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Sodium *N*-chloro-2-methylbenzene-sulfonamidate sesquihydrateB. Thimme Gowda,^{a*} Sabine Foro^b and Hartmut Fuess^b^aDepartment of Chemistry, Mangalore University, Mangalagangothri 574 199, Mangalore, India, and ^bInstitute of Materials Science, Darmstadt University of Technology, Petersenstrasse 23, D-64287 Darmstadt, Germany

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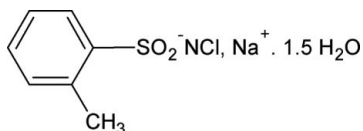
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Key indicators: single-crystal X-ray study; $T = 299$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.023; wR factor = 0.061; data-to-parameter ratio = 11.7.

In the title salt, $\text{Na}^+ \cdot \text{C}_7\text{H}_7\text{ClNO}_2\text{S}^- \cdot 1.5\text{H}_2\text{O}$, one of the water molecules lies on a twofold axis. The sodium ion shows an O_6 octahedral coordination defined by three water O atoms and three sulfonyl O atoms derived from three different anions. The S–N distance of 1.5898 (19) Å is consistent with an S=N double bond. The crystal structure is stabilized by N–H...O and O–H...Cl hydrogen bonds.

Related literature

For background to *N*-halo-arylsulfonamides, see: Gowda *et al.* (2005). For related structures, see: Gowda *et al.* (2007*a,b,c*); George *et al.* (2000); Olmstead & Power (1986).



Experimental

Crystal data

 $\text{Na}^+ \cdot \text{C}_7\text{H}_7\text{ClNO}_2\text{S}^- \cdot 1.5\text{H}_2\text{O}$ $M_r = 509.32$ Monoclinic, $C2$ $a = 11.011$ (1) Å $b = 6.6434$ (6) Å $c = 14.447$ (1) Å $\beta = 100.350$ (7)° $V = 1039.61$ (15) Å³ $Z = 2$ Mo $K\alpha$ radiation $\mu = 0.60$ mm⁻¹ $T = 299$ K $0.45 \times 0.32 \times 0.08$ mm

Data collection

Oxford Diffraction Xcalibur diffractometer with a Sapphire CCD detector

Absorption correction: multi-scan (*CrysAlis RED*; Oxford)

Diffraction, 2007)

 $T_{\min} = 0.776$, $T_{\max} = 0.954$

3268 measured reflections

1657 independent reflections

1613 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.018$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.023$ $wR(F^2) = 0.061$ $S = 1.02$

1657 reflections

142 parameters

1 restraint

H atoms treated by a mixture of independent and constrained refinement

 $\Delta\rho_{\text{max}} = 0.25$ e Å⁻³ $\Delta\rho_{\text{min}} = -0.16$ e Å⁻³

Absolute structure: Flack (1983),

617 Friedel pairs

Flack parameter: 0.02 (6)

Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$\text{O3}-\text{H31} \cdots \text{Cl1}^{\text{i}}$	0.83 (3)	2.62 (3)	3.4266 (19)	167 (3)
$\text{O3}-\text{H32} \cdots \text{N1}^{\text{ii}}$	0.77 (3)	2.19 (3)	2.951 (3)	168 (3)
$\text{O4}-\text{H41} \cdots \text{N1}^{\text{iii}}$	0.80 (3)	2.19 (3)	2.989 (2)	176 (3)

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2004); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2007); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); 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: TK2451).

