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Sodium (1*R*,2*S*,5*S*)-2-hydroxy-6,6-dimethylbicyclo[3.1.1]heptane-2-carboxylate pentahydrate

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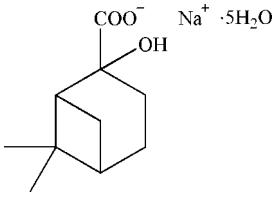
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.005 Å; R factor = 0.042; wR factor = 0.106; data-to-parameter ratio = 8.5.

In the title compound, $Na^+\cdot C_{10}H_{15}O_3^-\cdot 5H_2O$, the vertices of a distorted octahedron centred on the Na^+ cation are defined by six O atoms of water molecules. The edge-sharing $Na(H_2O)_6$ octahedra form a chain extended along the *b*-axis direction with adjacent Na^+ cations related by a twofold screw symmetry operation. The organic anion, which is not in close contact with the Na^+ cation, is hydrogen-bonded to an uncoordinated water molecule and to water molecules of the $Na(H_2O)_6$ octahedra.

Related literature

For a crystal structure with similar chains of edge-sharing $Na(H_2O)_6$ octahedra, see: Huang *et al.* (2005).



Experimental

Crystal data

$Na^+\cdot C_{10}H_{15}O_3^-\cdot 5H_2O$
M_r = 296.29
Monoclinic, $P2_1$
a = 6.647 (3) Å
b = 6.976 (3) Å
c = 16.608 (7) Å
β = 93.037 (7)°
V = 769.0 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.13 mm^{-1}
T = 295 K
0.15 × 0.12 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.981, T_{max} = 0.987
4017 measured reflections
1479 independent reflections
1284 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.107
S = 1.02
1479 reflections
173 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O8—H18···O3^{i}	0.85	1.90	2.737 (3)	170
O8—H17···O2	0.85	1.90	2.741 (3)	173
O7—H16···O1^{ii}	0.85	2.05	2.859 (4)	158
O7—H15···O4^{iii}	0.85	2.12	2.887 (4)	150
O6—H14···O8^{iv}	0.85	1.88	2.727 (3)	175
O6—H13···O2	0.85	1.96	2.776 (3)	161
O5—H12···O8^{iii}	0.85	1.98	2.805 (3)	164
O5—H11···O1^{v}	0.85	1.96	2.791 (3)	166
O4—H10···O2	0.85	2.06	2.879 (3)	161
O4—H9···O1^{v}	0.85	2.10	2.949 (4)	174
O3—H3···O7^{iii}	0.82	2.02	2.809 (3)	161

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2115).

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supporting information

Acta Cryst. (2008). E**64**, m92 [https://doi.org/10.1107/S1600536807063775]

Sodium (1*R*,2*S*,5*S*)-2-hydroxy-6,6-dimethylbicyclo[3.1.1]heptane-2-carboxylate pentahydrate

Shi-Ying Ma, Ze-Bao Zheng and Ji-Kun Li

S1. Comment

Sodium nopinate is an intermediate in the synthesis of nopinic acid. Hydroxyalkylamino salts of nopinic acid are new compounds useful in pharmaceutical compositions for alleviating ulcer conditions. In the course of synthesis of nopinic acid the crystal of sodium nopinate pentahydrate (I) was obtained in its crystallographic data are reported here (Fig.1). In the title compound the vertices of a distorted octahedron centred on Na^+ cation are defined by six O atoms of water molecules. The edge-sharing $Na(H_2O)_6$ octahedra form a chain extended along the **b** axis with the adjacent Na^+ cations related by twofold screw axis symmetry. Similar chains were observed in sodium pyridine-4-carboxylate tetrahydrate (Huang *et al.*, 2005).

