metal-organic compounds

Potassium N-bromo-4-chlorobenzenesulfonamidate monohydrate

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In the structure of the title compound, $K^+ \cdot C_6H_4BrClNO_2S^- \cdot H_2O$, the K^+ cation is heptacoordinated. It is connected to two water O atoms, four sulfonyl O atoms and one Br atom. Further, the sulfonyl and water O atoms in the structure are bridged in a bidentate fashion. The S—N distance of 1.584 (6) Å is consistent with an S—N double bond, The crystal structure is stabilized by intermolecular O—H···N hydrogen bonds.

Related literature

For our study of the effect of substituents on the structures of N-haloarylsulfonamides, see: Gowda et al. (2007, 2011a,b); and on the oxidative strengths of N-halolarylsulfonamides, see: Usha & Gowda (2006). For similar structures, see: George et al. (2000); Olmstead & Power (1986). For the preparation of the title compound, see: Gowda & Usha (2003).

$$Cl - \bigcirc - SO_2NBr^-, \; K^+ \cdot H_2O$$
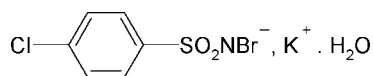
Experimental

Crystal data

$K^+ \cdot C_6H_4BrClNO_2S^- \cdot H_2O$
$M_r = 326.64$
Monoclinic, $P2_1/c$
$a = 15.596 (1)$ Å
$b = 10.188 (1)$ Å
$c = 6.7649 (7)$ Å
$\beta = 99.947 (9)°$

$V = 1058.73 (17)$ Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 4.70$ mm^{-1}
$T = 293$ K
$0.34 \times 0.34 \times 0.30$ mm

Data collection

Oxford Diffraction Xcalibur diffractometer with a Sapphire CCD detector
Absorption correction: multi-scan (CrysAlis RED; Oxford

Diffraction, 2009)
$T_{min} = 0.298$, $T_{max} = 0.333$
3796 measured reflections
2147 independent reflections
1984 reflections with $I > 2\sigma(I)$
$R_{int} = 0.035$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.057$
$wR(F^2) = 0.156$
$S = 1.19$
2147 reflections
134 parameters
2 restraints

H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max} = 1.22$ e Å^{-3}
$\Delta\rho_{min} = -0.95$ e Å^{-3}

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

$D - H \cdots A$	$D - H$	$H \cdots A$	$D \cdots A$	$D - H \cdots A$
O3—H31···N1[i]	0.82 (2)	2.25 (5)	3.005 (8)	152 (8)
O3—H32···N1[ii]	0.82 (2)	2.16 (3)	2.967 (8)	166 (9)

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

Data collection: CrysAlis CCD (Oxford Diffraction, 2009); cell refinement: CrysAlis RED (Oxford Diffraction, 2009); 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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supporting information

Potassium *N*-bromo-4-chlorobenzenesulfonamidate monohydrate

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S1. Comment

To explore the effect of substitution and replacing sodium ion by potassium ion in the solid state structures of *N*-chloro-arylsulfonamides (Gowda *et al.*, 2007; 2011*a,b*; Usha & Gowda, 2006), in the present work, the structure of potassium *N*-bromo-4-chloro- benzenesulfonamidate monohydrate (I) has been determined (Fig. 1). The structure of (I) resembles those of potassium *N*-bromo-2-chloro- benzenesulfonamidate sesquihydrate(II)(Gowda *et al.*, 2011*b*), potassium *N*,4-di-chloro-benzenesulfonamidate monohydrate (III) (Gowda *et al.*, 2011*a*), sodium *N*-bromo-4-chloro- benzenesulfonamidate sesquihydrate (IV)(Gowda *et al.*, 2007) and other sodium *N*-chloro-arylsulfonamdes (George *et al.*, 2000; Olmstead & Power, 1986). In particular, there is no interaction between the nitrogen and potassium atom in the molecule. Further, K^+ is hepta co-ordinated in contrast to hexa co-ordination with Na^+

K^+ hepta coordination involves two O atoms from water molecules, four sulfonyl O atoms of *N*-bromo-4-chloro-benzenesulfonamide anions and one Br, in contrast to octahedral coordination of Na^+ in (IV) by three O atoms of water molecules and by three sulfonyl O atoms of *N*-bromo-4-chloro- benzenesulfonamide anions (Gowda *et al.*, 2007).