References

- Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.
 George, E., Vivekanandan, S. & Sivakumar, K. (2000). *Acta Cryst.* **C56**, 1208–1209.
 Gowda, B. T., Damodara, N. & Jyothi, K. (2005). *Int. J. Chem. Kinet.* **37**, 572–582.
 Gowda, B. T., Jyothi, K., Foro, S., Kožisek, J. & Fuess, H. (2007*a*). *Acta Cryst.* **E63**, m1644–m1645.
 Gowda, B. T., Srilatha, Foro, S., Kozisek, J. & Fuess, H. (2007*b*). *Z. Naturforsch. Teil A*, **62**, 417–424.
 Gowda, B. T., Usha, K. M., Kožisek, J., Tokarčík, M. & Fuess, H. (2007*c*). *Acta Cryst.* **E63**, m1739–m1740.
 Olmstead, M. M. & Power, P. P. (1986). *Inorg. Chem.* **25**, 4057–4058.
 Oxford Diffraction (2004). *CrysAlis CCD*. Oxford Diffraction Ltd, Köln, Germany.
 Oxford Diffraction (2007). *CrysAlis RED*. Oxford Diffraction Ltd, Köln, Germany.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
 Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.

supporting information

Acta Cryst. (2009). E65, m700 [doi:10.1107/S1600536809019989]

Sodium *N*-chloro-2-methylbenzenesulfonamidate sesquihydrate

B. Thimme Gowda, Sabine Foro and Hartmut Fuess

S1. Comment

The chemistry of *N*-halo-arylsulfonamides is of interest due to their diverse characteristics (Gowda *et al.*, 2005). In the present work, the structure of sodium *N*-chloro-2-methylbenzenesulfonamidate (I) has been determined to explore substituent effects on the solid-state structures of *N*-halo arylsulfonamidates (Gowda *et al.*, 2007*a, b, c*). The structure of (I), Fig. 1, resembles the sodium salts of *N*-chloro-4-chloro-benzenesulfonamidate (Gowda *et al.*, 2007*a*), *N*-chloro-2-methyl-4-chloro-benzenesulfonamidate (Gowda *et al.*, 2007*b*), *N*-bromo-benzenesulfonamidate (Gowda *et al.*, 2007*c*), and other sodium *N*-chloro-arylsulfonamidates (George *et al.*, 2000; Olmstead & Power, 1986). The sodium ion shows octahedral coordination defined by three water-O atoms and by three sulfonyl-O atoms derived from three different anions. There is no interaction between the nitrogen and sodium ions in (I). The N1—S1 distance of 1.5898 (19) Å is consistent with a S—N double bond and is in agreement with those observed with related *N*-chloro arylsulfonamides. In this description, the negative charge on the anion is distributed over the oxygen atoms. With the association described above for the Na⁺ ion along with N-H···O and O-H···Cl hydrogen bonding, Table 1, the molecular packing comprises layers stacked along the *c* axis (Fig. 2).

S2. Experimental

The purity of the commercial sample (TCI Chemicals, Tokyo Kasei) was checked and characterized by recording its infrared and NMR spectra and estimating the amount of active chlorine present in it by the iodometric method (Gowda *et al.*, 2005). The single crystals used in X-ray diffraction studies were grown in a water solution of (I) by slow evaporation at room temperature.

S3. Refinement

The O-bound H atoms were located in difference map and their positional parameters were refined freely [O—H = 0.77 (3)–0.83 (3) Å]. The other H atoms were positioned in their idealized geometry using a riding model [C—H = 0.93–0.96 Å]. All H atoms were refined with isotropic displacement parameters set to 1.2 times of the U_{eq} of the parent atom.

