Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Sodium 2,4,*N*-trichlorobenzenesulfonamidate sesquihydrate

B. Thimme Gowda,[a]* M. B. Savitha,[a] Jozef Kožíšek,[b] Miroslav Tokarčík[c] and Hartmut Fuess[d]

[a]Department of Chemistry, Mangalore University, Mangalagangotri 574 199, Mangalore, India, [b]Department of Physical Chemistry, Slovak University of Technology, Radlinského 9, SK-812 37 Bratislava, Slovak Republic, [c]Department of Chemical Physics, Slovak University of Technology, Radlinského 9, 812 37 Bratislava, Slovak Republic, and [d]Institute of Materials Science, Darmstadt University of Technology, Petersenstrasse 23, D-64287 Darmstadt, Germany
Correspondence e-mail: gowdabt@yahoo.com

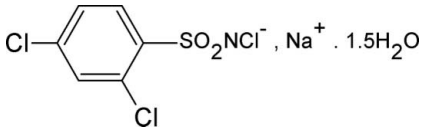
Received 6 May 2007; accepted 10 May 2007

Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.004 Å; R factor = 0.038; wR factor = 0.081; data-to-parameter ratio = 14.3.

The structure of the title compound, $Na^+\cdot C_6H_3Cl_3NO_2S^-\cdot 1.5H_2O$, is similar to those of sodium *N*-chlorobenzenesulfonamidate, sodium *N*-chloro-4-methylbenzenesulfonamidate, sodium 4,*N*-dichlorobenzenesulfonamidate and sodium 4,*N*-dichloro-2-methylbenzenesulfonamidate. There is no interaction between the N and Na atoms. The S—N distance of 1.583 (2) Å is consistent with an S=N double bond. One water molecule is located on a twofold rotation axis.

Related literature

For related literature, see: George *et al.* (2000); Gowda & Kumar (2003); Gowda & Shetty (2004); Gowda *et al.* (2002, 2005); Gowda, D'Souza & Kumar (2003); Gowda, Jyothi, Kozisek & Fuess (2003); Gowda, Jyothi, Kozisek, Tokarcik & Fuess (2007); Gowda, Srilatha, Foro, Kozisek & Fuess (2007); Olmstead & Power (1986).



Experimental

Crystal data

$Na^+\cdot C_6H_3Cl_3NO_2S^-\cdot 1.5H_2O$
M_r = 309.52
Monoclinic, $C2/c$
a = 11.033 (2) Å
b = 6.7410 (13) Å
c = 30.187 (6) Å
β = 98.51 (3)°
V = 2220.4 (8) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.04 mm^{-1}
T = 294 (2) K
0.46 × 0.32 × 0.16 mm

Data collection

Oxford Diffraction Xcalibur diffractometer
Absorption correction: analytical (*CrysAlis RED*; Oxford Diffraction, 2003)
T_{min} = 0.646, T_{max} = 0.851
3256 measured reflections
2162 independent reflections
1872 reflections with $I > 2\sigma(I)$
R_{int} = 0.047

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.081
S = 1.09
2162 reflections
151 parameters
7 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2003); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2003); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2002); software used to prepare material for publication: *SHELXL97*, *PLATON* (Spek, 2003) and *WinGX* (Farrugia, 1999).

BTG gratefully thanks the Alexander von Humboldt Foundation, Bonn, Germany for the extension of his research fellowship. JK and MT thank the Grant Agency of the Slovak Republic (grant No. 1/2449/05).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2359).

