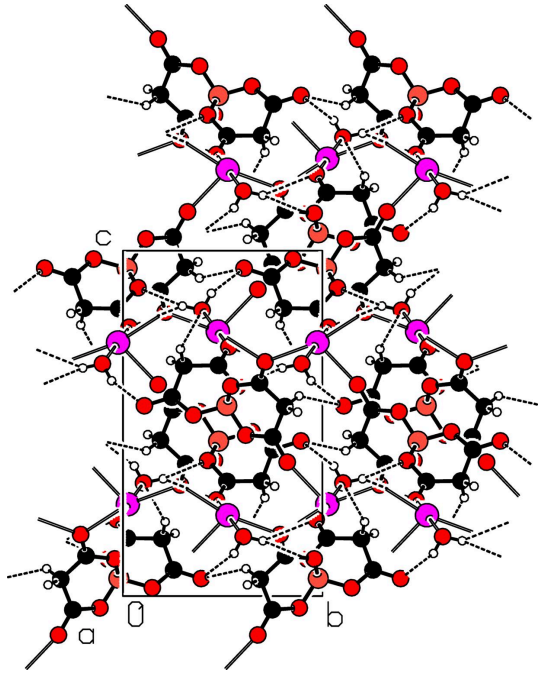

Figure 2
A packing diagram of (I), viewed along the *a*-axis direction (projection onto the *bc* plane), showing the C—H···O and O—H···O hydrogen bonds as black dashed lines.

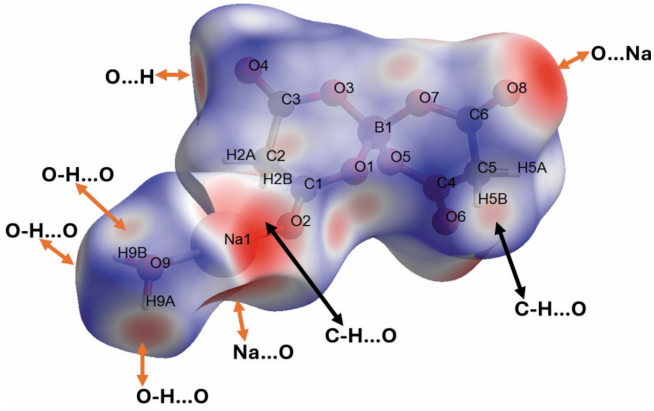

Figure 3
The Hirshfeld surface for (I). The surface is drawn with transparency and simplified for clarity, and the regions with the strongest intermolecular interactions are shown in red. (d_{norm} range: −0.66 to +0.93 a.u.)

regions denotes the longest (indicating possible repulsive interactions or regions with weak van der Waals interactions). Fig. 4 presents the two-dimensional fingerprint plots involving all the intermolecular interactions [Fig. 4(*a*)] and delineated into Na···O/O···Na = 16.1% [Fig. 4(*b*)], C···O/O···C = 7.3% [Fig. 4(*c*)], H···H = 10.7% [Fig. 4(*d*)], H···O/O···H = 49.7% [Fig. 4(*e*)] and O···O = 12.6% [Fig. 4(*f*)] interactions. The remaining interactions contribute less than 2.0%. The hydrogen bonds are indicated by pairs of characteristic wings in the fingerprint plot [Fig. 4(*e*)] representing H···O/O···H contacts. Pairs of scattered points of spikes are seen in the fingerprint plot delineated into H···O/O···H contacts (49.7% the maximum contribution to the Hirshfeld surface) [Fig. 4(*e*)].

4. Database survey

A search using CCDC *ConQuest* of the Cambridge Structural Database (CSD, Version 5.44, updated to June 2023; Groom *et al.*, 2016) for the bis(malonato)borate anion gave one hit (CSD refcode PITQUF; Zviedre & Belyakov, 2007), in which the bis(malonato)borate unit is similar to that in (I) and is charge balanced by potassium cations. The K^+ coordination geometry in PITQUF is an irregular nine-vertex polyhedron formed by the O atoms of seven complex anions.

