

# Potassium *N*,4-dichlorobenzene-sulfonamidate monohydrate

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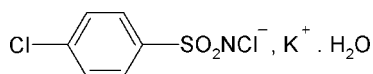
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Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.024;  $wR$  factor = 0.067; data-to-parameter ratio = 16.0.

The structure of the title salt hydrate,  $\text{K}^+ \cdot \text{C}_6\text{H}_4\text{Cl}_2\text{NO}_2\text{S}^- \cdot \text{H}_2\text{O}$ , shows each of the sulfonyl O and water O atoms to be bidentate bridging. The heptacoordinated  $\text{K}^+$  cation is connected to two water O atoms, four sulfonyl O atoms and one Cl atom. The crystal structure comprises sheets in the  $bc$  plane which are further stabilized by  $\text{O}-\text{H} \cdots \text{N}$  hydrogen bonds.

## Related literature

For our studies into the effect of substituents on the structures of *N*-haloarylsulfonamides, see: Gowda *et al.* (2007*a,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

$\text{K}^+ \cdot \text{C}_6\text{H}_4\text{Cl}_2\text{NO}_2\text{S} \cdot \text{H}_2\text{O}$   $V = 1044.84$  (13) Å<sup>3</sup>  
 $M_r = 282.18$   $Z = 4$   
 Monoclinic,  $P2_1/c$  Mo  $K\alpha$  radiation  
 $a = 15.487$  (1) Å  $\mu = 1.20$  mm<sup>-1</sup>  
 $b = 10.0620$  (8) Å  $T = 293$  K  
 $c = 6.8061$  (5) Å  $0.42 \times 0.42 \times 0.30$  mm  
 $\beta = 99.888$  (7)°

### Data collection

Oxford Diffraction Xcalibur Diffraction, 2009)  
 diffractometer with a Sapphire  $T_{\min} = 0.633$ ,  $T_{\max} = 0.715$   
 CCD detector 3796 measured reflections  
 Absorption correction: multi-scan 2139 independent reflections  
 (*CrysAlis RED*; Oxford 1962 reflections with  $I > 2\sigma(I)$ )  
 $R_{\text{int}} = 0.009$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.024$  H atoms treated by a mixture of  
 $wR(F^2) = 0.067$  independent and constrained  
 $S = 1.04$  refinement  
 2139 reflections  $\Delta\rho_{\text{max}} = 0.39$  e Å<sup>-3</sup>  
 134 parameters  $\Delta\rho_{\text{min}} = -0.28$  e Å<sup>-3</sup>  
 2 restraints

**Table 1**

Selected bond lengths (Å).

K1—O2	2.8576 (13)	K1—O3 <sup>iv</sup>	2.8714 (15)
K1—O2 <sup>i</sup>	2.6940 (13)	K1—O3 <sup>v</sup>	3.1905 (16)
K1—O1 <sup>ii</sup>	2.7965 (13)	K1—Cl2	3.3944 (6)
K1—O1 <sup>iii</sup>	2.8547 (13)		

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

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
O3—H31 <sup>v</sup> ···N1 <sup>v</sup>	0.81 (2)	2.22 (2)	2.987 (2)	160 (2)
O3—H32 <sup>v</sup> ···N1 <sup>vi</sup>	0.81 (2)	2.18 (2)	2.967 (2)	166 (2)

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

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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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2749).

## References

- George, E., Vivekanandan, S. & Sivakumar, K. (2000). *Acta Cryst.* **C56**, 1208–1209.
- Gowda, B. T., Foro, S., Kožíšek, J. & Fuess, H. (2007*a*). *Acta Cryst.* **E63**, m1688.
- Gowda, B. T., Jyothi, K., Foro, S., Kožíšek, J. & Fuess, H. (2007*b*). *Acta Cryst.* **E63**, m1644–m1645.
- Gowda, B. T. & Shetty, M. (2004). *J. Phys. Org. Chem.* **17**, 848–864.
- Jyothi, K. & Gowda, B. T. (2004). *Z. Naturforsch. Teil A*, **59**, 64–68.
- Olmstead, M. M. & Power, P. P. (1986). *Inorg. Chem.* **25**, 4057–4058.
- Oxford Diffraction (2009). *CrysAlis CCD* and *CrysAlis RED*. Oxford Diffraction Ltd, Yarnton, England.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.
- Usha, K. M. & Gowda, B. T. (2006). *J. Chem. Sci.* **118**, 351–359.

