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Sodium *N*-bromo-4-fluorobenzenesulfonamidate sesquihydrate

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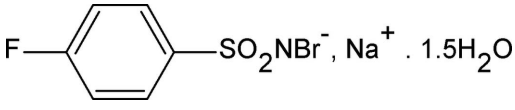
Key indicators: single-crystal X-ray study; T = 299 K; mean σ(C–C) = 0.015 Å; R factor = 0.070; wR factor = 0.151; data-to-parameter ratio = 14.2.

The structure of the title compound, $Na^+\cdot C_6H_4BrFNO_2S^-\cdot 1.5H_2O$, like other sodium *N*-bromoarylfonamidates, crystallizes with two cations, two anions and three water molecules in the asymmetric unit. The sodium cation shows octahedral coordination by three O atoms of three different water molecules and by three sulfonyl O atoms of three different *N*-bromo-4-fluorobenzenesulfonamide anions. There is no interaction between the nitrogen atom and sodium ion in the molecule. The S—N distance of 1.591 (6) Å is consistent with an S=N double bond. The crystal structure is stabilized by O—H···N hydrogen bonds.

Related literature

For related literature, see: George *et al.* (2000); Gowda & Usha (2003); Gowda, Jyothi *et al.* (2007); Gowda, Kožíšek *et al.* (2007*a*,*b*); Gowda, Usha *et al.* (2007); Usha & Gowda (2006).



Experimental

Crystal data

$Na^+\cdot C_6H_4BrFNO_2S^-\cdot 1.5H_2O$
M_r = 303.09
Monoclinic, $C2/c$
a = 10.3985 (8) Å
b = 6.7027 (4) Å
c = 29.892 (2) Å
β = 96.710 (8)°
V = 2069.1 (2) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 4.22 mm^{-1}
T = 299 (2) K
0.44 × 0.34 × 0.15 mm

Data collection

Oxford Diffraction Xcalibur diffractometer
Absorption correction: analytical (*CrysAlis RED*; Oxford Diffraction, 2006) using a multifaceted crystal model (Clark & Reid, 1995)
T_{min} = 0.187, T_{max} = 0.561
6114 measured reflections
2009 independent reflections
1798 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.070
$wR(F^2)$ = 0.151
S = 1.04
2009 reflections
141 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.60 e Å^{-3}
$\Delta\rho_{min}$ = −0.94 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3W—H31···N1^{i}	0.81 (5)	2.15 (4)	2.916 (7)	157 (8)
O4W—H41···N1^{ii}	0.82 (5)	2.05 (3)	2.846 (8)	165 (8)

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); 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).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2196).

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supplementary materials

Acta Cryst. (2007). E**63**, m1958 [**doi:10.1107/S1600536807029261**]

Sodium *N*-bromo-4-fluorobenzenesulfonamidate sesquihydrate

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Comment

The chemistry of *N*-bromo-arylsulfonamides is of interest due to their distinct physical, chemical and biological properties (Usha & Gowda, 2006). In the present work, the structure of sodium *N*-bromo-4-fluoro- benzenesulfonamidate (NaNB4FBSA) has been determined to study the substituent effects on the solid state structures of arylsulfonamides and N-halo arylsulfonamidates (Gowda, Jyothi *et al.*, 2007; Gowda *et al.*, 2007*a*,*b*; Gowda, Usha *et al.*, 2007). The structure of NaNB4FBSA (Fig. 1) is similar to those of sodium *N*-bromo-benzenesulfonamidate(NaNBBSA)(Gowda, Usha *et al.*, 2007) and sodium *N*-bromo-4-chloro-benzenesulfonamidate (NaNB4CBSA)(Gowda, Kožíšek *et al.*, 2007*a*) and sodium *N*-chloro-arylsulfonamidates (George *et al.*, 2000; Gowda, Jyothi *et al.*, 2007). NaNB4FBSA crystallizes with two cations, two anions and three water molecules in the asymmetric unit. 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-4-fluoro-benzenesulfonamide anions. There is no interaction between the nitrogen and sodium ions in the molecule. The S—N distances of N1—S1, 1.591 (6)Å is consistent with a S—N double bond and in agreement with those observed with NaNBBSA, NaNB4CBSA and sodium *N*-chloro- arylsulfonamidates. The occurrence of O—H···N hydrogen bonds between the wat er molecules and N atom associated with the presence of Na^+ result in the formation of thick layered structure parallel to the (0 0 1) plane (Table 1, Fig. 1). This thick layer may be described as build up from an internal layer containing Na atoms and water molecules sandwiched by the benzenesulfonamidate with the fluorobenzene pointing outward.

