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Sodium *N*-bromo-2,4-dichlorobenzenesulfonamidate sesquihydrate

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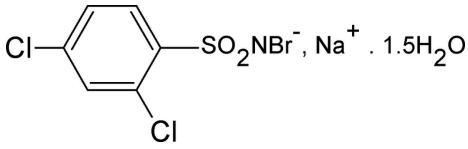
Key indicators: single-crystal X-ray study; T = 304 K; mean σ(C–C) = 0.011 Å; R factor = 0.062; wR factor = 0.177; data-to-parameter ratio = 14.9.

The title compound [systematic name: μ_2-aqua-diaquabis(μ_3-*N*-bromo-2,4-dichlorobenzenesulfonamidato)disodium(I)], $Na^+\cdot C_6H_3BrCl_2NO_2S^-\cdot 1.5H_2O$, crystallizes with two sodium cations, two *N*-bromo-2,4-dichlorobenzenesulfonamidate anions and three water molecules in the asymmetric unit, similar to sodium *N*-bromobenzenesulfonamidate, sodium *N*-bromo-4-chlorobenzenesulfonamidate and sodium *N*-bromo-2-methyl-4-chlorobenzenesulfonamidate. A crystallographic twofold rotation axis passes through one of the water molecules. There is no interaction between the nitrogen atoms and sodium ions. The sodium ion shows octahedral coordination by three O atoms of water molecules and by three sulfonyl O atoms of three different *N*-bromo-2,4-dichlorobenzenesulfonamidate anions. The S—N distance of 1.590 (6) Å is consistent with an S=N double bond. The Na^+ ion coordination in the structure gives rise to several hydrogen bonds between water molecules and N or Br atoms.

Related literature

For related literature, see: Gowda *et al.* (2007*a*,*b*); Gowda, Savitha *et al.* (2007); Gowda & Usha (2003); Gowda, Usha *et al.* (2007); Usha & Gowda (2006).



Experimental

Crystal data

$Na^+\cdot C_6H_3BrCl_2NO_2S^-\cdot 1.5H_2O$
M_r = 707.96
Monoclinic, $C2/c$
a = 11.1170 (15) Å
b = 6.780 (1) Å
c = 30.567 (4) Å
β = 99.124 (15)°
V = 2274.8 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 4.29 mm^{-1}
T = 304 (2) K
0.60 × 0.33 × 0.11 mm

Data collection

Oxford Diffraction Xcalibur CCD diffractometer
Absorption correction: analytical (*CrysAlis RED*; Oxford Diffraction, 2003; Clark & Reid, 1995)
T_{min} = 0.195, T_{max} = 0.627
3121 measured reflections
2200 independent reflections
2094 reflections with $I > 2\sigma(I)$
R_{int} = 0.065

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.177
S = 1.09
2200 reflections
148 parameters
5 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.06 e Å^{-3}
$\Delta\rho_{min}$ = −1.00 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O4W—H42···N1	0.80 (5)	2.13 (5)	2.925 (8)	169 (8)
O3W—H31···N1^{i}	0.88 (5)	2.18 (6)	3.010 (7)	158 (8)
O3W—H31···Br1^{i}	0.88 (5)	2.81 (6)	3.6109 (13)	152 (8)
O4W—H41···Br1^{ii}	0.82 (5)	2.69 (5)	3.493 (6)	165 (8)

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

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* (Sheldrick, 1997), *PLATON* (Spek, 2003) and *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2212).

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supplementary materials

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Sodium *N*-bromo-2,4-dichlorobenzenesulfonamidate sesquihydrate