## supporting information

*Acta Cryst.* (2011). E67, m918 [doi:10.1107/S1600536811020319]

## Potassium *N*,4-dichlorobenzenesulfonamidate monohydrate

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### S1. Comment

The chemistry of arylsulfonamides and their *N*-halo compounds is of interest in synthetic, mechanistic, analytical and biological chemistry (Gowda & Shetty, 2004; Usha & Gowda, 2006). To explore the effect of replacing the sodium ion by potassium ion on the solid state structures of *N*-chloroarylsulfonamides (Gowda *et al.*, 2007*a,b*), in the present work, the structure of potassium *N*-chloro-4-chloro-benzenesulfonamidate monohydrate (I) has been determined (Fig. 1). The structure of (I) resembles those of sodium *N*-chloro-benzenesulfonamide (George *et al.*, 2000) and other sodium *N*-chloro-arylsulfonamides (Olmstead & Power, 1986; Gowda *et al.*, 2007*a,b*). In particular, there is no interaction between the nitrogen and potassium atom in the molecule.

K<sup>+</sup> hepta coordination involves two O atoms from bridging water molecules, four sulfonyl O1 atoms from bridging *N*-chloro-4-chlorobenzenesulfonamide anions, and one Cl atom (Table 1). This is in contrast to octahedral coordination of K<sup>+</sup> in potassium *N*-chloro-benzenesulfonamidate monohydrate by two O atoms from water molecules and four sulfonyl O atoms of four different *N*-chlorobenzenesulfonamide anions (Gowda *et al.*, 2007*a*), and octahedral coordination of Na<sup>+</sup> in sodium *N*-chloro-4-chlorobenzenesulfonamidate sesquihydrate by three O atoms of water molecules and three sulfonyl O atoms of three different *N*-chloro-4-chlorobenzenesulfonamide anions (Gowda *et al.*, 2007*b*). The S—N distance of N1—S1, 1.588 (2) Å is consistent with a S—N double bond.

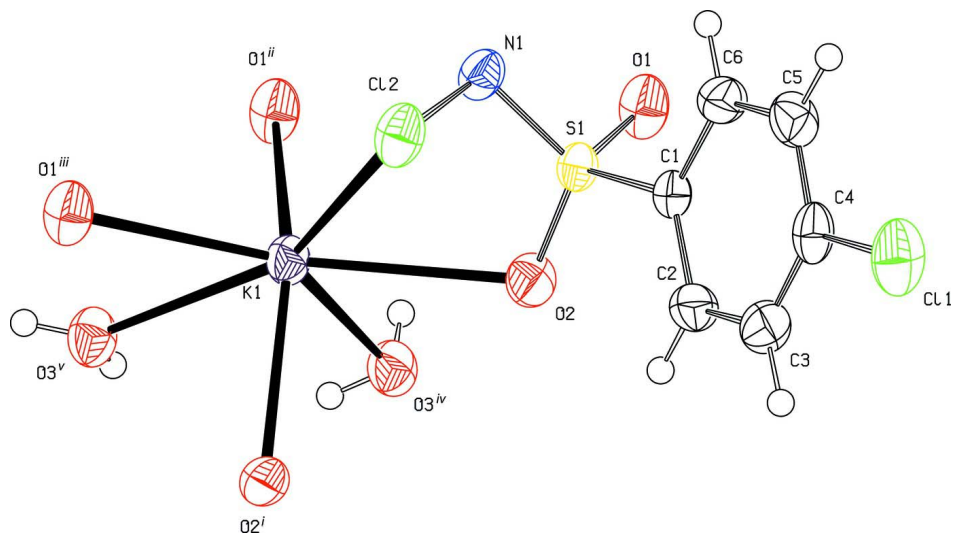
The crystal structure comprises sheets in the *bc* plane which are further stabilized by O—H···N hydrogen bonds (Table 2 and Fig. 2).

