metal-organic compounds

Potassium N,2-dichlorobenzene-sulfonamidate sesquihydrate

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In the title compound, $K^+ \cdot C_6H_4Cl_2NO_2S^- \cdot 1.5H_2O$, one water molecule has crystallographically imposed twofold symmetry. The K^+ ion is heptacoordinated by three O atoms from water molecules and by four sulfonyl O atoms of N-chloro-2-chlorobenzenesulfonamide anions. The S—N distance of 1.582 (2) Å is consistent with an S—N double bond. In the structure, the sulfonyl-O and the water-O atoms bridge the K^+ cations in a bidentate fashion. The crystal structure comprises sheets in the ac plane which are further stabilized by intermolecular O—H⋯Cl and O—H⋯N hydrogen bonds.

Related literature

For our studies of the effect of substituents on the structures of N-haloarylsulfonamides, see: Gowda et al. (2010, 2011a,b); and on the oxidative strengths of N-haloarylsulfonamides, see: Gowda & Shetty (2004); Usha & Gowda (2006). For similar structures, see: George et al. (2000); Olmstead & Power (1986). For the preparation of the title compound, see: Jyothi & Gowda (2004).
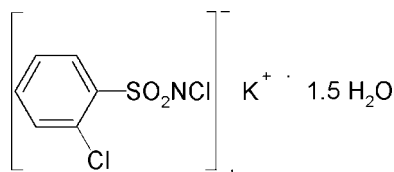
Experimental

Crystal data

$K^+ \cdot C_6H_4Cl_2NO_2S^- \cdot 1.5H_2O$
$M_r = 291.19$

Monoclinic, $C2/c$
$a = 12.301$ (2) Å
$b = 6.8277$ (6) Å
$c = 27.965$ (3) Å
$\beta = 106.28$ (1)°
$V = 2254.5$ (5) Å^3
$Z = 8$

Mo $K\alpha$ radiation
$\mu = 1.12$ mm^{-1}
$T = 293$ K
$0.44 \times 0.44 \times 0.38$ mm

Data collection

Oxford Diffraction Xcalibur diffractometer with Sapphire CCD detector
Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2009)
$T_{min} = 0.640$, $T_{max} = 0.677$

4174 measured reflections
2298 independent reflections
2181 reflections with $I > 2\sigma(I)$
$R_{int} = 0.015$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.105$
$S = 1.19$
2298 reflections
142 parameters
3 restraints

H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max} = 0.47$ e Å^{-3}
$\Delta\rho_{min} = -0.46$ e Å^{-3}

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O3—H31⋯N1^i	0.80 (2)	2.23 (2)	2.962 (3)	152 (4)
O3—H32⋯Cl1^{ii}	0.81 (2)	2.73 (2)	3.517 (3)	165 (4)
O4—H41⋯N1^i	0.81 (2)	2.19 (2)	2.978 (3)	165 (4)

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

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*,2-dichlorobenzenesulfonamidate sesquihydrate

B. Thimme Gowda, Sabine Foro and K. Shakuntala

S1. Comment

Arylsulfonamides and their N-halo compounds are of interest in synthetic, mechanistic and analytical chemistry (Gowda & Shetty, 2004; Usha & Gowda, 2006). To explore the substituent effects and the effect of replacing sodium ions by potassium ions on the solid state structures of *N*-halo- arylsulfonamides (Gowda *et al.*, 2010, 2011*a,b*), in the present work, the structure of potassium *N*,2-dichloro-benzenesulfonamidate sesquihydrate (I) has been determined (Fig. 1). The structure of (I) is isostructural with potassium *N*-bromo-2-chloro-benzenesulfonamidate sesquihydrate (II) (Gowda *et al.*, 2011*b*), and resembles those of potassium *N*,4-dichloro-benzenesulfonamidate monohydrate (III) (Gowda *et al.*, 2011*a*), sodium *N*,2-dichloro-benzenesulfonamidate sesquihydrate (IV) (Gowda *et al.*, 2010) and other sodium *N*-chloro-aryl-sulfonamides (George *et al.*, 2000; Olmstead & Power, 1986).

