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catena-Poly[[sodium-di-μ-aqua-μ-(boric acid)-μ-succinato-sodium-di-μ-aqua] boric acid monosolvate]

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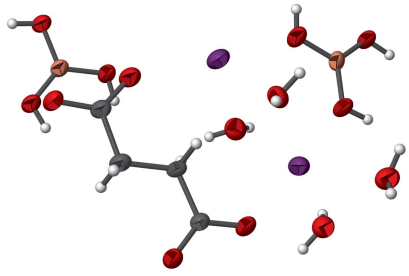
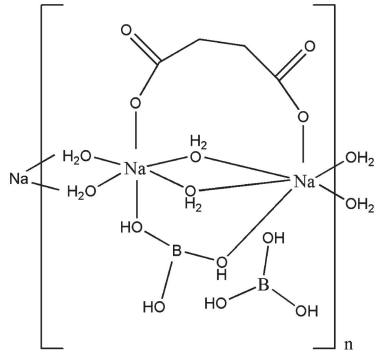
The title polymeric compound, $\{[Na_2(C_4H_4O_4)(H_3BO_3)(H_2O)_4]\cdot H_3BO_3\}_n$, comprises [101] chains of edge-sharing $[NaO_6]$ octahedra flanked by succinate and boric acid ligands. An intricate three-dimensional network is formed by O—H···O hydrogen bonds involving all components of the crystal. The crystal investigated was a non-merohedral twin; major component = 83%.

3D view



Chemical scheme



Structure description

Owing to their rich structural chemistry and potential applications in mineralogy (Grice *et al.*, 1999) and nonlinear optical materials (Touboul *et al.*, 2003), borates have provided an abounding area of research for over half a century. Hence, borates with various main groups and transition metals have been widely explored. However, less work has been carried out on inorganic–organic hybrid borates.

The asymmetric unit of the title compound contains two Na^+ cations (Na1 and Na2) which are octahedrally coordinated. Both cations are bonded to four bridging water molecules, one carboxylate O atom of the succinate anion and one O atom of a non-deprotonated boric acid ligand. In the crystal, the $[NaO_6]$ octahedra are linked through edge-sharing into chains extending parallel to [101] (Fig. 1). The succinato and boric acid ligands additionally bridge these chains. A pair of O—H···O hydrogen bonds [O5—H5···O7^{iii}; O9—H9···O11^{iii}; for the symmetry code, see: Table 1] generates an $R_2^2(8)$ ring motif. The chains exhibit intrachain hydrogen bonding and are linked through the boric acid solvent molecules by other O—H···O hydrogen bonds into a three-dimensional network (Table 1 and Fig. 2). Structures with boric acid as a solvent molecule with

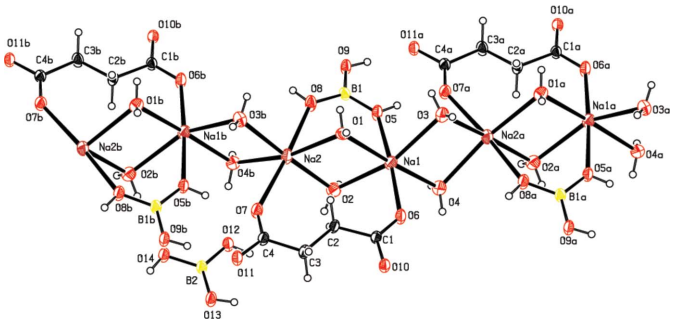


Figure 1
The chain structure of the title compound, with atom labelling and displacement ellipsoids drawn at the 30% probability level. [Symmetry codes: (*a*) $x-\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$; (*b*) $x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$.]

hydrogen-bonded networks have been reported by Li *et al.* (1999) and Shao *et al.*, (2010). Bond lengths and angles of the succinate anion in the title structure are comparable with those of a related structure (Sarr *et al.*, 2015).

