Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Sodium *N*-bromo-4-chlorobenzenesulfonamidate sesquihydrate

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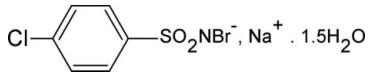
Received 16 May 2007; accepted 18 May 2007

Key indicators: single-crystal X-ray study; T = 300 K; mean σ(C–C) = 0.009 Å; R factor = 0.045; wR factor = 0.103; data-to-parameter ratio = 14.8.

In the structure of the title compound, $Na^+\cdot C_6H_4BrClNO_2S^-\cdot 1.5H_2O$, which crystallizes with two cations, two anions and three water molecules in the asymmetric unit, the sodium ions show octahedral coordination by three O atoms of water molecules and by three sulfonyl O atoms of three different *N*-bromobenzenesulfonamide anions. The S—N distances [1.574 (5) and 1.579 (4) Å] are consistent with an S=N double bond. The crystal structure is stabilized by O—H···Br, O—H···N, O—H···O and C—H···Br hydrogen bonds.

Related literature

For related literature, see: Gowda & Shetty (2004); Gowda & Usha (2003); Gowda *et al.* (2005); Gowda, Foro *et al.* (2007); Gowda, Jyothi, Foro *et al.* (2007); Gowda, Jyothi, Kozisek *et al.* (2003); Gowda, Kozisek *et al.* (2007); Gowda, Savitha *et al.* (2007); Gowda, Srilatha *et al.* (2007); Gowda, Usha *et al.*(2007); Usha & Gowda (2006).



Experimental

Crystal data

$Na^+\cdot C_6H_4BrClNO_2S^-\cdot 1.5H_2O$
M_r = 319.54
Orthorhombic, $P2_12_12_1$
a = 6.7510 (7) Å
b = 10.495 (1) Å
c = 30.286 (3) Å
V = 2145.8 (4) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 4.3 mm^{-1}
T = 300 (2) K
0.52 × 0.32 × 0.11 mm

Data collection

Oxford Diffraction Xcalibur diffractometer
Absorption correction: analytical (Clark & Reid, 1995)
T_{min} = 0.186, T_{max} = 0.543
13453 measured reflections
4156 independent reflections
3782 reflections with $I > 2\sigma(I)$
R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.103
S = 1.06
4156 reflections
280 parameters
9 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.63 e Å^{-3}
Absolute structure: Flack (1983), 1739 Friedel pairs
Flack parameter: 0.025 (12)

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

D—H···A	D—H	H···A	D···A	D—H···A
O3W—H31···Br1	0.82 (4)	2.81 (5)	3.610 (4)	167 (6)
O3W—H32···N2^{i}	0.82 (5)	2.08 (4)	2.875 (6)	166 (5)
O4W—H41···N2^{ii}	0.82 (4)	2.14 (5)	2.911 (6)	158 (4)
O4W—H42···O7W^{ii}	0.82 (4)	2.46 (4)	3.202 (6)	152 (5)
O7W—H71···Br2	0.82 (4)	2.62 (5)	3.392 (4)	157 (6)
O7W—H72···N1	0.82 (4)	2.02 (4)	2.840 (6)	174 (5)
C2—H2···Br2^{ii}	0.93	2.85	3.657 (6)	146

Symmetry codes: (i) $x+1, y+1, z$; (ii) $x, y+1, z$.

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), *DIAMOND* (Brandenburg, 2002); software used to prepare material for publication: *SHELXL97*, *PLATON* (Spek, 2003), *WinGX* (Farrugia, 1999).

BTG gratefully thanks the Alexander von Humboldt Foundation, Bonn, Germany for extensions 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: BT2373).

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supplementary materials

Acta Cryst. (2007). E**63**, m1647-m1648 [**doi:10.1107/S1600536807024531**]

