Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Potassium *N*-chlorobenzenesulfonamidate monohydrate

B. Thimme Gowda,[a]* Sabine Foro,[b] Jozef Kožíšek[c] and Hartmut Fuess[b]

[a]Department of Chemistry, Mangalore University, Mangalagangotri-574 199, Mangalore, India, [b]Institute of Materials Science, Darmstadt University of Technology, Petersenstrasse 23, D-64287, Darmstadt, Germany, and [c]Department of Physical Chemistry, Slovak University of Technology, Radlinského 9, SK-812 37 Bratislava, Slovak Republic.
Correspondence e-mail: gowdabt@yahoo.com

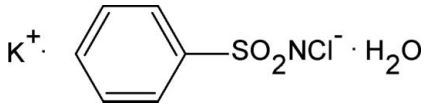
Received 12 May 2007; accepted 16 May 2007

Key indicators: single-crystal X-ray study; T = 303 K; mean σ(C–C) = 0.009 Å; R factor = 0.046; wR factor = 0.123; data-to-parameter ratio = 14.2.

In the title compound, $K^+\cdot C_6H_5ClNO_2S^-\cdot H_2O$, the S—N distance of 1.581 (4) Å is consistent with an S=N double bond. The ions and molecules in the crystal structure are held together by O—H···N hydrogen bonds.

Related literature

For related literature, see: George *et al.* (2000); Gowda & Shetty (2004); Gowda *et al.* (2003, 2005); Gowda, Jyothi *et al.* (2007); Gowda, Kozisek *et al.* (2007); Gowda, Savitha *et al.* (2007); Gowda, Srilatha *et al.* (2007); Jyothi & Gowda (2004); Olmstead & Power (1986).



Experimental

Crystal data

$K^+.C_6H_5ClNO_2S^-.H_2O$
M_r = 247.74
Orthorhombic, *Pbca*
a = 10.214 (1) Å
b = 6.8111 (4) Å
c = 28.336 (1) Å
V = 1971.3 (2) Å^3
Z = 8
Cu $K\alpha$ radiation
μ = 9.03 mm^{-1}
T = 303 (2) K
0.22 × 0.13 × 0.03 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.305, T_{max} = 0.798
1953 measured reflections
1756 independent reflections
1102 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
3 standard reflections
frequency: 120 min
intensity decay: 4.8%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.123
S = 0.99
1756 reflections
124 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H31O···N1^{i}	0.849 (10)	2.17 (3)	2.948 (5)	152 (5)
O3—H32O···N1^{ii}	0.846 (10)	2.21 (3)	3.007 (5)	156 (5)

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

Data collection: *CAD-4-PC* (Enraf–Nonius, 1996); cell refinement: *CAD-4-PC*; data reduction: *REDU4* (Stoe & Cie, 1987); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

BTG gratefully thanks the Alexander von Humboldt Foundation, Bonn, Germany for extensions of his research fellowship. JK thanks 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: BT2364).

References

George, E., Vivekanandan, S. & Sivakumar, K. (2000). *Acta Cryst.* C**56**, 1208–1209.
Gowda, B. T., Damodara, N. & Jyothi, K. (2005). *Int. J. Chem. Kinet.* **37**, 572–582.
Gowda, B. T., D'Souza, J. D. & Fuess, H. (2003). *Z. Naturforsch. Teil A*, **58**, 220–224.
Gowda, B. T., Jyothi, K., Foro, S., Kozisek, J. & Fuess, H. (2007). *Acta Cryst.* E**63**, m1644
Gowda, B. T., Kozisek, J., Tokarcik, M. & Fuess, H. (2007). *Acta Cryst.* E**63**, o2967
Gowda, B. T., Savitha, M. B., Kozisek, J., Tokarcik, M. & Fuess, H. (2007). *Acta Cryst.* E**63**, m1646.
Gowda, B. T. & Shetty, M. (2004). *J. Phys. Org. Chem.* **17**, 848–864.
Gowda, B. T., Srilatha, Foro, S., Kozisek, J. & Fuess, H. (2007). *Z. Naturforsch. Teil A*, **62**. In the press.
Jyothi, K. & Gowda, B. T. (2004). *Z. Naturforsch. Teil A*, **59**, 64–68.
Enraf–Nonius (1996). *CAD-4-PC*. Enraf–Nonius, Delft, The Netherlands.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Olmstead, M. M. & Power, P. P. (1986). *Inorg. Chem.* **25**, 4057–4058.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *PLATON*. *J. Appl. Cryst.* **36**, 7–13.
Stoe & Cie (1987). *REDU4*. Version 6.2c. Stoe & Cie GmbH, Darmstadt, Germany.