### S2. Experimental

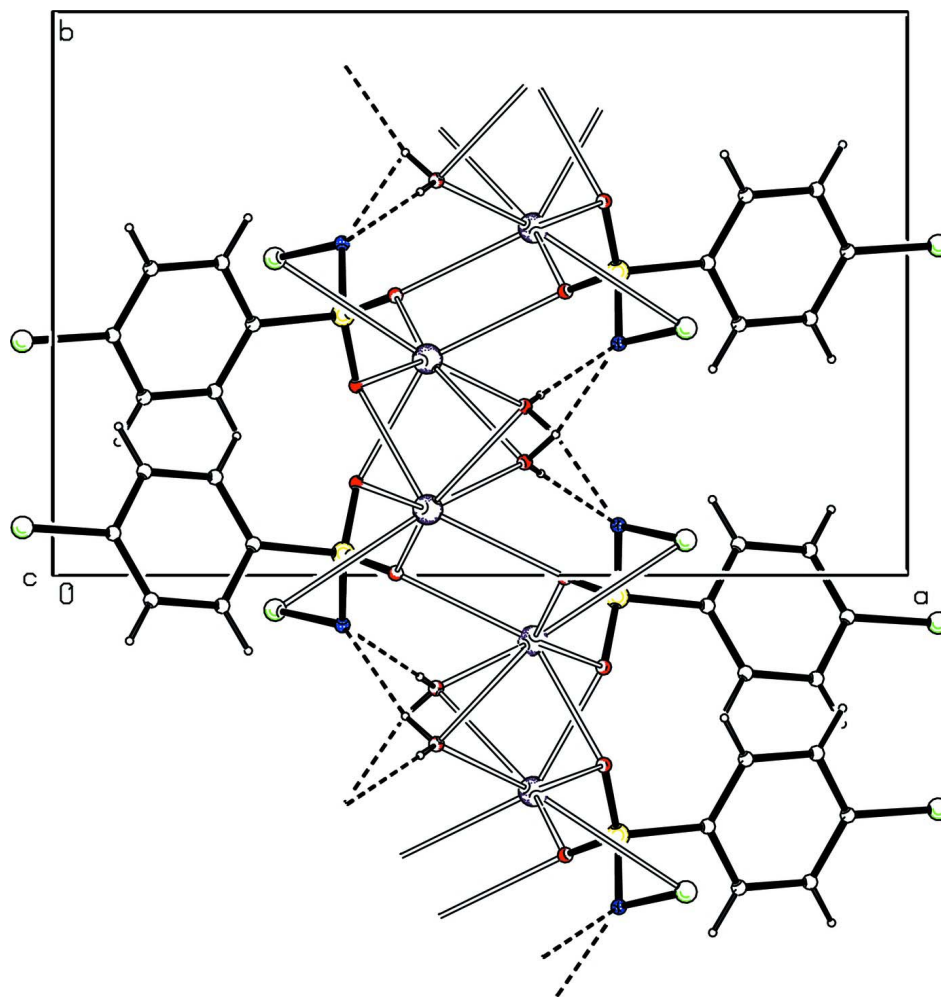
The title compound was prepared according to the literature method (Jyothi & Gowda, 2004). The purity of the compound was checked by determining its melting point. Yellow prisms of (I) were obtained from its aqueous solution at room temperature.

### 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 $U_{eq}$  of the parent atom.

**Figure 1**

Molecular structure of the title salt hydrate, showing the atom labelling scheme for the asymmetric unit and extended to show the coordination geometry for the  $K^+$  cation. The displacement ellipsoids are drawn at the 50% probability level. The H atoms are represented as small spheres of arbitrary radii. See Table 1 for symmetry operations.