Sodium *N*-bromo-4-chlorobenzenesulfonamidate sesquihydrate

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

Comment

The chemistry of N-halo arylsulfonamides is of interest in synthetic, mechanistic, analytical and biological chemistry (Gowda *et al.*, 2005; Gowda & Shetty, 2004; Usha & Gowda, 2006). In the present work, the structure of sodium *N*-bromo-4-chlorobenzenesulfonamde has been determined to explore the effect substituent on the solid state structures of sulfonamides and N-halo arylsulfonamides (Gowda *et al.*, 2003; Gowda, Foro *et al.*, 2007; Gowda, Jyothi *et al.*, 2007; Gowda, Kozisek *et al.*, 2007; Gowda, Savitha *et al.*, 2007; Gowda, Srilatha *et al.*, 2007; Gowda, Usha *et al.*, 2007). The structure of of the title compound (Fig. 1) resembles those of sodium *N*-bromo-benzenesulfonamde (Gowda, Usha *et al.*, 2007) and sodium *N*-chloro-4-chlorobenzenesulfonamde (Gowda, Jyothi *et al.*, 2007). The sodium ion shows octahedral coordination by three O atoms of water molecules and by three sulfonyl O atoms of three different *N*-bromobenzenesulfonamide anions. There is no interaction between the nitrogen and sodium atoms in the molecule and there are two molecules in the asymmetric unit. The S—N distances of N1—S1, 1.574 (5)Å and N2—S2 1.579 (4)Å are consistent with a S—N double bond. There are several hydrogen bonds in the crystal structure.

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

H atoms bonded to C were positioned geometrically and refined using a riding model with C—H = 0.93Å and with U_{iso}(H) = 1.2 U_{eq}(C). H atoms of water molecules (O3w, O4w, O7w) were visible in difference map and were subsequently treated as riding with U_{iso}(H) = 1.2 U_{eq}(O) and with the O—H bond length restrained to 0.82 (2) Å and the H···H distance restrained to 1.35 (2) Å.

Figures

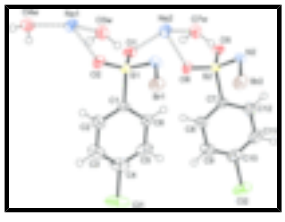

Fig. 1. Molecular structure of the title compound showing the atom labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radii.

Fig. 2. Packing diagram of the title compound viewed down the axis a, showing part of the crystal structure stabilized by hydrogen bonds O7w—H72···N1, O3w—H32···N2 and O4w—H41···N2.

Sodium *N*-Bromo-4-Chlorobenzenesulfonamide sesquihydrate

Crystal data

$Na^+.C_6H_4BrClNO_2S^-.1.5H_2O$	F_{000} = 1256
M_r = 319.54	D_x = 1.978 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2ac 2ab	Cell parameters from 2831 reflections
a = 6.7510 (7) Å	θ = 2.5–26.4º
b = 10.4950 (10) Å	μ = 4.3 mm^{-1}
c = 30.286 (3) Å	T = 300 (2) K
V = 2145.8 (4) Å^3	Block, yellow
Z = 8	0.52 × 0.32 × 0.11 mm

Data collection

Xcalibur System, Oxford Diffraction diffractometer	4156 independent reflections
Radiation source: fine-focus sealed tube	3782 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.043
T = 300(2) K	θ_{max} = 26.0º
Rotation method data acquisition using ω and phi scans	θ_{min} = 5.1º
Absorption correction: analytical (Clark & Reid, 1995)	h = −8→5
T_{min} = 0.186, T_{max} = 0.543	k = −12→12
13453 measured reflections	l = −36→37

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
$R[F^2 > 2\sigma(F^2)]$ = 0.045	$w = 1/[\sigma^2(F_o^2) + (0.0395P)^2 + 5.8841P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.103	$(\Delta/\sigma)_{max}$ = 0.011
S = 1.06	$\Delta\rho_{max}$ = 0.51 e Å^{-3}
4156 reflections	$\Delta\rho_{min}$ = −0.63 e Å^{-3}
280 parameters	Extinction correction: none
9 restraints	Absolute structure: Flack (1983), 1739 Friedel Pairs

Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Flack parameter: 0.025 (12)