  doi:10.1107/S1600536807024178

supplementary materials

Acta Cryst. (2007). E**63**, m1688 [**doi:10.1107/S1600536807024178**]

Potassium *N*-chlorobenzenesulfonamidate monohydrate

B. T. Gowda, S. Foro, J. Kozísek and H. Fuess

Comment

The chemistry of arylsulfonamides and their N-halo compounds is of interest as they show distinct physical, chemical and biological properties. Many of these compounds exhibit pharmacological, fungicidal and herbicidal activities due to their oxidizing action in aqueous, partial aqueous and non-aqueous media. Thus, N-halo arylsulfonamides are of interest in synthetic, mechanistic, analytical and biological chemistry (Gowda *et al.*, 2005; Gowda & Shetty, 2004). In the present work, the structure of potassium *N*- chlorobenzenesulfonamde has been determined to explore the effect of substitution and replacing a sodium ion by a potassium ion on the solid state structures of *N*-chloroarylsulfonamides (Gowda, Jyothi *et al.*, 2007; Gowda, Kozisek *et al.*, 2007; Gowda, Savitha *et al.*, 2007; Gowda, Srilatha *et al.*, 2007). The structure of the title compound (Fig. 1) resembles those of sodium *N*-chloro- benzenesulfonamde (George *et al.*, 2000) and other sodium *N*-chloro-arylsulfonamdes (Olmstead & Power, 1986; Gowda, Jyothi *et al.*, 2007; Gowda, Kozisek *et al.*, 2007; Gowda, Savitha *et al.*, 2007; Gowda, Srilatha *et al.*, 2007). The S—N distance of 1.581 (4)Å is consistent with a S—N double bond. The molecules in the structure are held together by O—H···N hydrogen bonds.

Experimental

The title compound was prepared according to the literature method (Gowda *et al.*, 2003; Jyothi & Gowda, 2004). The purity of the compound was checked by determining its melting point. It was characterized by recording its infrared, NMR (Jyothi & Gowda, 2004) and NQR spectra (Gowda *et al.*, 2003). Single crystals of the title compound were obtained from a slow evaporation of its chloroform 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 = 0.93 Å and with U_{iso}(H) = 1.2 U_{eq}(C,*O*). The coordinates of the H atoms bonded to O were refined with a distance restraint of 0.84 (1) Å.

Figures

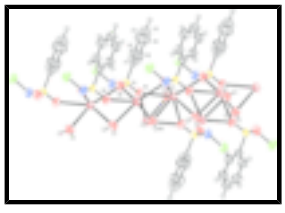


Fig. 1. Molecular structure of the title compound showing the atom labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

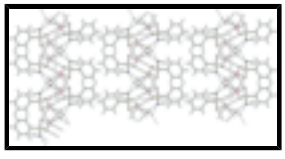


Fig. 2. Packing diagram viewed down the axis b

Potassium *N*-chlorobenzenesulfonamidate monohydrate

Crystal data

$K^+.C_6H_5ClNO_2S^-.H_2O$	F_{000} = 1008
M_r = 247.74	D_x = 1.669 Mg m^{-3}
Orthorhombic, *Pbca*	Cu *K*α radiation λ = 1.54180 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 25 reflections
a = 10.214 (1) Å	θ = 8.7–25.0º
b = 6.8111 (4) Å	μ = 9.03 mm^{-1}
c = 28.336 (1) Å	*T* = 303 (2) K
V = 1971.3 (2) Å^3	Laminar, colourless
Z = 8	0.22 × 0.13 × 0.03 mm

