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Disodium (2*RS*,3*SR*)-tartrate

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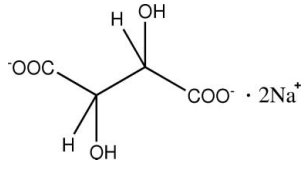
Key indicators: single-crystal X-ray study; T = 123 K; mean σ(C–C) = 0.002 Å; R factor = 0.028; wR factor = 0.072; data-to-parameter ratio = 16.5.

The asymmetric unit of the anhydrous title compound, $2Na^+\cdot C_4H_4O_6^{2-}$, contains two sodium cations and one tartrate anion. Each sodium ion is six coordinate, with bonding to six O atoms from both the carboxylate and hydroxyl groups of the anion. A three-dimensional coordination network is formed with sodium ions stacking in layers along the *c*-axis direction. This network is supported by additional O—H···O hydrogen bonds.

Related literature

For the preparation and structure of the equivalent anhydrous *meso*-tartrate salt, see: Blankensteyn & Kroon (1985). For similar hydrated tartrate salt examples using sodium or mixed sodium with lithium, potassium, rubidium or ammonium cations, see: Ambady & Kartha (1968); Suzuki *et al.* (1996); Buschmann & Luger (1985); Görbitz & Sagstuen (2008); Hinazumi & Mitsui (1972). For the use of tartrates as food additives, see: Vickers *et al.* (2007).



Experimental

Crystal data

$2Na^+\cdot C_4H_4O_6^{2-}$
M_r = 194.06
Orthorhombic, *Pbca*
a = 10.1160 (4) Å
b = 10.0049 (5) Å
c = 13.0821 (5) Å
V = 1324.03 (10) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.29 mm^{-1}
T = 123 K
0.24 × 0.15 × 0.09 mm

Data collection

Oxford Diffraction Gemini S CCD diffractometer
Absorption correction: multi-scan (ABSPACK; Oxford Diffraction, 2007)
T_{min} = 0.894, T_{max} = 1.000
7156 measured reflections
1934 independent reflections
1566 reflections with $I > 2/s(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.072
S = 1.05
1934 reflections
117 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H2···O2^{i}	0.900 (17)	1.752 (18)	2.6480 (12)	173.2 (17)
O6—H4···O5^{ii}	0.883 (17)	1.787 (17)	2.6643 (12)	172.0 (18)

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2007); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2539).

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supplementary materials

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Disodium (2*RS*,3*SR*)-tartrate

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Comment

Tartrate salts are often used as food additives due to their ability to act as anti-oxidants. Disodium tartrate dihydrate, additive number (E335), is used as an emulsifier and binding agent in food products such as jam and sugar syrup (Vickers *et al.*, 2007).

The anhydrous form of racemic disodium tartrate (I) was obtained from aqueous solution. The salt crystallizes in space group Pbca, with two sodium cations and one tartrate anion in the asymmetric unit, Fig. 1. Structures of anhydrous forms of similar materials are uncommon. The extensive structural literature on sodium tartrates and the historically important mixed cation double salts (Na/*X*, with *X* = Li, K, Rb & NH_4) is dominated by hydrated forms (Ambady & Kartha, 1968; Suzuki *et al.*, 1996; Buschmann & Luger, 1985; Görbitz & Sagstuen, 2008; Hinazumi & Mitsui, 1972). The only other known anhydrous sodium tartrate structure is that of disodium *meso*-tartrate salt (Blankensteyn & Kroon, 1985).

In the present anhydrate, (I), each Na ion forms six bonds to O and each O atom in turn forms two bonds to Na. The range of bond lengths found for Na—O_{OOC} interactions, 2.3097 (10) to 2.5370 (9), encompasses that found for Na—O_{OH} bonds, i.e. 2.3580 (9) to 2.4994 (9) Å. The bond lengths compare well with those observed for disodium D-tartrate dihydrate (Ambady & Kartha, 1968). Each tartrate anion bridges a total of 7 Na ions, see Fig. 2, giving a 3- dimensional coordination network. Figure 3 shows a view of the packed structure, looking down the *c* direction. Note the columns of Na atoms parallel to *c* and also that the apparently empty channels are only 2.5 Å wide and thus are in fact approximate to van der Waals contact distances. This network is supported by intermolecular hydrogen bonding from the OH groups to the carboxylate groups, see Table 1.