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	0.2141 (8)	0.1181 (5)	0.13313 (16)	0.0231 (11)
C2	0.2041 (11)	0.2388 (6)	0.1520 (2)	0.0425 (15)
H2	0.2513	0.3093	0.1367	0.051*
C3	0.1235 (10)	0.2537 (8)	0.1939 (2)	0.0488 (18)
H3	0.1168	0.3338	0.2069	0.059*
C4	0.0532 (9)	0.1474 (8)	0.2159 (2)	0.0429 (16)
C5	0.0622 (10)	0.0286 (7)	0.1971 (2)	0.0433 (16)
H5	0.0144	−0.0417	0.2124	0.052*
C6	0.1412 (9)	0.0129 (6)	0.15574 (18)	0.0340 (14)
H6	0.1461	−0.0676	0.1429	0.041*
C7	−0.2985 (8)	−0.4278 (5)	0.13144 (16)	0.0223 (10)
C8	−0.3727 (9)	−0.3308 (6)	0.15638 (19)	0.0327 (13)
H8	−0.3697	−0.2475	0.1459	0.039*
C9	−0.4532 (9)	−0.3576 (7)	0.1977 (2)	0.0391 (14)
H9	−0.5053	−0.2925	0.2150	0.047*
C10	−0.4546 (9)	−0.4807 (7)	0.2125 (2)	0.0388 (15)
C11	−0.3822 (10)	−0.5776 (7)	0.1881 (2)	0.0415 (16)
H11	−0.3856	−0.6605	0.1990	0.050*
C12	−0.3020 (10)	−0.5526 (5)	0.1466 (2)	0.0378 (13)
H12	−0.2519	−0.6184	0.1293	0.045*
N1	0.4811 (6)	−0.0033 (5)	0.08062 (15)	0.0296 (10)
N2	−0.0030 (6)	−0.4826 (4)	0.07372 (14)	0.0254 (10)
O1	0.1630 (6)	0.0484 (4)	0.05138 (11)	0.0298 (9)
O2	0.3802 (7)	0.2285 (4)	0.06782 (13)	0.0379 (10)
O3W	0.8614 (6)	0.2759 (4)	0.04069 (14)	0.0346 (10)
H31	0.843 (10)	0.219 (4)	0.0589 (14)	0.041*
H32	0.914 (9)	0.337 (4)	0.0526 (16)	0.041*
O4W	0.2557 (6)	0.4969 (4)	−0.00286 (12)	0.0322 (9)
H41	0.164 (6)	0.489 (5)	0.0146 (16)	0.039*
H42	0.312 (8)	0.565 (3)	0.0007 (18)	0.039*

O5	−0.3324 (6)	−0.4527 (4)	0.04617 (11)	0.0285 (8)
O6	−0.1679 (7)	−0.2632 (3)	0.07497 (12)	0.0330 (9)
O7W	0.3480 (6)	−0.2262 (4)	0.03649 (13)	0.0341 (9)
H71	0.344 (10)	−0.284 (4)	0.0549 (14)	0.041*
H72	0.394 (9)	−0.162 (3)	0.0481 (16)	0.041*
Na1	0.5364 (3)	0.3495 (2)	0.01446 (7)	0.0302 (5)
Na2	0.0188 (3)	−0.1502 (2)	0.01942 (8)	0.0319 (5)
S1	0.3149 (2)	0.10180 (12)	0.07971 (4)	0.0237 (3)
S2	−0.1963 (2)	−0.39892 (11)	0.07809 (4)	0.0222 (2)
Cl1	−0.0412 (3)	0.1656 (3)	0.26874 (6)	0.0739 (7)
Cl2	−0.5467 (3)	−0.5110 (2)	0.26505 (5)	0.0600 (5)
Br1	0.68840 (9)	0.04232 (6)	0.119227 (19)	0.03784 (16)
Br2	0.18659 (9)	−0.42882 (6)	0.11598 (2)	0.03978 (17)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.023 (3)	0.029 (3)	0.017 (2)	0.001 (2)	0.001 (2)	−0.0003 (19)
C2	0.058 (4)	0.033 (3)	0.037 (3)	0.000 (3)	0.008 (3)	−0.003 (3)
C3	0.047 (4)	0.055 (4)	0.044 (4)	−0.008 (3)	0.011 (3)	−0.017 (3)
C4	0.019 (3)	0.075 (5)	0.035 (3)	−0.004 (3)	0.003 (3)	−0.012 (3)
C5	0.042 (4)	0.059 (4)	0.029 (3)	−0.008 (3)	0.005 (3)	0.008 (3)
C6	0.047 (4)	0.029 (3)	0.026 (3)	0.001 (3)	0.003 (2)	0.004 (2)
C7	0.019 (2)	0.029 (3)	0.019 (2)	0.004 (2)	−0.002 (2)	0.0020 (18)
C8	0.039 (3)	0.030 (3)	0.029 (3)	0.002 (2)	0.008 (2)	0.001 (2)
C9	0.031 (3)	0.049 (4)	0.037 (3)	−0.002 (3)	0.015 (3)	−0.008 (3)
C10	0.027 (3)	0.055 (4)	0.034 (3)	−0.005 (3)	0.006 (3)	0.010 (3)
C11	0.042 (4)	0.041 (4)	0.042 (4)	0.005 (3)	0.005 (3)	0.014 (3)
C12	0.039 (3)	0.033 (3)	0.042 (3)	0.003 (3)	0.010 (3)	0.001 (2)
N1	0.024 (2)	0.035 (3)	0.030 (2)	0.005 (2)	−0.006 (2)	−0.006 (2)
N2	0.024 (2)	0.027 (2)	0.026 (2)	0.0013 (19)	0.0013 (18)	−0.0009 (18)
O1	0.030 (2)	0.041 (2)	0.0191 (17)	0.0012 (19)	−0.0054 (16)	−0.0017 (15)
O2	0.054 (3)	0.027 (2)	0.033 (2)	−0.0097 (19)	0.0062 (19)	0.0076 (17)
O3W	0.034 (2)	0.030 (2)	0.040 (2)	−0.0001 (18)	0.0043 (19)	0.0009 (18)
O4W	0.026 (2)	0.039 (2)	0.033 (2)	−0.0042 (16)	0.0051 (15)	−0.0017 (18)
O5	0.032 (2)	0.033 (2)	0.0204 (17)	−0.0013 (19)	−0.0038 (17)	0.0014 (15)
O6	0.050 (2)	0.0195 (18)	0.030 (2)	−0.0041 (19)	0.003 (2)	0.0057 (15)
O7W	0.037 (2)	0.026 (2)	0.039 (2)	0.0002 (19)	0.0000 (19)	0.0008 (17)
Na1	0.0320 (11)	0.0309 (11)	0.0276 (11)	−0.0076 (10)	−0.0022 (10)	0.0050 (9)
Na2	0.0282 (11)	0.0319 (12)	0.0355 (12)	−0.0040 (9)	−0.0018 (10)	0.0061 (10)
S1	0.0246 (6)	0.0272 (6)	0.0193 (6)	−0.0005 (6)	0.0002 (6)	0.0011 (5)
S2	0.0237 (6)	0.0235 (6)	0.0195 (6)	−0.0003 (6)	0.0000 (6)	0.0011 (5)
Cl1	0.0539 (11)	0.135 (2)	0.0328 (9)	−0.0077 (13)	0.0146 (9)	−0.0199 (11)
Cl2	0.0530 (10)	0.0954 (15)	0.0317 (8)	0.0015 (11)	0.0123 (8)	0.0159 (9)
Br1	0.0294 (3)	0.0519 (4)	0.0323 (3)	−0.0022 (3)	−0.0069 (3)	0.0015 (3)
Br2	0.0297 (3)	0.0512 (4)	0.0385 (3)	−0.0043 (3)	−0.0080 (3)	0.0075 (3)