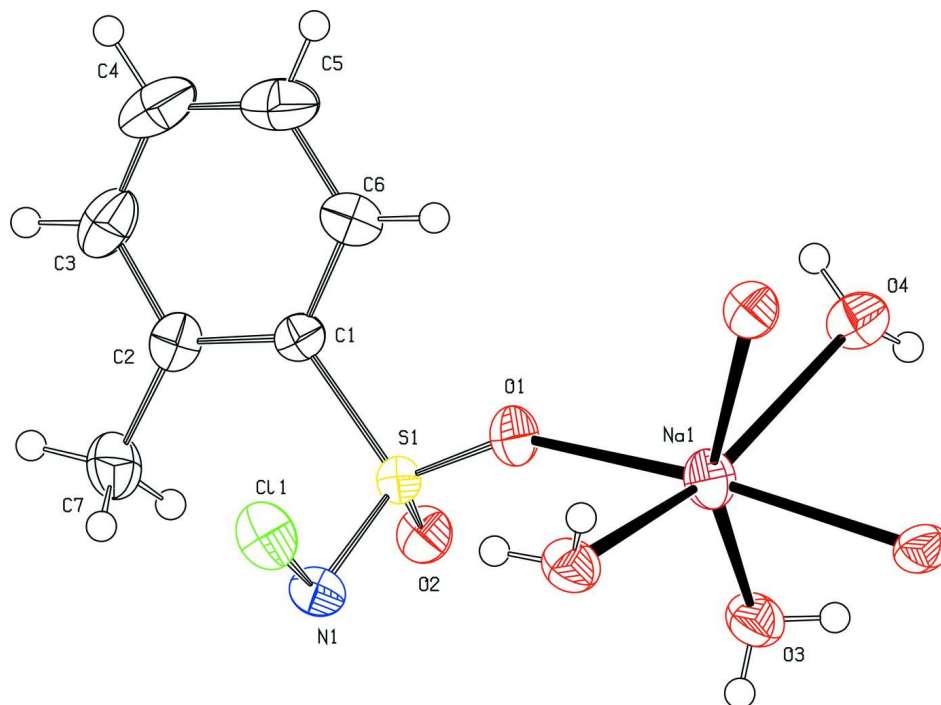


Figure 1

Molecular structure of (I), extended to show the immediate coordination geometry of the sodium cation. Only atoms comprising the asymmetric unit are labelled. Displacement ellipsoids are drawn at the 50% probability level.