Experimental

Compound (I) was obtained on treating an aqueous solution of (+/-)tartaric acid with an aqueous solution of sodium carbonate. Single-crystals were obtained by allowing the solvent of the reaction mixture to evaporate at 295 K.

Refinement

Hydroxyl-H atoms were found by difference synthesis and refined isotropically; see Table 1. All other H atoms were positioned geometrically with C—H = 1.00 Å, and with U_{iso}(H) = 1.2 times U_{eq}(C).

Figures

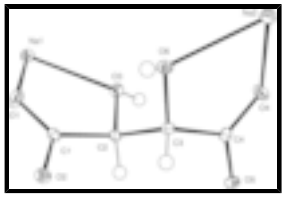

Fig. 1. The asymmetric unit and atomic labelling of (I), showing 50% probability displacement ellipsoids. H atoms are shown as spheres of arbitrary radius.

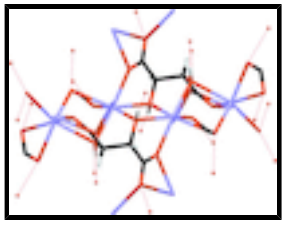

Fig. 2. Extended structure formed by bridging O atoms between the Na cations in (I). The Na atoms are purple, O atoms are red, and C atoms are black. Hydrogen bonds are shown as dashed lines.

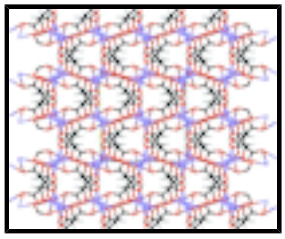

Fig. 3. Packed structure of (I) viewed down the *c*-axis.

Disodium (2*RS*,3*SR*)-tartrate

Crystal data

$2Na^{+}\cdot C_4H_4O_6^{2-}$	F_{000} = 784
M_r = 194.06	D_x = 1.947 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation, λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 3917 reflections
a = 10.1160 (4) Å	θ = 2.5–30.8°
b = 10.0049 (5) Å	μ = 0.29 mm^{-1}
c = 13.0821 (5) Å	*T* = 123 K
V = 1324.03 (10) Å^3	Block, colourless
Z = 8	0.24 × 0.15 × 0.09 mm

Data collection

Oxford Diffraction Gemini S CCD diffractometer	1934 independent reflections
Radiation source: fine-focus sealed tube	1566 reflections with $I > 2/s(I)$
Monochromator: graphite	R_{int} = 0.024
T = 123 K	θ_{max} = 30.8°
ω scans	θ_{min} = 3.1°
Absorption correction: multi-scan (ABSPACK; Oxford Diffraction, 2007)	*h* = −14→8
T_{min} = 0.894, T_{max} = 1.000	*k* = −14→14
7156 measured reflections	*l* = −17→18

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.028	H atoms treated by a mixture of independent and constrained refinement

$wR(F^2) = 0.072$	$w = 1/[\sigma^2(F_o^2) + (0.0412P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} = 0.001$
1934 reflections	$\Delta\rho_{max} = 0.39$ e Å^{-3}
117 parameters	$\Delta\rho_{min} = -0.31$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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	0.55185 (4)	−0.03963 (5)	−0.37266 (3)	0.01008 (12)
Na2	0.52569 (5)	−0.03323 (5)	0.12690 (3)	0.01163 (12)
O1	0.53147 (9)	−0.24500 (8)	−0.29356 (7)	0.0149 (2)
O2	0.61519 (8)	−0.40740 (8)	−0.19771 (6)	0.01028 (18)
O3	0.66678 (8)	−0.05364 (8)	−0.20387 (6)	0.00958 (17)
O4	0.73339 (8)	−0.01137 (9)	0.05789 (6)	0.01434 (19)
O5	0.89689 (8)	−0.12972 (8)	−0.01024 (6)	0.01052 (18)
O6	0.54400 (8)	−0.15557 (9)	−0.02943 (6)	0.00950 (17)
C1	0.60624 (11)	−0.28543 (11)	−0.22473 (8)	0.0082 (2)
C2	0.69680 (11)	−0.18581 (11)	−0.16939 (8)	0.0078 (2)
H1	0.7910	−0.2069	−0.1859	0.009*
C3	0.67622 (11)	−0.19485 (12)	−0.05305 (8)	0.0082 (2)
H3	0.6900	−0.2894	−0.0306	0.010*
C4	0.77515 (10)	−0.10399 (12)	0.00307 (8)	0.0087 (2)
H2	0.7378 (17)	0.0000 (17)	−0.1980 (13)	0.033 (5)*
H4	0.4958 (17)	−0.2286 (16)	−0.0224 (14)	0.026 (5)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Na1	0.0103 (2)	0.0103 (2)	0.0096 (2)	−0.00008 (18)	0.00033 (16)	0.00102 (17)
Na2	0.0123 (2)	0.0126 (2)	0.0100 (2)	0.0033 (2)	0.00156 (16)	0.00156 (17)
O1	0.0174 (4)	0.0114 (4)	0.0158 (4)	−0.0023 (4)	−0.0085 (3)	0.0021 (3)
O2	0.0111 (4)	0.0073 (4)	0.0124 (4)	0.0000 (3)	0.0002 (3)	0.0005 (3)
O3	0.0109 (4)	0.0069 (4)	0.0109 (4)	−0.0012 (3)	−0.0008 (3)	0.0019 (3)