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Comment

The chemistry of *N*-bromo-arylsulfonamides is of interest due to their diverse characteristics (Usha & Gowda, 2006). In the present work, the structure of sodium *N*-bromo-2,4-dichloro-benzenesulfonamidate (NaNB24DCBSA) has been determined to explore the substituent effects on the solid state structures of arylsulfonamides and N-halo arylsulfonamidates (Gowda *et al.*, 2007*a*,*b*; Gowda, Savitha *et al.* 2007; Gowda, Usha *et al.*, 2007). The structure of NaNB24DCBSA (Fig. 1) is similar to those of sodium *N*-chloro-2,4-dichloro-benzenesulfonamidate (NaNC24DCBSA) (Gowda, Savitha *et al.*, 2007), sodium *N*-bromo-benzenesulfonamidate (NaNBBSA) (Gowda *et al.*, 2007*d*), sodium *N*-bromo-4-chloro- benzenesulfonamidate (NaNB4CBSA) (Gowda *et al.*, 2007*a*) and sodium *N*-bromo-2-methyl-4-chloro-benzenesulfonamidate (Gowda *et al.*, 2007*b*). NaNB24DCBSA crystallizes with two sodium cations, two *N*-bromo-2,4-dichloro-benzenesulfonamidate anions and three water molecules in the asymmetric unit. One of the water molecules is located on a special position. Further, the sodium ion shows octahedral coordination by three O atoms of three different water molecules and by three sulfonyl O atoms of three different *N*-bromo-2,4-dichloro-benzenesulfonamidate anions. There is no interaction between the nitrogen and sodium ions in the molecule. The S—N distances of N1—S1, 1.590 (6)Å is consistent with a S—N double bond and in agreement with those observed with NaNBBSA, NaNB4CBSA, NaNB2M4CBSA and NaNC24DCBSA. The Na+ ion coordination in the structure gives rise to several hydrogen bonding between water hydrogen, oxygen and nitrogen or bromine atoms in the molecule (Table 1).

Experimental

The title compound was prepared according to the literature method (Gowda & Usha, 2003). The purity of the compound was checked by determining its melting point. It was characterized by recording its infrared and NMR spectra (Gowda & Usha, 2003). Single crystals of the title compound were obtained from its aqueous solution and used for X-ray diffraction studies at room temperature.

Refinement

Crystals of the tittle compound are monoclinic; space group *C*2/*c*. The crystal under study was refined as twinned. Non-merohedral twinning was detected and analysed using TWINROTM routine of the *WinGX* package. 26 percent of total 3121 reflections were found overlapped with rotation matrix (0.853 0.000 − 0.147) (0.000 − 1.000 0.000) (−1.853 0.000 − 0.853) Using this twin matrix a HKLF5 file was generated which was subsequently used in the *SHELXL97* refinement of the structure. Fractional contributions of the twin domains were refined to 76 and 24 percent. Benzene H atoms were positioned geometrically and refined using a riding model with C—H = 0.93 Å. H atoms of water molecules (O3w, O4w) were located in a difference map and refined with restraint on bond length O—H = 0.85 (5)Å and on mutual distance of H41, H42 H atoms 2.77 (8) Å. All H atoms have U_{iso}(H) = 1.2 U_{eq}(O,*C*).

Figures

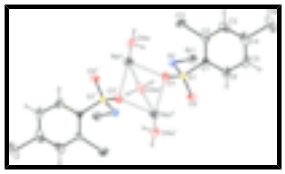


Fig. 1. *ORTEP* view of the title compound showing the atom labelling scheme. H atoms are represented as small spheres of arbitrary radii. Water molecule Ow3 is located on a two fold axis (1/2, 1/2 + *y*, 1/4). Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (i) 1 − *x*, *y*, 1/2 − *z*].

Sodium *N*-bromo-2,4-dichlorobenzenesulfonamidate sesquihydrate

Crystal data

$Na^+ \cdot C_6H_3BrCl_2NO_2S^- \cdot 1.5H_2O$	F_{000} = 1384
M_r = 707.96	D_x = 2.067 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 2198 reflections
a = 11.1170 (15) Å	θ = 2.5–26.4º
b = 6.7800 (10) Å	μ = 4.29 mm^{-1}
c = 30.567 (4) Å	*T* = 304 (2) K
β = 99.124 (15)º	Plate, yellow
V = 2274.8 (6) Å^3	0.60 × 0.33 × 0.11 mm
Z = 4	

Data collection

Oxford Diffraction Xcalibur CCD diffractometer	2094 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.065
T = 304(2) K	θ_{max} = 26.0º
Rotation method data acquisition using ω and phi scans	θ_{min} = 5.2º
Absorption correction: analytical (CrysAlis RED; Oxford Diffraction, 2003; Clark & Reid, 1995)	*h* = −13→13
T_{min} = 0.195, T_{max} = 0.627	*k* = −8→8
3121 measured reflections	*l* = −36→37
2200 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.062	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.177	$w = 1/[\sigma^2(F_o^2) + (0.0925P)^2 + 47.8P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.09	$(\Delta/\sigma)_{max}$ = 0.002