In the title compound, K^+ ion is hepta coordinated by three O atoms from water molecules and by four sulfonyl O atoms of *N*-chloro-2-chloro- benzenesulfonamidate anions. This is in contrast to hepta coordination of K^+ by two O atoms from water molecules, four sulfonyl O atoms from the *N*-chloro-4-chlorobenzenesulfonamidate anions and one Cl in (III), and octahedral coordination of Na^+ by three O atoms of water molecules and three sulfonyl O atoms of three different *N*-chloro-2-chloro- benzenesulfonamidate anions.

The S—N distance of 1.582 (4)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 1.588 (2) Å in (IV)

The crystal structure comprises sheets in the *ac* plane (Fig. 2). The molecular packing is stabilized by O3—H31···N1, O3—H32···Cl1 and O4—H41···N1 hydrogen bonds (Table 1).

S2. Experimental

The title compound was prepared by the method similar to that reported in literature (Jyothi & Gowda, 2004). The purity of the compound was checked by determining its melting point. Colourless prisms of (I) 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).
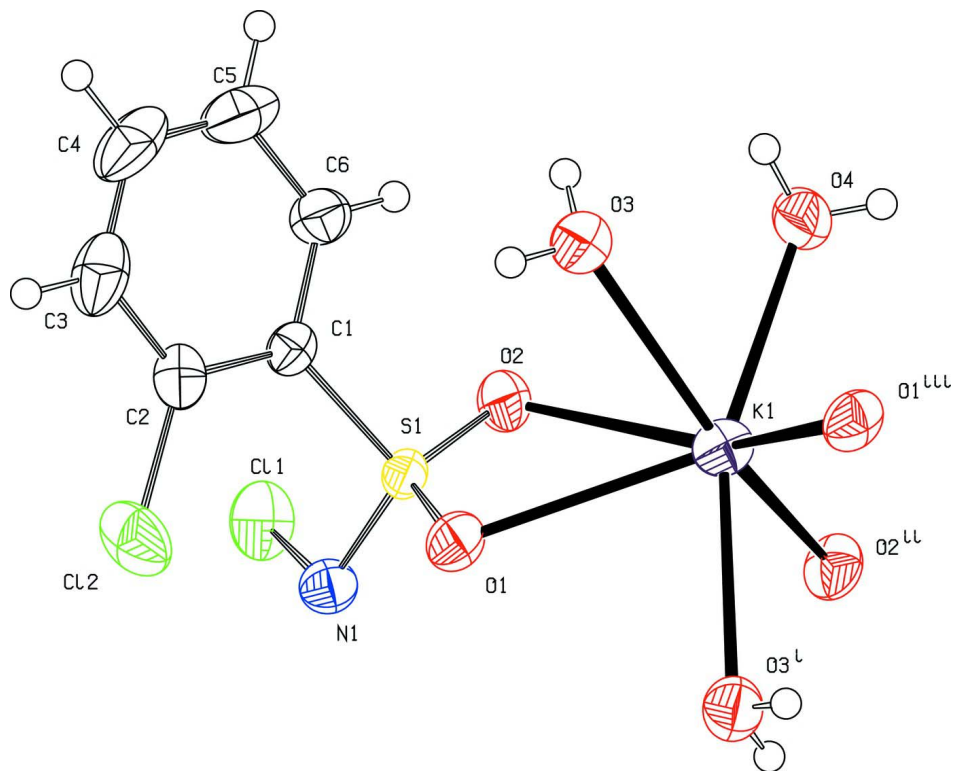
Figure 1