S2. Experimental

Potassium permanganate (0.03 mol) and NaOH (0.015 mol) were dissolved in the mixture of water (21 ml) and t-butyl-alcohol (9 ml).While stirring vigorously, enantiomerically pure (-)-*β*-pinene (0.01 mol) was dropped. The reaction mixture was maintained during 1 to 2 h at temperature of 283–293 K. The reaction was completed when the potassium permanganate reacted completely. The mixture was heated to 353 K,then filtered and the precipitate was washed with hot water. The filtrate was concentrated under vacuum to a volume of 10 ml. After standing for one night in refrigerator the product, sodium nopinate, was filtered and washed with ice water. The crude sodium nopinate was recrystallized from water. Analysis calculated for $C_{10}H_{15}O_3Na$: C 58.25, H 7.28, Na11.17%; found: C 58.23, H 7.25, N 11.15%. Crystals of (I) suitable for single-crystal X-ray analysis were selected directly from the sample after recrystallization.

S3. Refinement

In the absence of signifcant anomalous scattering effects, Friedel pairs were averaged. The chirality of atoms C2, C3 and C5 were assigned from the known hand of the starting material.The H-atoms were included in the riding-model approximation with C—H = 0.96–0.98 Å and O—H = 0.82 Å (*O*-hydroxy) and 0.85 Å (O-water), and with U_{iso}(H) = 1.2 or 1.5 U_{eq}(C) and U_{iso}(H) = 1.5 (*O*-hydroxy) or 1.2 (O-water) U_{eq}(O). Friedel pairs were merged for the refinement process.

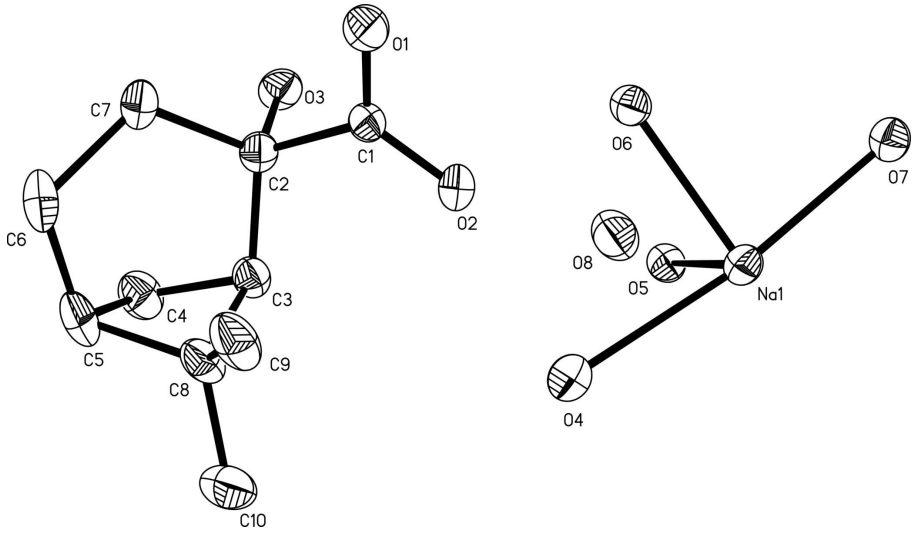

Figure 1

The molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level. H atoms are omitted and only asymmetric unit is labelled.

Sodium (1*R*,2*S*,5*S*)-2-hydroxy-6,6-dimethylbicyclo[3.1.1]heptane-2-carboxylate pentahydrate