**Figure 2**

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

### Potassium *N*,4-dichlorobenzenesulfonamidate monohydrate

#### Crystal data

$\text{K}^+ \cdot \text{C}_6\text{H}_4\text{Cl}_2\text{NO}_2\text{S} \cdot \text{H}_2\text{O}$

$M_r = 282.18$

Monoclinic,  $P2_1/c$

Hall symbol:  $-P\ 2_1/c$

$a = 15.487\ (1)\ \text{\AA}$

$b = 10.0620\ (8)\ \text{\AA}$

$c = 6.8061\ (5)\ \text{\AA}$

$\beta = 99.888\ (7)^\circ$

$V = 1044.84\ (13)\ \text{\AA}^3$

$Z = 4$

$F(000) = 568$

$D_x = 1.794\ \text{Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 2944 reflections

$\theta = 3.0\text{--}27.7^\circ$

$\mu = 1.20\ \text{mm}^{-1}$

$T = 293\ \text{K}$

Prism, yellow

$0.42 \times 0.42 \times 0.30\ \text{mm}$

#### Data collection

Oxford Diffraction Xcalibur

diffractometer with a Sapphire CCD detector

Radiation source: fine-focus sealed tube

Graphite monochromator

Rotation method data acquisition using  $\omega$  scans

Absorption correction: multi-scan

(*CrysAlis RED*; Oxford Diffraction, 2009)

$T_{\min} = 0.633$ ,  $T_{\max} = 0.715$

3796 measured reflections  
 2139 independent reflections  
 1962 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.009$

$\theta_{\text{max}} = 26.4^\circ$ ,  $\theta_{\text{min}} = 3.4^\circ$   
 $h = -18 \rightarrow 19$   
 $k = -8 \rightarrow 12$   
 $l = -6 \rightarrow 8$

*Refinement*

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.024$   
 $wR(F^2) = 0.067$   
 $S = 1.04$   
 2139 reflections  
 134 parameters  
 2 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  
 $w = 1/[\sigma^2(F_o^2) + (0.0355P)^2 + 0.5896P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.046$   
 $\Delta\rho_{\text{max}} = 0.39 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.28 \text{ e } \text{\AA}^{-3}$   
 Extinction correction: *SHELXL97* (Sheldrick,  
 2008),  $F_c^* = kFc^*[1 + 0.001x \text{Fc}^2 \lambda^3 / \sin(2\theta)]^{-1/4}$   
 Extinction coefficient: 0.0241 (14)

*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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.23433 (10)	0.44537 (16)	0.6229 (2)	0.0260 (3)
C2	0.18971 (12)	0.32599 (18)	0.5954 (3)	0.0342 (4)
H2	0.2152	0.2528	0.5447	0.041*
C3	0.10664 (13)	0.3162 (2)	0.6440 (3)	0.0394 (4)
H3	0.0760	0.2364	0.6266	0.047*
C4	0.07005 (11)	0.4256 (2)	0.7181 (3)	0.0346 (4)
C5	0.11456 (13)	0.5446 (2)	0.7494 (3)	0.0383 (4)
H5	0.0892	0.6170	0.8028	0.046*
C6	0.19736 (12)	0.55468 (18)	0.7003 (3)	0.0348 (4)
H6	0.2280	0.6344	0.7193	0.042*
N1	0.33843 (10)	0.58782 (15)	0.4143 (2)	0.0325 (3)
O1	0.40091 (8)	0.49624 (15)	0.73235 (19)	0.0411 (3)
O2	0.35592 (8)	0.33682 (13)	0.4620 (2)	0.0375 (3)
O3	0.55174 (9)	0.29958 (15)	-0.1344 (2)	0.0401 (3)
H31	0.5708 (15)	0.324 (2)	-0.231 (3)	0.048*
H32	0.5890 (13)	0.251 (2)	-0.076 (3)	0.048*
K1	0.43783 (2)	0.38377 (4)	0.12285 (5)	0.03214 (12)