Data collection

Enraf–Nonius CAD-4 diffractometer	R_{int} = 0.035
Radiation source: fine-focus sealed tube	θ_{max} = 66.9º
Monochromator: graphite	θ_{min} = 3.1º
T = 303(2) K	*h* = 0→12
ω/2θ scans	*k* = 0→8
Absorption correction: Psi-scan (North *et al.*, 1968)	*l* = −3→33
T_{min} = 0.305, T_{max} = 0.798	3 standard reflections
1953 measured reflections	every 120 min
1756 independent reflections	intensity decay: 4.8%
1102 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.046	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.123	$w = 1/[\sigma^2(F_o^2) + (0.0611P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.99	$(\Delta/\sigma)_{max} < 0.001$
1756 reflections	$\Delta\rho_{max}$ = 0.27 e Å^{-3}
124 parameters	$\Delta\rho_{min}$ = −0.38 e Å^{-3}
2 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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	0.9541 (5)	0.7329 (6)	0.35902 (15)	0.0416 (10)
C2	0.8421 (5)	0.7230 (8)	0.33231 (18)	0.0579 (14)
H2	0.7687	0.6566	0.3434	0.070*
C3	0.8404 (8)	0.8127 (10)	0.2891 (2)	0.083 (2)
H3	0.7651	0.8057	0.2707	0.100*
C4	0.9464 (10)	0.9120 (9)	0.2723 (2)	0.090 (2)
H4	0.9435	0.9736	0.2430	0.108*
C5	1.0569 (8)	0.9193 (9)	0.2992 (2)	0.081 (2)
H5	1.1301	0.9855	0.2879	0.097*
C6	1.0622 (5)	0.8313 (8)	0.34244 (19)	0.0566 (13)
H6	1.1381	0.8378	0.3605	0.068*
N1	1.0836 (4)	0.4749 (6)	0.41555 (14)	0.0477 (10)
O1	0.9920 (3)	0.7666 (5)	0.44928 (11)	0.0544 (9)
O2	0.8372 (3)	0.5189 (5)	0.42122 (12)	0.0524 (9)
O3	0.7965 (4)	−0.1477 (6)	0.52779 (12)	0.0558 (9)
H31O	0.744 (4)	−0.130 (8)	0.5507 (12)	0.067*
H32O	0.823 (5)	−0.260 (4)	0.5366 (19)	0.067*
S1	0.96138 (11)	0.61724 (16)	0.41499 (4)	0.0386 (3)
Cl1	1.06255 (14)	0.2980 (2)	0.37111 (5)	0.0634 (4)
K1	0.88083 (10)	0.14650 (14)	0.46609 (4)	0.0455 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.049 (2)	0.036 (2)	0.039 (2)	0.004 (2)	0.003 (2)	−0.001 (2)
C2	0.068 (3)	0.050 (3)	0.056 (3)	0.004 (3)	−0.009 (3)	0.001 (3)
C3	0.115 (6)	0.072 (4)	0.062 (4)	0.026 (4)	−0.034 (4)	−0.001 (4)
C4	0.170 (8)	0.054 (4)	0.046 (3)	0.026 (5)	0.008 (5)	0.005 (3)
C5	0.128 (6)	0.050 (3)	0.064 (4)	−0.001 (4)	0.046 (4)	0.011 (3)
C6	0.063 (3)	0.049 (3)	0.058 (3)	−0.007 (3)	0.006 (3)	−0.003 (3)
N1	0.049 (2)	0.039 (2)	0.055 (2)	0.0110 (18)	−0.011 (2)	−0.013 (2)
O1	0.071 (2)	0.0441 (18)	0.0480 (19)	0.0053 (18)	−0.0023 (17)	−0.0096 (16)

O2	0.0446 (17)	0.0498 (19)	0.063 (2)	−0.0084 (16)	0.0104 (16)	0.0080 (18)
O3	0.060 (2)	0.049 (2)	0.058 (2)	0.003 (2)	0.0111 (17)	0.007 (2)
S1	0.0419 (6)	0.0346 (5)	0.0392 (5)	0.0010 (5)	0.0016 (5)	−0.0005 (5)
Cl1	0.0751 (9)	0.0501 (7)	0.0651 (8)	0.0151 (7)	−0.0009 (7)	−0.0155 (7)
K1	0.0518 (6)	0.0368 (5)	0.0480 (5)	−0.0006 (5)	−0.0067 (5)	0.0033 (5)

Geometric parameters (Å, °)