References

Brandenburg, K. (2002). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
George, E., Vivekanandan, S. & Sivakumar, K. (2000). *Acta Cryst.* C**56**, 1208–1209.
Gowda, B. T., Damodara, N. & Jyothi, K. (2005). *Int. J. Chem. Kinet.* **37**, 572–582.
Gowda, B. T., D'Souza, J. D. & Kumar, B. H. A. (2003). *Z. Naturforsch. Teil A*, **58**, 51–56.
Gowda, B. T., Jyothi, K. & D'Souza, J. D. (2002). *Z. Naturforsch. Teil A*, **57**, 967–973.
Gowda, B. T., Jyothi, K., Kozisek, J. & Fuess, H. (2003). *Z. Naturforsch. Teil A*, **58**, 656–660.
Gowda, B. T., Jyothi, K., Kozisek, J., Tokarcik, M. T. & Fuess, H. (2007). *Acta Cryst.* E**63**. In the Press (bt2356).
Gowda, B. T. & Kumar, B. H. A. (2003). *Oxid. Commun.* **26**, 403–425.
Gowda, B. T. & Shetty, M. (2004). *J. Phys. Org. Chem.* **17**, 848–864.
Gowda, B. T., Srilatha, Foro, S., Kozisek, J. & Fuess, H. (2007). *Z. Naturforsch. Teil A*, **62**. In the press.
Olmstead, M. M. & Power, P. P. (1986). *Inorg. Chem.* **25**, 4057–4058.
Oxford Diffraction (2003). *CrysAlis CCD* & *CrysAlis RED*. Oxford Diffraction Ltd, Abingdon, Oxfordshire, England.
Sheldrick, G. M. (1997). *SHELXS97* & *SHELXL97* . University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

  doi:10.1107/S1600536807023045

supplementary materials

Acta Cryst. (2007). E**63**, m1646 [**doi:10.1107/S1600536807023045**]

Sodium 2,4,*N*-trichlorobenzenesulfonamidate sesquihydrate

B. T. Gowda, M. B. Savitha, J. Kozísek, M. Tokarcík and H. Fuess

Comment

The chemistry of arylsulfonamides and their N-halo compounds is of interest as they show distinct physical, chemical and biological properties. Many of these compounds exhibit pharmacological, fungicidal and herbicidal activities due to their oxidizing action in aqueous, partial aqueous and non-aqueous media. Thus N-halo arylsulfonamides are of interest in synthetic, mechanistic, analytical and biological chemistry (Gowda & Kumar, 2003; Gowda & Shetty, 2004; Gowda *et al.*, 2002; Gowda *et al.*,2005; Gowda, Srilatha *et al.*, 2007). In the present work, the structure of sodium *N*-chloro-2,4-dichlorobenzenesulfonamide has been determined to explore the substituent effects on the solid state structures of sulfonamides and N-halo arylsulfonamides (Gowda, Jyothi *et al.*, 2003; Gowda, Srilatha *et al.*, 2007).

The crystal structure of is complex similar to those of sodium *N*-chloro-benzenesulfonamide (George *et al.*, 2000), sodium *N*-chloro-4-chlorobenzenesulfonamide (Gowda, Srilatha, *et al.*, 2007), sodium *N*-chloro-4-methylbenzenesulfonamide (Olmstead & Power, 1986) and sodium *N*-chloro-2-methyl-4-chlorobenzenesulfonamide (Gowda, Jyothi *et al.*, 2007). There is no interaction between the nitrogen and sodium atoms in the molecule, and Na+ is attached to one of the sulfonyl oxygen atoms.

The effects of N-chlorination and substitution in the phenyl ring on the structural data of sulfonamides have been considered by comparing the geometric parameters of them. The comparison revealed that on mono N-chlorination of benzenesulfonamide (George *et al.*, 2000) and 4-chlorbenzenesulfonamide (Gowda, Jyothi *et al.*, 2003), the C—*S* and *S*—O bond lengths increased marginally, while the S—N bond length remained more or less the same or decreased marginally. Further, N-chlorination of *N*-chloro-4-chlorobenzenesulfonamide decreases the C—S, S—O and N—Cl, but increased the S—N bond length (Gowda, Jyothi *et al.*, 2007). The introduction of an additional Cl atom to the benzene ring at the *ortho* position marginally increased the C—S bond length and decreased the S—N bond length, while the S—O and N—Cl bond lengths remained more or less the same. The bond angles also changed on both N-chlorination and introduction of Cl atoms to the benzene ring.