Synthesis and crystallization

A mixture of boric acid (1.24 g; 0.02 mol) and succinic acid (1.18 g; 0.01 mol) in deionized water was heated at 353 K in a round bottom flask attached with a reflux condenser for 6 h. Then the temperature was reduced to 313 K before sodium carbonate (1.06 g; 0.01 mol) was added in small portions to the solution that was stirred for about 12 h. The resulting homogeneous solution was filtered through filter paper and was allowed to evaporate at a constant temperature of 313 K using a temperature bath. After a period of 9 to 10 weeks, crystals suitable for X-ray diffraction could be harvested.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Anisotropic displacement parameters of atoms O8, B1 and O10, C1 were restrained within 0.001 Å^2 by using the DELU command in *SHELXL* (Sheldrick, 2008). The crystal investigated was refined under consideration as a two-component twin by non-merohedry. The twin ratio refined to a value of 0.83:0.17.

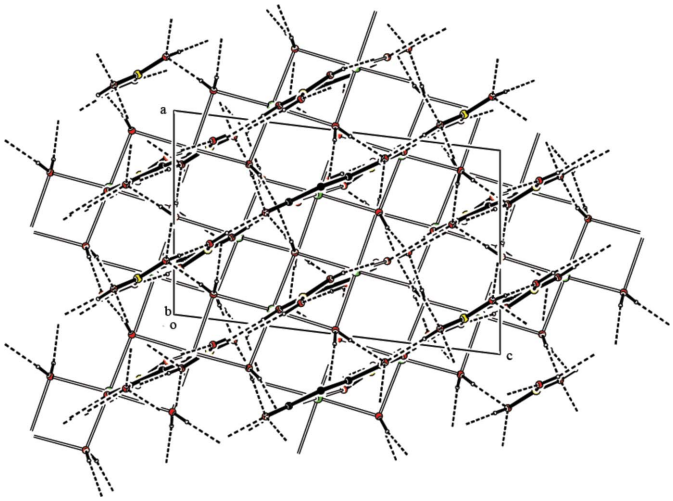


Figure 2
The crystal packing of the title compound viewed along the *b* axis. O—H···O hydrogen bonds are shown as dashed lines.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···O12^{i}	0.84 (1)	2.01 (1)	2.825 (2)	166 (2)
O1—H1*B*···O11^{ii}	0.85 (1)	2.00 (1)	2.825 (2)	164 (3)
O2—H2*C*···O14^{iii}	0.82 (1)	2.23 (1)	3.045 (2)	176 (2)
O2—H2*D*···O10^{iv}	0.81 (1)	2.01 (1)	2.822 (2)	175 (3)
O3—H3*C*···O14^{v}	0.82 (1)	2.02 (1)	2.840 (2)	173 (3)
O3—H3*D*···O10^{vi}	0.83 (1)	2.21 (1)	3.035 (2)	172 (3)
O4—H4*A*···O11^{iv}	0.83 (1)	2.12 (2)	2.923 (2)	164 (4)
O4—H4*B*···O12^{iii}	0.82 (1)	2.01 (1)	2.818 (2)	169 (2)
O5—H5···O7^{iii}	0.83 (1)	1.87 (1)	2.6888 (18)	173 (2)
O8—H8···O13^{vii}	0.83 (1)	1.89 (1)	2.711 (2)	174 (2)
O9—H9···O11^{iii}	0.82 (1)	1.79 (1)	2.6044 (18)	176 (2)
O12—H12···O10^{iv}	0.82 (1)	1.83 (1)	2.6261 (18)	167 (2)
O13—H13···O6^{iv}	0.81 (1)	1.81 (1)	2.6113 (19)	172 (3)
O14—H14···O9^{viii}	0.83 (1)	1.81 (1)	2.6384 (19)	175 (2)

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Na_2(C_4H_4O_4)(BH_3O_3)(H_2O)_4]\cdot BH_3O_3$
M_r	357.78
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	295
a, *b*, *c* (Å)	7.8524 (4), 14.8559 (9), 12.6646 (6)
β (°)	96.964 (5)
V (Å^3)	1466.48 (14)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.21
Crystal size (mm)	0.30 × 0.24 × 0.20
Data collection	
Diffractometer	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (*TWINABS*; Bruker, 2012)
T_{min}, T_{max}	0.941, 0.960
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	24155, 24155, 14052
R_{int}	0.000
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.597
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.069, 0.164, 1.09
No. of reflections	24155
No. of parameters	257
No. of restraints	16
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, −0.44