O4	0.0116 (4)	0.0154 (4)	0.0161 (4)	−0.0004 (4)	0.0013 (3)	−0.0077 (3)
O5	0.0078 (3)	0.0112 (4)	0.0125 (4)	0.0004 (3)	0.0002 (3)	0.0009 (3)
O6	0.0074 (4)	0.0097 (4)	0.0114 (4)	−0.0004 (3)	0.0017 (3)	0.0003 (3)
C1	0.0085 (5)	0.0086 (5)	0.0075 (4)	0.0003 (4)	0.0019 (4)	−0.0012 (4)
C2	0.0087 (5)	0.0066 (5)	0.0082 (4)	0.0002 (4)	−0.0003 (4)	0.0002 (4)
C3	0.0073 (5)	0.0081 (5)	0.0092 (4)	0.0009 (4)	0.0000 (4)	0.0001 (4)
C4	0.0100 (5)	0.0092 (5)	0.0069 (5)	−0.0004 (4)	−0.0004 (4)	0.0020 (4)

Geometric parameters (Å, °)

Na1—O1	2.3097 (10)	O2—C1	1.2737 (14)
Na1—O2^{i}	2.3352 (9)	O2—Na1^{viii}	2.3352 (9)
Na1—O5^{ii}	2.3699 (9)	O2—Na2^{vii}	2.5370 (9)
Na1—O4^{iii}	2.4095 (9)	O3—C2	1.4298 (14)
Na1—O3	2.4994 (9)	O3—Na2^{iv}	2.3580 (9)
Na1—O5^{iii}	2.5257 (9)	O3—H2	0.900 (17)
Na1—C4^{iii}	2.7875 (12)	O4—C4	1.2457 (13)
Na1—Na2^{iv}	3.3886 (6)	O4—Na1^{ix}	2.4095 (9)
Na1—Na1^{v}	3.5820 (8)	O5—C4	1.2701 (13)
Na2—O4	2.2973 (9)	O5—Na1^{x}	2.3699 (9)
Na2—O3^{iv}	2.3580 (9)	O5—Na1^{ix}	2.5257 (9)
Na2—O6^{iv}	2.3856 (9)	O6—C3	1.4279 (13)
Na2—O6	2.3907 (9)	O6—Na2^{iv}	2.3856 (9)
Na2—O1^{vi}	2.4513 (10)	O6—H4	0.883 (17)
Na2—O2^{vi}	2.5370 (9)	C1—C2	1.5352 (16)
Na2—C1^{vi}	2.7790 (12)	C1—Na2^{vii}	2.7790 (12)
Na2—C4	3.0813 (12)	C2—C3	1.5389 (14)
Na2—Na1^{iv}	3.3886 (6)	C2—H1	1.0000
Na2—Na2^{iv}	3.4259 (9)	C3—C4	1.5385 (15)
O1—C1	1.2435 (13)	C3—H3	1.0000
O1—Na2^{vii}	2.4513 (10)	C4—Na1^{ix}	2.7875 (12)
O1—Na1—O2^{i}	105.24 (3)	O6—Na2—Na1^{iv}	160.01 (3)
O1—Na1—O5^{ii}	83.81 (3)	O1^{vi}—Na2—Na1^{iv}	78.32 (2)
O2^{i}—Na1—O5^{ii}	89.52 (3)	O2^{vi}—Na2—Na1^{iv}	43.53 (2)
O1—Na1—O4^{iii}	115.96 (4)	C1^{vi}—Na2—Na1^{iv}	62.98 (3)
O2^{i}—Na1—O4^{iii}	132.93 (4)	C4—Na2—Na1^{iv}	137.55 (3)
O5^{ii}—Na1—O4^{iii}	115.67 (3)	O4—Na2—Na2^{iv}	74.89 (3)
O1—Na1—O3	66.16 (3)	O3^{iv}—Na2—Na2^{iv}	102.54 (3)
O2^{i}—Na1—O3	91.15 (3)	O6^{iv}—Na2—Na2^{iv}	44.23 (2)
O5^{ii}—Na1—O3	149.03 (3)	O6—Na2—Na2^{iv}	44.11 (2)
O4^{iii}—Na1—O3	85.73 (3)	O1^{vi}—Na2—Na2^{iv}	126.20 (3)
O1—Na1—O5^{iii}	159.12 (4)	O2^{vi}—Na2—Na2^{iv}	167.44 (3)
O2^{i}—Na1—O5^{iii}	92.83 (3)	C1^{vi}—Na2—Na2^{iv}	148.01 (3)