Cl1	-0.03614 (3)	0.41509 (7)	0.76911 (8)	0.05237 (17)
Cl2	0.26012 (3)	0.56182 (5)	0.19737 (7)	0.04134 (14)
S1	0.33942 (3)	0.46167 (4)	0.55495 (6)	0.02637 (12)

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0254 (8)	0.0310 (8)	0.0227 (7)	-0.0002 (6)	0.0072 (6)	0.0017 (6)
C2	0.0348 (9)	0.0327 (9)	0.0374 (9)	-0.0024 (7)	0.0129 (7)	-0.0040 (7)
C3	0.0363 (10)	0.0435 (10)	0.0399 (10)	-0.0129 (8)	0.0110 (8)	-0.0030 (8)
C4	0.0251 (8)	0.0527 (11)	0.0274 (8)	-0.0012 (8)	0.0084 (6)	0.0046 (8)
C5	0.0378 (10)	0.0415 (10)	0.0390 (10)	0.0068 (8)	0.0161 (8)	-0.0020 (8)
C6	0.0359 (10)	0.0314 (9)	0.0393 (9)	-0.0032 (7)	0.0131 (8)	-0.0025 (7)
N1	0.0300 (7)	0.0362 (8)	0.0309 (7)	-0.0066 (6)	0.0045 (6)	0.0050 (6)
O1	0.0301 (6)	0.0599 (8)	0.0312 (7)	-0.0064 (6)	-0.0004 (5)	0.0055 (6)
O2	0.0377 (7)	0.0361 (7)	0.0424 (7)	0.0091 (5)	0.0172 (6)	0.0027 (5)
O3	0.0370 (7)	0.0464 (8)	0.0401 (7)	0.0061 (6)	0.0154 (6)	0.0044 (6)
K1	0.0309 (2)	0.0366 (2)	0.0309 (2)	-0.00472 (15)	0.01105 (14)	-0.00100 (15)
Cl1	0.0282 (2)	0.0845 (4)	0.0475 (3)	-0.0038 (2)	0.0153 (2)	0.0031 (3)
Cl2	0.0344 (2)	0.0542 (3)	0.0339 (2)	0.00022 (19)	0.00135 (17)	0.0115 (2)
S1	0.0224 (2)	0.0318 (2)	0.0258 (2)	0.00090 (15)	0.00658 (15)	0.00292 (15)

*Geometric parameters (Å, °)*

C1—C6	1.385 (2)	O1—K1 <sup>i</sup>	2.7965 (13)
C1—C2	1.382 (2)	O1—K1 <sup>ii</sup>	2.8547 (13)
C1—S1	1.7742 (16)	O2—S1	1.4489 (13)
C2—C3	1.386 (3)	O2—K1 <sup>iii</sup>	2.6940 (13)
C2—H2	0.9300	O2—K1	2.8576 (13)
C3—C4	1.373 (3)	O3—K1	2.8204 (14)
C3—H3	0.9300	O3—K1 <sup>iv</sup>	2.8714 (15)
C4—C5	1.380 (3)	O3—K1 <sup>v</sup>	3.1905 (16)
C4—Cl1	1.7414 (18)	O3—H31	0.808 (16)
C5—C6	1.383 (3)	O3—H32	0.808 (16)
C5—H5	0.9300	K1—O2 <sup>iv</sup>	2.6940 (13)
C6—H6	0.9300	K1—O1 <sup>i</sup>	2.7965 (13)
N1—S1	1.5883 (15)	K1—O1 <sup>vi</sup>	2.8547 (13)
N1—Cl2	1.7620 (15)	K1—O3 <sup>iii</sup>	2.8714 (15)
N1—K1	3.4014 (16)	K1—O3 <sup>v</sup>	3.1905 (16)
O1—S1	1.4460 (13)	K1—Cl2	3.3944 (6)
C6—C1—C2	120.77 (15)	O2 <sup>iv</sup> —K1—O1 <sup>vi</sup>	86.74 (4)
C6—C1—S1	118.90 (13)	O1 <sup>i</sup> —K1—O1 <sup>vi</sup>	100.42 (3)
C2—C1—S1	120.32 (13)	O3—K1—O1 <sup>vi</sup>	65.66 (4)
C3—C2—C1	119.51 (17)	O2 <sup>iv</sup> —K1—O2	87.06 (3)
C3—C2—H2	120.2	O1 <sup>i</sup> —K1—O2	106.27 (4)
C1—C2—H2	120.2	O3—K1—O2	149.71 (4)
C4—C3—C2	119.30 (17)	O1 <sup>vi</sup> —K1—O2	140.52 (4)