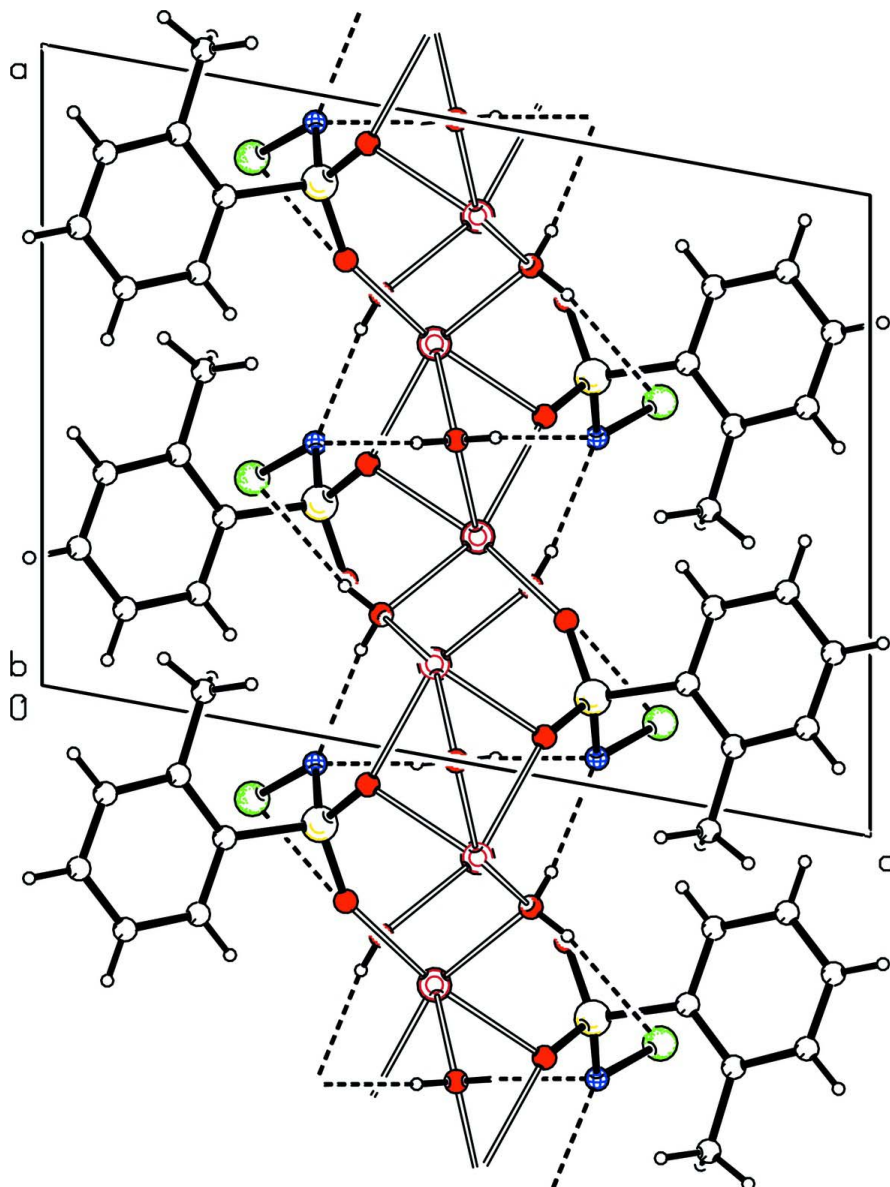


Figure 2

Part of the crystal structure of (I) as viewed down the *b* axis, showing the O3W—H31...Cl1, O3W—H32...N1 and O4W—H41...N1 hydrogen bonds as dashed lines.

Sodium *N*-chloro-2-methylbenzenesulfonamidate sesquihydrate

Crystal data

$\text{Na}^+ \cdot \text{C}_7\text{H}_7\text{ClNO}_2\text{S}^- \cdot 1.5\text{H}_2\text{O}$

$M_r = 509.32$

Monoclinic, *C*2

Hall symbol: *C* 2y

$a = 11.011$ (1) Å

$b = 6.6434$ (6) Å

$c = 14.447$ (1) Å

$\beta = 100.350$ (7)°

$V = 1039.61$ (15) Å³

$Z = 2$

$F(000) = 524$

$D_x = 1.627$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 3049 reflections

$\theta = 2.6$ – 27.5 °

$\mu = 0.60$ mm⁻¹

$T = 299$ K $0.45 \times 0.32 \times 0.08$ mm
 Plate, colourless

Data collection

Oxford Diffraction Xcalibur	3268 measured reflections
diffractometer with a Sapphire CCD detector	1657 independent reflections
Radiation source: fine-focus sealed tube	1613 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{\text{int}} = 0.018$
Rotation method data acquisition using ω and ϕ scans	$\theta_{\text{max}} = 25.3^\circ$, $\theta_{\text{min}} = 2.9^\circ$
Absorption correction: multi-scan	$h = -13 \rightarrow 12$
(<i>CrysAlis RED</i> ; Oxford Diffraction, 2007)	$k = -7 \rightarrow 8$
$T_{\text{min}} = 0.776$, $T_{\text{max}} = 0.954$	$l = -16 \rightarrow 17$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.023$	$w = 1/[\sigma^2(F_o^2) + (0.041P)^2 + 0.5427P]$
$wR(F^2) = 0.061$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{\text{max}} = 0.017$
1657 reflections	$\Delta\rho_{\text{max}} = 0.25 \text{ e } \text{\AA}^{-3}$
142 parameters	$\Delta\rho_{\text{min}} = -0.16 \text{ e } \text{\AA}^{-3}$
1 restraint	Absolute structure: Flack (1983), 617 Friedel pairs
Primary atom site location: structure-invariant direct methods	Absolute structure parameter: 0.02 (6)
Secondary atom site location: difference Fourier map	

Special details

Experimental. Absorption correction: *CrysAlis RED*, Oxford Diffraction Ltd., 2007 Empirical absorption correction using spherical harmonics, implemented in *SCALE3 ABSPACK* scaling algorithm.