C1—C2	1.373 (7)	O2—S1	1.445 (3)
C1—C6	1.375 (7)	O2—K1^{iii}	2.708 (3)
C1—S1	1.772 (4)	O2—K1	2.872 (4)
C2—C3	1.370 (8)	O3—K1	2.795 (4)
C2—H2	0.9300	O3—K1^{iv}	2.881 (4)
C3—C4	1.362 (10)	O3—K1^{v}	3.301 (4)
C3—H3	0.9300	O3—H31O	0.849 (10)
C4—C5	1.362 (9)	O3—H32O	0.846 (10)
C4—H4	0.9300	S1—K1	3.6130 (15)
C5—C6	1.366 (8)	S1—K1^{iii}	3.7886 (15)
C5—H5	0.9300	Cl1—K1	3.4285 (18)
C6—H6	0.9300	K1—O2^{iv}	2.708 (3)
N1—S1	1.581 (4)	K1—O1^{i}	2.791 (3)
N1—Cl1	1.756 (4)	K1—O1^{vi}	2.865 (3)
N1—K1	3.368 (4)	K1—O3^{iii}	2.881 (4)
O1—S1	1.441 (3)	K1—O3^{v}	3.301 (4)
O1—K1^{i}	2.791 (3)	K1—K1^{v}	3.688 (2)
O1—K1^{ii}	2.865 (3)	K1—S1^{iv}	3.7886 (15)
C2—C1—C6	120.3 (5)	O1^{i}—K1—O2	105.39 (11)
C2—C1—S1	120.4 (4)	O3—K1—O2	149.56 (10)
C6—C1—S1	119.2 (4)	O1^{vi}—K1—O2	141.75 (10)
C3—C2—C1	118.8 (6)	O2^{iv}—K1—O3^{iii}	85.65 (11)
C3—C2—H2	120.6	O1^{i}—K1—O3^{iii}	70.61 (10)
C1—C2—H2	120.6	O3—K1—O3^{iii}	77.03 (8)
C4—C3—C2	121.6 (6)	O1^{vi}—K1—O3^{iii}	142.11 (10)
C4—C3—H3	119.2	O2—K1—O3^{iii}	75.02 (10)
C2—C3—H3	119.2	O2^{iv}—K1—O3^{v}	147.86 (11)
C5—C4—C3	118.7 (6)	O1^{i}—K1—O3^{v}	59.30 (10)
C5—C4—H4	120.6	O3—K1—O3^{v}	106.07 (9)
C3—C4—H4	120.6	O1^{vi}—K1—O3^{v}	67.38 (10)
C4—C5—C6	121.3 (6)	O2—K1—O3^{v}	100.14 (10)
C4—C5—H5	119.4	O3^{iii}—K1—O3^{v}	126.49 (7)
C6—C5—H5	119.4	O2^{iv}—K1—N1	121.29 (10)
C5—C6—C1	119.3 (6)	O1^{i}—K1—N1	86.46 (10)
C5—C6—H6	120.4	O3—K1—N1	158.67 (10)