C4—C3—H3	120.4	O2 <sup>iv</sup> —K1—O3 <sup>iii</sup>	84.52 (4)
C2—C3—H3	120.4	O1 <sup>i</sup> —K1—O3 <sup>iii</sup>	69.60 (4)
C3—C4—C5	121.72 (16)	O3—K1—O3 <sup>iii</sup>	77.07 (3)
C3—C4—Cl1	119.22 (15)	O1 <sup>vi</sup> —K1—O3 <sup>iii</sup>	142.71 (4)
C5—C4—Cl1	119.05 (15)	O2—K1—O3 <sup>iii</sup>	75.11 (4)
C4—C5—C6	119.05 (17)	O2 <sup>iv</sup> —K1—O3 <sup>v</sup>	148.33 (4)
C4—C5—H5	120.5	O1 <sup>i</sup> —K1—O3 <sup>v</sup>	61.43 (4)
C6—C5—H5	120.5	O3—K1—O3 <sup>v</sup>	106.31 (3)
C1—C6—C5	119.64 (17)	O1 <sup>vi</sup> —K1—O3 <sup>v</sup>	68.17 (4)
C1—C6—H6	120.2	O2—K1—O3 <sup>v</sup>	99.95 (4)
C5—C6—H6	120.2	O3 <sup>iii</sup> —K1—O3 <sup>v</sup>	127.16 (3)
S1—N1—Cl2	108.69 (8)	O2 <sup>iv</sup> —K1—Cl2	99.11 (3)
S1—N1—K1	84.87 (6)	O1 <sup>i</sup> —K1—Cl2	114.67 (3)
Cl2—N1—K1	74.75 (5)	O3—K1—Cl2	149.42 (3)
S1—O1—K1 <sup>i</sup>	144.92 (8)	O1 <sup>vi</sup> —K1—Cl2	83.80 (3)
S1—O1—K1 <sup>ii</sup>	132.84 (8)	O2—K1—Cl2	58.85 (3)
K1 <sup>i</sup> —O1—K1 <sup>ii</sup>	79.58 (3)	O3 <sup>iii</sup> —K1—Cl2	133.39 (3)
S1—O2—K1 <sup>iii</sup>	130.01 (8)	O3 <sup>v</sup> —K1—Cl2	60.54 (3)
S1—O2—K1	110.21 (7)	O2 <sup>iv</sup> —K1—N1	120.37 (4)
K1 <sup>iii</sup> —O2—K1	102.77 (4)	O1 <sup>i</sup> —K1—N1	90.00 (4)
K1—O3—K1 <sup>iv</sup>	99.34 (4)	O3—K1—N1	159.60 (4)
K1—O3—K1 <sup>v</sup>	73.69 (3)	O1 <sup>vi</sup> —K1—N1	105.39 (4)
K1 <sup>iv</sup> —O3—K1 <sup>v</sup>	132.78 (5)	O2—K1—N1	47.20 (4)