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 of the benzene ring were positioned geometrically and refined using a riding model with C—H = 0.93 Å and U_{iso}(H) = 1.2 U_{eq}(C). H atoms of the water molecules (O3w, O4w) were visible in difference map and were subsequently treated as riding with mutual distance restrained to 1.35 (5) Å and O—H bond length 0.82 (5) Å. No restraints were applied to non-hydrogen atoms.

Figures

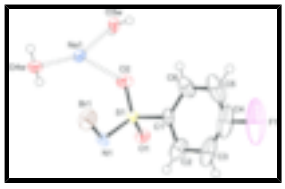

Fig. 1. *ORTEP* view of the title compound showing the atom labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. Na—O contacts are shown as dashed lines. H atoms are represented as small spheres of arbitrary radii.

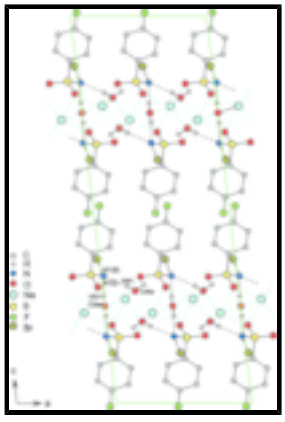

Fig. 2. Partial packing view down the *b* axis of the title compound showing the formation of layers through O—H···N hydrogen bonds. H bonds are represented as dashed lines. H atoms not involved in H bonds have been omitted for clarity. [Symmetry codes:(i) $x - 1/2, y + 1/2, z$; (ii) $x - 1/2, y - 1/2, z$]

Sodium *N*-bromo-4-fluorobenzenesulfonamidate sesquihydrate

Crystal data

$Na^{+}\cdot C_6H_4BrFNO_2S^{-}\cdot 1.5H_2O$	$Z = 8$
$M_r = 303.09$	$F_{000} = 1192$
Monoclinic, *C*2/*c*	$D_x = 1.946$ Mg m^{-3}
Hall symbol: -C 2yc	Mo *K*α radiation λ = 0.71073 Å
a = 10.3985 (8) Å	μ = 4.22 mm^{-1}
b = 6.7027 (4) Å	*T* = 299 (2) K
c = 29.892 (2) Å	Plate, yellow
β = 96.710 (8)º	0.44 × 0.34 × 0.15 mm
V = 2069.1 (2) Å^3	

Data collection

Oxford Diffraction Xcalibur diffractometer	2009 independent reflections
Radiation source: Enhance (Mo) X-ray Source	1798 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.025$
T = 299(2) K	$\theta_{max} = 26.0$º
Rotation method data acquisition using ω and φ scans	$\theta_{min} = 5.2$º
Absorption correction: analytical (CrysAlis RED; Oxford Diffraction, 2006) using a multifaceted crystal model (Clark & Reid, 1995)	*h* = −12→12
$T_{min} = 0.187$, $T_{max} = 0.561$	*k* = −8→7

6114 measured reflections

$l = -36 \rightarrow 36$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.070$

$wR(F^2) = 0.151$

$S = 1.04$

2009 reflections

141 parameters

4 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.021P)^2 + 67.2P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.60$ e Å^{-3}

$\Delta\rho_{min} = -0.94$ e Å^{-3}

Extinction correction: none

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 $F^2 > 2$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	0.4571 (7)	0.5495 (10)	0.3857 (2)	0.0287 (15)
C2	0.5860 (10)	0.5823 (15)	0.4020 (3)	0.052 (2)
H2	0.6509	0.5469	0.3846	0.062*
C3	0.6180 (14)	0.6670 (16)	0.4437 (4)	0.070 (3)
H3	0.704	0.6891	0.455	0.084*
C4	0.5215 (18)	0.7165 (16)	0.4674 (4)	0.078 (4)
C5	0.3931 (16)	0.6915 (18)	0.4527 (3)	0.078 (4)
H5	0.3296	0.7311	0.4703	0.093*
C6	0.3601 (10)	0.6044 (14)	0.4102 (3)	0.051 (2)
H6	0.2738	0.5846	0.399	0.061*
N1	0.5170 (6)	0.2609 (9)	0.3281 (2)	0.0274 (13)
O1	0.4650 (4)	0.5891 (8)	0.29942 (16)	0.0280 (11)
O2	0.2871 (5)	0.4018 (9)	0.32575 (17)	0.0350 (12)
O3W	0	0.4971 (10)	0.25	0.0273 (15)
H31	0.000 (8)	0.541 (12)	0.2754 (12)	0.033*