C1—C6—H6	120.4	O1^{vi}—K1—N1	106.57 (10)
S1—N1—Cl1	108.5 (2)	O2—K1—N1	47.22 (9)
S1—N1—K1	85.74 (16)	O3^{iii}—K1—N1	108.76 (10)
Cl1—N1—K1	76.94 (14)	O3^{v}—K1—N1	53.59 (9)
S1—O1—K1^{i}	146.1 (2)	O2^{iv}—K1—Cl1	99.98 (8)
S1—O1—K1^{ii}	131.57 (19)	O1^{i}—K1—Cl1	111.02 (8)
K1^{i}—O1—K1^{ii}	81.38 (9)	O3—K1—Cl1	150.88 (8)
S1—O2—K1^{iii}	129.1 (2)	O1^{vi}—K1—Cl1	85.80 (8)
S1—O2—K1	109.11 (17)	O2—K1—Cl1	58.04 (7)
K1^{iii}—O2—K1	101.73 (10)	O3^{iii}—K1—Cl1	132.09 (8)
K1—O3—K1^{iv}	99.38 (11)	O3^{v}—K1—Cl1	59.99 (7)
K1—O3—K1^{v}	73.93 (9)	N1—K1—Cl1	29.93 (7)
K1^{iv}—O3—K1^{v}	131.37 (13)	O2^{iv}—K1—S1	106.50 (8)
K1—O3—H31O	125 (4)	O1^{i}—K1—S1	92.88 (8)
K1^{iv}—O3—H31O	98 (4)	O3—K1—S1	163.14 (9)
K1^{v}—O3—H31O	126 (4)	O1^{vi}—K1—S1	130.12 (8)
K1—O3—H32O	137 (4)	O2—K1—S1	22.21 (6)
K1^{iv}—O3—H32O	87 (4)	O3^{iii}—K1—S1	87.40 (8)
K1^{v}—O3—H32O	71 (4)	O3^{v}—K1—S1	77.96 (7)
H31O—O3—H32O	96 (5)	N1—K1—S1	25.88 (6)
O1—S1—O2	115.8 (2)	Cl1—K1—S1	45.17 (3)
O1—S1—N1	104.8 (2)	O2^{iv}—K1—K1^{v}	127.87 (8)
O2—S1—N1	114.1 (2)	O1^{i}—K1—K1^{v}	50.19 (7)
O1—S1—C1	107.4 (2)	O3—K1—K1^{v}	59.32 (8)
O2—S1—C1	106.2 (2)	O1^{vi}—K1—K1^{v}	48.43 (7)
N1—S1—C1	108.4 (2)	O2—K1—K1^{v}	144.19 (8)
O1—S1—K1	113.93 (14)	O3^{iii}—K1—K1^{v}	111.22 (8)
O2—S1—K1	48.69 (14)	O3^{v}—K1—K1^{v}	46.75 (7)
N1—S1—K1	68.38 (16)	N1—K1—K1^{v}	100.07 (7)
C1—S1—K1	138.02 (15)	Cl1—K1—K1^{v}	102.39 (5)
O1—S1—K1^{iii}	84.57 (15)	S1—K1—K1^{v}	122.60 (5)
O2—S1—K1^{iii}	33.70 (14)	O2^{iv}—K1—S1^{iv}	17.23 (7)
N1—S1—K1^{iii}	139.20 (16)	O1^{i}—K1—S1^{iv}	140.27 (8)
C1—S1—K1^{iii}	106.24 (16)	O3—K1—S1^{iv}	85.24 (8)
K1—S1—K1^{iii}	71.54 (3)	O1^{vi}—K1—S1^{iv}	104.75 (8)
N1—Cl1—K1	73.13 (14)	O2—K1—S1^{iv}	74.58 (7)
O2^{iv}—K1—O1^{i}	148.70 (11)	O3^{iii}—K1—S1^{iv}	71.19 (8)
O2^{iv}—K1—O3	79.05 (11)	O3^{v}—K1—S1^{iv}	160.31 (7)
O1^{i}—K1—O3	76.00 (11)	N1—K1—S1^{iv}	116.09 (7)
O2^{iv}—K1—O1^{vi}	87.59 (10)	Cl1—K1—S1^{iv}	102.43 (4)
O1^{i}—K1—O1^{vi}	98.62 (9)	S1—K1—S1^{iv}	95.94 (4)