K1—O3—H31	140.3 (17)	O3 <sup>iii</sup> —K1—N1	110.31 (4)
K1 <sup>iv</sup> —O3—H31	90.1 (17)	O3 <sup>v</sup> —K1—N1	53.77 (3)
K1 <sup>v</sup> —O3—H31	71.8 (17)	Cl2—K1—N1	30.05 (3)
K1—O3—H32	110.2 (17)	N1—Cl2—K1	75.20 (5)
K1 <sup>iv</sup> —O3—H32	102.1 (17)	O1—S1—O2	115.65 (8)
K1 <sup>v</sup> —O3—H32	124.4 (17)	O1—S1—N1	104.35 (8)
H31—O3—H32	105 (2)	O2—S1—N1	114.45 (8)
O2 <sup>iv</sup> —K1—O1 <sup>i</sup>	145.96 (4)	O1—S1—C1	107.86 (8)
O2 <sup>iv</sup> —K1—O3	78.54 (4)	O2—S1—C1	105.79 (8)
O1 <sup>i</sup> —K1—O3	74.49 (4)	N1—S1—C1	108.45 (8)
C6—C1—C2—C3	0.7 (3)	Cl2—N1—K1—O1 <sup>i</sup>	146.44 (5)
S1—C1—C2—C3	-178.16 (14)	S1—N1—K1—O3	-142.50 (10)
C1—C2—C3—C4	0.2 (3)	Cl2—N1—K1—O3	106.52 (12)
C2—C3—C4—C5	-1.4 (3)	S1—N1—K1—O1 <sup>vi</sup>	156.60 (5)
C2—C3—C4—Cl1	177.31 (14)	Cl2—N1—K1—O1 <sup>vi</sup>	45.63 (6)
C3—C4—C5—C6	1.6 (3)	S1—N1—K1—O2	9.86 (5)
Cl1—C4—C5—C6	-177.09 (14)	Cl2—N1—K1—O2	-101.12 (6)
C2—C1—C6—C5	-0.5 (3)	S1—N1—K1—O3 <sup>iii</sup>	-34.41 (7)
S1—C1—C6—C5	178.40 (14)	Cl2—N1—K1—O3 <sup>iii</sup>	-145.38 (5)
C4—C5—C6—C1	-0.6 (3)	S1—N1—K1—O3 <sup>v</sup>	-156.23 (8)
K1 <sup>iv</sup> —O3—K1—O2 <sup>iv</sup>	15.72 (4)	Cl2—N1—K1—O3 <sup>v</sup>	92.80 (6)
K1 <sup>v</sup> —O3—K1—O2 <sup>iv</sup>	147.72 (4)	S1—N1—K1—Cl2	110.97 (8)
K1 <sup>iv</sup> —O3—K1—O1 <sup>i</sup>	174.75 (5)	S1—N1—Cl2—K1	-79.04 (8)
K1 <sup>v</sup> —O3—K1—O1 <sup>i</sup>	-53.25 (3)	O2 <sup>iv</sup> —K1—Cl2—N1	138.20 (6)