The S—N distance of N1—S1, 1.584 (6) Å is consistent with an S—N double bond and is in agreement with the observed values of 1.582 (4) Å in (II), 1.588 (2)Å in (III), and N1—S1, 1.574 (5)Å and N2—S2 1.579 (4)Å in (IV).

K^+ ion coordination in the structure gives rise to several hydrogen bonding between coordinated water molecules and nitrogen atoms. The packing diagram consists of a two-dimensional polymeric layer running parallel to the *b*-axis (Fig. 2). The molecular packing is stabilized by O3—H31···N1 and O3—H32···N1 hydrogen bonds (Table 1).

S2. Experimental

The title compound was prepared similar to the literature method (Gowda & Usha, 2003). The purity of the compound was checked by determining its melting point (184 ° C). It was characterized by recording its infrared and NMR spectra.

Yellow prisms of the title compound used in X-ray diffraction studies were obtained from its aqueous solution at room temperature.

S3. Refinement

The O bound H atoms were located in difference map and later restrained to O—H = 0.82 (2) Å The other H atoms were positioned with idealized geometry using a riding model with C—H = 0.93 Å. All H atoms were refined with isotropic displacement parameters (set to 1.2 times of the U_{eq} of the parent atom).

The residual electron-density features are located in the region of Br1. The highest peak and the deepest hole are 1.70 and 0.93 Å from Br1, respectively.
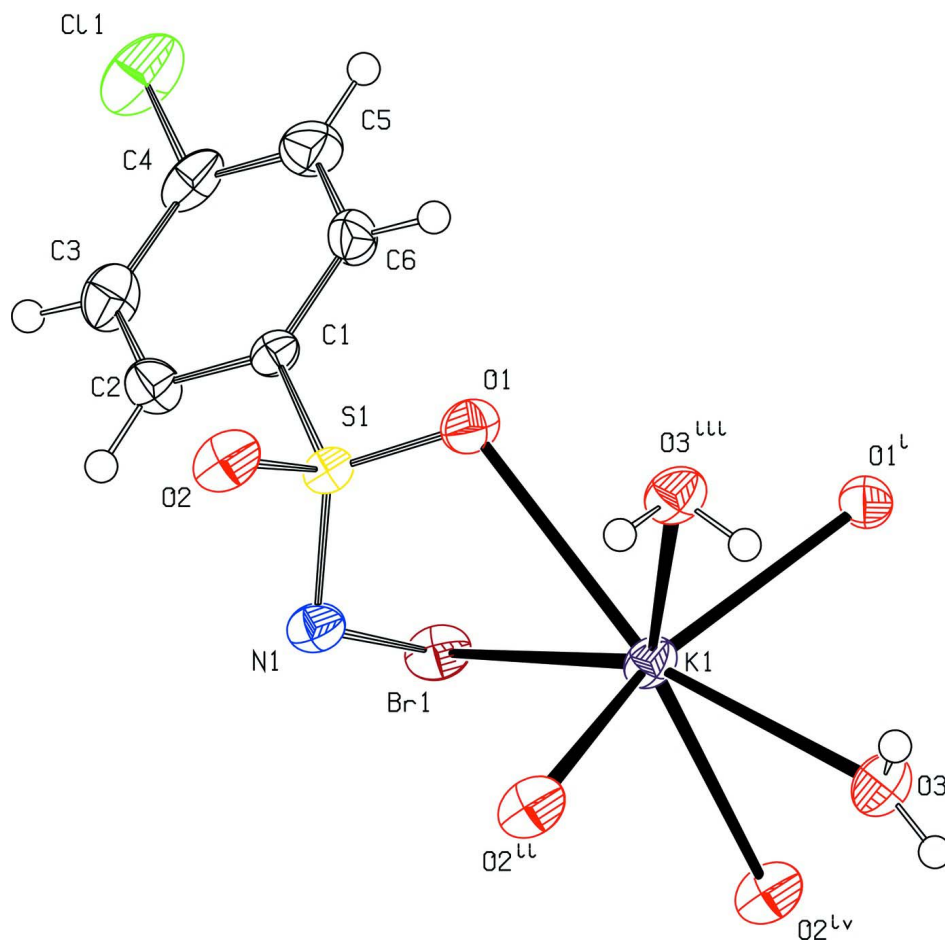
Figure 1