Experimental

The title compound was prepared according to the literature method (Gowda, D'Souza *et al.*, 2003 *a*). The purity of the compound was checked by determining its melting point. It was characterized by recording its infrared, and NMR spectra (Gowda, D'Souza *et al.*, 2003 *a*). Single crystals of the title compound were obtained from a slow evaporation of its chloroform solution and used for X-ray diffraction studies at room temperature.

Refinement

Crystals of the title compound are monoclinic; space group *C*2/*c*. H atoms were positioned geometrically and refined using a riding model with C—H = 0.93 Å and with U_{iso}(H) = 1.2 U_{eq}(C). No restraints were applied for non-hydrogen atoms. Friedel equivalents were merged prior to the final refinements.

H atoms bonded to O atoms were found in fourier map and finally refined with O—H bond length restrained to 0.82 (1)Å and U_{iso}(H) = 1.2 U_{eq}(O).

Figures

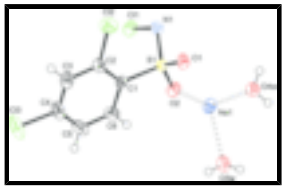


Fig. 1. *ORTEP* view of the title compound showing the atom labelling scheme (50% probability displacement ellipsoids)

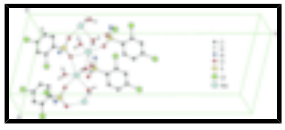


Fig. 2. Packing diagram of the title compound viewed down the axis b.

Sodium 2,4,*N*-trichlorobenzenesulfonamidate sesquihydrate

Crystal data

$Na^+ \cdot C_6H_3Cl_3NO_2S^- \cdot 1.5H_2O$	F_{000} = 1240.0
M_r = 309.52	D_x = 1.834 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 3687 reflections
a = 11.033 (2) Å	θ = 3.6–30.1°
b = 6.7410 (13) Å	μ = 1.04 mm^{-1}
c = 30.187 (6) Å	*T* = 294 (2) K
β = 98.51 (3)°	Block, yellow
V = 2220.4 (8) Å^3	0.46 × 0.32 × 0.16 mm
Z = 8	

Data collection

Oxford Diffraction Xcalibur System diffractometer	2162 independent reflections
Radiation source: fine-focus sealed tube	1872 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.047
T = 294(2) K	θ_{max} = 26.2°
Rotation method data acquisition using ω and phi scans	θ_{min} = 6.8°
Absorption correction: analytical (CrysAlis RED; Oxford Diffraction, 2003)	*h* = −13→13
T_{min} = 0.646, T_{max} = 0.851	*k* = 0→8
3256 measured reflections	*l* = 0→37

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0305P)^2 + 4.9463P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.038$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.081$	$\Delta\rho_{max} = 0.40$ e Å^{-3}
$S = 1.09$	$\Delta\rho_{min} = -0.41$ e Å^{-3}
2162 reflections	Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
151 parameters	Extinction coefficient: 0.0083 (6)
7 restraints	