$O5^{ii}$—Na1—$O5^{iii}$	86.00 (3)	C4—Na2—$Na2^{iv}$	70.08 (2)
$O4^{iii}$—Na1—$O5^{iii}$	53.42 (3)	$Na1^{iv}$—Na2—$Na2^{iv}$	147.42 (2)
O3—Na1—$O5^{iii}$	124.87 (3)	C1—O1—Na1	124.02 (7)
O1—Na1—$C4^{iii}$	140.88 (4)	C1—O1—$Na2^{vii}$	91.57 (7)
$O2^{i}$—Na1—$C4^{iii}$	113.09 (4)	Na1—O1—$Na2^{vii}$	128.11 (4)
$O5^{ii}$—Na1—$C4^{iii}$	103.55 (3)	C1—O2—$Na1^{viii}$	126.92 (7)
$O4^{iii}$—Na1—$C4^{iii}$	26.47 (3)	C1—O2—$Na2^{vii}$	87.02 (6)
O3—Na1—$C4^{iii}$	104.60 (3)	$Na1^{viii}$—O2—$Na2^{vii}$	88.03 (3)
$O5^{iii}$—Na1—$C4^{iii}$	27.09 (3)	C2—O3—$Na2^{iv}$	112.43 (6)
O1—Na1—$Na2^{iv}$	75.27 (3)	C2—O3—Na1	115.43 (6)
$O2^{i}$—Na1—$Na2^{iv}$	48.44 (2)	$Na2^{iv}$—O3—Na1	88.42 (3)
$O5^{ii}$—Na1—$Na2^{iv}$	122.82 (3)	C2—O3—H2	110.8 (11)
$O4^{iii}$—Na1—$Na2^{iv}$	121.39 (3)	$Na2^{iv}$—O3—H2	113.8 (11)
O3—Na1—$Na2^{iv}$	44.07 (2)	Na1—O3—H2	114.4 (11)
$O5^{iii}$—Na1—$Na2^{iv}$	125.40 (3)	C4—O4—Na2	117.75 (7)
$C4^{iii}$—Na1—$Na2^{iv}$	126.00 (3)	C4—O4—$Na1^{ix}$	93.95 (7)
O1—Na1—$Na1^{v}$	125.98 (3)	Na2—O4—$Na1^{ix}$	134.16 (4)
$O2^{i}$—Na1—$Na1^{v}$	91.68 (3)	C4—O5—$Na1^{x}$	130.76 (7)
$O5^{ii}$—Na1—$Na1^{v}$	44.70 (2)	C4—O5—$Na1^{ix}$	88.02 (7)
$O4^{iii}$—Na1—$Na1^{v}$	82.32 (2)	$Na1^{x}$—O5—$Na1^{ix}$	94.00 (3)
O3—Na1—$Na1^{v}$	166.03 (3)	C3—O6—$Na2^{iv}$	112.27 (6)
$O5^{iii}$—Na1—$Na1^{v}$	41.30 (2)	C3—O6—Na2	113.49 (6)
$C4^{iii}$—Na1—$Na1^{v}$	61.79 (2)	$Na2^{iv}$—O6—Na2	91.66 (3)
$Na2^{iv}$—Na1—$Na1^{v}$	140.09 (2)	C3—O6—H4	108.1 (11)
O4—Na2—$O3^{iv}$	152.61 (4)	$Na2^{iv}$—O6—H4	123.2 (11)
O4—Na2—$O6^{iv}$	89.13 (3)	Na2—O6—H4	107.0 (12)
$O3^{iv}$—Na2—$O6^{iv}$	72.09 (3)	O1—C1—O2	123.77 (10)
O4—Na2—O6	69.00 (3)	O1—C1—C2	119.55 (10)
$O3^{iv}$—Na2—O6	128.17 (3)	O2—C1—C2	116.66 (9)
$O6^{iv}$—Na2—O6	88.34 (3)	O1—C1—$Na2^{vii}$	61.86 (6)
O4—Na2—$O1^{vi}$	103.37 (3)	O2—C1—$Na2^{vii}$	65.74 (6)
$O3^{iv}$—Na2—$O1^{vi}$	99.91 (3)	C2—C1—$Na2^{vii}$	158.15 (7)
$O6^{iv}$—Na2—$O1^{vi}$	161.92 (4)	O3—C2—C1	108.96 (9)
O6—Na2—$O1^{vi}$	84.14 (3)	O3—C2—C3	109.73 (9)
O4—Na2—$O2^{vi}$	92.94 (3)	C1—C2—C3	110.33 (9)
$O3^{iv}$—Na2—$O2^{vi}$	89.70 (3)	O3—C2—H1	109.3
$O6^{iv}$—Na2—$O2^{vi}$	140.73 (3)	C1—C2—H1	109.3
O6—Na2—$O2^{vi}$	128.77 (3)	C3—C2—H1	109.3
$O1^{vi}$—Na2—$O2^{vi}$	52.82 (3)	O6—C3—C4	110.09 (9)
O4—Na2—$C1^{vi}$	93.93 (3)	O6—C3—C2	108.94 (8)
$O3^{iv}$—Na2—$C1^{vi}$	100.63 (3)	C4—C3—C2	110.44 (9)