Molecular structure of the title compound, showing the atom labelling scheme for the asymmetric unit and extended to show the coordination geometry for the K^+. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radii.
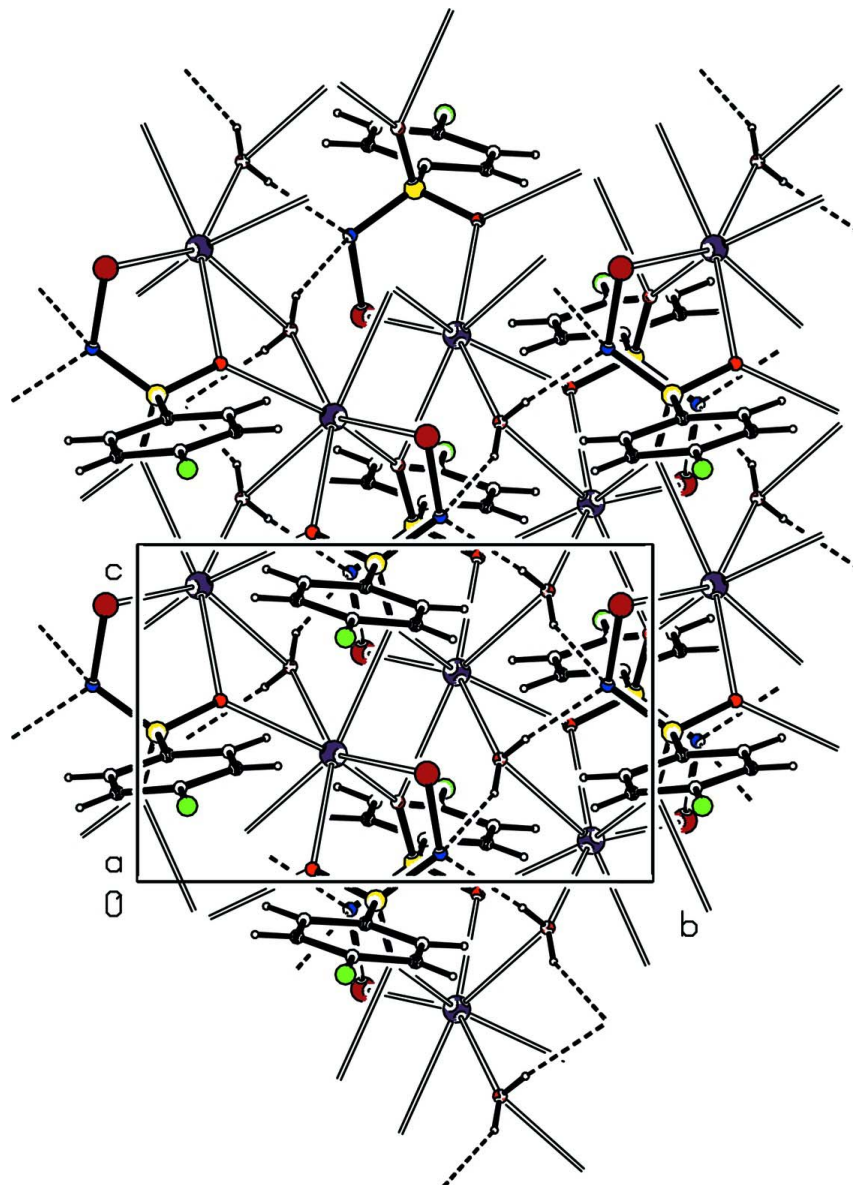
Figure 2

Molecular packing of the title compound with hydrogen bonding shown as dashed lines.