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.3266 (2)	0.3152 (3)	0.61865 (8)	0.0221 (5)
C2	0.4082 (2)	0.3777 (4)	0.59049 (8)	0.0260 (5)
C3	0.3651 (3)	0.4513 (4)	0.54803 (9)	0.0348 (6)
H3	0.4198	0.4937	0.5293	0.042*
C4	0.2411 (3)	0.4607 (4)	0.53402 (9)	0.0374 (7)
C5	0.1587 (3)	0.4044 (5)	0.56120 (10)	0.0413 (7)
H5	0.0749	0.4146	0.5514	0.05*
C6	0.2020 (2)	0.3320 (4)	0.60359 (9)	0.0329 (6)
H6	0.1463	0.2939	0.6223	0.039*
N1	0.46541 (19)	0.0345 (3)	0.66974 (7)	0.0267 (5)
O1	0.44434 (16)	0.3586 (3)	0.70026 (6)	0.0317 (4)
O2	0.25872 (17)	0.1563 (3)	0.68763 (6)	0.0359 (5)
S1	0.37271 (5)	0.21142 (9)	0.672848 (19)	0.02257 (18)
Cl1	0.39467 (6)	−0.15130 (10)	0.63434 (2)	0.0345 (2)
Cl2	0.56526 (6)	0.36763 (12)	0.60616 (3)	0.0424 (2)
Cl3	0.18902 (9)	0.53791 (12)	0.47951 (3)	0.0579 (3)
Na1	0.14565 (9)	−0.00688 (16)	0.73657 (3)	0.0328 (3)
O3	0	0.2632 (4)	0.75	0.0346 (6)
H31	−0.010 (3)	0.339 (3)	0.7290 (7)	0.041*
O4	0.28754 (17)	0.1707 (3)	0.79286 (6)	0.0350 (5)
H41	0.247 (2)	0.196 (4)	0.8128 (6)	0.042*
H42	0.3478 (17)	0.111 (4)	0.8039 (8)	0.042*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0252 (12)	0.0203 (12)	0.0208 (11)	0.0009 (10)	0.0029 (9)	−0.0014 (9)
C2	0.0301 (13)	0.0220 (12)	0.0255 (12)	−0.0008 (10)	0.0031 (10)	−0.0002 (10)
C3	0.0514 (18)	0.0274 (14)	0.0264 (13)	−0.0040 (13)	0.0084 (12)	0.0034 (11)
C4	0.0562 (19)	0.0245 (14)	0.0272 (13)	0.0024 (13)	−0.0080 (13)	0.0030 (11)
C5	0.0357 (16)	0.0397 (16)	0.0429 (17)	0.0060 (13)	−0.0124 (13)	0.0002 (14)
C6	0.0288 (14)	0.0348 (15)	0.0343 (14)	0.0027 (11)	0.0025 (11)	0.0006 (12)
N1	0.0279 (11)	0.0251 (11)	0.0259 (11)	0.0004 (9)	−0.0003 (9)	−0.0017 (9)
O1	0.0341 (10)	0.0343 (10)	0.0258 (9)	−0.0022 (8)	0.0010 (8)	−0.0077 (8)
O2	0.0307 (10)	0.0484 (12)	0.0314 (10)	−0.0019 (9)	0.0142 (8)	0.0066 (9)
S1	0.0237 (3)	0.0258 (3)	0.0183 (3)	−0.0003 (2)	0.0035 (2)	−0.0003 (2)
Cl1	0.0408 (4)	0.0289 (4)	0.0344 (4)	−0.0029 (3)	0.0080 (3)	−0.0068 (3)
Cl2	0.0277 (4)	0.0522 (5)	0.0487 (4)	−0.0044 (3)	0.0104 (3)	0.0122 (4)
Cl3	0.0932 (7)	0.0384 (4)	0.0331 (4)	−0.0024 (4)	−0.0209 (4)	0.0076 (3)
Na1	0.0320 (6)	0.0350 (6)	0.0330 (6)	−0.0054 (4)	0.0105 (4)	0.0002 (5)
O3	0.0487 (16)	0.0275 (15)	0.0256 (14)	0	−0.0007 (12)	0
O4	0.0287 (10)	0.0442 (12)	0.0321 (10)	0.0026 (9)	0.0047 (8)	−0.0021 (9)

Geometric parameters (Å, °)