O6^{iv}—Na2—C1^{vi}	167.66 (4)	O6—C3—H3	109.1
O6—Na2—C1^{vi}	103.92 (4)	C4—C3—H3	109.1
O1^{vi}—Na2—C1^{vi}	26.57 (3)	C2—C3—H3	109.1
O2^{vi}—Na2—C1^{vi}	27.24 (3)	O4—C4—O5	123.96 (10)
O4—Na2—C4	20.96 (3)	O4—C4—C3	119.58 (10)
O3^{iv}—Na2—C4	170.22 (3)	O5—C4—C3	116.46 (10)
O6^{iv}—Na2—C4	98.22 (3)	O4—C4—Na1^{ix}	59.58 (6)
O6—Na2—C4	50.89 (3)	O5—C4—Na1^{ix}	64.89 (6)
O1^{vi}—Na2—C4	89.75 (3)	C3—C4—Na1^{ix}	172.43 (7)
O2^{vi}—Na2—C4	97.44 (3)	O4—C4—Na2	41.28 (5)
C1^{vi}—Na2—C4	88.69 (3)	O5—C4—Na2	155.89 (7)
O4—Na2—Na1^{iv}	124.34 (3)	C3—C4—Na2	81.60 (6)
O3^{iv}—Na2—Na1^{iv}	47.50 (2)	Na1^{ix}—C4—Na2	95.11 (3)
O6^{iv}—Na2—Na1^{iv}	105.57 (3)		
O2^{i}—Na1—O1—C1	−103.88 (9)	Na2^{iv}—O3—C2—C1	78.38 (8)
O5^{ii}—Na1—O1—C1	168.31 (9)	Na1—O3—C2—C1	−21.02 (10)
O4^{iii}—Na1—O1—C1	52.72 (10)	Na2^{iv}—O3—C2—C3	−42.52 (10)
O3—Na1—O1—C1	−19.48 (9)	Na1—O3—C2—C3	−141.92 (7)
O5^{iii}—Na1—O1—C1	107.05 (12)	O1—C1—C2—O3	5.65 (14)
C4^{iii}—Na1—O1—C1	64.41 (11)	O2—C1—C2—O3	−175.83 (9)
Na2^{iv}—Na1—O1—C1	−65.38 (9)	Na2^{vii}—C1—C2—O3	93.2 (2)
Na1^{v}—Na1—O1—C1	152.51 (8)	O1—C1—C2—C3	126.19 (11)
O2^{i}—Na1—O1—Na2^{vii}	131.26 (5)	O2—C1—C2—C3	−55.30 (13)
O5^{ii}—Na1—O1—Na2^{vii}	43.45 (5)	Na2^{vii}—C1—C2—C3	−146.27 (17)
O4^{iii}—Na1—O1—Na2^{vii}	−72.13 (6)	Na2^{iv}—O6—C3—C4	80.01 (8)
O3—Na1—O1—Na2^{vii}	−144.34 (6)	Na2—O6—C3—C4	−22.24 (10)
O5^{iii}—Na1—O1—Na2^{vii}	−17.81 (13)	Na2^{iv}—O6—C3—C2	−41.23 (10)
C4^{iii}—Na1—O1—Na2^{vii}	−60.45 (7)	Na2—O6—C3—C2	−143.48 (7)
Na2^{iv}—Na1—O1—Na2^{vii}	169.76 (5)	O3—C2—C3—O6	56.23 (12)
Na1^{v}—Na1—O1—Na2^{vii}	27.65 (7)	C1—C2—C3—O6	−63.83 (12)
O1—Na1—O3—C2	20.93 (7)	O3—C2—C3—C4	−64.79 (11)
O2^{i}—Na1—O3—C2	127.10 (7)	C1—C2—C3—C4	175.14 (9)
O5^{ii}—Na1—O3—C2	36.12 (11)	Na2—O4—C4—O5	−154.27 (9)
O4^{iii}—Na1—O3—C2	−99.92 (7)	Na1^{ix}—O4—C4—O5	−8.65 (11)
O5^{iii}—Na1—O3—C2	−138.64 (7)	Na2—O4—C4—C3	25.69 (12)
C4^{iii}—Na1—O3—C2	−118.66 (7)	Na1^{ix}—O4—C4—C3	171.31 (8)
Na2^{iv}—Na1—O3—C2	114.18 (8)	Na2—O4—C4—Na1^{ix}	−145.62 (7)
Na1^{v}—Na1—O3—C2	−131.23 (13)	Na1^{ix}—O4—C4—Na2	145.62 (7)
O1—Na1—O3—Na2^{iv}	−93.25 (4)	Na1^{x}—O5—C4—O4	−85.34 (13)
O2^{i}—Na1—O3—Na2^{iv}	12.92 (3)	Na1^{ix}—O5—C4—O4	8.23 (11)
O5^{ii}—Na1—O3—Na2^{iv}	−78.06 (7)	Na1^{x}—O5—C4—C3	94.70 (11)