Geometric parameters (Å, °)

C1—C6	1.389 (8)	O2—S1	1.446 (4)
C1—C2	1.392 (8)	O2—Na1	2.311 (4)
C1—S1	1.764 (5)	O3W—Na1^{ii}	2.433 (5)
C2—C3	1.387 (9)	O3W—Na1	2.458 (5)
C2—H2	0.9300	O3W—H31	0.82 (5)
C3—C4	1.384 (10)	O3W—H32	0.82 (5)
C3—H3	0.9300	O4W—Na2^{ii}	2.448 (5)
C4—C5	1.373 (10)	O4W—Na1	2.502 (5)
C4—Cl1	1.733 (6)	O4W—H41	0.82 (5)
C5—C6	1.370 (8)	O4W—H42	0.82 (5)
C5—H5	0.9300	O5—S2	1.448 (4)
C6—H6	0.9300	O5—Na1^{iii}	2.453 (4)
C7—C8	1.363 (7)	O5—Na2^{iv}	2.474 (4)
C7—C12	1.387 (7)	O6—S2	1.440 (4)
C7—S2	1.783 (5)	O6—Na2	2.414 (4)
C8—C9	1.392 (8)	O7W—Na2	2.417 (5)
C8—H8	0.9300	O7W—Na2^{v}	2.425 (5)
C9—C10	1.368 (9)	O7W—H71	0.82 (5)
C9—H9	0.9300	O7W—H72	0.82 (5)
C10—C11	1.348 (9)	Na1—O1^{ii}	2.420 (4)
C10—Cl2	1.738 (6)	Na1—O3W^{i}	2.433 (5)
C11—C12	1.396 (9)	Na1—O5^{vi}	2.453 (4)
C11—H11	0.9300	Na1—Na2^{ii}	3.321 (3)
C12—H12	0.9300	Na1—Na1^{i}	4.065 (3)
N1—S1	1.574 (5)	Na1—Na1^{ii}	4.065 (3)
N1—Br1	1.885 (4)	Na2—O7W^{iv}	2.425 (5)
N2—S2	1.579 (4)	Na2—O4W^{i}	2.448 (5)
N2—Br2	1.896 (4)	Na2—O5^{v}	2.474 (4)
O1—S1	1.450 (4)	Na2—Na1^{i}	3.321 (3)
O1—Na1^{i}	2.420 (4)	Na2—Na2^{iv}	4.143 (3)
O1—Na2	2.495 (4)	Na2—Na2^{v}	4.143 (3)
C6—C1—C2	120.2 (5)	O3W^{i}—Na1—Na2^{ii}	106.53 (13)
C6—C1—S1	120.8 (4)	O5^{vi}—Na1—Na2^{ii}	47.90 (10)
C2—C1—S1	119.0 (4)	O3W—Na1—Na2^{ii}	115.51 (13)
C3—C2—C1	119.8 (6)	O4W—Na1—Na2^{ii}	47.19 (11)
C3—C2—H2	120.1	O2—Na1—Na1^{i}	59.27 (12)
C1—C2—H2	120.1	O1^{ii}—Na1—Na1^{i}	110.07 (13)
C4—C3—C2	119.0 (7)	O3W^{i}—Na1—Na1^{i}	33.98 (11)
C4—C3—H3	120.5	O5^{vi}—Na1—Na1^{i}	144.99 (13)
C2—C3—H3	120.5	O3W—Na1—Na1^{i}	130.49 (14)