C1—C6	1.387 (4)	O2—S1	1.4440 (19)
C1—C2	1.392 (3)	O2—Na1	2.344 (2)
C1—S1	1.783 (2)	S1—Na1^{i}	3.3597 (13)
C2—C3	1.391 (4)	Na1—O4	2.446 (2)
C2—Cl2	1.729 (3)	Na1—O1^{iii}	2.450 (2)
C3—C4	1.372 (4)	Na1—O1^{iv}	2.497 (2)
C3—H3	0.93	Na1—O4^{iii}	2.500 (2)
C4—C5	1.366 (4)	Na1—O3	2.501 (2)
C4—Cl3	1.741 (3)	Na1—S1^{iii}	3.3597 (13)
C5—C6	1.387 (4)	Na1—Na1^{v}	3.429 (2)
C5—H5	0.93	Na1—Na1^{i}	4.0948 (13)
C6—H6	0.93	Na1—Na1^{iii}	4.0948 (13)
N1—S1	1.583 (2)	O3—Na1^{v}	2.501 (2)
N1—Cl1	1.753 (2)	O3—H31	0.809 (10)
O1—S1	1.4493 (18)	O4—Na1^{i}	2.500 (2)
O1—Na1^{i}	2.450 (2)	O4—H41	0.817 (10)
O1—Na1^{ii}	2.497 (2)	O4—H42	0.806 (10)
C6—C1—C2	118.3 (2)	O4—Na1—O3	83.78 (6)
C6—C1—S1	117.86 (19)	O1^{iii}—Na1—O3	78.42 (6)
C2—C1—S1	123.82 (19)	O1^{iv}—Na1—O3	77.55 (6)
C3—C2—C1	120.5 (2)	O4^{iii}—Na1—O3	157.05 (7)
C3—C2—Cl2	117.3 (2)	O2—Na1—S1^{iii}	151.64 (6)

C1—C2—Cl2	122.25 (19)	O4—Na1—S1^{iii}	79.67 (6)
C4—C3—C2	119.3 (3)	O1^{iii}—Na1—S1^{iii}	22.68 (4)
C4—C3—H3	120.3	O1^{iv}—Na1—S1^{iii}	89.73 (6)
C2—C3—H3	120.3	O4^{iii}—Na1—S1^{iii}	81.63 (6)
C5—C4—C3	121.6 (3)	O3—Na1—S1^{iii}	99.33 (5)
C5—C4—Cl3	119.7 (2)	O2—Na1—Na1^{v}	138.93 (7)
C3—C4—Cl3	118.7 (2)	O4—Na1—Na1^{v}	111.20 (6)
C4—C5—C6	118.9 (3)	O1^{iii}—Na1—Na1^{v}	46.70 (5)
C4—C5—H5	120.6	O1^{iv}—Na1—Na1^{v}	45.57 (5)
C6—C5—H5	120.6	O4^{iii}—Na1—Na1^{v}	114.84 (5)
C5—C6—C1	121.4 (3)	O3—Na1—Na1^{v}	46.72 (5)
C5—C6—H6	119.3	S1^{iii}—Na1—Na1^{v}	68.66 (4)
C1—C6—H6	119.3	O2—Na1—Na1^{i}	53.30 (6)
S1—N1—Cl1	109.95 (12)	O4—Na1—Na1^{i}	34.54 (5)
S1—O1—Na1^{i}	116.63 (10)	O1^{iii}—Na1—Na1^{i}	115.54 (6)
S1—O1—Na1^{ii}	150.88 (11)	O1^{iv}—Na1—Na1^{i}	145.42 (6)
Na1^{i}—O1—Na1^{ii}	87.74 (7)	O4^{iii}—Na1—Na1^{i}	126.81 (6)
S1—O2—Na1	152.22 (13)	O3—Na1—Na1^{i}	74.01 (5)
O2—S1—O1	115.22 (11)	S1^{iii}—Na1—Na1^{i}	113.82 (5)
O2—S1—N1	115.11 (12)	Na1^{v}—Na1—Na1^{i}	118.20 (3)
O1—S1—N1	104.31 (11)	O2—Na1—Na1^{iii}	100.07 (7)
O2—S1—C1	103.96 (11)	O4—Na1—Na1^{iii}	88.97 (7)
O1—S1—C1	108.23 (11)	O1^{iii}—Na1—Na1^{iii}	79.75 (5)
N1—S1—C1	109.90 (11)	O1^{iv}—Na1—Na1^{iii}	103.04 (5)
O2—S1—Na1^{i}	74.56 (9)	O4^{iii}—Na1—Na1^{iii}	33.70 (4)
O1—S1—Na1^{i}	40.69 (8)	O3—Na1—Na1^{iii}	157.39 (5)
N1—S1—Na1^{i}	126.25 (8)	S1^{iii}—Na1—Na1^{iii}	58.23 (3)
C1—S1—Na1^{i}	118.80 (8)	Na1^{v}—Na1—Na1^{iii}	118.20 (3)
O2—Na1—O4	82.10 (8)	Na1^{i}—Na1—Na1^{iii}	110.80 (5)
O2—Na1—O1^{iii}	168.19 (8)	Na1^{v}—O3—Na1	86.55 (10)
O4—Na1—O1^{iii}	86.09 (7)	Na1^{v}—O3—H31	125 (2)
O2—Na1—O1^{iv}	114.55 (8)	Na1—O3—H31	110 (2)
O4—Na1—O1^{iv}	156.75 (8)	Na1—O4—Na1^{i}	111.76 (8)
O1^{iii}—Na1—O1^{iv}	76.75 (8)	Na1—O4—H41	104.5 (19)
O2—Na1—O4^{iii}	88.36 (8)	Na1^{i}—O4—H41	108 (2)
O4—Na1—O4^{iii}	118.70 (6)	Na1—O4—H42	117 (2)
O1^{iii}—Na1—O4^{iii}	97.45 (7)	Na1^{i}—O4—H42	108 (2)
O1^{iv}—Na1—O4^{iii}	79.53 (7)	H41—O4—H42	108 (2)
O2—Na1—O3	100.09 (8)		
C6—C1—C2—C3	−1.3 (4)	C2—C1—S1—O1	61.2 (2)
S1—C1—C2—C3	177.9 (2)	C6—C1—S1—N1	127.0 (2)