O4W	0.2379 (5)	−0.0996 (8)	0.28949 (18)	0.0339 (12)
H41	0.183 (5)	−0.158 (12)	0.302 (2)	0.041*
H42	0.307 (4)	−0.102 (13)	0.306 (2)	0.041*
Na1	0.1560 (3)	0.2298 (4)	0.26819 (9)	0.0285 (6)
S1	0.42385 (15)	0.4474 (3)	0.33121 (5)	0.0214 (4)
F1	0.5471 (12)	0.7988 (13)	0.5096 (2)	0.141 (4)
Br1	0.48476 (9)	0.06776 (13)	0.37091 (3)	0.0481 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.046 (4)	0.018 (3)	0.022 (3)	0.006 (3)	0.001 (3)	0.001 (3)
C2	0.059 (6)	0.054 (6)	0.037 (5)	−0.011 (5)	−0.016 (4)	0.000 (4)
C3	0.107 (10)	0.041 (6)	0.051 (6)	−0.006 (6)	−0.035 (6)	−0.006 (5)
C4	0.150 (13)	0.035 (6)	0.040 (6)	−0.003 (7)	−0.025 (7)	−0.002 (5)
C5	0.139 (12)	0.064 (7)	0.036 (5)	0.024 (8)	0.038 (7)	−0.003 (5)
C6	0.067 (6)	0.051 (6)	0.039 (5)	0.014 (5)	0.020 (4)	0.000 (4)
N1	0.031 (3)	0.021 (3)	0.032 (3)	0.010 (3)	0.008 (2)	0.004 (2)
O1	0.027 (2)	0.028 (3)	0.029 (2)	0.000 (2)	0.0027 (19)	0.009 (2)
O2	0.022 (2)	0.042 (3)	0.040 (3)	−0.002 (2)	0.001 (2)	0.001 (2)
O3W	0.038 (4)	0.021 (3)	0.023 (3)	0	0.006 (3)	0
O4W	0.020 (2)	0.032 (3)	0.050 (3)	0.001 (2)	0.007 (2)	0.003 (2)
Na1	0.0212 (13)	0.0253 (15)	0.0383 (15)	−0.0031 (11)	0.0001 (11)	0.0013 (12)
S1	0.0207 (8)	0.0201 (8)	0.0230 (8)	−0.0002 (6)	0.0006 (6)	0.0019 (6)
F1	0.275 (13)	0.089 (6)	0.045 (4)	0.023 (7)	−0.039 (5)	−0.030 (4)
Br1	0.0596 (6)	0.0303 (4)	0.0524 (5)	−0.0024 (4)	−0.0012 (4)	0.0134 (4)

Geometric parameters (Å, °)

C1—C6	1.365 (11)	O1—S1	1.444 (5)
C1—C2	1.388 (12)	O1—Na1^{i}	2.442 (5)
C1—S1	1.764 (7)	O1—Na1^{ii}	2.478 (5)
C2—C3	1.374 (13)	O2—S1	1.445 (5)
C2—H2	0.93	O2—Na1	2.367 (6)
C3—C4	1.338 (19)	O3W—Na1	2.435 (6)
C3—H3	0.93	O3W—H31	0.81 (5)
C4—C5	1.366 (19)	O4W—Na1	2.425 (6)
C4—F1	1.373 (12)	O4W—H41	0.82 (5)
C5—C6	1.402 (14)	O4W—H42	0.82 (5)
C5—H5	0.93	Na1—O4W^{i}	2.438 (6)
C6—H6	0.93	Na1—Na1^{iii}	3.299 (5)
N1—S1	1.591 (6)	Na1—Na1^{i}	4.091 (3)
N1—Br1	1.879 (6)	Na1—H31	2.66 (8)
C6—C1—C2	120.9 (8)	O2—Na1—O1^{v}	109.3 (2)
C6—C1—S1	121.5 (7)	O4W—Na1—O1^{v}	80.03 (18)
C2—C1—S1	117.5 (6)	O3W—Na1—O1^{v}	79.74 (16)
C3—C2—C1	120.3 (11)	O4W^{i}—Na1—O1^{v}	153.4 (2)

