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Sodium 3-chloro-2-hydroxyethanesulfonate hemihydrate

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The title compound, $Na^+ \cdot C_3H_6ClO_4S^- \cdot 0.5H_2O$, was synthesized from sodium hydrogen sulfite and 2-(chloromethyl)oxirane in aqueous solution. The Na^+ ion is coordinated by six O atoms in a distorted octahedral manner.

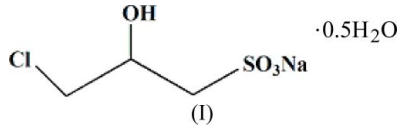
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.040
wR factor = 0.105
Data-to-parameter ratio = 17.7

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

Comment

The crystal structure of the title compound, (I), an important organic intermediate, has been determined in order to elucidate the molecular conformation. The structure is shown in Fig. 1.



(I)

In the structure of (I), the Na^+ ion is coordinated by O1,O2(x, $-y$, $z+\frac{1}{2}$), O3($-x$, $-y$, $-z$), O3(x, $y-1$, z), O4(x, $y-1$, z) and O5 of the water molecule in a distorted octahedral geometry. The average Na—O bond length is 2.3795 Å (Table 1). The Na^+ ion forms a six-membered ring with O3(x, $y-1$, z), S1(x, $y-1$, z), C1(x, $y-1$, z), C2(x, $y-1$, z) and O4(x, $y-1$, z) in the structure. This may contribute to the structural stability.

In the crystal structure, anions and water molecules are linked though O—H···O hydrogen bonds (Table 2). In addition,there are some weak interactions between the chlorine atoms (Fig. 2).

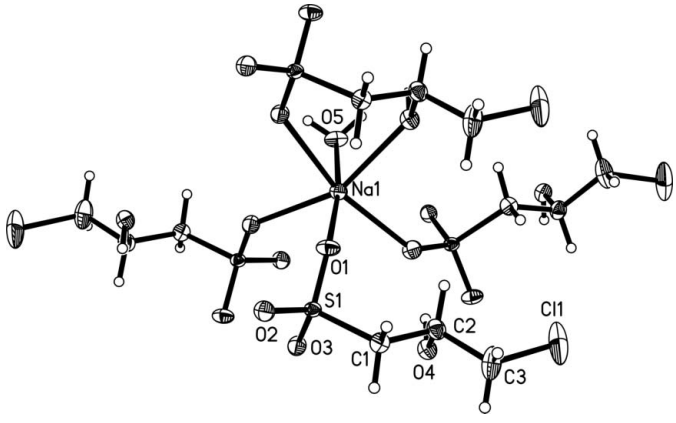


Figure 1
The title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented by circles of arbitrary size.