Potassium *N*-bromo-4-chlorobenzenesulfonamidate monohydrate

Crystal data

$K^+ \cdot C_6H_4BrClNO_2S^- \cdot H_2O$	$F(000) = 640$
$M_r = 326.64$	$D_x = 2.049$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 2989 reflections
$a = 15.596$ (1) Å	$\theta = 3.0–27.8°$
$b = 10.188$ (1) Å	$\mu = 4.70$ mm^{-1}
$c = 6.7649$ (7) Å	$T = 293$ K
$\beta = 99.947$ (9)°	Prism, yellow
$V = 1058.73$ (17) Å^3	$0.34 \times 0.34 \times 0.30$ mm
$Z = 4$	

Data collection

Oxford Diffraction Xcalibur diffractometer with a Sapphire CCD detector	3796 measured reflections
Radiation source: fine-focus sealed tube	2147 independent reflections
Graphite monochromator	1984 reflections with $I > 2\sigma(I)$
Rotation method data acquisition using ω scans	$R_{int} = 0.035$
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2009)	$\theta_{max} = 26.4°$, $\theta_{min} = 3.7°$
$T_{min} = 0.298$, $T_{max} = 0.333$	$h = -19\rightarrow17$
	$k = -5\rightarrow12$
	$l = -8\rightarrow6$

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
$R[F^2 > 2\sigma(F^2)] = 0.057$	
$wR(F^2) = 0.156$	
$S = 1.19$	$w = 1/[\sigma^2(F_o^2) + (0.0614P)^2 + 8.645P]$ where $P = (F_o^2 + 2F_c^2)/3$
2147 reflections	
134 parameters	$(\Delta/\sigma)_{max} = 0.014$
2 restraints	$\Delta\rho_{max} = 1.22$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{min} = -0.95$ e Å^{-3}
Secondary atom site location: difference Fourier map	Extinction correction: *SHELXL97* (Sheldrick, 2008), Fc*=kFc[1+0.001xFc²λ³/sin(2θ)]$^{-1/4}$
	Extinction coefficient: 0.044 (3)

Special details

Experimental. CrysAlis RED (Oxford Diffraction, 2009) 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Br1	0.25575 (4)	0.43815 (7)	−0.31985 (10)	0.0299 (3)
K1	0.44027 (9)	0.61960 (15)	−0.3785 (2)	0.0252 (4)
Cl1	−0.02963 (13)	0.5964 (3)	0.2758 (3)	0.0534 (6)
S1	0.34113 (9)	0.53777 (15)	0.0566 (2)	0.0190 (4)
O1	0.3587 (3)	0.6607 (5)	−0.0369 (7)	0.0310 (11)
O2	0.4024 (3)	0.5053 (6)	0.2355 (7)	0.0329 (11)
O3	0.5513 (3)	0.7034 (5)	−0.6370 (8)	0.0318 (11)
H31	0.572 (5)	0.692 (9)	−0.739 (8)	0.038*
H32	0.589 (4)	0.753 (7)	−0.578 (12)	0.038*
N1	0.3390 (4)	0.4126 (6)	−0.0831 (8)	0.0258 (12)
C1	0.2367 (4)	0.5577 (6)	0.1250 (9)	0.0197 (12)
C2	0.1965 (4)	0.4475 (7)	0.1854 (11)	0.0278 (14)
H2	0.2239	0.3662	0.1914	0.033*