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cl1	0.38269 (5)	0.04628 (9)	0.25363 (4)	0.03904 (16)
S1	0.36260 (4)	0.41295 (8)	0.33507 (3)	0.02316 (13)
Na1	0.14461 (8)	0.19582 (15)	0.47389 (6)	0.0333 (2)
O1	0.24978 (13)	0.3583 (3)	0.36677 (10)	0.0367 (4)
O2	0.43766 (13)	0.5621 (3)	0.39333 (10)	0.0320 (4)
O3	0.29326 (15)	0.3727 (3)	0.59025 (12)	0.0365 (4)
H31	0.258 (3)	0.402 (5)	0.6345 (18)	0.044*
H32	0.354 (3)	0.324 (5)	0.615 (2)	0.044*
O4	0.0000	0.4675 (4)	0.5000	0.0358 (6)
H41	-0.015 (3)	0.534 (5)	0.4534 (18)	0.043*

N1	0.45553 (16)	0.2319 (3)	0.32989 (12)	0.0286 (4)
C1	0.31412 (18)	0.5172 (3)	0.22046 (13)	0.0254 (4)
C2	0.3987 (2)	0.5799 (4)	0.16471 (15)	0.0310 (5)
C3	0.3489 (3)	0.6595 (4)	0.07650 (16)	0.0442 (6)
H3	0.4026	0.7045	0.0380	0.053*
C4	0.2246 (3)	0.6740 (5)	0.04438 (17)	0.0533 (7)
H4	0.1954	0.7255	-0.0153	0.064*
C5	0.1428 (3)	0.6125 (5)	0.10021 (19)	0.0503 (7)
H5	0.0582	0.6233	0.0788	0.060*
C6	0.1876 (2)	0.5343 (4)	0.18857 (16)	0.0367 (5)
H6	0.1328	0.4930	0.2268	0.044*
C7	0.5365 (2)	0.5657 (5)	0.19499 (17)	0.0410 (6)
H7A	0.5600	0.4270	0.2040	0.049*
H7B	0.5610	0.6378	0.2529	0.049*
H7C	0.5763	0.6233	0.1473	0.049*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0411 (3)	0.0278 (3)	0.0496 (3)	-0.0037 (2)	0.0118 (2)	-0.0106 (3)
S1	0.0232 (2)	0.0237 (3)	0.0231 (2)	-0.0006 (2)	0.00549 (16)	-0.0007 (2)
Na1	0.0316 (5)	0.0327 (5)	0.0374 (4)	-0.0053 (4)	0.0114 (4)	-0.0002 (4)
O1	0.0316 (8)	0.0456 (12)	0.0360 (8)	-0.0025 (7)	0.0143 (6)	0.0047 (7)
O2	0.0343 (8)	0.0302 (10)	0.0305 (7)	-0.0028 (7)	0.0034 (6)	-0.0084 (6)
O3	0.0270 (8)	0.0421 (12)	0.0396 (8)	0.0008 (7)	0.0040 (6)	-0.0010 (7)
O4	0.0457 (14)	0.0257 (14)	0.0342 (11)	0.000	0.0025 (10)	0.000
N1	0.0262 (9)	0.0240 (11)	0.0342 (9)	-0.0005 (7)	0.0016 (7)	-0.0019 (7)
C1	0.0296 (10)	0.0206 (12)	0.0250 (9)	-0.0003 (9)	0.0024 (7)	-0.0009 (8)
C2	0.0383 (12)	0.0250 (14)	0.0306 (10)	-0.0045 (9)	0.0091 (8)	-0.0017 (9)
C3	0.0646 (17)	0.0364 (17)	0.0332 (11)	-0.0040 (13)	0.0132 (11)	0.0056 (11)
C4	0.076 (2)	0.0450 (18)	0.0334 (12)	0.0053 (15)	-0.0048 (13)	0.0079 (12)
C5	0.0449 (15)	0.0508 (18)	0.0478 (14)	0.0069 (12)	-0.0115 (11)	-0.0001 (12)
C6	0.0319 (11)	0.0337 (14)	0.0432 (11)	0.0019 (10)	0.0033 (9)	0.0007 (11)
C7	0.0357 (12)	0.0449 (17)	0.0457 (12)	-0.0071 (11)	0.0163 (10)	0.0029 (12)