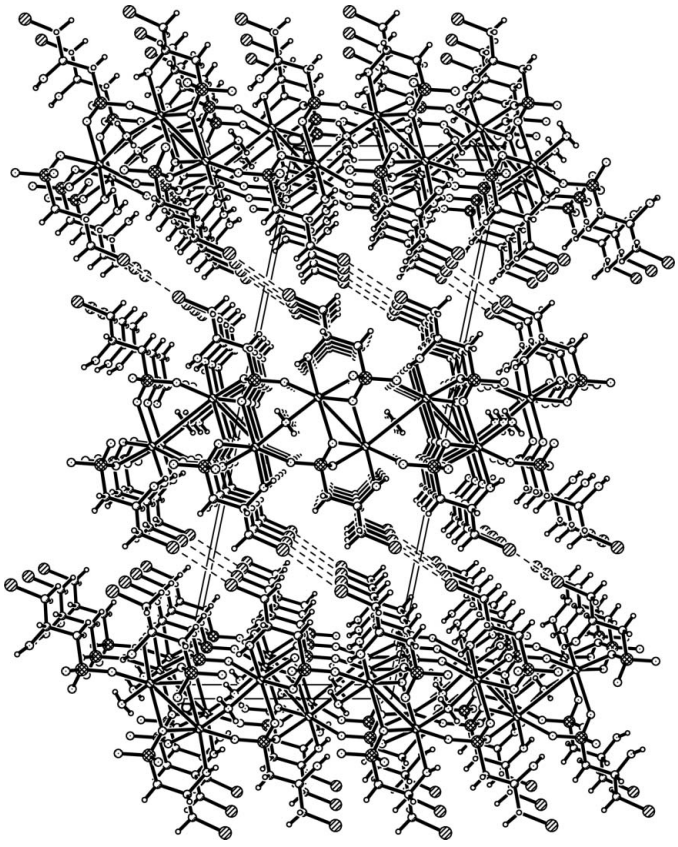


Figure 2
The packing of (I), viewed along the *c* axis. Dashed lines indicate hydrogen-bonding and Cl···Cl interactions.

Experimental

To an aqueous solution (100 ml) of sodium hydrogen sulfite (10.40 g, 100 mmol), 2-(chloromethyl)oxirane (9.25 g, 100 mmol) was added at 333 K over a period of 1 h. The reaction was stirred at 333–335 K for 2 h. The mass was then cooled in a ice–water bath and filtered. The resulting solid was recrystallized from water. A colorless single crystal suitable for X-ray analysis was obtained (m.p. 533 K).

Crystal data

$Na^+·C_3H_6ClNaO_4S^-·0.5H_2O$
M_r = 205.59
Monoclinic, $C2/c$
a = 28.523 (6) Å
b = 5.2756 (11) Å
c = 10.722 (2) Å
β = 101.67 (3)°
V = 1580.1 (6) Å^3
Z = 8
D_x = 1.728 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.77 mm^{-1}
T = 293 (2) K
Block, colorless
0.26 × 0.20 × 0.18 mm

Data collection

Rigaku Saturn diffractometer
ω scans
Absorption correction: multi-scan (Jacobson, 1998)
T_{min} = 0.737, T_{max} = 0.873
8844 measured reflections
1860 independent reflections
1583 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 27.9°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.105
S = 1.06
1860 reflections
105 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0564P)^2 + 1.454P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.64 e Å^{-3}
$\Delta\rho_{min}$ = −0.72 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0057 (17)

Table 1
Selected geometric parameters (Å, °).

Na1—O1	2.3152 (17)	Na1—Na1^{iv}	3.5642 (19)
Na1—O2^{i}	2.3575 (17)	Na1—Na1^{v}	3.8834 (18)
Na1—O5	2.3785 (15)	Cl1—C3	1.784 (3)
Na1—O3^{ii}	2.3986 (17)	C1—C2	1.538 (3)
Na1—O4^{iii}	2.4486 (18)	C2—C3	1.511 (3)
Na1—O3^{iii}	2.4536 (16)		
O1—Na1—O2^{i}	91.00 (6)	O5—Na1—O4^{iii}	85.13 (6)
O1—Na1—O5	172.96 (5)	O3^{ii}—Na1—O4^{iii}	156.57 (6)
O2^{i}—Na1—O5	94.10 (6)	O1—Na1—O3^{iii}	88.48 (6)
O1—Na1—O3^{ii}	92.26 (6)	O2^{i}—Na1—O3^{iii}	164.55 (6)
O2^{i}—Na1—O3^{ii}	109.98 (6)	O5—Na1—O3^{iii}	87.90 (6)
O5—Na1—O3^{ii}	81.43 (5)	O3^{ii}—Na1—O3^{iii}	85.47 (6)
O1—Na1—O4^{iii}	99.75 (6)	O4^{iii}—Na1—O3^{iii}	74.91 (6)
O2^{i}—Na1—O4^{iii}	89.98 (6)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5A···O1^{vi}	0.84 (5)	2.51 (4)	3.286 (2)	155 (5)
O5—H5A···O2^{vi}	0.84 (5)	2.40 (5)	3.121 (2)	145 (5)
O4—H4···O2^{i}	0.90 (3)	1.94 (3)	2.832 (2)	169 (3)

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

All H atoms were initially located in a difference Fourier map. They were then constrained to an ideal geometry, with O—H = 84 (5)–0.90 (3) and C—H = 0.97–0.98 Å, and with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *CrystalStructure* (Rigaku/MSC, 2005).

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