C3	0.1148 (5)	0.4602 (8)	0.2370 (11)	0.0341 (16)
H3	0.0867	0.3879	0.2806	0.041*
C4	0.0755 (4)	0.5829 (8)	0.2223 (10)	0.0306 (15)
C5	0.1156 (5)	0.6906 (8)	0.1639 (11)	0.0371 (17)
H5	0.0885	0.7721	0.1573	0.044*
C6	0.1977 (5)	0.6771 (7)	0.1141 (10)	0.0286 (14)
H6	0.2260	0.7499	0.0733	0.034*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0227 (4)	0.0383 (5)	0.0267 (4)	−0.0011 (3)	−0.0019 (3)	−0.0082 (3)
K1	0.0199 (7)	0.0332 (8)	0.0234 (7)	0.0037 (5)	0.0062 (5)	0.0010 (6)
Cl1	0.0198 (9)	0.0954 (18)	0.0479 (11)	0.0083 (10)	0.0137 (8)	0.0025 (11)
S1	0.0136 (7)	0.0251 (8)	0.0178 (7)	−0.0009 (5)	0.0013 (5)	−0.0026 (5)
O1	0.032 (3)	0.029 (2)	0.034 (3)	−0.009 (2)	0.014 (2)	−0.005 (2)
O2	0.019 (2)	0.052 (3)	0.024 (2)	0.006 (2)	−0.0043 (18)	−0.003 (2)
O3	0.023 (2)	0.042 (3)	0.032 (3)	−0.005 (2)	0.008 (2)	0.000 (2)
N1	0.021 (3)	0.032 (3)	0.024 (3)	0.005 (2)	0.002 (2)	−0.003 (2)
C1	0.018 (3)	0.025 (3)	0.016 (3)	0.000 (2)	0.001 (2)	−0.002 (2)
C2	0.020 (3)	0.027 (3)	0.037 (4)	0.002 (2)	0.007 (3)	0.002 (3)
C3	0.028 (4)	0.040 (4)	0.036 (4)	−0.010 (3)	0.009 (3)	0.002 (3)
C4	0.016 (3)	0.056 (5)	0.020 (3)	0.003 (3)	0.003 (2)	0.000 (3)
C5	0.036 (4)	0.040 (4)	0.036 (4)	0.015 (3)	0.010 (3)	0.002 (3)
C6	0.029 (3)	0.026 (3)	0.033 (3)	0.002 (3)	0.012 (3)	0.006 (3)

Geometric parameters (Å, º)

Br1—N1	1.897 (5)	O2—K1ii	2.784 (5)
Br1—K1	3.5001 (16)	O2—K1vi	2.827 (5)
K1—O1i	2.704 (5)	O3—K1i	2.818 (6)
K1—O2ii	2.784 (5)	O3—K1v	3.295 (6)
K1—O3	2.799 (5)	O3—H31	0.82 (2)
K1—O3iii	2.818 (6)	O3—H32	0.82 (2)
K1—O2iv	2.827 (5)	C1—C6	1.356 (9)
K1—O1	2.855 (5)	C1—C2	1.382 (9)
K1—O3v	3.295 (6)	C2—C3	1.384 (10)
K1—N1	3.468 (6)	C2—H2	0.9300
Cl1—C4	1.745 (7)	C3—C4	1.388 (11)
S1—O2	1.446 (5)	C3—H3	0.9300
S1—O1	1.450 (5)	C4—C5	1.355 (11)
S1—N1	1.584 (6)	C5—C6	1.386 (10)
S1—C1	1.780 (6)	C5—H5	0.9300
O1—K1iii	2.704 (5)	C6—H6	0.9300
N1—Br1—K1	73.28 (18)	O2—S1—C1	108.1 (3)
O1i—K1—O2ii	147.39 (17)	O1—S1—C1	105.3 (3)
O1i—K1—O3	78.43 (15)	N1—S1—C1	108.7 (3)