C5—C4—C3	121.1 (6)	O4W—Na1—Na1^{i}	69.12 (10)
C5—C4—Cl1	120.0 (6)	Na2^{ii}—Na1—Na1^{i}	113.08 (8)
C3—C4—Cl1	118.9 (6)	O2—Na1—Na1^{ii}	104.32 (15)
C6—C5—C4	120.4 (6)	O1^{ii}—Na1—Na1^{ii}	75.93 (11)
C6—C5—H5	119.8	O3W^{i}—Na1—Na1^{ii}	88.71 (14)
C4—C5—H5	119.8	O5^{vi}—Na1—Na1^{ii}	102.68 (11)
C5—C6—C1	119.5 (6)	O3W—Na1—Na1^{ii}	33.58 (10)
C5—C6—H6	120.2	O4W—Na1—Na1^{ii}	154.36 (13)
C1—C6—H6	120.2	Na2^{ii}—Na1—Na1^{ii}	116.84 (8)
C8—C7—C12	121.0 (5)	Na1^{i}—Na1—Na1^{ii}	112.28 (11)
C8—C7—S2	121.2 (4)	O6—Na2—O7W	99.72 (16)
C12—C7—S2	117.8 (4)	O6—Na2—O7W^{iv}	88.60 (15)
C7—C8—C9	119.4 (6)	O7W—Na2—O7W^{iv}	114.21 (13)
C7—C8—H8	120.3	O6—Na2—O4W^{i}	94.98 (16)
C9—C8—H8	120.3	O7W—Na2—O4W^{i}	158.08 (16)
C10—C9—C8	119.3 (6)	O7W^{iv}—Na2—O4W^{i}	82.15 (15)
C10—C9—H9	120.4	O6—Na2—O5^{v}	170.44 (17)
C8—C9—H9	120.4	O7W—Na2—O5^{v}	86.71 (15)
C11—C10—C9	122.0 (6)	O7W^{iv}—Na2—O5^{v}	82.29 (15)
C11—C10—Cl2	119.5 (5)	O4W^{i}—Na2—O5^{v}	80.98 (14)
C9—C10—Cl2	118.4 (5)	O6—Na2—O1	110.10 (15)
C10—C11—C12	119.5 (6)	O7W—Na2—O1	80.45 (15)
C10—C11—H11	120.3	O7W^{iv}—Na2—O1	154.57 (17)
C12—C11—H11	120.3	O4W^{i}—Na2—O1	79.27 (14)
C7—C12—C11	118.8 (6)	O5^{v}—Na2—O1	77.79 (14)
C7—C12—H12	120.6	O6—Na2—Na1^{i}	134.52 (13)
C11—C12—H12	120.6	O7W—Na2—Na1^{i}	110.29 (12)
S1—N1—Br1	111.2 (3)	O7W^{iv}—Na2—Na1^{i}	108.04 (13)
S2—N2—Br2	109.6 (2)	O4W^{i}—Na2—Na1^{i}	48.57 (11)
S1—O1—Na1^{i}	124.5 (2)	O5^{v}—Na2—Na1^{i}	47.35 (10)
S1—O1—Na2	145.9 (2)	O1—Na2—Na1^{i}	46.54 (10)
Na1^{i}—O1—Na2	84.99 (14)	O6—Na2—Na2^{iv}	61.57 (11)
S1—O2—Na1	145.0 (3)	O7W—Na2—Na2^{iv}	130.01 (14)
Na1^{ii}—O3W—Na1	112.44 (17)	O4W^{i}—Na2—Na2^{iv}	71.51 (10)
Na2^{ii}—O4W—Na1	84.24 (14)	O5^{v}—Na2—Na2^{iv}	108.88 (13)
S2—O5—Na1^{iii}	145.1 (2)	O1—Na2—Na2^{iv}	148.22 (12)
S2—O5—Na2^{iv}	128.6 (2)	Na1^{i}—Na2—Na2^{iv}	114.96 (8)
Na1^{iii}—O5—Na2^{iv}	84.75 (14)	O6—Na2—Na2^{v}	112.02 (14)
S2—O6—Na2	126.9 (2)	O7W^{iv}—Na2—Na2^{v}	85.34 (14)
Na2—O7W—Na2^{v}	117.67 (17)	O4W^{i}—Na2—Na2^{v}	149.90 (14)
O2—Na1—O1^{ii}	168.85 (17)	O5^{v}—Na2—Na2^{v}	70.25 (11)