C6—C1—C2—Cl2	178.9 (2)	C2—C1—S1—N1	−52.1 (2)
S1—C1—C2—Cl2	−2.0 (3)	C6—C1—S1—Na1^{i}	−76.5 (2)
C1—C2—C3—C4	−0.4 (4)	C2—C1—S1—Na1^{i}	104.3 (2)
Cl2—C2—C3—C4	179.5 (2)	S1—O2—Na1—O4	51.6 (3)
C2—C3—C4—C5	1.8 (4)	S1—O2—Na1—O1^{iii}	52.1 (6)
C2—C3—C4—Cl3	−175.9 (2)	S1—O2—Na1—O1^{iv}	−145.4 (3)
C3—C4—C5—C6	−1.5 (4)	S1—O2—Na1—O4^{iii}	−67.7 (3)
Cl3—C4—C5—C6	176.1 (2)	S1—O2—Na1—O3	133.8 (3)
C4—C5—C6—C1	−0.2 (4)	S1—O2—Na1—S1^{iii}	1.2 (4)
C2—C1—C6—C5	1.6 (4)	S1—O2—Na1—Na1^{v}	165.0 (2)
S1—C1—C6—C5	−177.6 (2)	S1—O2—Na1—Na1^{i}	72.6 (3)
Na1—O2—S1—O1	−73.5 (3)	S1—O2—Na1—Na1^{iii}	−35.9 (3)
Na1—O2—S1—N1	47.9 (3)	O2—Na1—O3—Na1^{v}	152.16 (7)
Na1—O2—S1—C1	168.2 (3)	O4—Na1—O3—Na1^{v}	−127.04 (6)
Na1—O2—S1—Na1^{i}	−75.3 (3)	O1^{iii}—Na1—O3—Na1^{v}	−39.77 (5)
Na1^{i}—O1—S1—O2	−2.58 (16)	O1^{iv}—Na1—O3—Na1^{v}	39.03 (5)
Na1^{ii}—O1—S1—O2	141.4 (2)	O4^{iii}—Na1—O3—Na1^{v}	41.92 (16)
Na1^{i}—O1—S1—N1	−129.75 (11)	S1^{iii}—Na1—O3—Na1^{v}	−48.61 (3)
Na1^{ii}—O1—S1—N1	14.3 (3)	Na1^{i}—Na1—O3—Na1^{v}	−160.87 (5)
Na1^{i}—O1—S1—C1	113.26 (12)	Na1^{iii}—Na1—O3—Na1^{v}	−55.04 (13)
Na1^{ii}—O1—S1—C1	−102.7 (2)	O2—Na1—O4—Na1^{i}	30.41 (8)
Na1^{ii}—O1—S1—Na1^{i}	144.0 (3)	O1^{iii}—Na1—O4—Na1^{i}	−149.48 (8)
Cl1—N1—S1—O2	56.49 (15)	O1^{iv}—Na1—O4—Na1^{i}	−107.28 (19)
Cl1—N1—S1—O1	−176.27 (11)	O4^{iii}—Na1—O4—Na1^{i}	114.16 (12)
Cl1—N1—S1—C1	−60.44 (15)	O3—Na1—O4—Na1^{i}	−70.72 (7)
Cl1—N1—S1—Na1^{i}	145.30 (7)	S1^{iii}—Na1—O4—Na1^{i}	−171.42 (8)
C6—C1—S1—O2	3.3 (2)	Na1^{v}—Na1—O4—Na1^{i}	−109.28 (7)
C2—C1—S1—O2	−175.8 (2)	Na1^{iii}—Na1—O4—Na1^{i}	130.72 (8)
C6—C1—S1—O1	−119.6 (2)		