Crystal data

$Na^+ \cdot C_{10}H_{15}O_3^- \cdot 5H_2O$
$M_r = 296.29$
Monoclinic, $P2_1$
Hall symbol: P 2yb
$a = 6.647\ (3)$ Å
$b = 6.976\ (3)$ Å
$c = 16.608\ (7)$ Å
$\beta = 93.037\ (7)°$
$V = 769.0\ (6)$ Å^3
$Z = 2$
$F(000) = 320$
$D_x = 1.280$ Mg m^{-3}
Melting point: 350 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1420 reflections
$\theta = 3.1–22.4°$
$\mu = 0.13$ mm^{-1}
$T = 295$ K
Block, colourless
0.15 × 0.12 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.981$, $T_{max} = 0.987$
4017 measured reflections
1479 independent reflections
1284 reflections with $I > 2\sigma(I)$
$R_{int} = 0.039$
$\theta_{max} = 25.1°$, $\theta_{min} = 2.5°$
$h = -7 \rightarrow 7$
$k = -5 \rightarrow 8$
$l = -16 \rightarrow 19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.107$
$S = 1.03$
1479 reflections
173 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-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.069P)^2 + 0.001P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.21$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ 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	−0.00585 (18)	0.5552 (2)	1.00549 (8)	0.0409 (3)
O1	0.6546 (3)	0.2810 (4)	0.82272 (12)	0.0526 (6)
O2	0.3527 (3)	0.4065 (3)	0.83467 (12)	0.0430 (6)
O3	0.3247 (3)	−0.0018 (3)	0.77372 (14)	0.0440 (6)
H3	0.2070	0.0084	0.7855	0.066*
O4	−0.0358 (3)	0.5789 (4)	0.85286 (14)	0.0507 (6)
H9	−0.1268	0.4968	0.8404	0.061*
H10	0.0723	0.5321	0.8360	0.061*
O5	−0.2377 (3)	0.3046 (4)	0.98716 (11)	0.0426 (5)
H11	−0.2909	0.2932	0.9397	0.051*
H12	−0.3323	0.2808	1.0182	0.051*
O6	0.2300 (3)	0.3093 (4)	0.98658 (11)	0.0417 (5)
H13	0.2944	0.3309	0.9446	0.050*
H14	0.3195	0.2885	1.0240	0.050*
O7	0.0435 (3)	0.4926 (3)	1.15078 (13)	0.0474 (6)
H15	0.0819	0.3783	1.1605	0.057*
H16	0.1382	0.5627	1.1707	0.057*
O8	0.4976 (3)	0.7554 (3)	0.88678 (12)	0.0493 (6)
H17	0.4586	0.6483	0.8672	0.059*
H18	0.4541	0.8403	0.8536	0.059*
C1	0.4727 (4)	0.2977 (5)	0.80066 (15)	0.0352 (6)
C2	0.3845 (5)	0.1694 (4)	0.73196 (18)	0.0356 (7)
C3	0.2004 (4)	0.2543 (5)	0.68807 (17)	0.0384 (7)
H3A	0.0894	0.2849	0.7224	0.046*
C4	0.1419 (5)	0.1285 (6)	0.6148 (2)	0.0527 (9)
H4A	0.1791	−0.0053	0.6212	0.063*
H4B	0.0028	0.1423	0.5948	0.063*
C5	0.2921 (5)	0.2488 (6)	0.56934 (18)	0.0541 (10)
H5	0.2527	0.2741	0.5126	0.065*
C6	0.4990 (6)	0.1655 (7)	0.58425 (18)	0.0586 (11)
H6A	0.5982	0.2592	0.5692	0.070*
H6B	0.5124	0.0540	0.5501	0.070*