Geometric parameters (Å, °)

Cl1—N1	1.7491 (19)	O3—H31	0.83 (3)
S1—O1	1.4454 (15)	O3—H32	0.77 (3)
S1—O2	1.4571 (16)	O4—Na1 ^{iv}	2.480 (2)
S1—N1	1.5898 (19)	O4—H41	0.80 (3)
S1—C1	1.785 (2)	C1—C6	1.391 (3)
S1—Na1 ⁱ	3.3517 (10)	C1—C2	1.399 (3)
Na1—O1	2.3549 (17)	C2—C3	1.397 (3)
Na1—O3	2.4283 (18)	C2—C7	1.505 (3)
Na1—O2 ⁱⁱ	2.4319 (16)	C3—C4	1.367 (4)
Na1—O4	2.480 (2)	C3—H3	0.9300
Na1—O3 ⁱⁱⁱ	2.483 (2)	C4—C5	1.375 (4)

Na1—O2 ⁱⁱⁱ	2.5266 (16)	C4—H4	0.9300
Na1—S1 ⁱⁱ	3.3517 (10)	C5—C6	1.384 (4)
Na1—Na1 ^{iv}	3.4021 (16)	C5—H5	0.9300
Na1—Na1 ⁱ	4.0447 (10)	C6—H6	0.9300
Na1—Na1 ⁱⁱ	4.0447 (10)	C7—H7A	0.9600
O2—Na1 ⁱ	2.4319 (16)	C7—H7B	0.9600
O2—Na1 ^v	2.5266 (16)	C7—H7C	0.9600
O3—Na1 ⁱ	2.483 (2)		
O1—S1—O2	114.72 (9)	O3—Na1—Na1 ⁱⁱ	88.59 (6)
O1—S1—N1	114.96 (10)	O2 ⁱⁱ —Na1—Na1 ⁱⁱ	80.53 (5)
O2—S1—N1	103.80 (9)	O4—Na1—Na1 ⁱⁱ	158.72 (5)
O1—S1—C1	105.10 (9)	O3 ⁱⁱ —Na1—Na1 ⁱⁱ	34.12 (4)
O2—S1—C1	108.43 (10)	O2 ⁱⁱⁱ —Na1—Na1 ⁱⁱ	103.70 (5)
N1—S1—C1	109.72 (9)	S1 ⁱⁱ —Na1—Na1 ⁱⁱ	58.91 (2)
O1—S1—Na1 ⁱ	74.39 (7)	Na1 ^{iv} —Na1—Na1 ⁱⁱ	119.16 (2)
N1—S1—Na1 ⁱ	125.01 (7)	Na1 ⁱ —Na1—Na1 ⁱⁱ	110.42 (4)
C1—S1—Na1 ⁱ	119.92 (8)	S1—O1—Na1	151.10 (10)
O1—Na1—O3	83.29 (6)	S1—O2—Na1 ⁱ	116.81 (8)
O1—Na1—O2 ⁱⁱ	169.34 (7)	S1—O2—Na1 ^v	151.20 (10)