2200 reflections	$\Delta\rho_{max}$ = 1.06 e Å^{-3}
148 parameters	$\Delta\rho_{min}$ = −1.00 e Å^{-3}
5 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 $F^2 > 2\text{sigma}(F^2)$ 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}
C1	0.3275 (6)	0.1809 (9)	0.1192 (2)	0.0183 (12)
C2	0.4084 (7)	0.1212 (10)	0.0912 (2)	0.0219 (13)
C3	0.3665 (8)	0.0504 (11)	0.0492 (2)	0.0319 (17)
H3	0.4213	0.0098	0.031	0.038*
C4	0.2426 (8)	0.0402 (11)	0.0345 (3)	0.0354 (18)
C5	0.1588 (7)	0.0946 (12)	0.0613 (3)	0.0354 (18)
H5	0.0755	0.0843	0.0514	0.042*
C6	0.2028 (6)	0.1643 (11)	0.1032 (3)	0.0279 (16)
H6	0.1475	0.2018	0.1215	0.033*
N1	0.4651 (5)	0.4579 (8)	0.17108 (18)	0.0203 (11)
O1	0.4400 (5)	0.1331 (7)	0.20070 (16)	0.0254 (10)
O2	0.2573 (5)	0.3374 (8)	0.18720 (17)	0.0292 (12)
O3W	0.5	−0.2706 (11)	0.25	0.0289 (15)
H31	0.529 (8)	−0.332 (12)	0.275 (2)	0.035*
O4W	0.7099 (5)	0.3237 (9)	0.20865 (19)	0.0318 (12)
H41	0.745 (8)	0.302 (11)	0.187 (2)	0.038*
H42	0.647 (5)	0.369 (10)	0.196 (3)	0.038*
S1	0.37118 (14)	0.2828 (2)	0.17335 (5)	0.0174 (4)
Na1	0.6445 (3)	−0.0014 (4)	0.23596 (10)	0.0287 (6)
Cl1	0.56406 (16)	0.1333 (3)	0.10764 (7)	0.0358 (5)
Cl2	0.1903 (3)	−0.0354 (3)	−0.01953 (7)	0.0553 (7)
Br1	0.39296 (7)	0.65862 (11)	0.13323 (2)	0.0301 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.019 (3)	0.018 (3)	0.018 (3)	−0.003 (2)	0.001 (2)	0.000 (2)

C2	0.033 (4)	0.019 (3)	0.014 (3)	0.003 (3)	0.006 (3)	0.000 (2)
C3	0.055 (5)	0.018 (3)	0.024 (4)	0.006 (3)	0.010 (3)	−0.008 (3)
C4	0.051 (5)	0.016 (3)	0.033 (4)	−0.004 (3)	−0.010 (4)	−0.003 (3)
C5	0.029 (4)	0.033 (4)	0.038 (4)	−0.005 (3)	−0.012 (3)	−0.003 (3)
C6	0.020 (3)	0.031 (4)	0.032 (4)	−0.004 (3)	−0.001 (3)	0.001 (3)
N1	0.019 (3)	0.019 (3)	0.022 (3)	0.000 (2)	0.003 (2)	0.003 (2)
O1	0.029 (2)	0.024 (2)	0.023 (2)	0.002 (2)	0.001 (2)	0.0059 (19)
O2	0.023 (2)	0.041 (3)	0.027 (3)	0.007 (2)	0.014 (2)	−0.005 (2)
O3W	0.041 (4)	0.025 (4)	0.018 (3)	0	−0.003 (3)	0
O4W	0.022 (3)	0.038 (3)	0.036 (3)	0.002 (2)	0.005 (2)	0.000 (2)
S1	0.0200 (7)	0.0177 (7)	0.0153 (7)	0.0002 (6)	0.0051 (6)	0.0010 (6)
Na1	0.0290 (14)	0.0299 (15)	0.0292 (15)	0.0037 (12)	0.0107 (12)	−0.0006 (12)
Cl1	0.0228 (8)	0.0442 (11)	0.0429 (11)	0.0029 (7)	0.0124 (7)	−0.0097 (9)
Cl2	0.0911 (19)	0.0350 (11)	0.0295 (10)	0.0023 (12)	−0.0216 (11)	−0.0077 (8)
Br1	0.0347 (5)	0.0246 (4)	0.0323 (4)	0.0024 (3)	0.0090 (3)	0.0059 (3)