O4^{iii}—Na1—O3—Na2^{iv}	145.90 (3)	Na1^{ix}—O5—C4—C3	−171.72 (8)
O5^{iii}—Na1—O3—Na2^{iv}	107.18 (4)	Na1^{x}—O5—C4—Na1^{ix}	−93.57 (8)
C4^{iii}—Na1—O3—Na2^{iv}	127.16 (3)	Na1^{x}—O5—C4—Na2	−129.86 (16)
Na1^{v}—Na1—O3—Na2^{iv}	114.59 (13)	Na1^{ix}—O5—C4—Na2	−36.3 (2)
O3^{iv}—Na2—O4—C4	−161.78 (8)	O6—C3—C4—O4	−1.01 (13)
O6^{iv}—Na2—O4—C4	−116.05 (8)	C2—C3—C4—O4	119.33 (11)
O6—Na2—O4—C4	−27.50 (7)	O6—C3—C4—O5	178.95 (9)
O1^{vi}—Na2—O4—C4	50.75 (8)	C2—C3—C4—O5	−60.71 (13)
O2^{vi}—Na2—O4—C4	103.18 (8)	O6—C3—C4—Na1^{ix}	80.5 (6)
C1^{vi}—Na2—O4—C4	75.91 (8)	C2—C3—C4—Na1^{ix}	−159.2 (5)
Na1^{iv}—Na2—O4—C4	135.61 (7)	O6—C3—C4—Na2	15.80 (7)
Na2^{iv}—Na2—O4—C4	−73.63 (7)	C2—C3—C4—Na2	136.14 (8)
O3^{iv}—Na2—O4—Na1^{ix}	69.96 (10)	O3^{iv}—Na2—C4—O4	57.9 (2)
O6^{iv}—Na2—O4—Na1^{ix}	115.68 (6)	O6^{iv}—Na2—C4—O4	65.18 (8)
O6—Na2—O4—Na1^{ix}	−155.76 (6)	O6—Na2—C4—O4	146.25 (9)
O1^{vi}—Na2—O4—Na1^{ix}	−77.51 (6)	O1^{vi}—Na2—C4—O4	−131.11 (8)
O2^{vi}—Na2—O4—Na1^{ix}	−25.08 (6)	O2^{vi}—Na2—C4—O4	−78.70 (8)
C1^{vi}—Na2—O4—Na1^{ix}	−52.35 (6)	C1^{vi}—Na2—C4—O4	−104.56 (8)
C4—Na2—O4—Na1^{ix}	−128.26 (11)	Na1^{iv}—Na2—C4—O4	−58.85 (9)
Na1^{iv}—Na2—O4—Na1^{ix}	7.34 (7)	Na2^{iv}—Na2—C4—O4	99.85 (8)
Na2^{iv}—Na2—O4—Na1^{ix}	158.11 (6)	O4—Na2—C4—O5	61.8 (2)
O4—Na2—O6—C3	25.51 (7)	O3^{iv}—Na2—C4—O5	119.7 (2)
O3^{iv}—Na2—O6—C3	−179.25 (7)	O6^{iv}—Na2—C4—O5	127.0 (2)
O6^{iv}—Na2—O6—C3	115.22 (8)	O6—Na2—C4—O5	−151.9 (2)
O1^{vi}—Na2—O6—C3	−81.24 (7)	O1^{vi}—Na2—C4—O5	−69.3 (2)
O2^{vi}—Na2—O6—C3	−50.74 (9)	O2^{vi}—Na2—C4—O5	−16.9 (2)
C1^{vi}—Na2—O6—C3	−63.37 (8)	C1^{vi}—Na2—C4—O5	−42.7 (2)
C4—Na2—O6—C3	13.22 (7)	Na1^{iv}—Na2—C4—O5	3.0 (2)
Na1^{iv}—Na2—O6—C3	−109.91 (9)	Na2^{iv}—Na2—C4—O5	161.7 (2)
Na2^{iv}—Na2—O6—C3	115.22 (8)	O4—Na2—C4—C3	−157.60 (11)
O4—Na2—O6—Na2^{iv}	−89.70 (3)	O3^{iv}—Na2—C4—C3	−99.7 (2)
O3^{iv}—Na2—O6—Na2^{iv}	65.53 (4)	O6^{iv}—Na2—C4—C3	−92.43 (6)
O6^{iv}—Na2—O6—Na2^{iv}	0.0	O6—Na2—C4—C3	−11.35 (6)
O1^{vi}—Na2—O6—Na2^{iv}	163.54 (4)	O1^{vi}—Na2—C4—C3	71.29 (6)
O2^{vi}—Na2—O6—Na2^{iv}	−165.95 (4)	O2^{vi}—Na2—C4—C3	123.70 (6)
C1^{vi}—Na2—O6—Na2^{iv}	−178.59 (4)	C1^{vi}—Na2—C4—C3	97.84 (6)
C4—Na2—O6—Na2^{iv}	−102.00 (4)	Na1^{iv}—Na2—C4—C3	143.55 (5)
Na1^{iv}—Na2—O6—Na2^{iv}	134.88 (8)	Na2^{iv}—Na2—C4—C3	−57.75 (5)
Na1—O1—C1—O2	−163.11 (8)	O4—Na2—C4—Na1^{ix}	29.27 (7)
Na2^{vii}—O1—C1—O2	−23.34 (11)	O3^{iv}—Na2—C4—Na1^{ix}	87.1 (2)
Na1—O1—C1—C2	15.30 (14)	O6^{iv}—Na2—C4—Na1^{ix}	94.44 (4)