Computer programs: *APEX2* and *SAINT* (Bruker, 2004), *SHELXS97* and *SHELXL97* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x160948 [doi:10.1107/S2414314616009482]

catena-Poly[[sodium-di-μ-aqua-μ-(boric acid)-μ-succinato-sodium-di-μ-aqua] boric acid monosolvate]

Gunasekaran Rajasekar, Panchanathan Vinothkumar, Sakkarapani Sudhahar, Ganesan Chakkaravarthi and Arumugam Bhaskaran

***catena*-Poly[[sodium-di-μ-aqua-μ-(boric acid)-μ-succinato-sodium-di-μ-aqua] boric acid monosolvate]**

Crystal data

$[Na_2(C_4H_4O_4)(BH_3O_3)(H_2O)_4]\cdot BH_3O_3$
M_r = 357.78
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 7.8524 (4) Å
b = 14.8559 (9) Å
c = 12.6646 (6) Å
β = 96.964 (5)°
V = 1466.48 (14) Å^3
Z = 4
$F(000)$ = 744
D_x = 1.621 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9068 reflections
θ = 2.7–23.6°
μ = 0.21 mm^{-1}
T = 295 K
Block, colourless
0.30 × 0.24 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scan
Absorption correction: multi-scan (*TWINABS*; Bruker, 2012)
T_{min} = 0.941, T_{max} = 0.960
24155 measured reflections
24155 independent reflections
14052 reflections with $I > 2\sigma(I)$
R_{int} = 0.000
θ_{max} = 25.1°, θ_{min} = 2.1°
h = −9→9
k = −17→17
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.164
S = 1.09
24155 reflections
257 parameters
16 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
$w = 1/[\sigma^2(F_o^2) + (0.0211P)^2 + 6.2176P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}
Extinction correction: SHELXL97 (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00222 (15)

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.

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.1246 (2)	−0.02094 (12)	0.36401 (15)	0.0295 (4)
C2	0.2195 (2)	0.01759 (12)	0.46482 (15)	0.0342 (5)
H2A	0.3162	0.0521	0.4458	0.041*
H2B	0.1435	0.0593	0.4950	0.041*
C3	0.2852 (3)	−0.04843 (12)	0.54944 (15)	0.0369 (5)
H3A	0.3621	−0.0903	0.5204	0.044*
H3B	0.1894	−0.0827	0.5701	0.044*
C4	0.3792 (2)	−0.00422 (13)	0.64725 (15)	0.0318 (5)
B1	0.1614 (3)	0.41227 (15)	0.39628 (17)	0.0341 (6)
B2	0.1553 (3)	0.09750 (15)	0.88974 (17)	0.0300 (5)
O1	0.37630 (19)	0.19833 (11)	0.37142 (12)	0.0371 (4)
O2	0.0207 (2)	0.21732 (12)	0.49534 (13)	0.0413 (4)
O3	0.1223 (2)	0.24810 (12)	0.12148 (13)	0.0433 (4)
O4	−0.21781 (19)	0.20360 (12)	0.23010 (12)	0.0394 (4)
O9	0.1317 (2)	0.50134 (9)	0.38965 (11)	0.0417 (4)
O5	0.08776 (19)	0.35194 (9)	0.32262 (11)	0.0393 (4)
O8	0.2674 (2)	0.37719 (10)	0.47929 (11)	0.0441 (4)
O6	0.06469 (18)	0.03609 (8)	0.29602 (10)	0.0442 (4)
O10	0.10757 (17)	−0.10483 (8)	0.35306 (10)	0.0352 (3)
O7	0.38951 (17)	0.07937 (9)	0.65379 (10)	0.0402 (4)
O11	0.44516 (17)	−0.05839 (8)	0.71869 (10)	0.0378 (4)
O12	0.09010 (19)	0.16059 (9)	0.81646 (11)	0.0370 (4)
O13	0.1246 (2)	0.00877 (9)	0.87999 (12)	0.0432 (4)
O14	0.25890 (19)	0.13058 (9)	0.97609 (11)	0.0389 (4)
Na1	0.07984 (10)	0.19493 (5)	0.30174 (6)	0.0365 (2)
Na2	0.32232 (10)	0.22915 (5)	0.55892 (6)	0.0401 (2)
H1A	0.428 (3)	0.2458 (10)	0.360 (2)	0.081 (10)*
H1B	0.446 (3)	0.1637 (15)	0.346 (2)	0.107 (12)*
H2C	−0.048 (3)	0.2588 (12)	0.4929 (19)	0.066 (9)*
H2D	−0.020 (4)	0.1874 (16)	0.5400 (18)	0.107 (13)*
H3C	0.162 (3)	0.2105 (13)	0.0836 (18)	0.077 (10)*
H3D	0.188 (3)	0.2916 (13)	0.131 (2)	0.109 (13)*
H4A	−0.268 (5)	0.1556 (15)	0.240 (4)	0.24 (2)*
H4B	−0.264 (2)	0.2419 (10)	0.2627 (14)	0.029 (6)*
H5	0.027 (2)	0.3771 (13)	0.2735 (13)	0.058 (8)*