Geometric parameters (Å, °)

C1—C2	1.397 (9)	O1—Na1	2.526 (6)
C1—C6	1.399 (9)	O2—S1	1.445 (5)
C1—S1	1.788 (7)	O2—Na1^{ii}	2.363 (5)
C2—C3	1.380 (10)	O3W—Na1	2.513 (6)
C2—Cl1	1.726 (7)	O3W—Na1^{i}	2.513 (6)
C3—C4	1.381 (12)	O3W—H31	0.88 (5)
C3—H3	0.93	O4W—Na1^{iii}	2.454 (6)
C4—C5	1.386 (13)	O4W—Na1	2.505 (7)
C4—Cl2	1.739 (8)	O4W—H41	0.82 (5)
C5—C6	1.378 (11)	O4W—H42	0.80 (5)
C5—H5	0.93	Na1—O2^{iv}	2.363 (5)
C6—H6	0.93	Na1—O4W^{v}	2.454 (6)
N1—S1	1.590 (6)	Na1—O1^{i}	2.458 (6)
N1—Br1	1.881 (5)	Na1—Na1^{i}	3.455 (5)
O1—S1	1.453 (5)	Na1—Na1^{iii}	4.134 (3)
O1—Na1^{i}	2.458 (6)	Na1—Na1^{v}	4.134 (3)
C2—C1—C6	117.4 (6)	N1—S1—C1	109.4 (3)
C2—C1—S1	124.9 (5)	O2^{iv}—Na1—O4W^{v}	81.6 (2)
C6—C1—S1	117.7 (5)	O2^{iv}—Na1—O1^{i}	167.5 (2)
C3—C2—C1	121.1 (7)	O4W^{v}—Na1—O1^{i}	85.9 (2)
C3—C2—Cl1	117.6 (6)	O2^{iv}—Na1—O4W	89.2 (2)
C1—C2—Cl1	121.4 (5)	O4W^{v}—Na1—O4W	117.42 (17)
C2—C3—C4	119.5 (7)	O1^{i}—Na1—O4W	95.9 (2)
C2—C3—H3	120.2	O2^{iv}—Na1—O3W	100.9 (2)
C4—C3—H3	120.2	O4W^{v}—Na1—O3W	84.32 (17)
C3—C4—C5	121.5 (7)	O1^{i}—Na1—O3W	78.48 (17)
C3—C4—Cl2	119.4 (7)	O4W—Na1—O3W	157.4 (2)