O2ii—K1—O3	75.72 (16)	S1—O1—K1iii	130.8 (3)
O1i—K1—O3iii	84.28 (16)	S1—O1—K1	111.7 (3)
O2ii—K1—O3iii	71.01 (15)	K1iii—O1—K1	101.36 (15)
O3—K1—O3iii	77.42 (11)	S1—O2—K1ii	144.2 (3)
O1i—K1—O2iv	88.05 (16)	S1—O2—K1vi	133.0 (3)
O2ii—K1—O2iv	99.40 (13)	K1ii—O2—K1vi	80.60 (12)
O3—K1—O2iv	66.52 (15)	K1—O3—K1i	99.95 (16)
O3iii—K1—O2iv	143.94 (16)	K1—O3—K1v	72.59 (13)
O1i—K1—O1	87.38 (13)	K1i—O3—K1v	132.42 (18)
O2ii—K1—O1	105.97 (15)	K1—O3—H31	149 (6)
O3—K1—O1	150.63 (16)	K1i—O3—H31	84 (6)
O3iii—K1—O1	75.66 (14)	K1v—O3—H31	82 (6)
O2iv—K1—O1	139.19 (15)	K1—O3—H32	110 (6)
O1i—K1—O3v	148.56 (15)	K1i—O3—H32	102 (6)
O2ii—K1—O3v	60.31 (15)	K1v—O3—H32	125 (6)
O3—K1—O3v	107.41 (13)	H31—O3—H32	98 (9)
O3iii—K1—O3v	127.12 (10)	S1—N1—Br1	109.5 (3)
O2iv—K1—O3v	67.58 (15)	S1—N1—K1	83.6 (2)
O1—K1—O3v	98.14 (14)	Br1—N1—K1	75.12 (18)
O1i—K1—N1	120.12 (14)	C6—C1—C2	121.5 (6)
O2ii—K1—N1	89.06 (15)	C6—C1—S1	120.7 (5)
O3—K1—N1	159.76 (16)	C2—C1—S1	117.8 (5)
O3iii—K1—N1	110.52 (14)	C1—C2—C3	118.9 (6)
O2iv—K1—N1	103.80 (15)	C1—C2—H2	120.6
O1—K1—N1	46.50 (13)	C3—C2—H2	120.6
O3v—K1—N1	52.68 (13)	C2—C3—C4	118.7 (7)
O1i—K1—Br1	98.17 (12)	C2—C3—H3	120.7
O2ii—K1—Br1	114.30 (12)	C4—C3—H3	120.7
O3—K1—Br1	147.31 (12)	C5—C4—C3	122.0 (7)
O3iii—K1—Br1	135.01 (11)	C5—C4—Cl1	119.6 (6)
O2iv—K1—Br1	80.94 (11)	C3—C4—Cl1	118.4 (6)
O1—K1—Br1	59.70 (10)	C4—C5—C6	118.8 (7)
O3v—K1—Br1	59.85 (9)	C4—C5—H5	120.6
N1—K1—Br1	31.60 (9)	C6—C5—H5	120.6
O2—S1—O1	114.6 (3)	C1—C6—C5	120.1 (7)
O2—S1—N1	105.0 (3)	C1—C6—H6	120.0
O1—S1—N1	114.9 (3)	C5—C6—H6	120.0
N1—Br1—K1—O1i	−137.2 (2)	O3iii—K1—O3—K1v	125.32 (11)
N1—Br1—K1—O2ii	39.8 (2)	O2iv—K1—O3—K1v	−55.11 (13)
N1—Br1—K1—O3	141.5 (3)	O1—K1—O3—K1v	149.3 (3)
N1—Br1—K1—O3iii	−47.2 (2)	O3v—K1—O3—K1v	0.0
N1—Br1—K1—O2iv	136.1 (2)	N1—K1—O3—K1v	9.7 (4)
N1—Br1—K1—O1	−55.1 (2)	Br1—K1—O3—K1v	−60.9 (2)
N1—Br1—K1—O3v	66.8 (2)	O2—S1—N1—Br1	177.0 (3)
O2—S1—O1—K1iii	−27.2 (5)	O1—S1—N1—Br1	−56.3 (4)
N1—S1—O1—K1iii	−148.9 (3)	C1—S1—N1—Br1	61.5 (4)
C1—S1—O1—K1iii	91.5 (4)	O2—S1—N1—K1	−111.3 (2)