5. Synthesis and crystallization

The title compound was synthesized by mixing malonic acid ($C_3H_4O_4$), boric acid (H_3BO_3) and sodium carbonate (Na_2CO_3) in a 4:2:1 molar ratio, using deionized water as the solvent. Initially, malonic acid (4.1264 g) was dissolved in deionized water. This was followed by the addition of a boric acid solution (1.236 g) and then a sodium carbonate solution (1.382 g) was added. The mixture was stirred thoroughly to ensure a uniform solution. The beaker containing the solution was then covered with a perforated sheet and left undisturbed. Over three months, due to slow evaporation of the solvent, small clear crystals of (I) formed at the bottom of the container [yield: 2.744 g, 40.6%; m.p. 527–529 K (decomposition)]. FT–IR (cm^{-1}): 3928, 3856, 3419, 3014, 2908, 2542,

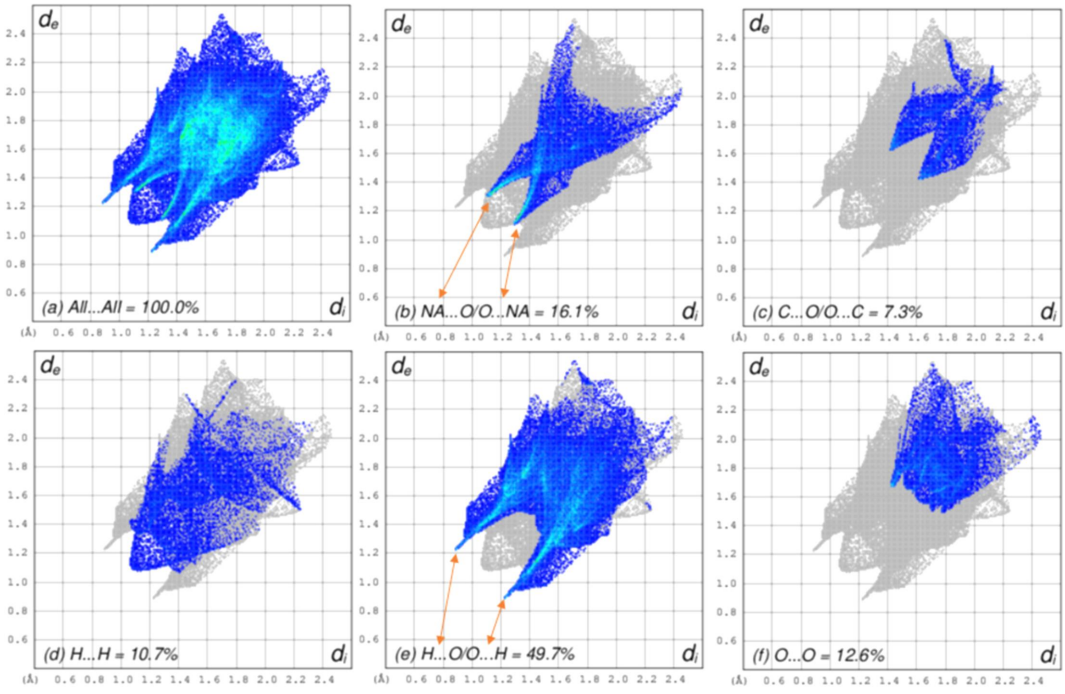

Figure 4
A view of the two-dimensional fingerprint plots for title compound (I), showing (*a*) all interactions, and those delineated into (*b*) Na···O/O···Na, (*c*) C···O/O···C, (*d*) H···H, (*e*) H···O/O···H and (*f*) O···O interactions. The d_i (*x* axis) and d_e (*y* axis) values are the closest internal and external distances (in Å) from given points on the Hirshfeld surface.

2016, 1711, 1635, 1400, 1334, 1271, 1069, 1019, 958, 914, 859, 833, 657, 634, 561, 478, 457, 423.

6. Refinement

Crystal data and structure refinement details are summarized in Table 3. The H atoms attached to C atoms were placed in calculated positions (C—H = 0.97 Å) and refined as riding atoms with U_{iso}(H) = 1.2U_{eq}(C). The water H atoms were located in difference maps and refined with restraints (O—H = 0.84 ± 0.02 Å and H···H = 1.36 ± 0.02 Å) to ensure a realistic geometry.

Acknowledgements

The authors thank the Sophisticated Analytical Instrument Facility (SAIF), Indian Institute of Technology Madras (IITM), Chennai, Tamilnadu, India, for the single-crystal X-ray diffraction data.

Table 3
Experimental details.

Crystal data	
Chemical formula	$[Na(C_6H_4BO_8)(H_2O)]$
M_r	255.91
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	298
a, b, c (Å)	7.9058 (4), 8.2979 (5), 14.6473 (9)
β (°)	101.565 (2)
V (Å^3)	941.38 (9)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.21
Crystal size (mm)	0.35 × 0.27 × 0.27
Data collection	
Diffractometer	Bruker D8 VENTURE diffractometer with a PHOTON II detector
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.917, 0.958
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	32209, 2864, 2494
R_{int}	0.030
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.714
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.038, 0.105, 1.08
No. of reflections	2864
No. of parameters	162
No. of restraints	4
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.53, −0.60

Computer programs: *APEX4*, *SAINT* and *XPREP* (Bruker, 2021), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012), *PLATON* (Spek, 2020) and *publCIF* (Westrip, 2010).