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$^+$ cation. Displacement ellipsoids are drawn at the 50% probability level and H atoms are represented as small spheres of arbitrary radii (i) -x+1/2, y-1/2, -z+3/2; (ii) -x+1, y, -z+3/2; (iii) -x+1/2, y+1/2, -z+3/2.
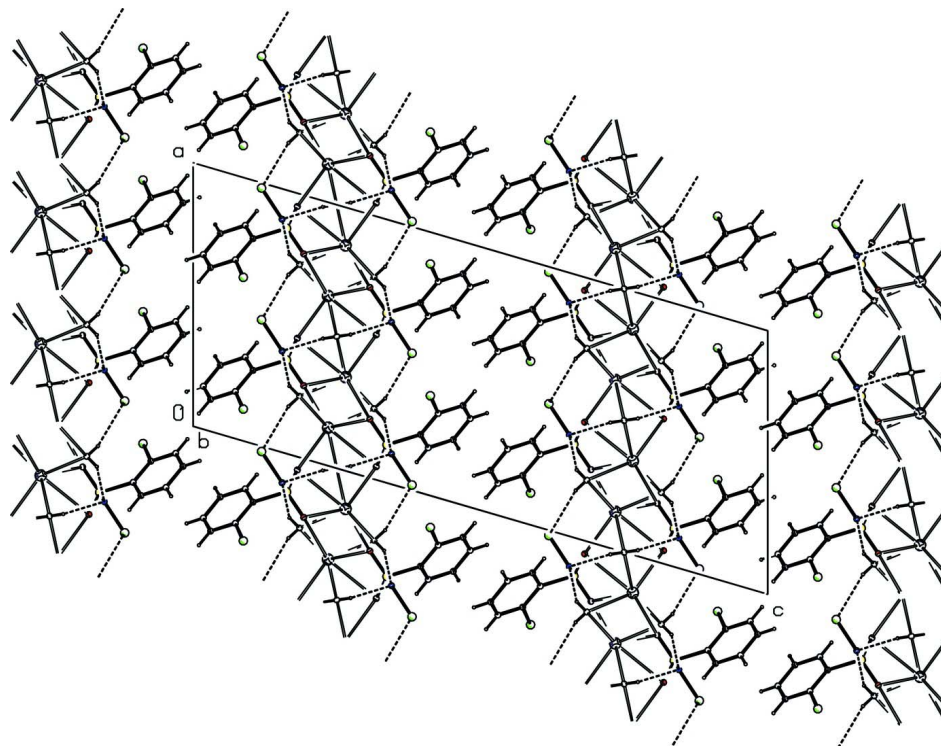
Figure 2

Molecular packing of the title compound with hydrogen bonds drawn as dashed lines.

Potassium *N*,2-dichlorobenzenesulfonamidate sesquihydrate

Crystal data

K$^+$·C$_6$H$_4$Cl$_2$NO$_2$S$^-$·1.5H$_2$O
M_r = 291.19
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
a = 12.301 (2) Å
b = 6.8277 (6) Å
c = 27.965 (3) Å
β = 106.28 (1)°
V = 2254.5 (5) Å^3
Z = 8

$F(000)$ = 1176
D_x = 1.716 Mg m^{-3}
Mo *Kα* radiation, λ = 0.71073 Å
Cell parameters from 2350 reflections
θ = 3.0–27.8°
μ = 1.12 mm^{-1}
T = 293 K
Prism, colourless
0.44 × 0.44 × 0.38 mm

Data collection

Oxford Diffraction Xcalibur
   diffractometer with Sapphire CCD detector
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans.
Absorption correction: multi-scan
   (*CrysAlis RED*; Oxford Diffraction, 2009)
T_{min} = 0.640, T_{max} = 0.677

4174 measured reflections
2298 independent reflections
2181 reflections with $I > 2\sigma(I)$
R_{int} = 0.015
θ_{max} = 26.4°, θ_{min} = 3.0°
$h = -15 \rightarrow 10$
$k = -6 \rightarrow 8$
$l = -34 \rightarrow 34$