O3—K1—O1^{vi}	65.09 (10)	K1^{v}—K1—S1^{iv}	141.23 (5)
O2^{iv}—K1—O2	87.02 (9)		
C6—C1—C2—C3	0.0 (8)	S1—O2—K1—S1^{iv}	−163.7 (2)
S1—C1—C2—C3	−179.4 (4)	K1^{iii}—O2—K1—S1^{iv}	57.42 (9)
C1—C2—C3—C4	−0.5 (9)	S1—N1—K1—O2^{iv}	60.56 (19)
C2—C3—C4—C5	0.8 (10)	Cl1—N1—K1—O2^{iv}	−49.51 (17)
C3—C4—C5—C6	−0.7 (10)	S1—N1—K1—O1^{i}	−104.06 (16)
C4—C5—C6—C1	0.2 (9)	Cl1—N1—K1—O1^{i}	145.87 (14)
C2—C1—C6—C5	0.1 (7)	S1—N1—K1—O3	−138.5 (3)
S1—C1—C6—C5	179.6 (4)	Cl1—N1—K1—O3	111.4 (3)
K1^{i}—O1—S1—O2	94.6 (4)	S1—N1—K1—O1^{vi}	158.00 (14)
K1^{ii}—O1—S1—O2	−69.3 (3)	Cl1—N1—K1—O1^{vi}	47.93 (15)
K1^{i}—O1—S1—N1	−31.9 (4)	S1—N1—K1—O2	10.75 (13)
K1^{ii}—O1—S1—N1	164.2 (2)	Cl1—N1—K1—O2	−99.32 (17)
K1^{i}—O1—S1—C1	−147.0 (4)	S1—N1—K1—O3^{iii}	−35.91 (17)
K1^{ii}—O1—S1—C1	49.1 (3)	Cl1—N1—K1—O3^{iii}	−145.98 (13)
K1^{i}—O1—S1—K1	40.6 (4)	S1—N1—K1—O3^{v}	−157.9 (2)
K1^{ii}—O1—S1—K1	−123.28 (19)	Cl1—N1—K1—O3^{v}	92.03 (15)
K1^{i}—O1—S1—K1^{iii}	107.7 (3)	S1—N1—K1—Cl1	110.1 (2)
K1^{ii}—O1—S1—K1^{iii}	−56.2 (2)	Cl1—N1—K1—S1	−110.1 (2)
K1^{iii}—O2—S1—O1	23.9 (3)	S1—N1—K1—K1^{v}	−152.57 (13)
K1—O2—S1—O1	−100.1 (2)	Cl1—N1—K1—K1^{v}	97.36 (12)
K1^{iii}—O2—S1—N1	145.6 (2)	S1—N1—K1—S1^{iv}	41.80 (16)
K1—O2—S1—N1	21.6 (3)	Cl1—N1—K1—S1^{iv}	−68.27 (13)
K1^{iii}—O2—S1—C1	−95.2 (3)	N1—Cl1—K1—O2^{iv}	138.71 (15)
K1—O2—S1—C1	140.88 (18)	N1—Cl1—K1—O1^{i}	−36.86 (15)
K1^{iii}—O2—S1—K1	123.9 (3)	N1—Cl1—K1—O3	−135.9 (2)
K1—O2—S1—K1^{iii}	−123.9 (3)	N1—Cl1—K1—O1^{vi}	−134.49 (15)
Cl1—N1—S1—O1	−175.0 (2)	N1—Cl1—K1—O2	58.61 (15)
K1—N1—S1—O1	110.29 (16)	N1—Cl1—K1—O3^{iii}	45.55 (17)
Cl1—N1—S1—O2	57.4 (3)	N1—Cl1—K1—O3^{v}	−68.25 (15)
K1—N1—S1—O2	−17.3 (2)	N1—Cl1—K1—S1	35.31 (13)
Cl1—N1—S1—C1	−60.6 (3)	N1—Cl1—K1—K1^{v}	−88.70 (13)
K1—N1—S1—C1	−135.32 (17)	N1—Cl1—K1—S1^{iv}	121.32 (13)
Cl1—N1—S1—K1	74.7 (2)	O1—S1—K1—O2^{iv}	133.79 (18)
Cl1—N1—S1—K1^{iii}	86.1 (3)	O2—S1—K1—O2^{iv}	29.67 (14)
K1—N1—S1—K1^{iii}	11.4 (2)	N1—S1—K1—O2^{iv}	−129.09 (17)
C2—C1—S1—O1	−122.0 (4)	C1—S1—K1—O2^{iv}	−35.3 (3)
C6—C1—S1—O1	58.6 (4)	K1^{iii}—S1—K1—O2^{iv}	58.70 (9)
C2—C1—S1—O2	2.5 (4)	O1—S1—K1—O1^{i}	−21.3 (2)
C6—C1—S1—O2	−177.0 (4)	O2—S1—K1—O1^{i}	−125.4 (2)