O2—Na1—O3W^{i}	87.76 (16)	O1—Na2—Na2^{v}	102.39 (11)
O1^{ii}—Na1—O3W^{i}	81.10 (15)	Na1^{i}—Na2—Na2^{v}	111.32 (8)
O2—Na1—O5^{vi}	110.88 (16)	Na2^{iv}—Na2—Na2^{v}	109.12 (11)
O1^{ii}—Na1—O5^{vi}	79.65 (14)	O2—S1—O1	115.1 (2)
O3W^{i}—Na1—O5^{vi}	154.43 (17)	O2—S1—N1	115.6 (3)
O2—Na1—O3W	90.50 (17)	O1—S1—N1	104.1 (2)
O1^{ii}—Na1—O3W	95.20 (15)	O2—S1—C1	104.9 (2)
O3W^{i}—Na1—O3W	119.04 (13)	O1—S1—C1	107.9 (2)
O5^{vi}—Na1—O3W	79.47 (15)	N1—S1—C1	109.1 (2)
O2—Na1—O4W	98.09 (16)	O6—S2—O5	115.2 (2)
O1^{ii}—Na1—O4W	79.67 (14)	O6—S2—N2	115.8 (3)
O3W^{i}—Na1—O4W	79.78 (15)	O5—S2—N2	104.6 (2)
O5^{vi}—Na1—O4W	80.34 (14)	O6—S2—C7	106.2 (2)
O3W—Na1—O4W	159.76 (16)	O5—S2—C7	107.0 (2)
O2—Na1—Na2^{ii}	136.25 (15)	N2—S2—C7	107.5 (2)
O1^{ii}—Na1—Na2^{ii}	48.47 (11)		
C6—C1—C2—C3	0.9 (10)	Na2^{v}—O7W—Na2—Na1^{i}	−97.92 (19)
S1—C1—C2—C3	179.4 (5)	Na2^{v}—O7W—Na2—Na2^{iv}	56.0 (2)
C1—C2—C3—C4	−0.4 (11)	S1—O1—Na2—O6	74.8 (4)
C2—C3—C4—C5	0.0 (10)	Na1^{i}—O1—Na2—O6	−132.98 (15)
C2—C3—C4—Cl1	178.3 (5)	S1—O1—Na2—O7W	−22.1 (4)
C3—C4—C5—C6	−0.1 (10)	Na1^{i}—O1—Na2—O7W	130.08 (15)
Cl1—C4—C5—C6	−178.4 (5)	S1—O1—Na2—O7W^{iv}	−150.0 (4)
C4—C5—C6—C1	0.6 (10)	Na1^{i}—O1—Na2—O7W^{iv}	2.2 (4)
C2—C1—C6—C5	−1.0 (9)	S1—O1—Na2—O4W^{i}	166.2 (4)
S1—C1—C6—C5	−179.5 (5)	Na1^{i}—O1—Na2—O4W^{i}	−41.57 (13)
C12—C7—C8—C9	0.1 (9)	S1—O1—Na2—O5^{v}	−110.8 (4)
S2—C7—C8—C9	179.3 (5)	Na1^{i}—O1—Na2—O5^{v}	41.41 (14)
C7—C8—C9—C10	0.5 (9)	S1—O1—Na2—Na1^{i}	−152.2 (5)
C8—C9—C10—C11	−0.7 (10)	S1—O1—Na2—Na2^{iv}	143.0 (3)
C8—C9—C10—Cl2	177.4 (5)	Na1^{i}—O1—Na2—Na2^{iv}	−64.8 (3)
C9—C10—C11—C12	0.3 (10)	S1—O1—Na2—Na2^{v}	−44.5 (4)
Cl2—C10—C11—C12	−177.8 (5)	Na1^{i}—O1—Na2—Na2^{v}	107.73 (12)
C8—C7—C12—C11	−0.4 (10)	Na1—O2—S1—O1	−64.3 (6)
S2—C7—C12—C11	−179.7 (5)	Na1—O2—S1—N1	57.1 (6)
C10—C11—C12—C7	0.3 (10)	Na1—O2—S1—C1	177.3 (5)
S1—O2—Na1—O1^{ii}	41.3 (13)	Na1^{i}—O1—S1—O2	4.2 (4)
S1—O2—Na1—O3W^{i}	39.5 (5)	Na2—O1—S1—O2	149.9 (4)
S1—O2—Na1—O5^{vi}	−158.4 (5)	Na1^{i}—O1—S1—N1	−123.3 (3)
S1—O2—Na1—O3W	−79.5 (5)	Na2—O1—S1—N1	22.4 (5)
S1—O2—Na1—O4W	118.9 (5)	Na1^{i}—O1—S1—C1	120.9 (3)
S1—O2—Na1—Na2^{ii}	151.3 (4)	Na2—O1—S1—C1	−93.4 (4)