C5—C4—Cl2	119.1 (6)	O2^{iv}—Na1—O1	115.4 (2)
C6—C5—C4	117.9 (7)	O4W^{v}—Na1—O1	156.8 (2)
C6—C5—H5	121.1	O1^{i}—Na1—O1	76.8 (2)
C4—C5—H5	121.1	O4W—Na1—O1	80.15 (19)
C5—C6—C1	122.6 (7)	O3W—Na1—O1	77.22 (17)
C5—C6—H6	118.7	O2^{iv}—Na1—Na1^{i}	139.86 (18)
C1—C6—H6	118.7	O4W^{v}—Na1—Na1^{i}	111.49 (17)
S1—N1—Br1	110.4 (3)	O1^{i}—Na1—Na1^{i}	46.95 (13)
S1—O1—Na1^{i}	118.7 (3)	O4W—Na1—Na1^{i}	114.39 (14)
S1—O1—Na1	148.6 (3)	O3W—Na1—Na1^{i}	46.58 (13)
Na1^{i}—O1—Na1	87.74 (18)	O1—Na1—Na1^{i}	45.31 (13)
S1—O2—Na1^{ii}	151.7 (3)	O2^{iv}—Na1—Na1^{iii}	99.78 (18)
Na1—O3W—Na1^{i}	86.8 (3)	O4W^{v}—Na1—Na1^{iii}	87.84 (18)
Na1—O3W—H31	109 (6)	O1^{i}—Na1—Na1^{iii}	78.90 (14)
Na1^{i}—O3W—H31	111 (6)	O4W—Na1—Na1^{iii}	33.14 (13)
Na1^{iii}—O4W—Na1	112.9 (2)	O3W—Na1—Na1^{iii}	156.51 (15)
Na1^{iii}—O4W—H41	106 (6)	O1—Na1—Na1^{iii}	103.59 (13)
Na1—O4W—H41	108 (5)	Na1^{i}—Na1—Na1^{iii}	117.89 (8)
Na1^{iii}—O4W—H42	125 (6)	O2^{iv}—Na1—Na1^{v}	53.92 (15)
Na1—O4W—H42	103 (5)	O4W^{v}—Na1—Na1^{v}	33.93 (15)
H41—O4W—H42	100 (10)	O1^{i}—Na1—Na1^{v}	114.58 (17)
O2—S1—O1	114.6 (3)	O4W—Na1—Na1^{v}	127.28 (18)
O2—S1—N1	115.7 (3)	O3W—Na1—Na1^{v}	74.09 (12)
O1—S1—N1	104.9 (3)	O1—Na1—Na1^{v}	145.79 (16)
O2—S1—C1	104.4 (3)	Na1^{i}—Na1—Na1^{v}	117.89 (8)
O1—S1—C1	107.7 (3)	Na1^{iii}—Na1—Na1^{v}	110.17 (13)
C6—C1—C2—C3	0.5 (10)	C6—C1—S1—N1	−127.7 (5)
S1—C1—C2—C3	−177.7 (5)	Na1^{iii}—O4W—Na1—O2^{iv}	−109.4 (3)
C6—C1—C2—Cl1	−179.5 (5)	Na1^{iii}—O4W—Na1—O4W^{v}	−29.3 (3)
S1—C1—C2—Cl1	2.3 (9)	Na1^{iii}—O4W—Na1—O1^{i}	59.1 (2)
C1—C2—C3—C4	0.7 (11)	Na1^{iii}—O4W—Na1—O3W	133.3 (4)
Cl1—C2—C3—C4	−179.3 (6)	Na1^{iii}—O4W—Na1—O1	134.6 (3)
C2—C3—C4—C5	−1.8 (12)	Na1^{iii}—O4W—Na1—Na1^{i}	104.2 (2)
C2—C3—C4—Cl2	176.3 (5)	Na1^{iii}—O4W—Na1—Na1^{v}	−68.1 (3)
C3—C4—C5—C6	1.6 (12)	Na1^{i}—O3W—Na1—O2^{iv}	−152.8 (2)
Cl2—C4—C5—C6	−176.5 (6)	Na1^{i}—O3W—Na1—O4W^{v}	126.95 (18)
C4—C5—C6—C1	−0.3 (12)	Na1^{i}—O3W—Na1—O1^{i}	39.98 (13)
C2—C1—C6—C5	−0.7 (11)	Na1^{i}—O3W—Na1—O4W	−37.6 (5)
S1—C1—C6—C5	177.6 (6)	Na1^{i}—O3W—Na1—O1	−38.90 (13)
Na1^{ii}—O2—S1—O1	73.5 (8)	Na1^{i}—O3W—Na1—Na1^{iii}	55.8 (3)
Na1^{ii}—O2—S1—N1	−48.8 (8)	Na1^{i}—O3W—Na1—Na1^{v}	159.94 (14)