C2—C1—S1—N1	125.4 (4)	N1—S1—K1—O1^{i}	75.80 (17)
C6—C1—S1—N1	−54.1 (4)	C1—S1—K1—O1^{i}	169.6 (2)
C2—C1—S1—K1	47.6 (5)	K1^{iii}—S1—K1—O1^{i}	−96.41 (7)
C6—C1—S1—K1	−131.9 (3)	O1—S1—K1—O3	26.7 (3)
C2—C1—S1—K1^{iii}	−32.7 (4)	O2—S1—K1—O3	−77.4 (4)
C6—C1—S1—K1^{iii}	147.9 (4)	N1—S1—K1—O3	123.8 (3)
S1—N1—Cl1—K1	−80.9 (2)	C1—S1—K1—O3	−142.4 (4)
K1^{iv}—O3—K1—O2^{iv}	16.83 (11)	K1^{iii}—S1—K1—O3	−48.4 (3)
K1^{v}—O3—K1—O2^{iv}	147.33 (11)	O1—S1—K1—O1^{vi}	−125.1 (2)
K1^{iv}—O3—K1—O1^{i}	177.77 (13)	O2—S1—K1—O1^{vi}	130.8 (2)
K1^{v}—O3—K1—O1^{i}	−51.73 (8)	N1—S1—K1—O1^{vi}	−28.01 (18)
K1^{iv}—O3—K1—O1^{vi}	−75.61 (12)	C1—S1—K1—O1^{vi}	65.8 (3)
K1^{v}—O3—K1—O1^{vi}	54.89 (9)	K1^{iii}—S1—K1—O1^{vi}	159.78 (10)
K1^{iv}—O3—K1—O2	81.1 (2)	O1—S1—K1—O2	104.1 (3)
K1^{v}—O3—K1—O2	−148.38 (19)	N1—S1—K1—O2	−158.8 (2)
K1^{iv}—O3—K1—O3^{iii}	104.84 (16)	C1—S1—K1—O2	−65.0 (3)
K1^{v}—O3—K1—O3^{iii}	−124.66 (8)	K1^{iii}—S1—K1—O2	29.03 (19)
K1^{iv}—O3—K1—O3^{v}	−130.50 (13)	O1—S1—K1—O3^{iii}	49.11 (18)
K1^{v}—O3—K1—O3^{v}	0.0	O2—S1—K1—O3^{iii}	−55.0 (2)
K1^{iv}—O3—K1—N1	−146.7 (2)	N1—S1—K1—O3^{iii}	146.23 (17)
K1^{v}—O3—K1—N1	−16.2 (3)	C1—S1—K1—O3^{iii}	−120.0 (2)
K1^{iv}—O3—K1—Cl1	−74.04 (19)	K1^{iii}—S1—K1—O3^{iii}	−25.98 (7)
K1^{v}—O3—K1—Cl1	56.46 (18)	O1—S1—K1—O3^{v}	−79.09 (17)
K1^{iv}—O3—K1—S1	127.9 (3)	O2—S1—K1—O3^{v}	176.8 (2)
K1^{v}—O3—K1—S1	−101.6 (3)	N1—S1—K1—O3^{v}	18.03 (16)
K1^{iv}—O3—K1—K1^{v}	−130.50 (13)	C1—S1—K1—O3^{v}	111.8 (2)
K1^{iv}—O3—K1—S1^{iv}	33.07 (9)	K1^{iii}—S1—K1—O3^{v}	−154.17 (7)
K1^{v}—O3—K1—S1^{iv}	163.57 (7)	O1—S1—K1—N1	−97.1 (2)
S1—O2—K1—O2^{iv}	−151.62 (13)	O2—S1—K1—N1	158.8 (2)
K1^{iii}—O2—K1—O2^{iv}	69.51 (17)	C1—S1—K1—N1	93.8 (3)
S1—O2—K1—O1^{i}	57.6 (2)	K1^{iii}—S1—K1—N1	−172.21 (16)
K1^{iii}—O2—K1—O1^{i}	−81.31 (12)	O1—S1—K1—Cl1	−138.48 (17)
S1—O2—K1—O3	146.03 (19)	O2—S1—K1—Cl1	117.4 (2)
K1^{iii}—O2—K1—O3	7.2 (3)	N1—S1—K1—Cl1	−41.36 (15)
S1—O2—K1—O1^{vi}	−69.3 (3)	C1—S1—K1—Cl1	52.4 (2)
K1^{iii}—O2—K1—O1^{vi}	151.81 (13)	K1^{iii}—S1—K1—Cl1	146.43 (5)
S1—O2—K1—O3^{iii}	122.1 (2)	O1—S1—K1—K1^{v}	−64.54 (17)
K1^{iii}—O2—K1—O3^{iii}	−16.78 (11)	O2—S1—K1—K1^{v}	−168.7 (2)
S1—O2—K1—O3^{v}	−3.2 (2)	N1—S1—K1—K1^{v}	32.58 (16)
K1^{iii}—O2—K1—O3^{v}	−142.05 (10)	C1—S1—K1—K1^{v}	126.4 (2)
S1—O2—K1—N1	−12.44 (15)	K1^{iii}—S1—K1—K1^{v}	−139.63 (4)