C7	0.5440 (5)	0.1063 (5)	0.67306 (18)	0.0451 (8)
H7A	0.5565	−0.0321	0.6755	0.054*
H7B	0.6730	0.1603	0.6913	0.054*
C8	0.2550 (5)	0.4173 (5)	0.62814 (18)	0.0463 (8)
C9	0.4265 (6)	0.5520 (6)	0.6499 (2)	0.0581 (9)
H9A	0.3882	0.6371	0.6919	0.087*
H9B	0.4581	0.6253	0.6033	0.087*
H9C	0.5426	0.4794	0.6685	0.087*
C10	0.0681 (7)	0.5319 (7)	0.6031 (3)	0.0742 (12)
H10A	0.0984	0.6187	0.5605	0.111*
H10B	0.0250	0.6035	0.6485	0.111*
H10C	−0.0373	0.4462	0.5845	0.111*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Na1	0.0433 (6)	0.0359 (7)	0.0437 (6)	0.0011 (5)	0.0047 (4)	−0.0013 (6)
O1	0.0472 (12)	0.0610 (16)	0.0483 (12)	0.0079 (13)	−0.0090 (9)	−0.0138 (12)
O2	0.0484 (12)	0.0462 (14)	0.0348 (11)	0.0040 (11)	0.0068 (9)	−0.0075 (10)
O3	0.0505 (13)	0.0341 (13)	0.0482 (13)	0.0017 (10)	0.0094 (10)	0.0087 (10)
O4	0.0494 (12)	0.0487 (15)	0.0547 (13)	0.0013 (12)	0.0076 (10)	−0.0040 (12)
O5	0.0366 (10)	0.0505 (13)	0.0409 (10)	−0.0013 (12)	0.0025 (8)	0.0008 (12)
O6	0.0373 (10)	0.0504 (13)	0.0378 (10)	0.0015 (11)	0.0056 (8)	0.0033 (12)
O7	0.0507 (13)	0.0440 (15)	0.0478 (13)	−0.0012 (11)	0.0050 (10)	−0.0024 (11)
O8	0.0604 (13)	0.0484 (16)	0.0381 (11)	−0.0009 (12)	−0.0061 (9)	−0.0015 (11)
C1	0.0416 (15)	0.0360 (16)	0.0282 (13)	0.0043 (16)	0.0039 (11)	0.0026 (15)
C2	0.0421 (16)	0.0299 (17)	0.0352 (15)	−0.0014 (13)	0.0051 (12)	0.0011 (13)
C3	0.0433 (15)	0.038 (2)	0.0336 (14)	−0.0013 (14)	0.0033 (11)	0.0007 (14)
C4	0.059 (2)	0.053 (2)	0.0450 (19)	−0.0102 (18)	−0.0072 (15)	−0.0052 (17)
C5	0.073 (2)	0.062 (3)	0.0261 (15)	−0.011 (2)	0.0004 (14)	−0.0043 (17)
C6	0.070 (2)	0.072 (3)	0.0349 (17)	−0.006 (2)	0.0152 (16)	−0.0166 (18)
C7	0.0505 (17)	0.047 (2)	0.0384 (17)	0.0018 (16)	0.0111 (14)	−0.0071 (15)
C8	0.064 (2)	0.041 (2)	0.0325 (16)	−0.0047 (18)	−0.0039 (15)	0.0069 (15)
C9	0.093 (2)	0.044 (2)	0.0376 (17)	−0.016 (2)	0.0028 (16)	0.0096 (17)
C10	0.101 (3)	0.062 (3)	0.058 (2)	0.018 (3)	−0.014 (2)	0.010 (2)

Geometric parameters (Å, º)

Na1—O5	2.340 (3)	C2—C7	1.544 (4)
Na1—O6	2.356 (3)	C3—C4	1.534 (5)
Na1—O7	2.457 (3)	C3—C8	1.566 (4)
Na1—O4	2.538 (3)	C3—H3A	0.9800
Na1—Na1^{i}	3.4939 (15)	C4—C5	1.533 (5)
Na1—Na1^{ii}	3.4939 (15)	C4—H4A	0.9700
O1—C1	1.250 (3)	C4—H4B	0.9700
O2—C1	1.257 (4)	C5—C6	1.502 (5)
O3—C2	1.447 (4)	C5—C8	1.556 (5)
O3—H3	0.8200	C5—H5	0.9800

O4—H9	0.8500	C6—C7	1.545 (5)
O4—H10	0.8500	C6—H6A	0.9700
O5—Na1^{i}	2.375 (3)	C6—H6B	0.9700
O5—H11	0.8500	C7—H7A	0.9700
O5—H12	0.8499	C7—H7B	0.9700
O6—Na1^{i}	2.324 (3)	C8—C9	1.507 (5)
O6—H13	0.8500	C8—C10	1.517 (6)
O6—H14	0.8499	C9—H9A	0.9600
O7—H15	0.8500	C9—H9B	0.9600
O7—H16	0.8501	C9—H9C	0.9600
O8—H17	0.8499	C10—H10A	0.9600
O8—H18	0.8498	C10—H10B	0.9600
C1—C2	1.541 (4)	C10—H10C	0.9600
C2—C3	1.512 (4)		