K1 <sup>iv</sup> —O3—K1—O1 <sup>vi</sup>	-75.88 (5)	O1 <sup>i</sup> —K1—Cl2—N1	-37.47 (6)
K1 <sup>v</sup> —O3—K1—O1 <sup>vi</sup>	56.11 (4)	O3—K1—Cl2—N1	-138.93 (8)
K1 <sup>iv</sup> —O3—K1—O2	78.94 (9)	O1 <sup>vi</sup> —K1—Cl2—N1	-136.11 (6)
K1 <sup>v</sup> —O3—K1—O2	-149.06 (7)	O2—K1—Cl2—N1	57.27 (6)
K1 <sup>iv</sup> —O3—K1—O3 <sup>iii</sup>	102.66 (7)	O3 <sup>iii</sup> —K1—Cl2—N1	47.15 (7)
K1 <sup>v</sup> —O3—K1—O3 <sup>iii</sup>	-125.35 (3)	O3 <sup>v</sup> —K1—Cl2—N1	-67.72 (6)
K1 <sup>iv</sup> —O3—K1—O3 <sup>v</sup>	-132.00 (5)	K1 <sup>i</sup> —O1—S1—O2	85.59 (16)
K1 <sup>v</sup> —O3—K1—O3 <sup>v</sup>	0.0	K1 <sup>ii</sup> —O1—S1—O2	-67.43 (12)
K1 <sup>iv</sup> —O3—K1—Cl2	-72.81 (7)	K1 <sup>i</sup> —O1—S1—N1	-41.06 (17)
K1 <sup>v</sup> —O3—K1—Cl2	59.19 (7)	K1 <sup>ii</sup> —O1—S1—N1	165.92 (10)
K1 <sup>iv</sup> —O3—K1—N1	-143.50 (10)	K1 <sup>i</sup> —O1—S1—C1	-156.25 (14)
K1 <sup>v</sup> —O3—K1—N1	-11.50 (12)	K1 <sup>ii</sup> —O1—S1—C1	50.73 (13)
S1—O2—K1—O2 <sup>iv</sup>	-149.02 (5)	K1 <sup>iii</sup> —O2—S1—O1	26.81 (12)
K1 <sup>iii</sup> —O2—K1—O2 <sup>iv</sup>	69.17 (7)	K1—O2—S1—O1	-101.25 (8)
S1—O2—K1—O1 <sup>i</sup>	62.84 (8)	K1 <sup>iii</sup> —O2—S1—N1	148.17 (8)
K1 <sup>iii</sup> —O2—K1—O1 <sup>i</sup>	-78.97 (5)	K1—O2—S1—N1	20.11 (10)
S1—O2—K1—O3	149.81 (7)	K1 <sup>iii</sup> —O2—S1—C1	-92.49 (10)
K1 <sup>iii</sup> —O2—K1—O3	8.00 (11)	K1—O2—S1—C1	139.44 (7)
S1—O2—K1—O1 <sup>vi</sup>	-67.75 (10)	Cl2—N1—S1—O1	-176.41 (8)
K1 <sup>iii</sup> —O2—K1—O1 <sup>vi</sup>	150.44 (5)	K1—N1—S1—O1	111.60 (6)
S1—O2—K1—O3 <sup>iii</sup>	125.88 (8)	Cl2—N1—S1—O2	56.20 (11)
K1 <sup>iii</sup> —O2—K1—O3 <sup>iii</sup>	-15.93 (4)	K1—N1—S1—O2	-15.79 (8)
S1—O2—K1—O3 <sup>v</sup>	-0.13 (8)	Cl2—N1—S1—C1	-61.63 (10)
K1 <sup>iii</sup> —O2—K1—O3 <sup>v</sup>	-141.94 (4)	K1—N1—S1—C1	-133.62 (6)
S1—O2—K1—Cl2	-46.53 (6)	C6—C1—S1—O1	61.22 (16)
K1 <sup>iii</sup> —O2—K1—Cl2	171.66 (5)	C2—C1—S1—O1	-119.88 (15)
S1—O2—K1—N1	-11.49 (6)	C6—C1—S1—O2	-174.45 (14)
K1 <sup>iii</sup> —O2—K1—N1	-153.30 (7)	C2—C1—S1—O2	4.44 (16)
S1—N1—K1—O2 <sup>iv</sup>	61.26 (7)	C6—C1—S1—N1	-51.24 (16)
Cl2—N1—K1—O2 <sup>iv</sup>	-49.71 (6)	C2—C1—S1—N1	127.66 (14)
S1—N1—K1—O1 <sup>i</sup>	-102.59 (6)		

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

#### Hydrogen-bond geometry ( $\text{\AA}, ^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O3—H31 $\cdots$ N1 <sup>v</sup>	0.81 (2)	2.22 (2)	2.987 (2)	160 (2)
O3—H32 $\cdots$ N1 <sup>vii</sup>	0.81 (2)	2.18 (2)	2.967 (2)	166 (2)

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