H8	0.306 (3)	0.4183 (12)	0.5194 (16)	0.080 (9)*
H12	0.031 (3)	0.1355 (14)	0.7680 (14)	0.074 (9)*
H13	0.075 (3)	−0.0056 (15)	0.8227 (11)	0.080 (9)*
H14	0.291 (3)	0.0877 (10)	1.0157 (14)	0.055 (8)*
H9	0.069 (2)	0.5193 (14)	0.3373 (12)	0.068 (8)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0335 (12)	0.0268 (8)	0.0264 (11)	−0.0020 (9)	−0.0041 (9)	−0.0013 (9)
C2	0.0378 (12)	0.0273 (11)	0.0329 (12)	−0.0043 (9)	−0.0143 (9)	0.0004 (9)
C3	0.0444 (13)	0.0315 (12)	0.0316 (12)	−0.0057 (10)	−0.0080 (10)	−0.0037 (9)
C4	0.0362 (13)	0.0281 (12)	0.0290 (11)	−0.0001 (9)	−0.0046 (9)	−0.0038 (9)
B1	0.0509 (16)	0.0244 (13)	0.0249 (12)	−0.0006 (11)	−0.0041 (9)	0.0036 (9)
B2	0.0390 (14)	0.0258 (13)	0.0238 (12)	0.0012 (10)	−0.0022 (10)	−0.0037 (9)
O1	0.0373 (9)	0.0296 (9)	0.0437 (9)	−0.0029 (8)	0.0024 (7)	0.0058 (7)
O2	0.0407 (10)	0.0381 (10)	0.0445 (10)	0.0016 (8)	0.0026 (8)	0.0026 (8)
O3	0.0455 (11)	0.0465 (11)	0.0371 (10)	−0.0040 (9)	0.0015 (8)	−0.0044 (8)
O4	0.0386 (9)	0.0385 (10)	0.0409 (9)	0.0039 (8)	0.0036 (7)	−0.0013 (8)
O9	0.0624 (11)	0.0236 (8)	0.0326 (9)	0.0031 (7)	−0.0205 (8)	−0.0004 (6)
O5	0.0528 (10)	0.0274 (8)	0.0323 (9)	0.0040 (7)	−0.0174 (7)	−0.0022 (6)
O8	0.0639 (11)	0.0274 (9)	0.0348 (8)	0.0053 (7)	−0.0184 (7)	0.0007 (7)
O6	0.0649 (11)	0.0272 (8)	0.0339 (8)	−0.0020 (7)	−0.0210 (7)	0.0012 (6)
O10	0.0489 (9)	0.0232 (6)	0.0302 (8)	0.0013 (6)	−0.0091 (6)	−0.0009 (6)
O7	0.0532 (10)	0.0276 (8)	0.0356 (8)	0.0011 (7)	−0.0124 (7)	−0.0030 (6)
O11	0.0529 (9)	0.0273 (8)	0.0290 (8)	0.0015 (7)	−0.0122 (7)	−0.0008 (6)
O12	0.0547 (10)	0.0232 (8)	0.0294 (8)	0.0014 (7)	−0.0100 (7)	−0.0007 (6)
O13	0.0660 (11)	0.0247 (8)	0.0329 (9)	−0.0023 (7)	−0.0175 (8)	−0.0021 (7)
O14	0.0529 (10)	0.0267 (9)	0.0326 (8)	−0.0007 (7)	−0.0132 (7)	−0.0020 (7)
Na1	0.0379 (5)	0.0293 (5)	0.0395 (5)	−0.0016 (4)	−0.0062 (4)	−0.0003 (4)
Na2	0.0425 (5)	0.0421 (5)	0.0328 (5)	0.0004 (4)	−0.0077 (4)	−0.0043 (4)