S1—O2—Na1—Na1^{i}	59.1 (5)	Br1—N1—S1—O2	56.7 (3)
S1—O2—Na1—Na1^{ii}	−48.6 (5)	Br1—N1—S1—O1	−176.1 (2)
Na1^{ii}—O3W—Na1—O2	115.7 (2)	Br1—N1—S1—C1	−61.1 (3)
Na1^{ii}—O3W—Na1—O1^{ii}	−54.67 (19)	C6—C1—S1—O2	−178.1 (5)
Na1^{ii}—O3W—Na1—O3W^{i}	28.02 (19)	C2—C1—S1—O2	3.5 (6)
Na1^{ii}—O3W—Na1—O5^{vi}	−133.1 (2)	C6—C1—S1—O1	58.8 (5)
Na1^{ii}—O3W—Na1—O4W	−128.8 (4)	C2—C1—S1—O1	−119.7 (5)
Na1^{ii}—O3W—Na1—Na2^{ii}	−100.70 (17)	C6—C1—S1—N1	−53.7 (5)
Na1^{ii}—O3W—Na1—Na1^{i}	67.4 (2)	C2—C1—S1—N1	127.8 (5)
Na2^{ii}—O4W—Na1—O2	149.64 (15)	Na2—O6—S2—O5	−74.1 (4)
Na2^{ii}—O4W—Na1—O1^{ii}	−41.42 (13)	Na2—O6—S2—N2	48.4 (4)
Na2^{ii}—O4W—Na1—O3W^{i}	−124.13 (15)	Na2—O6—S2—C7	167.6 (3)
Na2^{ii}—O4W—Na1—O5^{vi}	39.70 (13)	Na1^{iii}—O5—S2—O6	170.2 (4)
Na2^{ii}—O4W—Na1—O3W	35.4 (5)	Na2^{iv}—O5—S2—O6	10.4 (4)
Na2^{ii}—O4W—Na1—Na1^{i}	−157.71 (13)	Na1^{iii}—O5—S2—N2	41.9 (5)
Na2^{ii}—O4W—Na1—Na1^{ii}	−59.5 (3)	Na2^{iv}—O5—S2—N2	−117.9 (3)
S2—O6—Na2—O7W	−66.0 (3)	Na1^{iii}—O5—S2—C7	−72.0 (4)
S2—O6—Na2—O7W^{iv}	48.3 (3)	Na2^{iv}—O5—S2—C7	128.2 (3)
S2—O6—Na2—O4W^{i}	130.3 (3)	Br2—N2—S2—O6	55.0 (3)
S2—O6—Na2—O1	−149.4 (3)	Br2—N2—S2—O5	−177.0 (2)
S2—O6—Na2—Na1^{i}	162.5 (2)	Br2—N2—S2—C7	−63.5 (3)
S2—O6—Na2—Na2^{iv}	64.4 (3)	C8—C7—S2—O6	13.9 (6)
S2—O6—Na2—Na2^{v}	−36.1 (3)	C12—C7—S2—O6	−166.9 (5)
Na2^{v}—O7W—Na2—O6	116.8 (2)	C8—C7—S2—O5	−109.7 (5)
Na2^{v}—O7W—Na2—O7W^{iv}	23.96 (18)	C12—C7—S2—O5	69.6 (5)
Na2^{v}—O7W—Na2—O4W^{i}	−111.8 (4)	C8—C7—S2—N2	138.4 (5)
Na2^{v}—O7W—Na2—O5^{v}	−56.06 (19)	C12—C7—S2—N2	−42.3 (6)
Na2^{v}—O7W—Na2—O1	−134.2 (2)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3W—H31···Br1	0.82 (4)	2.81 (5)	3.610 (4)	167 (6)
O3W—H32···N2^{vi}	0.82 (5)	2.08 (4)	2.875 (6)	166 (5)
O4W—H41···N2^{vii}	0.82 (4)	2.14 (5)	2.911 (6)	158 (4)
O4W—H42···O7W^{vii}	0.82 (4)	2.46 (4)	3.202 (6)	152 (5)
O7W—H71···Br2	0.82 (4)	2.62 (5)	3.392 (4)	157 (6)
O7W—H72···N1	0.82 (4)	2.02 (4)	2.840 (6)	174 (5)
C2—H2···Br2^{vii}	0.93	2.85	3.657 (6)	146