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supporting information

Acta Cryst. (2024). E**80**, 180-183 [https://doi.org/10.1107/S2056989024000537]

Synthesis, crystal structure and Hirshfeld surface analysis of sodium bis-(malonato)borate monohydrate

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Computing details

Poly[aqua[μ_4-bis(malonato)borato]sodium]

Crystal data

$[Na(C_6H_4BO_8)(H_2O)]$
M_r = 255.91
Monoclinic, $P2_1/n$
a = 7.9058 (4) Å
b = 8.2979 (5) Å
c = 14.6473 (9) Å
β = 101.565 (2)°
V = 941.38 (9) Å^3
Z = 4
$F(000)$ = 520
D_x = 1.806 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9951 reflections
θ = 2.8–30.5°
μ = 0.21 mm^{-1}
T = 298 K
Block, colourless
0.35 × 0.27 × 0.27 mm

Data collection

Bruker D8 VENTURE diffractometer with a PHOTON II detector
Radiation source: fine-focus sealed tube
ω and φ scan
Absorption correction: multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min} = 0.917, T_{max} = 0.958
32209 measured reflections
2864 independent reflections
2494 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 30.5°, θ_{min} = 3.6°
h = −10→11
k = −11→11
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.105
S = 1.08
2864 reflections
162 parameters
4 restraints
Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0503P)^2 + 0.3262P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.60 e Å^{-3}

Special details

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Na1	0.24488 (7)	0.47538 (7)	0.76584 (4)	0.03728 (15)
B1	0.76757 (17)	0.52073 (15)	0.55156 (9)	0.0271 (2)
C1	0.59169 (15)	0.47853 (15)	0.66789 (9)	0.0294 (2)
C2	0.64385 (17)	0.30481 (15)	0.66658 (9)	0.0331 (3)
H2A	0.551966	0.239128	0.681940	0.040*
H2B	0.745590	0.288268	0.715054	0.040*
C3	0.68228 (16)	0.24605 (14)	0.57587 (9)	0.0309 (2)
C4	1.01449 (13)	0.68524 (13)	0.61701 (7)	0.0235 (2)
C5	0.93606 (17)	0.81205 (14)	0.54883 (9)	0.0340 (3)
H5A	1.028548	0.875823	0.532601	0.041*
H5B	0.867448	0.883229	0.579401	0.041*
C6	0.82428 (16)	0.75128 (16)	0.46059 (9)	0.0331 (3)
O1	0.64336 (12)	0.57513 (11)	0.60743 (7)	0.0337 (2)
O2	0.50736 (14)	0.53111 (13)	0.72169 (8)	0.0451 (3)
O3	0.74511 (13)	0.35276 (11)	0.52435 (7)	0.0358 (2)
O4	0.66050 (17)	0.10738 (13)	0.55087 (9)	0.0518 (3)
O5	0.94362 (11)	0.54098 (10)	0.60778 (6)	0.02768 (18)
O6	1.13921 (12)	0.71217 (11)	0.67822 (6)	0.0329 (2)
O7	0.74022 (12)	0.61563 (12)	0.46608 (6)	0.0366 (2)
O8	0.80823 (17)	0.82359 (17)	0.38773 (8)	0.0577 (3)
O9	0.00848 (15)	0.39690 (13)	0.82757 (8)	0.0448 (3)
H9A	−0.008 (4)	0.443 (3)	0.8765 (14)	0.088 (9)*
H9B	0.019 (4)	0.2983 (16)	0.8397 (19)	0.100 (10)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Na1	0.0334 (3)	0.0373 (3)	0.0430 (3)	0.0070 (2)	0.0124 (2)	0.0112 (2)
B1	0.0289 (6)	0.0257 (6)	0.0283 (6)	−0.0034 (4)	0.0090 (5)	−0.0002 (4)
C1	0.0242 (5)	0.0316 (6)	0.0337 (6)	−0.0052 (4)	0.0089 (4)	−0.0065 (4)
C2	0.0401 (6)	0.0291 (6)	0.0316 (6)	−0.0021 (5)	0.0107 (5)	0.0008 (4)
C3	0.0322 (5)	0.0252 (5)	0.0360 (6)	−0.0037 (4)	0.0086 (4)	−0.0039 (4)
C4	0.0255 (4)	0.0238 (5)	0.0219 (4)	0.0022 (4)	0.0062 (4)	0.0025 (4)
C5	0.0391 (6)	0.0234 (5)	0.0355 (6)	−0.0004 (4)	−0.0022 (5)	0.0087 (5)
C6	0.0310 (5)	0.0382 (6)	0.0286 (6)	0.0004 (5)	0.0025 (4)	0.0120 (5)
O1	0.0349 (4)	0.0249 (4)	0.0456 (5)	0.0004 (3)	0.0180 (4)	−0.0013 (4)
O2	0.0423 (5)	0.0478 (6)	0.0527 (6)	−0.0066 (4)	0.0272 (5)	−0.0150 (5)
O3	0.0458 (5)	0.0288 (4)	0.0375 (5)	−0.0077 (4)	0.0198 (4)	−0.0079 (4)
O4	0.0722 (8)	0.0270 (5)	0.0611 (7)	−0.0110 (5)	0.0249 (6)	−0.0122 (5)