Refinement

Refinement on F^2	Hydrogen site location: inferred from
Least-squares matrix: full	neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.042$	H atoms treated by a mixture of independent
$wR(F^2) = 0.105$	and constrained refinement
$S = 1.19$	$w = 1/[\sigma^2(F_o^2) + (0.0457P)^2 + 5.0762P]$
2298 reflections	where $P = (F_o^2 + 2F_c^2)/3$
142 parameters	$(\Delta/\sigma)_{max} = 0.002$
3 restraints	$\Delta\rho_{max} = 0.47$ e Å^{-3}
Primary atom site location: structure-invariant	$\Delta\rho_{min} = -0.46$ e Å^{-3}
direct methods	Extinction correction: *SHELXL*,
Secondary atom site location: difference Fourier	$Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
map	Extinction coefficient: 0.0234 (10)

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 $F^2 > \sigma(F^2)$ 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	0.2790 (2)	0.2499 (4)	0.60429 (9)	0.0268 (5)
C2	0.1789 (2)	0.1729 (4)	0.57347 (10)	0.0346 (6)
C3	0.1218 (3)	0.2695 (6)	0.53041 (12)	0.0510 (8)
H3	0.0551	0.2173	0.5100	0.061*
C4	0.1633 (4)	0.4426 (6)	0.51767 (13)	0.0599 (10)
H4	0.1241	0.5075	0.4887	0.072*
C5	0.2620 (3)	0.5203 (5)	0.54735 (13)	0.0545 (9)
H5	0.2899	0.6373	0.5384	0.065*
C6	0.3204 (3)	0.4242 (4)	0.59073 (11)	0.0383 (6)
H6	0.3874	0.4769	0.6108	0.046*
N1	0.38459 (19)	−0.0793 (3)	0.65478 (9)	0.0328 (5)
O1	0.27693 (18)	0.1323 (3)	0.69244 (7)	0.0380 (5)
O2	0.45006 (17)	0.2695 (3)	0.68135 (7)	0.0402 (5)
O3	0.2321 (2)	0.6414 (3)	0.68516 (8)	0.0431 (5)
H31	0.260 (3)	0.704 (5)	0.6675 (12)	0.052*
H32	0.181 (3)	0.584 (5)	0.6658 (12)	0.052*
O4	0.5000	0.7199 (5)	0.7500	0.0478 (8)
H41	0.477 (3)	0.791 (5)	0.7260 (10)	0.057*
K1	0.35556 (5)	0.42956 (9)	0.76528 (2)	0.0342 (2)
Cl1	0.48019 (7)	−0.09326 (13)	0.61910 (3)	0.0478 (2)
Cl2	0.12087 (7)	−0.04411 (13)	0.58723 (4)	0.0561 (3)
S1	0.35458 (5)	0.14187 (9)	0.66219 (2)	0.0262 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0265 (11)	0.0307 (13)	0.0240 (11)	0.0051 (10)	0.0085 (9)	0.0003 (10)
C2	0.0302 (13)	0.0381 (14)	0.0329 (13)	0.0059 (11)	0.0047 (11)	−0.0060 (11)
C3	0.0414 (17)	0.067 (2)	0.0359 (16)	0.0174 (16)	−0.0028 (13)	−0.0059 (15)
C4	0.072 (2)	0.069 (2)	0.0342 (17)	0.032 (2)	0.0082 (16)	0.0163 (16)
C5	0.071 (2)	0.0499 (19)	0.0461 (18)	0.0114 (17)	0.0224 (17)	0.0192 (15)
C6	0.0433 (16)	0.0370 (15)	0.0360 (14)	0.0002 (12)	0.0133 (12)	0.0035 (12)
N1	0.0325 (12)	0.0327 (12)	0.0339 (12)	0.0018 (9)	0.0104 (9)	0.0021 (9)
O1	0.0449 (11)	0.0444 (11)	0.0309 (10)	−0.0048 (9)	0.0208 (9)	−0.0007 (8)
O2	0.0373 (11)	0.0430 (11)	0.0341 (10)	−0.0127 (9)	−0.0002 (8)	−0.0018 (9)
O3	0.0455 (12)	0.0427 (12)	0.0387 (12)	−0.0017 (10)	0.0079 (9)	0.0016 (9)
O4	0.0565 (19)	0.0343 (16)	0.0420 (17)	0.000	−0.0038 (15)	0.000
K1	0.0325 (3)	0.0354 (3)	0.0366 (3)	0.0065 (2)	0.0129 (2)	0.0028 (2)
Cl1	0.0399 (4)	0.0590 (5)	0.0472 (4)	0.0057 (3)	0.0164 (3)	−0.0102 (4)
Cl2	0.0364 (4)	0.0480 (5)	0.0718 (6)	−0.0112 (3)	−0.0049 (4)	−0.0054 (4)
S1	0.0271 (3)	0.0299 (3)	0.0206 (3)	−0.0043 (2)	0.0053 (2)	0.0000 (2)