O3—Na1—O2 ⁱⁱ	86.05 (6)	Na1 ⁱ —O2—Na1 ^v	86.63 (5)
O1—Na1—O4	99.86 (6)	Na1—O3—Na1 ⁱ	110.90 (7)
O3—Na1—O4	85.06 (6)	Na1—O3—H31	107 (2)
O2 ⁱⁱ —Na1—O4	78.79 (5)	Na1 ⁱ —O3—H31	107 (2)
O1—Na1—O3 ⁱⁱ	87.14 (7)	Na1—O3—H32	123 (2)
O3—Na1—O3 ⁱⁱ	118.69 (5)	Na1 ⁱ —O3—H32	105 (2)
O2 ⁱⁱ —Na1—O3 ⁱⁱ	98.34 (7)	H31—O3—H32	103 (3)
O4—Na1—O3 ⁱⁱ	156.00 (6)	Na1 ^{iv} —O4—Na1	86.61 (9)
O1—Na1—O2 ⁱⁱⁱ	111.58 (6)	Na1 ^{iv} —O4—H41	119 (2)
O3—Na1—O2 ⁱⁱⁱ	158.28 (7)	Na1—O4—H41	108 (2)
O2 ⁱⁱ —Na1—O2 ⁱⁱⁱ	78.57 (6)	S1—N1—C11	109.69 (10)
O4—Na1—O2 ⁱⁱⁱ	77.02 (5)	C6—C1—C2	121.0 (2)
O3 ⁱⁱ —Na1—O2 ⁱⁱⁱ	79.06 (6)	C6—C1—S1	116.98 (16)
O1—Na1—S1 ⁱⁱ	152.30 (5)	C2—C1—S1	122.02 (15)
O3—Na1—S1 ⁱⁱ	79.28 (5)	C3—C2—C1	116.5 (2)
O2 ⁱⁱ —Na1—S1 ⁱⁱ	22.83 (4)	C3—C2—C7	119.9 (2)
O4—Na1—S1 ⁱⁱ	99.90 (4)	C1—C2—C7	123.7 (2)
O3 ⁱⁱ —Na1—S1 ⁱⁱ	82.61 (5)	C4—C3—C2	122.7 (2)
O2 ⁱⁱⁱ —Na1—S1 ⁱⁱ	91.68 (5)	C4—C3—H3	118.6
O1—Na1—Na1 ^{iv}	137.40 (5)	C2—C3—H3	118.6
O3—Na1—Na1 ^{iv}	112.82 (5)	C3—C4—C5	120.1 (2)
O2 ⁱⁱ —Na1—Na1 ^{iv}	47.85 (4)	C3—C4—H4	119.9
O4—Na1—Na1 ^{iv}	46.69 (4)	C5—C4—H4	119.9
O3 ⁱⁱ —Na1—Na1 ^{iv}	114.48 (5)	C4—C5—C6	119.3 (2)
O2 ⁱⁱⁱ —Na1—Na1 ^{iv}	45.53 (4)	C4—C5—H5	120.3
S1 ⁱⁱ —Na1—Na1 ^{iv}	69.87 (2)	C6—C5—H5	120.3
O1—Na1—Na1 ⁱ	54.03 (5)	C5—C6—C1	120.4 (2)
O3—Na1—Na1 ⁱ	34.99 (5)	C5—C6—H6	119.8