O6^{ii}—Na1—O5	99.06 (9)	O3—C2—C7	106.5 (3)
O5—Na1—O6	82.94 (9)	C3—C2—C7	111.8 (3)
O6^{ii}—Na1—O5^{ii}	82.86 (9)	C1—C2—C7	112.8 (3)
O6—Na1—O5^{ii}	94.79 (9)	C2—C3—C4	108.8 (3)
O6^{ii}—Na1—O7	97.62 (9)	C2—C3—C8	112.5 (2)
O5—Na1—O7	92.74 (9)	C4—C3—C8	88.2 (2)
O6—Na1—O7	86.92 (8)	C2—C3—H3A	114.8
O5^{ii}—Na1—O7	91.40 (9)	C4—C3—H3A	114.8
O6^{ii}—Na1—O4	89.44 (9)	C8—C3—H3A	114.8
O5—Na1—O4	84.40 (9)	C5—C4—C3	86.2 (3)
O6—Na1—O4	86.10 (9)	C5—C4—H4A	114.3
O5^{ii}—Na1—O4	91.19 (9)	C3—C4—H4A	114.3
O7—Na1—O4	172.73 (11)	C5—C4—H4B	114.3
O6^{ii}—Na1—Na1^{i}	141.31 (8)	C3—C4—H4B	114.3
O5—Na1—Na1^{i}	42.58 (6)	H4A—C4—H4B	111.4
O6—Na1—Na1^{i}	41.36 (6)	C6—C5—C4	108.8 (3)
O5^{ii}—Na1—Na1^{i}	135.80 (8)	C6—C5—C8	111.3 (3)
O7—Na1—Na1^{i}	82.63 (8)	C4—C5—C8	88.6 (3)
O4—Na1—Na1^{i}	90.79 (8)	C6—C5—H5	115.1
O6^{ii}—Na1—Na1^{ii}	42.06 (6)	C4—C5—H5	115.1
O5—Na1—Na1^{ii}	139.07 (8)	C8—C5—H5	115.1
O6—Na1—Na1^{ii}	134.67 (9)	C5—C6—C7	113.0 (3)
O5^{ii}—Na1—Na1^{ii}	41.80 (6)	C5—C6—H6A	109.0
O7—Na1—Na1^{ii}	103.09 (8)	C7—C6—H6A	109.0
O4—Na1—Na1^{ii}	83.32 (8)	C5—C6—H6B	109.0
Na1^{i}—Na1—Na1^{ii}	173.37 (8)	C7—C6—H6B	109.0
C2—O3—H3	109.5	H6A—C6—H6B	107.8
Na1—O4—H9	102.5	C2—C7—C6	115.1 (3)
Na1—O4—H10	106.3	C2—C7—H7A	108.5
H9—O4—H10	105.3	C6—C7—H7A	108.5
Na1—O5—H11	115.4	C2—C7—H7B	108.5
Na1^{i}—O5—H11	103.2	C6—C7—H7B	108.5
Na1—O5—H12	124.7	H7A—C7—H7B	107.5

Na1^{i}—O5—H12	110.5	C9—C8—C10	109.6 (3)
H11—O5—H12	105.0	C9—C8—C5	118.6 (3)
Na1^{i}—O6—H13	122.3	C10—C8—C5	112.4 (3)
Na1—O6—H13	110.3	C9—C8—C3	119.9 (3)
Na1^{i}—O6—H14	104.7	C10—C8—C3	110.1 (3)
Na1—O6—H14	118.1	C5—C8—C3	84.3 (2)
H13—O6—H14	105.5	C8—C9—H9A	109.5
Na1—O7—H15	112.1	C8—C9—H9B	109.5
Na1—O7—H16	109.8	H9A—C9—H9B	109.5
H15—O7—H16	104.8	C8—C9—H9C	109.5
H17—O8—H18	106.1	H9A—C9—H9C	109.5
O1—C1—O2	123.5 (3)	H9B—C9—H9C	109.5
O1—C1—O2	123.5 (3)	C8—C10—H10A	109.5
O1—C1—C2	119.1 (3)	C8—C10—H10B	109.5
O2—C1—C2	117.2 (2)	H10A—C10—H10B	109.5
O2—C1—C2	117.2 (2)	C8—C10—H10C	109.5
O3—C2—C3	108.6 (2)	H10A—C10—H10C	109.5
O3—C2—C1	103.2 (2)	H10B—C10—H10C	109.5
C3—C2—C1	113.3 (3)		