C3—C2—H2	119.9	O1^{iv}—Na1—O1^{v}	78.8 (2)
C1—C2—H2	119.9	O2—Na1—Na1^{iii}	134.46 (17)
C4—C3—C2	117.8 (11)	O4W—Na1—Na1^{iii}	112.85 (14)
C4—C3—H3	121.1	O3W—Na1—Na1^{iii}	47.37 (13)
C2—C3—H3	121.1	O4W^{i}—Na1—Na1^{iii}	106.01 (17)
C3—C4—C5	124.3 (10)	O1^{iv}—Na1—Na1^{iii}	48.35 (13)
C3—C4—F1	120.7 (14)	O1^{v}—Na1—Na1^{iii}	47.43 (13)
C5—C4—F1	115.0 (15)	O2—Na1—Na1^{iv}	109.86 (17)
C4—C5—C6	118.0 (11)	O4W—Na1—Na1^{iv}	32.82 (13)
C4—C5—H5	121	O3W—Na1—Na1^{iv}	150.46 (15)
C6—C5—H5	121	O4W^{i}—Na1—Na1^{iv}	85.78 (17)
C1—C6—C5	118.6 (10)	O1^{iv}—Na1—Na1^{iv}	71.32 (14)
C1—C6—H6	120.7	O1^{v}—Na1—Na1^{iv}	102.55 (14)
C5—C6—H6	120.7	Na1^{iii}—Na1—Na1^{iv}	113.24 (9)
S1—N1—Br1	110.0 (3)	O2—Na1—Na1^{i}	62.71 (15)
S1—O1—Na1^{i}	129.4 (3)	O4W—Na1—Na1^{i}	130.67 (17)
S1—O1—Na1^{ii}	144.2 (3)	O3W—Na1—Na1^{i}	70.39 (11)
Na1^{i}—O1—Na1^{ii}	84.22 (17)	O4W^{i}—Na1—Na1^{i}	32.63 (14)
S1—O2—Na1	131.4 (3)	O1^{iv}—Na1—Na1^{i}	108.21 (17)
Na1^{iii}—O3W—Na1	85.3 (3)	O1^{v}—Na1—Na1^{i}	147.25 (16)
Na1^{iii}—O3W—H31	114 (6)	Na1^{iii}—Na1—Na1^{i}	113.24 (9)
Na1—O3W—H31	97 (6)	Na1^{iv}—Na1—Na1^{i}	110.02 (12)
Na1—O4W—Na1^{iv}	114.6 (2)	O2—Na1—H31	82.2 (12)
Na1—O4W—H41	108 (6)	O4W—Na1—H31	152.8 (15)
Na1^{iv}—O4W—H41	120 (6)	O3W—Na1—H31	17.7 (8)
Na1—O4W—H42	116 (6)	O4W^{i}—Na1—H31	91.2 (16)
Na1^{iv}—O4W—H42	88 (6)	O1^{iv}—Na1—H31	96.3 (11)
H41—O4W—H42	109 (3)	O1^{v}—Na1—H31	75.3 (18)
O2—Na1—O4W	95.6 (2)	Na1^{iii}—Na1—H31	56.2 (15)
O2—Na1—O3W	96.66 (19)	Na1^{iv}—Na1—H31	167.6 (10)
O4W—Na1—O3W	158.9 (2)	Na1^{i}—Na1—H31	72.2 (18)
O2—Na1—O4W^{i}	90.9 (2)	O1—S1—O2	115.4 (3)
O4W—Na1—O4W^{i}	116.02 (17)	O1—S1—N1	104.4 (3)
O3W—Na1—O4W^{i}	80.89 (16)	O2—S1—N1	115.2 (3)
O2—Na1—O1^{iv}	170.9 (2)	O1—S1—C1	108.2 (3)
O4W—Na1—O1^{iv}	89.8 (2)	O2—S1—C1	105.7 (3)
O3W—Na1—O1^{iv}	80.45 (17)	N1—S1—C1	107.7 (3)
O4W^{i}—Na1—O1^{iv}	80.09 (19)		
C6—C1—C2—C3	1.5 (14)	Na1^{iii}—O3W—Na1—O4W^{i}	121.82 (17)
S1—C1—C2—C3	178.1 (8)	Na1^{iii}—O3W—Na1—O1^{iv}	40.44 (13)
C1—C2—C3—C4	−0.3 (16)	Na1^{iii}—O3W—Na1—O1^{v}	−39.84 (12)