Na2^{vii}—O1—C1—C2	155.06 (9)	O6—Na2—C4—Na1^{ix}	175.52 (5)
Na1—O1—C1—Na2^{vii}	−139.77 (8)	O1^{vi}—Na2—C4—Na1^{ix}	−101.84 (3)
Na1^{viii}—O2—C1—O1	−62.75 (14)	O2^{vi}—Na2—C4—Na1^{ix}	−49.43 (4)
Na2^{vii}—O2—C1—O1	22.53 (11)	C1^{vi}—Na2—C4—Na1^{ix}	−75.29 (4)
Na1^{viii}—O2—C1—C2	118.80 (9)	Na1^{iv}—Na2—C4—Na1^{ix}	−29.59 (5)
Na2^{vii}—O2—C1—C2	−155.91 (9)	Na2^{iv}—Na2—C4—Na1^{ix}	129.12 (3)
Na1^{viii}—O2—C1—Na2^{vii}	−85.29 (7)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H2···O2^{xi}	0.900 (17)	1.752 (18)	2.6480 (12)	173.2 (17)
O6—H4···O5^{xii}	0.883 (17)	1.787 (17)	2.6643 (12)	172.0 (18)

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

Fig. 1

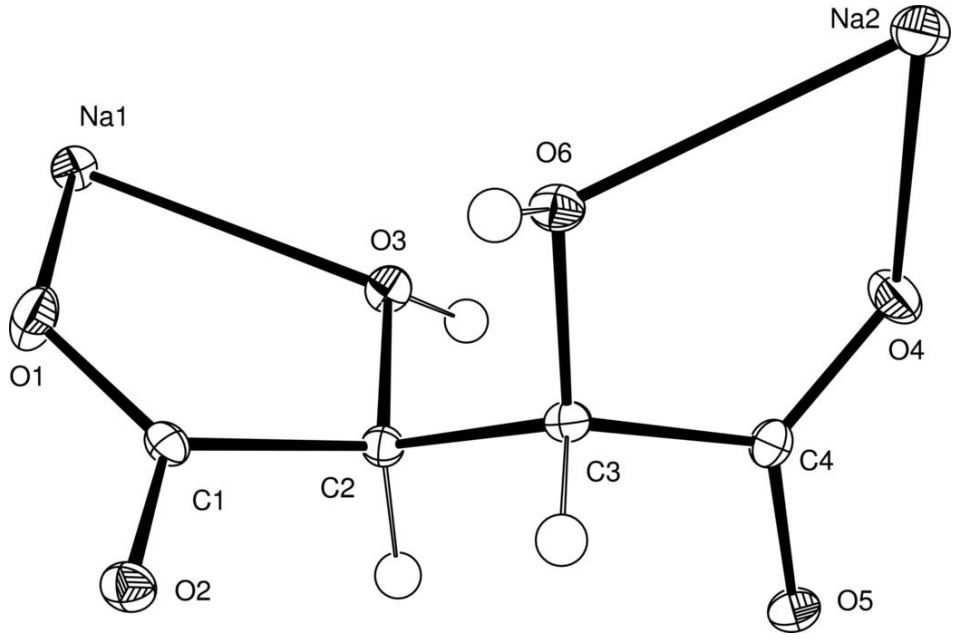

Fig. 2

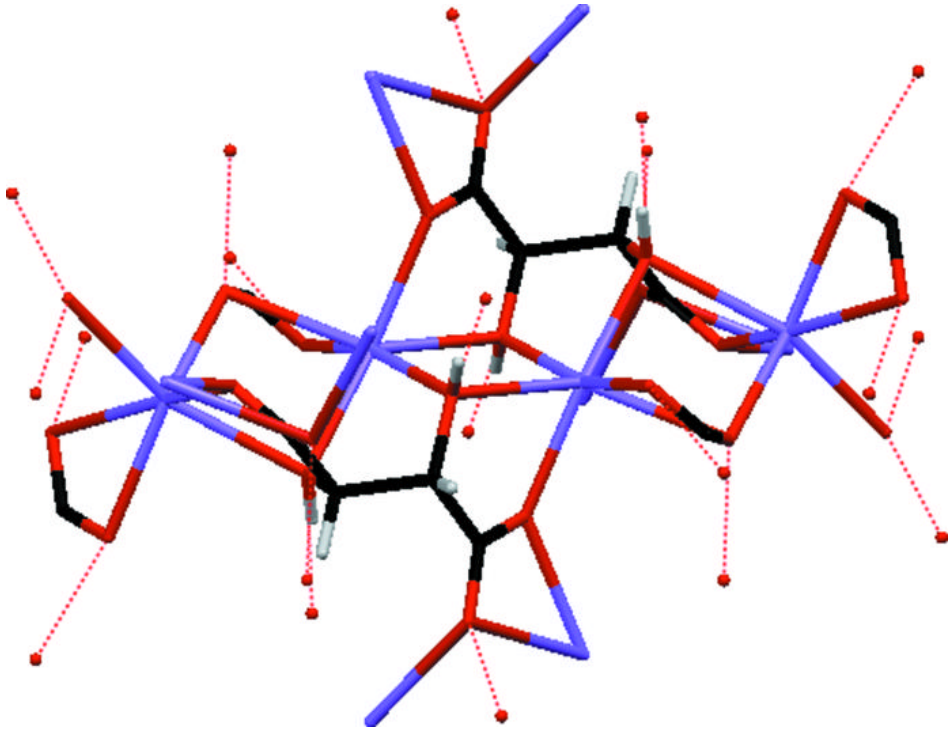

Fig. 3