Geometric parameters (Å, º)

C1—O6	1.258 (2)	O2—H2C	0.816 (9)
C1—O10	1.259 (2)	O2—H2D	0.814 (9)
C1—C2	1.511 (2)	O3—Na2^{i}	2.4161 (19)
C2—C3	1.497 (2)	O3—Na1	2.4761 (18)
C2—H2A	0.9700	O3—H3C	0.822 (9)
C2—H2B	0.9700	O3—H3D	0.828 (9)
C3—C4	1.513 (2)	O4—Na1	2.4059 (17)
C3—H3A	0.9700	O4—Na2^{i}	2.4419 (17)
C3—H3B	0.9700	O4—H4A	0.830 (10)
C4—O7	1.247 (2)	O4—H4B	0.815 (9)
C4—O11	1.273 (2)	O9—H9	0.820 (9)
B1—O9	1.345 (2)	O5—Na1	2.3474 (15)
B1—O8	1.363 (3)	O5—H5	0.826 (9)
B1—O5	1.370 (3)	O8—Na2	2.4361 (16)

B2—O13	1.343 (2)	O8—H8	0.829 (9)
B2—O14	1.372 (2)	O6—Na1	2.3634 (14)
B2—O12	1.374 (3)	O7—Na2	2.5533 (15)
O1—Na1	2.3879 (17)	O12—H12	0.815 (9)
O1—Na2	2.5044 (17)	O13—H13	0.810 (9)
O1—H1A	0.836 (9)	O14—H14	0.831 (9)
O1—H1B	0.845 (9)	Na1—Na2	3.6039 (11)
O2—Na2	2.4135 (18)	Na1—Na2^{i}	3.6483 (11)
O2—Na1	2.5716 (18)		