C2—C3—C4—C5	−1.1 (18)	Na1^{iii}—O3W—Na1—Na1^{iv}	57.5 (2)
C2—C3—C4—F1	179.0 (10)	Na1^{iii}—O3W—Na1—Na1^{i}	153.79 (13)
C3—C4—C5—C6	1.4 (18)	Na1^{i}—O1—S1—O2	−9.1 (5)
F1—C4—C5—C6	−178.7 (9)	Na1^{ii}—O1—S1—O2	−165.6 (5)
C2—C1—C6—C5	−1.2 (13)	Na1^{i}—O1—S1—N1	118.3 (4)
S1—C1—C6—C5	−177.6 (8)	Na1^{ii}—O1—S1—N1	−38.2 (6)
C4—C5—C6—C1	−0.2 (16)	Na1^{i}—O1—S1—C1	−127.2 (4)
S1—O2—Na1—O4W	73.4 (5)	Na1^{ii}—O1—S1—C1	76.3 (6)
S1—O2—Na1—O3W	−123.8 (4)	Na1—O2—S1—O1	68.3 (5)
S1—O2—Na1—O1^{v}	154.8 (4)	Na1—O2—S1—N1	−53.5 (5)
S1—O2—Na1—Na1^{iii}	−156.5 (3)	Na1—O2—S1—C1	−172.3 (4)
S1—O2—Na1—Na1^{iv}	43.0 (5)	Br1—N1—S1—O1	175.7 (3)
Na1^{iv}—O4W—Na1—O2	−118.5 (2)	Br1—N1—S1—O2	−56.8 (4)
Na1^{iv}—O4W—Na1—O3W	116.1 (5)	Br1—N1—S1—C1	60.9 (4)
Na1^{iv}—O4W—Na1—O4W^{i}	−24.8 (2)	C6—C1—S1—O1	112.3 (7)
Na1^{iv}—O4W—Na1—O1^{iv}	54.1 (2)	C2—C1—S1—O1	−64.2 (7)
Na1^{iv}—O4W—Na1—O1^{v}	132.8 (3)	C6—C1—S1—O2	−11.8 (8)
Na1^{iv}—O4W—Na1—Na1^{iii}	97.9 (2)	C2—C1—S1—O2	171.7 (7)
Na1^{iv}—O4W—Na1—Na1^{i}	−60.1 (3)	C6—C1—S1—N1	−135.4 (7)
Na1^{iii}—O3W—Na1—O2	−148.33 (19)	C2—C1—S1—N1	48.1 (7)
Na1^{iii}—O3W—Na1—O4W	−23.1 (5)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3W—H31···N1^{vi}	0.81 (5)	2.15 (4)	2.916 (7)	157 (8)
O4W—H41···N1^{v}	0.82 (5)	2.05 (3)	2.846 (8)	165 (8)

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

Fig. 1

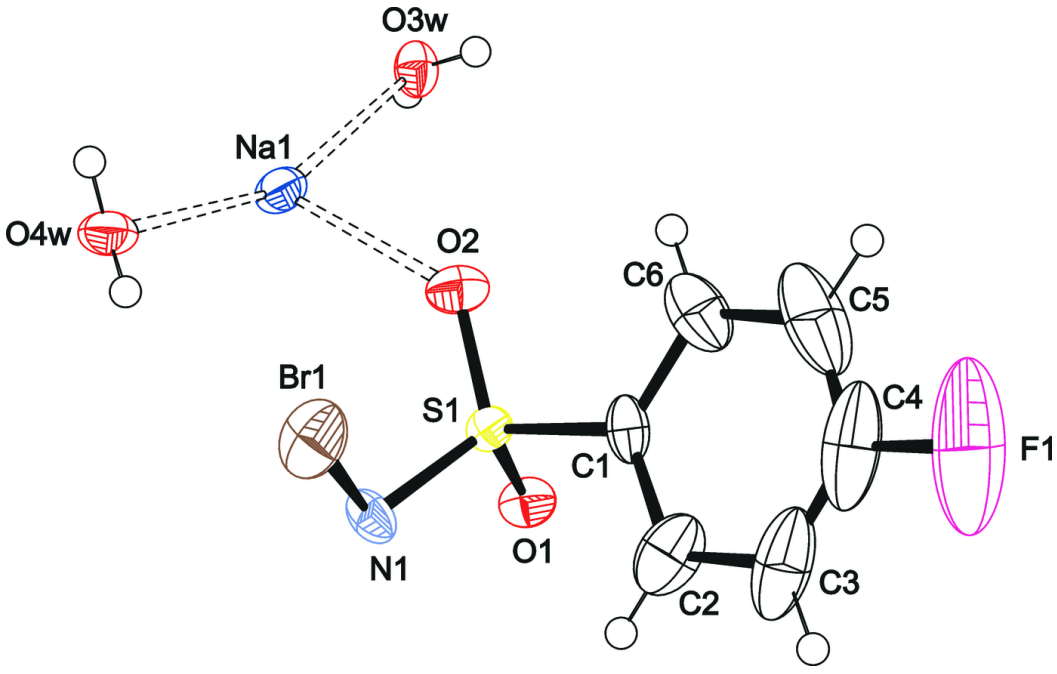

Fig. 2