Geometric parameters (Å, º)

C1—C6	1.388 (4)	O1—K1	2.846 (2)
C1—C2	1.393 (4)	O2—S1	1.440 (2)
C1—S1	1.785 (2)	O2—K1ii	2.672 (2)
C2—C3	1.380 (4)	O2—K1	3.096 (2)
C2—Cl2	1.734 (3)	O3—K1	2.741 (2)
C3—C4	1.373 (6)	O3—K1iii	2.791 (2)
C3—H3	0.9300	O3—H31	0.797 (19)
C4—C5	1.372 (6)	O3—H32	0.806 (19)
C4—H4	0.9300	O4—K1	2.774 (2)
C5—C6	1.389 (4)	O4—K1ii	2.774 (2)
C5—H5	0.9300	O4—H41	0.811 (18)
C6—H6	0.9300	K1—O1iii	2.655 (2)
N1—S1	1.582 (2)	K1—O2ii	2.672 (2)
N1—Cl1	1.745 (2)	K1—O3i	2.791 (2)
O1—S1	1.4442 (19)	K1—S1	3.4859 (9)
O1—K1i	2.655 (2)		
C6—C1—C2	118.9 (2)	O2ii—K1—O3	151.25 (7)
C6—C1—S1	117.7 (2)	O1iii—K1—O4	101.28 (7)
C2—C1—S1	123.4 (2)	O2ii—K1—O4	82.34 (6)
C3—C2—C1	120.3 (3)	O3—K1—O4	74.28 (6)
C3—C2—Cl2	117.5 (2)	O1iii—K1—O3i	77.05 (7)
C1—C2—Cl2	122.2 (2)	O2ii—K1—O3i	81.03 (7)
C4—C3—C2	120.2 (3)	O3—K1—O3i	125.11 (4)
C4—C3—H3	119.9	O4—K1—O3i	158.97 (5)
C2—C3—H3	119.9	O1iii—K1—O1	124.24 (4)
C5—C4—C3	120.4 (3)	O2ii—K1—O1	100.34 (7)