O6—C1—O10	124.41 (17)	Na1—O4—H4B	108.8 (15)
O6—C1—C2	115.38 (16)	Na2^{i}—O4—H4B	106.2 (14)
O10—C1—C2	120.20 (16)	H4A—O4—H4B	106 (3)
C3—C2—C1	116.65 (15)	B1—O9—H9	117.0 (16)
C3—C2—H2A	108.1	B1—O5—Na1	136.87 (13)
C1—C2—H2A	108.1	B1—O5—H5	111.9 (15)
C3—C2—H2B	108.1	Na1—O5—H5	111.1 (15)
C1—C2—H2B	108.1	B1—O8—Na2	136.51 (14)
H2A—C2—H2B	107.3	B1—O8—H8	109.7 (17)
C2—C3—C4	113.16 (16)	Na2—O8—H8	112.1 (17)
C2—C3—H3A	108.9	C1—O6—Na1	129.66 (12)
C4—C3—H3A	108.9	C4—O7—Na2	145.98 (12)
C2—C3—H3B	108.9	B2—O12—H12	109.2 (17)
C4—C3—H3B	108.9	B2—O13—H13	113.8 (17)
H3A—C3—H3B	107.8	B2—O14—H14	108.4 (16)
O7—C4—O11	124.39 (17)	O5—Na1—O6	174.95 (6)
O7—C4—C3	120.54 (17)	O5—Na1—O1	85.76 (6)
O11—C4—C3	115.07 (16)	O6—Na1—O1	94.34 (6)
O9—B1—O8	120.64 (19)	O5—Na1—O4	90.03 (6)
O9—B1—O5	123.06 (19)	O6—Na1—O4	89.94 (6)
O8—B1—O5	116.30 (19)	O1—Na1—O4	175.69 (7)
O13—B2—O14	120.48 (18)	O5—Na1—O3	77.42 (6)
O13—B2—O12	124.03 (18)	O6—Na1—O3	107.58 (6)
O14—B2—O12	115.49 (18)	O1—Na1—O3	95.73 (6)
Na1—O1—Na2	94.86 (6)	O4—Na1—O3	82.44 (6)
Na1—O1—H1A	115.2 (18)	O5—Na1—O2	76.67 (6)
Na2—O1—H1A	98.8 (18)	O6—Na1—O2	98.29 (6)
Na1—O1—H1B	120 (2)	O1—Na1—O2	85.73 (6)
Na2—O1—H1B	132 (2)	O4—Na1—O2	94.20 (6)
H1A—O1—H1B	95 (2)	O3—Na1—O2	153.87 (7)
Na2—O2—Na1	92.54 (6)	O2—Na2—O3^{ii}	176.13 (7)
Na2—O2—H2C	124.9 (18)	O2—Na2—O8	79.06 (6)
Na1—O2—H2C	104.8 (17)	O3^{ii}—Na2—O8	97.25 (6)
Na2—O2—H2D	105 (2)	O2—Na2—O4^{ii}	95.68 (6)
Na1—O2—H2D	136 (2)	O3^{ii}—Na2—O4^{ii}	82.95 (6)
H2C—O2—H2D	97 (2)	O8—Na2—O4^{ii}	87.86 (6)
Na2^{i}—O3—Na1	96.44 (6)	O2—Na2—O1	86.70 (6)
Na2^{i}—O3—H3C	109.1 (18)	O3^{ii}—Na2—O1	93.80 (6)