Na1^{ii}—O2—S1—C1	−169.0 (7)	S1—O1—Na1—O2^{iv}	−74.9 (6)
Na1^{i}—O1—S1—O2	0.2 (4)	Na1^{i}—O1—Na1—O2^{iv}	136.06 (18)
Na1—O1—S1—O2	−143.9 (6)	S1—O1—Na1—O4W^{v}	150.9 (6)
Na1^{i}—O1—S1—N1	128.2 (3)	Na1^{i}—O1—Na1—O4W^{v}	1.8 (6)
Na1—O1—S1—N1	−16.0 (7)	S1—O1—Na1—O1^{i}	108.0 (5)
Na1^{i}—O1—S1—C1	−115.4 (3)	Na1^{i}—O1—Na1—O1^{i}	−41.1 (2)
Na1—O1—S1—C1	100.5 (6)	S1—O1—Na1—O4W	9.5 (6)
Br1—N1—S1—O2	−56.7 (4)	Na1^{i}—O1—Na1—O4W	−139.6 (2)
Br1—N1—S1—O1	176.0 (3)	S1—O1—Na1—O3W	−171.0 (6)
Br1—N1—S1—C1	60.8 (4)	Na1^{i}—O1—Na1—O3W	39.91 (15)
C2—C1—S1—O2	174.8 (6)	S1—O1—Na1—Na1^{i}	149.1 (7)
C6—C1—S1—O2	−3.4 (6)	S1—O1—Na1—Na1^{iii}	33.1 (6)
C2—C1—S1—O1	−63.0 (6)	Na1^{i}—O1—Na1—Na1^{iii}	−115.97 (17)
C6—C1—S1—O1	118.8 (6)	S1—O1—Na1—Na1^{v}	−137.5 (5)
C2—C1—S1—N1	50.5 (7)	Na1^{i}—O1—Na1—Na1^{v}	73.5 (3)

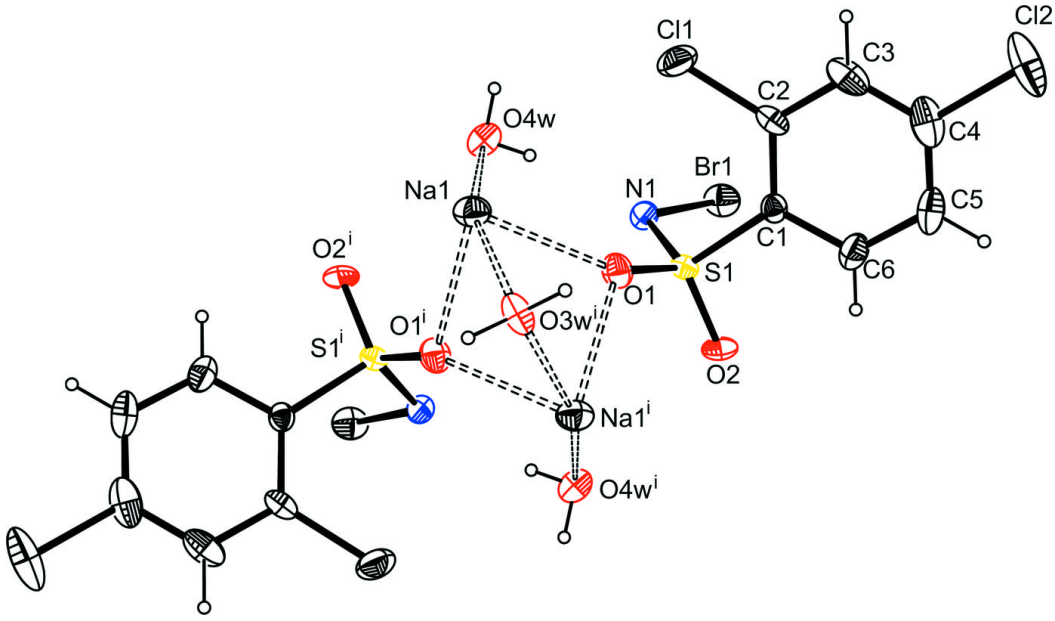
Symmetry codes: (i) −*x*+1, *y*, −*z*+1/2; (ii) *x*−1/2, *y*+1/2, *z*; (iii) −*x*+3/2, *y*+1/2, −*z*+1/2; (iv) *x*+1/2, *y*−1/2, *z*; (v) −*x*+3/2, *y*−1/2, −*z*+1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4W—H42···N1	0.80 (5)	2.13 (5)	2.925 (8)	169 (8)
O3W—H31···N1^{vi}	0.88 (5)	2.18 (6)	3.010 (7)	158 (8)
O3W—H31···Br1^{vi}	0.88 (5)	2.81 (6)	3.6109 (13)	152 (8)
O4W—H41···Br1^{iv}	0.82 (5)	2.69 (5)	3.493 (6)	165 (8)

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

Fig. 1


Cl1
C3
Cl2
C2
C4
O4w
Br1
Na1
N1
C5
C1
O2i
S1
C6
O1
O3wi
O1i
S1i
O2
Na1i
O4wi