C5—C4—H4	119.8	O3—K1—O1	77.99 (7)
C3—C4—H4	119.8	O4—K1—O1	120.21 (5)
C4—C5—C6	119.9 (3)	O3ⁱ—K1—O1	75.62 (6)
C4—C5—H5	120.0	O1ⁱⁱⁱ—K1—O2	158.33 (6)
C6—C5—H5	120.0	O2ⁱⁱ—K1—O2	79.15 (7)
C1—C6—C5	120.3 (3)	O3—K1—O2	78.84 (6)
C1—C6—H6	119.9	O4—K1—O2	75.08 (6)
C5—C6—H6	119.9	O3ⁱ—K1—O2	114.01 (7)
S1—N1—Cl1	110.28 (13)	O1—K1—O2	47.94 (5)
S1—O1—K1ⁱ	150.89 (13)	O1ⁱⁱⁱ—K1—S1	143.30 (5)
S1—O1—K1	103.85 (10)	O2ⁱⁱ—K1—S1	91.52 (5)
K1ⁱ—O1—K1	100.43 (6)	O3—K1—S1	75.44 (5)
S1—O2—K1ⁱⁱ	164.66 (13)	O4—K1—S1	97.42 (4)
S1—O2—K1	93.17 (10)	O3ⁱ—K1—S1	95.81 (5)
K1ⁱⁱ—O2—K1	84.23 (6)	O1—K1—S1	23.72 (4)
K1—O3—K1ⁱⁱⁱ	99.72 (7)	O2—K1—S1	24.36 (4)
K1—O3—H31	124 (3)	O2—S1—O1	114.44 (12)
K1ⁱⁱⁱ—O3—H31	103 (3)	O2—S1—N1	115.50 (13)
K1—O3—H32	116 (3)	O1—S1—N1	104.51 (12)
K1ⁱⁱⁱ—O3—H32	110 (3)	O2—S1—C1	104.51 (12)
H31—O3—H32	103 (4)	O1—S1—C1	106.75 (12)
K1—O4—K1ⁱⁱ	88.78 (10)	N1—S1—C1	110.93 (12)
K1—O4—H41	118 (3)	O2—S1—K1	62.47 (9)
K1ⁱⁱ—O4—H41	113 (3)	O1—S1—K1	52.43 (9)
O1ⁱⁱⁱ—K1—O2ⁱⁱ	121.97 (7)	N1—S1—K1	134.37 (9)
O1ⁱⁱⁱ—K1—O3	79.63 (7)	C1—S1—K1	113.42 (8)
C6—C1—C2—C3	−0.4 (4)	K1—O2—S1—O1	−7.24 (13)
S1—C1—C2—C3	176.7 (2)	K1ⁱⁱ—O2—S1—N1	−49.0 (5)
C6—C1—C2—Cl2	179.9 (2)	K1—O2—S1—N1	−128.69 (10)
S1—C1—C2—Cl2	−3.0 (3)	K1ⁱⁱ—O2—S1—C1	−171.1 (5)
C1—C2—C3—C4	−0.1 (5)	K1—O2—S1—C1	109.15 (9)
Cl2—C2—C3—C4	179.6 (3)	K1ⁱⁱ—O2—S1—K1	79.7 (5)
C2—C3—C4—C5	0.5 (5)	K1ⁱ—O1—S1—O2	−137.6 (2)
C3—C4—C5—C6	−0.4 (6)	K1—O1—S1—O2	8.11 (15)
C2—C1—C6—C5	0.6 (4)	K1ⁱ—O1—S1—N1	−10.2 (3)
S1—C1—C6—C5	−176.7 (2)	K1—O1—S1—N1	135.42 (10)
C4—C5—C6—C1	−0.2 (5)	K1ⁱ—O1—S1—C1	107.3 (3)
K1ⁱⁱⁱ—O3—K1—O1ⁱⁱⁱ	16.67 (7)	K1—O1—S1—C1	−106.99 (11)
K1ⁱⁱⁱ—O3—K1—O2ⁱⁱ	−125.10 (13)	K1ⁱ—O1—S1—K1	−145.7 (3)
K1ⁱⁱⁱ—O3—K1—O4	−88.29 (7)	Cl1—N1—S1—O2	−52.68 (17)
K1ⁱⁱⁱ—O3—K1—O3ⁱ	82.64 (12)	Cl1—N1—S1—O1	−179.33 (13)
K1ⁱⁱⁱ—O3—K1—O1	145.25 (8)	Cl1—N1—S1—C1	65.98 (16)
K1ⁱⁱⁱ—O3—K1—O2	−165.75 (8)	Cl1—N1—S1—K1	−128.22 (10)
K1ⁱⁱⁱ—O3—K1—S1	169.49 (7)	C6—C1—S1—O2	−2.1 (2)
K1ⁱⁱ—O4—K1—O1ⁱⁱⁱ	164.53 (5)	C2—C1—S1—O2	−179.2 (2)
K1ⁱⁱ—O4—K1—O2ⁱⁱ	43.34 (5)	C6—C1—S1—O1	119.5 (2)
K1ⁱⁱ—O4—K1—O3	−119.75 (6)	C2—C1—S1—O1	−57.6 (2)