O2—S1—O1—K1	101.4 (3)	O1—S1—N1—K1	15.5 (3)
N1—S1—O1—K1	−20.3 (4)	C1—S1—N1—K1	133.2 (2)
C1—S1—O1—K1	−139.9 (3)	K1—Br1—N1—S1	77.5 (3)
O1ⁱ—K1—O1—S1	148.80 (19)	O1ⁱ—K1—N1—S1	−61.2 (3)
O2ⁱⁱ—K1—O1—S1	−61.4 (3)	O2ⁱⁱ—K1—N1—S1	103.5 (2)
O3—K1—O1—S1	−150.6 (3)	O3—K1—N1—S1	144.3 (4)
O3ⁱⁱⁱ—K1—O1—S1	−126.4 (3)	O3ⁱⁱⁱ—K1—N1—S1	34.2 (2)
O2ⁱᵛ—K1—O1—S1	64.8 (4)	O2ⁱᵛ—K1—N1—S1	−157.0 (2)
O3ᵛ—K1—O1—S1	−0.1 (3)	O1—K1—N1—S1	−9.74 (19)
N1—K1—O1—S1	11.4 (2)	O3ᵛ—K1—N1—S1	155.9 (3)
Br1—K1—O1—S1	47.7 (2)	Br1—K1—N1—S1	−112.2 (3)
O1ⁱ—K1—O1—K1ⁱⁱⁱ	−68.3 (3)	O1ⁱ—K1—N1—Br1	51.0 (2)
O2ⁱⁱ—K1—O1—K1ⁱⁱⁱ	81.47 (19)	O2ⁱⁱ—K1—N1—Br1	−144.32 (18)
O3—K1—O1—K1ⁱⁱⁱ	−7.7 (4)	O3—K1—N1—Br1	−103.5 (4)
O3ⁱⁱⁱ—K1—O1—K1ⁱⁱⁱ	16.46 (16)	O3ⁱⁱⁱ—K1—N1—Br1	146.39 (17)
O2ⁱᵛ—K1—O1—K1ⁱⁱⁱ	−152.3 (2)	O2ⁱᵛ—K1—N1—Br1	−44.9 (2)
O3ᵛ—K1—O1—K1ⁱⁱⁱ	142.81 (15)	O1—K1—N1—Br1	102.4 (2)
N1—K1—O1—K1ⁱⁱⁱ	154.3 (3)	O3ᵛ—K1—N1—Br1	−91.9 (2)
Br1—K1—O1—K1ⁱⁱⁱ	−169.3 (2)	O2—S1—C1—C6	112.9 (6)
O1—S1—O2—K1ⁱⁱ	−88.7 (6)	O1—S1—C1—C6	−10.0 (6)
N1—S1—O2—K1ⁱⁱ	38.3 (6)	N1—S1—C1—C6	−133.7 (6)
C1—S1—O2—K1ⁱⁱ	154.2 (5)	O2—S1—C1—C2	−68.3 (6)
O1—S1—O2—K1ᵛⁱ	66.9 (5)	O1—S1—C1—C2	168.8 (5)
N1—S1—O2—K1ᵛⁱ	−166.1 (4)	N1—S1—C1—C2	45.1 (6)
C1—S1—O2—K1ᵛⁱ	−50.2 (5)	C6—C1—C2—C3	−0.4 (10)
O1ⁱ—K1—O3—K1ⁱ	−16.53 (16)	S1—C1—C2—C3	−179.2 (5)
O2ⁱⁱ—K1—O3—K1ⁱ	−176.5 (2)	C1—C2—C3—C4	1.2 (11)
O3ⁱⁱⁱ—K1—O3—K1ⁱ	−103.2 (2)	C2—C3—C4—C5	−1.6 (11)
O2ⁱᵛ—K1—O3—K1ⁱ	76.40 (17)	C2—C3—C4—Cl1	176.9 (6)
O1—K1—O3—K1ⁱ	−79.2 (3)	C3—C4—C5—C6	1.1 (11)
O3ᵛ—K1—O3—K1ⁱ	131.51 (17)	Cl1—C4—C5—C6	−177.4 (6)
N1—K1—O3—K1ⁱ	141.2 (4)	C2—C1—C6—C5	−0.1 (10)
Br1—K1—O3—K1ⁱ	70.6 (3)	S1—C1—C6—C5	178.6 (5)
O1ⁱ—K1—O3—K1ᵛ	−148.04 (15)	C4—C5—C6—C1	−0.2 (11)
O2ⁱⁱ—K1—O3—K1ᵛ	52.01 (12)		

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

Hydrogen-bond geometry (Å, °)

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O3—H31⋯N1ᵛ	0.82 (2)	2.25 (5)	3.005 (8)	152 (8)
O3—H32⋯N1ᵛⁱⁱ	0.82 (2)	2.16 (3)	2.967 (8)	166 (9)

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