O6^{ii}—Na1—O5—Na1^{i}	−174.16 (10)	C1—C2—C3—C8	76.8 (3)
O6—Na1—O5—Na1^{i}	10.56 (7)	C7—C2—C3—C8	−52.0 (4)
O7—Na1—O5—Na1^{i}	−76.00 (9)	C2—C3—C4—C5	−86.5 (3)
O4—Na1—O5—Na1^{i}	97.30 (9)	C8—C3—C4—C5	26.7 (3)
Na1^{ii}—Na1—O5—Na1^{i}	170.35 (13)	C3—C4—C5—C6	85.2 (3)
O5—Na1—O6—Na1^{i}	−10.82 (7)	C3—C4—C5—C8	−26.9 (2)
O5^{ii}—Na1—O6—Na1^{i}	173.48 (10)	C4—C5—C6—C7	−42.5 (4)
O7—Na1—O6—Na1^{i}	82.33 (9)	C8—C5—C6—C7	53.6 (4)
O4—Na1—O6—Na1^{i}	−95.64 (9)	O3—C2—C7—C6	126.2 (3)
Na1^{ii}—Na1—O6—Na1^{i}	−172.26 (12)	C3—C2—C7—C6	7.8 (4)
O2—O2—C1—O1	0.0 (7)	C1—C2—C7—C6	−121.3 (3)
O2—O2—C1—C2	0.0 (6)	C5—C6—C7—C2	−8.5 (5)
O1—C1—C2—O3	87.1 (3)	C6—C5—C8—C9	37.7 (4)
O2—C1—C2—O3	−88.8 (3)	C4—C5—C8—C9	147.3 (3)
O2—C1—C2—O3	−88.8 (3)	C6—C5—C8—C10	167.4 (3)
O1—C1—C2—C3	−155.6 (3)	C4—C5—C8—C10	−83.0 (4)
O2—C1—C2—C3	28.4 (4)	C6—C5—C8—C3	−83.3 (3)
O2—C1—C2—C3	28.4 (4)	C4—C5—C8—C3	26.3 (2)
O1—C1—C2—C7	−27.4 (4)	C2—C3—C8—C9	−36.5 (4)
O2—C1—C2—C7	156.7 (3)	C4—C3—C8—C9	−146.1 (3)
O2—C1—C2—C7	156.7 (3)	C2—C3—C8—C10	−164.9 (3)
O3—C2—C3—C4	−73.2 (3)	C4—C3—C8—C10	85.4 (3)
C1—C2—C3—C4	172.8 (3)	C2—C3—C8—C5	83.3 (3)
C7—C2—C3—C4	44.0 (3)	C4—C3—C8—C5	−26.3 (2)
O3—C2—C3—C8	−169.2 (2)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O8—H18···O3^{iii}	0.85	1.90	2.737 (3)	170
O8—H17···O2	0.85	1.90	2.741 (3)	173
O7—H16···O1^{iv}	0.85	2.05	2.859 (4)	158
O7—H15···O4^{i}	0.85	2.12	2.887 (4)	150
O6—H14···O8^{v}	0.85	1.88	2.727 (3)	175
O6—H13···O2	0.85	1.96	2.776 (3)	161
O5—H12···O8^{i}	0.85	1.98	2.805 (3)	164
O5—H11···O1^{vi}	0.85	1.96	2.791 (3)	166
O4—H10···O2	0.85	2.06	2.879 (3)	161
O4—H9···O1^{vi}	0.85	2.10	2.949 (4)	174
O3—H3···O7^{i}	0.82	2.02	2.809 (3)	161

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