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

Fig. 1

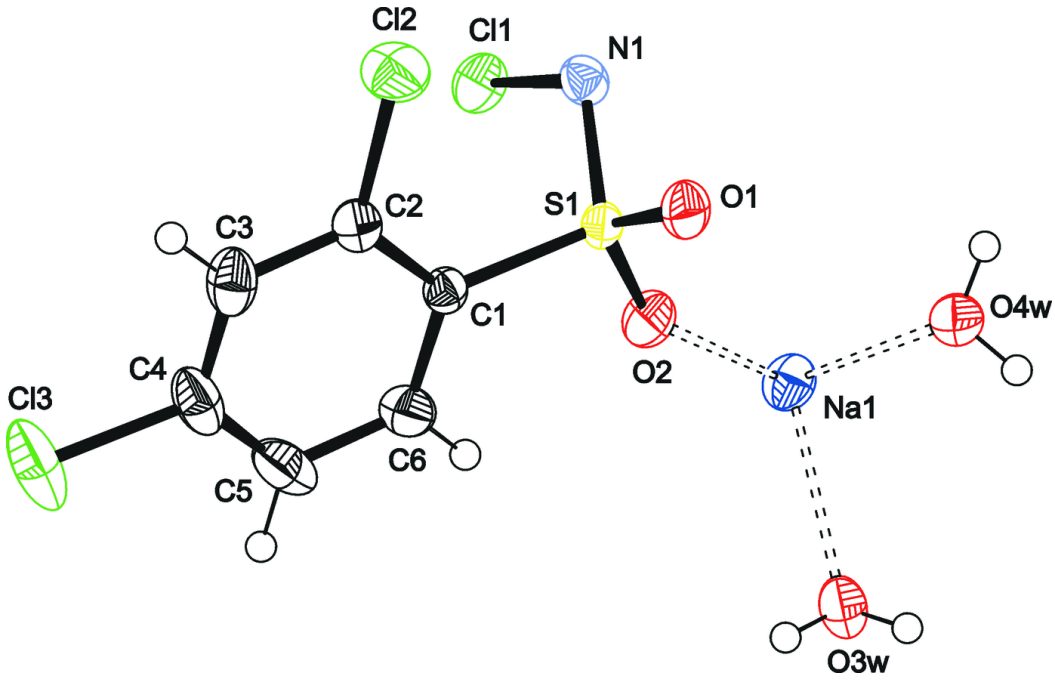


Fig. 2