O5	0.0295 (4)	0.0236 (4)	0.0292 (4)	−0.0007 (3)	0.0042 (3)	0.0075 (3)
O6	0.0332 (4)	0.0349 (4)	0.0274 (4)	−0.0009 (3)	−0.0016 (3)	0.0013 (3)
O7	0.0369 (4)	0.0411 (5)	0.0282 (4)	−0.0087 (4)	−0.0017 (3)	0.0066 (4)
O8	0.0601 (7)	0.0713 (8)	0.0370 (6)	−0.0081 (6)	−0.0020 (5)	0.0315 (6)
O9	0.0525 (6)	0.0366 (5)	0.0487 (6)	−0.0035 (4)	0.0181 (5)	0.0039 (5)

Geometric parameters (Å, º)

Na1—O9	2.3264 (12)	C2—H2A	0.9700
Na1—O2	2.3402 (11)	C2—H2B	0.9700
Na1—O6^{i}	2.4032 (10)	C3—O4	1.2094 (16)
Na1—O8^{ii}	2.4213 (12)	C3—O3	1.3231 (15)
Na1—O6^{iii}	2.4455 (11)	C4—O6	1.2130 (14)
Na1—O5^{i}	3.0195 (10)	C4—O5	1.3171 (13)
B1—O3	1.4508 (15)	C4—C5	1.4969 (15)
B1—O7	1.4581 (16)	C5—C6	1.4993 (18)
B1—O1	1.4697 (15)	C5—H5A	0.9700
B1—O5	1.4779 (15)	C5—H5B	0.9700
C1—O2	1.2109 (15)	C6—O8	1.2086 (15)
C1—O1	1.3186 (15)	C6—O7	1.3177 (16)
C1—C2	1.5005 (17)	O9—H9A	0.846 (13)
C2—C3	1.5024 (17)	O9—H9B	0.838 (13)
O9—Na1—O2	171.38 (5)	O4—C3—C2	122.33 (12)
O9—Na1—O6^{i}	102.48 (4)	O3—C3—C2	116.93 (10)
O2—Na1—O6^{i}	85.61 (4)	O6—C4—O5	120.62 (10)
O9—Na1—O8^{ii}	88.27 (5)	O6—C4—C5	122.02 (10)
O2—Na1—O8^{ii}	90.22 (5)	O5—C4—C5	117.36 (10)
O6^{i}—Na1—O8^{ii}	80.15 (4)	O6—C4—Na1^{iv}	45.91 (6)
O9—Na1—O6^{iii}	84.03 (4)	O5—C4—Na1^{iv}	74.82 (6)
O2—Na1—O6^{iii}	88.60 (4)	C5—C4—Na1^{iv}	167.29 (8)
O6^{i}—Na1—O6^{iii}	167.40 (3)	C4—C5—C6	115.62 (10)
O8^{ii}—Na1—O6^{iii}	111.10 (5)	C4—C5—H5A	108.4
O9—Na1—O5^{i}	77.10 (4)	C6—C5—H5A	108.4
O2—Na1—O5^{i}	111.06 (4)	C4—C5—H5B	108.4
O6^{i}—Na1—O5^{i}	46.12 (3)	C6—C5—H5B	108.4
O8^{ii}—Na1—O5^{i}	117.12 (4)	H5A—C5—H5B	107.4
O6^{iii}—Na1—O5^{i}	127.08 (4)	O8—C6—O7	120.86 (13)
O3—B1—O7	107.10 (10)	O8—C6—C5	122.25 (13)
O3—B1—O1	112.92 (9)	O7—C6—C5	116.88 (10)
O7—B1—O1	108.16 (10)	C1—O1—B1	121.25 (10)
O3—B1—O5	108.18 (10)	C1—O2—Na1	137.99 (9)
O7—B1—O5	112.21 (9)	C3—O3—B1	121.70 (10)
O1—B1—O5	108.33 (10)	C4—O5—B1	119.62 (9)
O2—C1—O1	120.21 (12)	C4—O5—Na1^{iv}	80.28 (6)
O2—C1—C2	122.89 (12)	B1—O5—Na1^{iv}	156.45 (7)
O1—C1—C2	116.90 (10)	C4—O6—Na1^{iv}	112.84 (8)
C1—C2—C3	115.33 (11)	C4—O6—Na1^{v}	127.34 (8)