Symmetry codes: (vi) *x*+1, *y*+1, *z*; (vii) *x*, *y*+1, *z*.

Fig. 1

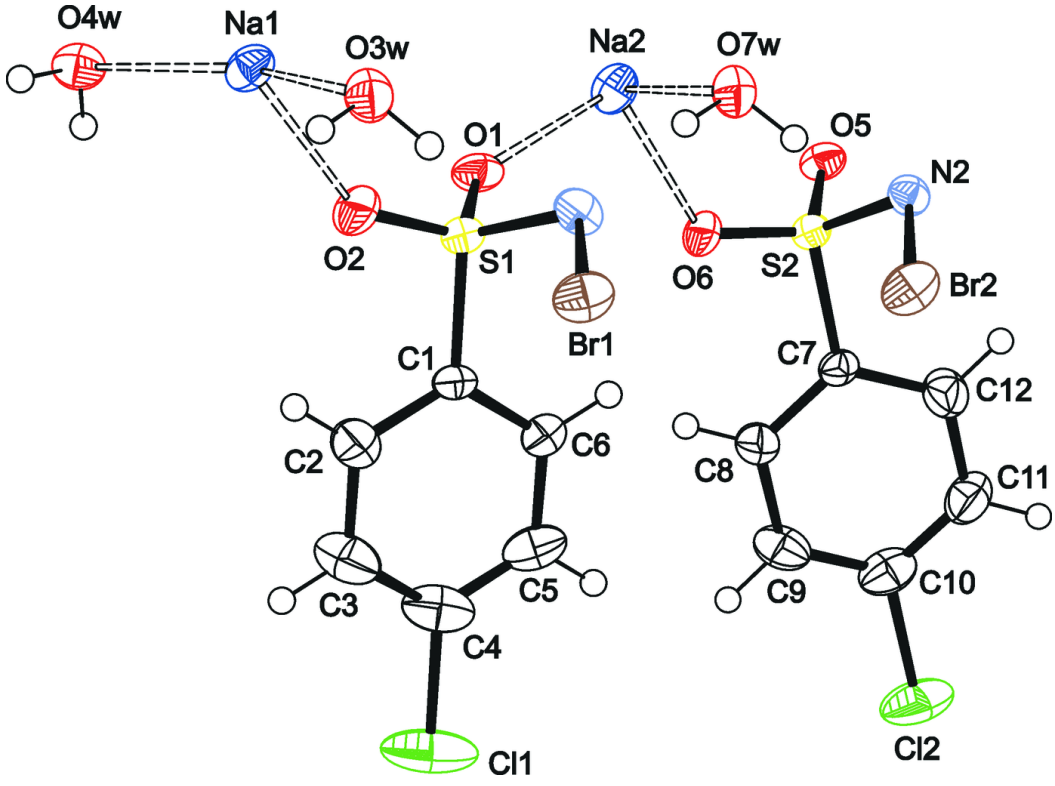
O4w
Na1
O3w
Na2
O7w
O1
O5
N2
O2
S1
O6
S2
Br2
Br1
C1
C7
C12
C2
C6
C8
C11
C3
C5
C9
C10
C4
Cl1
Cl2

Fig. 2