K1^{iii}—O2—K1—N1	−151.31 (18)	O1—S1—K1—S1^{iv}	119.89 (16)
S1—O2—K1—Cl1	−47.91 (15)	O2—S1—K1—S1^{iv}	15.8 (2)
K1^{iii}—O2—K1—Cl1	173.22 (14)	N1—S1—K1—S1^{iv}	−142.99 (15)
K1^{iii}—O2—K1—S1	−138.9 (3)	C1—S1—K1—S1^{iv}	−49.2 (2)
S1—O2—K1—K1^{v}	16.4 (3)	K1^{iii}—S1—K1—S1^{iv}	44.80 (4)
K1^{iii}—O2—K1—K1^{v}	−122.42 (10)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H31O···N1^{vii}	0.849 (10)	2.17 (3)	2.948 (5)	152 (5)
O3—H32O···N1^{v}	0.846 (10)	2.21 (3)	3.007 (5)	156 (5)

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

Fig. 1

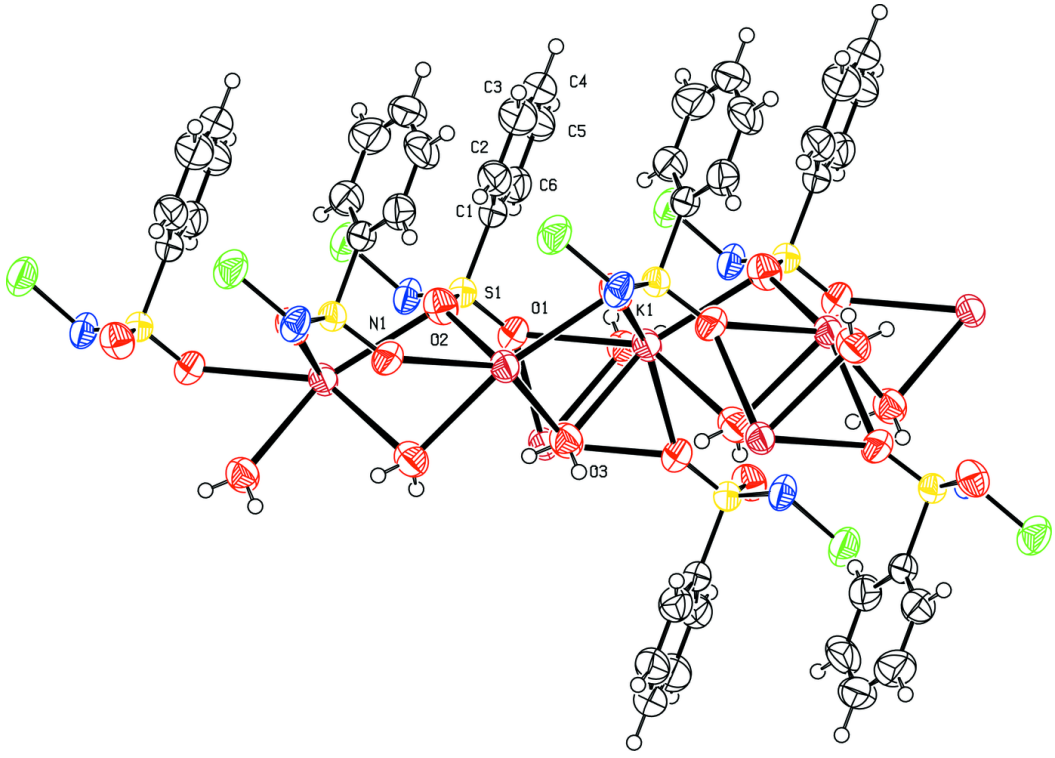


Fig. 2