C1—C2—H2A	108.4	Na1^{iv}—O6—Na1^{v}	118.98 (3)
C3—C2—H2A	108.4	C6—O7—B1	121.60 (10)
C1—C2—H2B	108.4	C6—O8—Na1^{vi}	164.30 (13)
C3—C2—H2B	108.4	Na1—O9—H9A	118 (2)
H2A—C2—H2B	107.5	Na1—O9—H9B	108 (2)
O4—C3—O3	120.73 (12)	H9A—O9—H9B	107 (2)
O2—C1—C2—C3	156.38 (13)	C5—C4—O5—B1	−17.36 (15)
O1—C1—C2—C3	−24.22 (16)	Na1^{iv}—C4—O5—B1	166.54 (9)
C1—C2—C3—O4	−150.74 (13)	O6—C4—O5—Na1^{iv}	−3.33 (10)
C1—C2—C3—O3	30.58 (17)	C5—C4—O5—Na1^{iv}	176.10 (10)
O6—C4—C5—C6	160.61 (11)	O3—B1—O5—C4	159.43 (9)
O5—C4—C5—C6	−18.81 (16)	O7—B1—O5—C4	41.49 (14)
Na1^{iv}—C4—C5—C6	143.8 (3)	O1—B1—O5—C4	−77.85 (12)
C4—C5—C6—O8	−150.46 (14)	O3—B1—O5—Na1^{iv}	−55.6 (2)
C4—C5—C6—O7	30.90 (17)	O7—B1—O5—Na1^{iv}	−173.55 (12)
O2—C1—O1—B1	170.39 (12)	O1—B1—O5—Na1^{iv}	67.1 (2)
C2—C1—O1—B1	−9.02 (16)	O5—C4—O6—Na1^{iv}	4.47 (13)
O3—B1—O1—C1	35.76 (16)	C5—C4—O6—Na1^{iv}	−174.93 (9)
O7—B1—O1—C1	154.11 (10)	O5—C4—O6—Na1^{v}	−164.81 (7)
O5—B1—O1—C1	−84.03 (13)	C5—C4—O6—Na1^{v}	15.79 (16)
O1—C1—O2—Na1	126.39 (13)	Na1^{iv}—C4—O6—Na1^{v}	−169.29 (12)
C2—C1—O2—Na1	−54.2 (2)	O8—C6—O7—B1	175.44 (14)
O4—C3—O3—B1	178.15 (13)	C5—C6—O7—B1	−5.90 (18)
C2—C3—O3—B1	−3.14 (18)	O3—B1—O7—C6	−147.33 (11)
O7—B1—O3—C3	−147.88 (11)	O1—B1—O7—C6	90.69 (14)
O1—B1—O3—C3	−28.92 (17)	O5—B1—O7—C6	−28.75 (16)
O5—B1—O3—C3	90.96 (13)	O7—C6—O8—Na1^{vi}	117.5 (4)
O6—C4—O5—B1	163.22 (10)	C5—C6—O8—Na1^{vi}	−61.0 (5)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2*B*···O9^{iv}	0.97	2.54	3.4247 (18)	151
C5—H5*B*···O4^{vii}	0.97	2.46	3.2830 (18)	143
O9—H9*A*···O4^{viii}	0.85 (1)	2.23 (2)	2.9932 (17)	151 (3)
O9—H9*B*···O1^{ix}	0.84 (1)	2.46 (2)	3.1520 (14)	140 (3)
O9—H9*B*···O2^{ix}	0.84 (1)	2.39 (2)	3.1166 (17)	146 (3)

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