O2 ⁱⁱ —Na1—Na1 ⁱ	115.82 (6)	C1—C6—H6	119.8
O4—Na1—Na1 ⁱ	74.73 (4)	C2—C7—H7A	109.5
O3 ⁱⁱ —Na1—Na1 ⁱ	126.33 (6)	C2—C7—H7B	109.5
O2 ⁱⁱⁱ —Na1—Na1 ⁱ	144.54 (5)	H7A—C7—H7B	109.5
S1 ⁱⁱ —Na1—Na1 ⁱ	113.86 (3)	C2—C7—H7C	109.5
Na1 ^{iv} —Na1—Na1 ⁱ	119.16 (2)	H7A—C7—H7C	109.5
O1—Na1—Na1 ⁱⁱ	99.54 (6)	H7B—C7—H7C	109.5
O2—S1—O1—Na1	-71.5 (3)	O2 ⁱⁱ —Na1—O4—Na1 ^{iv}	-41.12 (4)
N1—S1—O1—Na1	48.8 (2)	O3 ⁱⁱ —Na1—O4—Na1 ^{iv}	44.21 (14)
C1—S1—O1—Na1	169.5 (2)	O2 ⁱⁱⁱ —Na1—O4—Na1 ^{iv}	39.58 (4)
Na1 ⁱ —S1—O1—Na1	-73.0 (2)	S1 ⁱⁱ —Na1—O4—Na1 ^{iv}	-49.86 (2)
O3—Na1—O1—S1	49.7 (2)	Na1 ⁱ —Na1—O4—Na1 ^{iv}	-162.08 (4)
O2 ⁱⁱ —Na1—O1—S1	51.7 (5)	Na1 ⁱⁱ —Na1—O4—Na1 ^{iv}	-54.89 (12)
O4—Na1—O1—S1	133.4 (2)	O1—S1—N1—C11	58.78 (12)
O3 ⁱⁱ —Na1—O1—S1	-69.7 (2)	O2—S1—N1—C11	-175.11 (9)
O2 ⁱⁱⁱ —Na1—O1—S1	-146.7 (2)	C1—S1—N1—C11	-59.39 (13)
S1 ⁱⁱ —Na1—O1—S1	-1.5 (3)	Na1 ⁱ —S1—N1—C11	146.70 (6)
Na1 ^{iv} —Na1—O1—S1	166.35 (18)	O1—S1—C1—C6	3.1 (2)
Na1 ⁱ —Na1—O1—S1	70.6 (2)	O2—S1—C1—C6	-119.99 (19)
Na1 ⁱⁱ —Na1—O1—S1	-37.8 (2)	N1—S1—C1—C6	127.3 (2)
O1—S1—O2—Na1 ⁱ	-2.28 (14)	Na1 ⁱ —S1—C1—C6	-77.3 (2)
N1—S1—O2—Na1 ⁱ	-128.55 (10)	O1—S1—C1—C2	-177.07 (18)
C1—S1—O2—Na1 ⁱ	114.82 (10)	O2—S1—C1—C2	59.8 (2)
O1—S1—O2—Na1 ^v	139.18 (19)	N1—S1—C1—C2	-52.9 (2)
N1—S1—O2—Na1 ^v	12.9 (2)	Na1 ⁱ —S1—C1—C2	102.50 (18)
C1—S1—O2—Na1 ^v	-103.7 (2)	C6—C1—C2—C3	0.0 (3)
Na1 ⁱ —S1—O2—Na1 ^v	141.5 (3)	S1—C1—C2—C3	-179.79 (19)
O1—Na1—O3—Na1 ⁱ	30.30 (8)	C6—C1—C2—C7	179.9 (2)
O2 ⁱⁱ —Na1—O3—Na1 ⁱ	-149.33 (8)	S1—C1—C2—C7	0.2 (3)
O4—Na1—O3—Na1 ⁱ	-70.26 (7)	C1—C2—C3—C4	-0.9 (4)
O3 ⁱⁱ —Na1—O3—Na1 ⁱ	113.32 (11)	C7—C2—C3—C4	179.1 (3)
O2 ⁱⁱⁱ —Na1—O3—Na1 ⁱ	-104.58 (18)	C2—C3—C4—C5	1.3 (5)
S1 ⁱⁱ —Na1—O3—Na1 ⁱ	-171.33 (7)	C3—C4—C5—C6	-0.6 (5)
Na1 ^{iv} —Na1—O3—Na1 ⁱ	-108.70 (6)	C4—C5—C6—C1	-0.3 (5)
Na1 ⁱⁱ —Na1—O3—Na1 ⁱ	130.07 (7)	C2—C1—C6—C5	0.6 (4)
O1—Na1—O4—Na1 ^{iv}	149.64 (6)	S1—C1—C6—C5	-179.6 (2)
O3—Na1—O4—Na1 ^{iv}	-128.06 (5)		

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

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O3—H31 \cdots C11 ⁱ	0.83 (3)	2.62 (3)	3.4266 (19)	167 (3)
O3—H32 \cdots N1 ^{vi}	0.77 (3)	2.19 (3)	2.951 (3)	168 (3)
O4—H41 \cdots N1 ^{vii}	0.80 (3)	2.19 (3)	2.989 (2)	176 (3)

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