Na1—O3—H3C	115.1 (19)	O8—Na2—O1	79.30 (6)
Na2^{i}—O3—H3D	121 (2)	O4^{ii}—Na2—O1	166.28 (7)
Na1—O3—H3D	105 (2)	O2—Na2—O7	103.41 (6)
H3C—O3—H3D	110 (3)	O3^{ii}—Na2—O7	80.21 (6)
Na1—O4—Na2^{i}	97.63 (6)	O8—Na2—O7	176.09 (6)
Na1—O4—H4A	111 (3)	O4^{ii}—Na2—O7	88.87 (6)
Na2^{i}—O4—H4A	127 (3)	O1—Na2—O7	103.76 (5)
O6—C1—C2—C3	177.20 (18)	Na2^{i}—O4—Na1—O2	148.34 (6)
O10—C1—C2—C3	−1.7 (3)	Na2^{i}—O3—Na1—O5	−86.09 (6)
C1—C2—C3—C4	179.70 (17)	Na2^{i}—O3—Na1—O6	93.17 (7)
C2—C3—C4—O7	3.1 (3)	Na2^{i}—O3—Na1—O1	−170.43 (7)
C2—C3—C4—O11	−176.34 (17)	Na2^{i}—O3—Na1—O4	5.64 (6)
O9—B1—O5—Na1	−174.98 (14)	Na2^{i}—O3—Na1—O2	−78.46 (15)
O8—B1—O5—Na1	4.3 (3)	Na2—O2—Na1—O5	−83.43 (6)
O9—B1—O8—Na2	162.69 (15)	Na2—O2—Na1—O6	96.98 (6)
O5—B1—O8—Na2	−16.6 (3)	Na2—O2—Na1—O1	3.22 (6)
O10—C1—O6—Na1	179.34 (13)	Na2—O2—Na1—O4	−172.46 (7)
C2—C1—O6—Na1	0.5 (3)	Na2—O2—Na1—O3	−91.08 (14)
O11—C4—O7—Na2	175.26 (14)	Na1—O2—Na2—O8	76.67 (6)
C3—C4—O7—Na2	−4.1 (4)	Na1—O2—Na2—O4^{ii}	163.38 (6)
B1—O5—Na1—O1	−39.8 (2)	Na1—O2—Na2—O1	−3.06 (6)
B1—O5—Na1—O4	141.1 (2)	Na1—O2—Na2—O7	−106.42 (6)
B1—O5—Na1—O3	−136.7 (2)	B1—O8—Na2—O2	−31.8 (2)
B1—O5—Na1—O2	46.8 (2)	B1—O8—Na2—O3^{ii}	149.4 (2)
C1—O6—Na1—O1	43.80 (18)	B1—O8—Na2—O4^{ii}	−128.0 (2)
C1—O6—Na1—O4	−136.74 (17)	B1—O8—Na2—O1	56.9 (2)
C1—O6—Na1—O3	141.21 (17)	Na1—O1—Na2—O2	3.31 (6)
C1—O6—Na1—O2	−42.50 (18)	Na1—O1—Na2—O3^{ii}	−172.84 (6)
Na2—O1—Na1—O5	73.82 (6)	Na1—O1—Na2—O8	−76.18 (6)
Na2—O1—Na1—O6	−101.12 (6)	Na1—O1—Na2—O4^{ii}	−97.1 (3)
Na2—O1—Na1—O3	150.70 (6)	Na1—O1—Na2—O7	106.31 (6)
Na2—O1—Na1—O2	−3.11 (6)	C4—O7—Na2—O2	51.3 (2)
Na2^{i}—O4—Na1—O5	71.71 (6)	C4—O7—Na2—O3^{ii}	−130.1 (2)
Na2^{i}—O4—Na1—O6	−113.35 (6)	C4—O7—Na2—O4^{ii}	146.9 (2)
Na2^{i}—O4—Na1—O3	−5.60 (6)	C4—O7—Na2—O1	−38.5 (2)

Symmetry codes: (i) $x-1/2, -y+1/2, z-1/2$; (ii) $x+1/2, -y+1/2, z+1/2$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···O12^{iii}	0.84 (1)	2.01 (1)	2.825 (2)	166 (2)
O1—H1*B*···O11^{iv}	0.85 (1)	2.00 (1)	2.825 (2)	164 (3)
O2—H2*C*···O14^{i}	0.82 (1)	2.23 (1)	3.045 (2)	176 (2)
O2—H2*D*···O10^{v}	0.81 (1)	2.01 (1)	2.822 (2)	175 (3)
O3—H3*C*···O14^{vi}	0.82 (1)	2.02 (1)	2.840 (2)	173 (3)
O3—H3*D*···O10^{vii}	0.83 (1)	2.21 (1)	3.035 (2)	172 (3)

O4—H4*A*···O11^{v}	0.83 (1)	2.12 (2)	2.923 (2)	164 (4)
O4—H4*B*···O12^{i}	0.82 (1)	2.01 (1)	2.818 (2)	169 (2)
O5—H5···O7^{i}	0.83 (1)	1.87 (1)	2.6888 (18)	173 (2)
O8—H8···O13^{viii}	0.83 (1)	1.89 (1)	2.711 (2)	174 (2)
O9—H9···O11^{i}	0.82 (1)	1.79 (1)	2.6044 (18)	176 (2)
O12—H12···O10^{v}	0.82 (1)	1.83 (1)	2.6261 (18)	167 (2)
O13—H13···O6^{v}	0.81 (1)	1.81 (1)	2.6113 (19)	172 (3)
O14—H14···O9^{ix}	0.83 (1)	1.81 (1)	2.6384 (19)	175 (2)

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