K1ii—O4—K1—O3i	81.31 (19)	C6—C1—S1—N1	−127.2 (2)
K1ii—O4—K1—O1	−54.21 (6)	C2—C1—S1—N1	55.7 (2)
K1ii—O4—K1—O2	−37.41 (4)	C6—C1—S1—K1	63.8 (2)
K1ii—O4—K1—S1	−47.208 (16)	C2—C1—S1—K1	−113.3 (2)
S1—O1—K1—O1iii	149.55 (9)	O1iii—K1—S1—O2	143.82 (13)
K1i—O1—K1—O1iii	−46.65 (10)	O2ii—K1—S1—O2	−58.97 (8)
S1—O1—K1—O2ii	−69.62 (12)	O3—K1—S1—O2	95.08 (11)
K1i—O1—K1—O2ii	94.17 (7)	O4—K1—S1—O2	23.50 (11)
S1—O1—K1—O3	81.10 (11)	O3i—K1—S1—O2	−140.10 (11)
K1i—O1—K1—O3	−115.10 (8)	O1—K1—S1—O2	−171.67 (15)
S1—O1—K1—O4	17.48 (14)	O1iii—K1—S1—O1	−44.51 (11)
K1i—O1—K1—O4	−178.72 (6)	O2ii—K1—S1—O1	112.70 (12)
S1—O1—K1—O3i	−147.47 (12)	O3—K1—S1—O1	−93.24 (12)
K1i—O1—K1—O3i	16.33 (7)	O4—K1—S1—O1	−164.82 (12)
S1—O1—K1—O2	−4.61 (8)	O3i—K1—S1—O1	31.57 (12)
K1i—O1—K1—O2	159.19 (11)	O2—K1—S1—O1	171.67 (15)
K1i—O1—K1—S1	163.80 (15)	O1iii—K1—S1—N1	−116.44 (14)
S1—O2—K1—O1iii	−72.9 (2)	O2ii—K1—S1—N1	40.78 (13)
K1ii—O2—K1—O1iii	122.30 (16)	O3—K1—S1—N1	−165.17 (13)
S1—O2—K1—O2ii	119.28 (6)	O4—K1—S1—N1	123.25 (13)
K1ii—O2—K1—O2ii	−45.55 (9)	O3i—K1—S1—N1	−40.36 (13)
S1—O2—K1—O3	−79.32 (10)	O1—K1—S1—N1	−71.93 (16)
K1ii—O2—K1—O3	115.85 (7)	O2—K1—S1—N1	99.75 (16)
S1—O2—K1—O4	−155.84 (10)	O1iii—K1—S1—C1	49.10 (13)
K1ii—O2—K1—O4	39.33 (5)	O2ii—K1—S1—C1	−153.68 (10)
S1—O2—K1—O3i	44.31 (12)	O3—K1—S1—C1	0.37 (11)
K1ii—O2—K1—O3i	−120.52 (7)	O4—K1—S1—C1	−71.21 (10)
S1—O2—K1—O1	4.50 (8)	O3i—K1—S1—C1	125.18 (10)
K1ii—O2—K1—O1	−160.33 (10)	O1—K1—S1—C1	93.61 (15)
K1ii—O2—K1—S1	−164.83 (13)	O2—K1—S1—C1	−94.71 (13)
K1ii—O2—S1—O1	72.5 (5)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H31···N1iv	0.80 (2)	2.23 (2)	2.962 (3)	152 (4)
O3—H32···Cl1v	0.81 (2)	2.73 (2)	3.517 (3)	165 (4)
O4—H41···N1iv	0.81 (2)	2.19 (2)	2.978 (3)	165 (4)

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