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Potassium 4-chlorobenzenesulfonate

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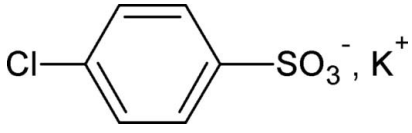
Key indicators: single-crystal X-ray study; T = 303 K; mean σ(S–C) = 0.002 Å; disorder in main residue; R factor = 0.037; wR factor = 0.098; data-to-parameter ratio = 12.5.

The structure of the title compound (K4CBS), poly[μ_4-4-chlorobenzenesulfonato-potassium(I)], $[K(C_6H_4ClO_3S)]_n$, resembles that of silver 4-chlorobenzenesulfonate with somewhat different geometric parameters. The supramolecular structure is constructed by Cl atoms bridging the K^+ ions. Each K^+ ion is heptacoordinated by two Cl ligands and four sulfonate groups, one of them in a monodentate and three in a bidentate fashion. Thus, each sulfonate group coordinates four K^+ ions.

Related literature

For related literature, see: Bernardinelli *et al.* (1991); Gowda *et al.* (2002, 2003); Gowda, Jyothi *et al.* (2007); Gowda, Kožíšek *et al.* (2007); Gowda, Nayak *et al.* (2007); Oae *et al.* (1981).



Experimental

Crystal data

$[K(C_6H_4ClO_3S)]$
M_r = 230.70
Monoclinic, $P2_1/m$
a = 6.1688 (6) Å
b = 6.813 (1) Å
c = 9.804 (1) Å
β = 97.236 (8)°
V = 408.76 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.19 mm^{-1}
T = 303 (2) K
0.44 × 0.32 × 0.06 mm

Data collection

Oxford Diffraction Xcalibur diffractometer with Sapphire CCD detector
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2006), based on Clark & Reid (1995)
T_{min} = 0.623, T_{max} = 0.932
6343 measured reflections
912 independent reflections
799 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.098
S = 1.09
912 reflections
73 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.55 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 e Å^{-3}

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: *PLATON* (Spek 2003) and *ORTEP-3* (Farrugia, 1997); 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: IM2021).

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supplementary materials

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Potassium 4-chlorobenzenesulfonate

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Comment

As part of a study on the substituent effects on the solid state structures of chemically and biologically significant compounds (Gowda *et al.*, 2003, Gowda, Jyothi *et al.*, 2007; Gowda, Kozisek *et al.*, 2007; Gowda, Nayak *et al.*, 2007), in the present work, the structure of potassium 4-chloro-benzenesulfonate (K4CBS) has been determined. The structure of K4CBS (Fig. 1) resembles that of silver 4-chloro-benzenesulfonate (Ag4CBS) with somewhat different geometric parameters (Bernardinelli *et al.*, 1991). K4CBS crystallizes in monoclinic $P2_1/m$ space group compared to the monoclinic $P2_1/c$ space group observed for Ag4CBS ((Bernardinelli *et al.*, 1991). The potassium ion shows hepta coordination with two Chloro ligands and five sulfonato O atoms of four different 4-chloro-benzenesulfonato anions, one of them in a monodentate and three in a bidentate way (Fig. 2). This potassium coordination therefore results in a three dimensional supramolecular structure (Fig. 2). The benzene rings are disordered over two different conformations with site occupation factors of 0.5 each.

Experimental

The title compound was prepared from 4-chloro-sulfonylchloride prepared as an intermediate compound in the preparation of 4-chloro-benzenesulfonamide (Gowda *et al.*, 2002). 4-Chlorosulfonylchloride was hydrolysed by treating with aqueous KOH to obtain the title compound. The purity of the compound was checked by determining its melting point (Oae *et al.*, 1981) and by recording its infrared spectra. 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 = 0.93Å and with U_{iso}(H) = 1.2 U_{eq}(C). No restraints were applied to non-hydrogen atoms.

Figures

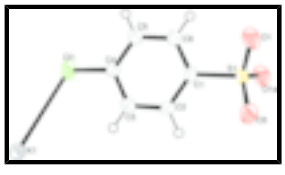

Fig. 1. Molecular structure of a monomeric unit of the title compound showing the atom labeling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radii.

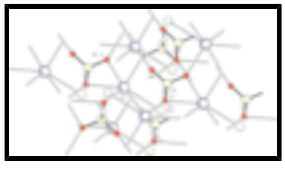

Fig. 2. Crystal structure of the title compound.

poly[μ4-4-chlorobenzenesulfonato-potassium(I)]

Crystal data

[K($C_6H_4ClO_3S$)]	F_{000} = 232
M_r = 230.70	D_x = 1.874 Mg m^{-3}
Monoclinic, $P2_1/m$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P2yb	Cell parameters from 3635 reflections
a = 6.1688 (6) Å	θ = 2.1–27.4º
b = 6.813 (1) Å	μ = 1.19 mm^{-1}
c = 9.804 (1) Å	T = 303 (2) K
β = 97.236 (8)º	Prism, colourless
V = 408.76 (8) Å^3	0.44 × 0.32 × 0.06 mm
Z = 2	

Data collection

Oxford Diffraction Xcalibur diffractometer with Sapphire CCD detector	912 independent reflections
Radiation source: Enhance (Mo) X-ray Source	799 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.031
Detector resolution: 8.4012 pixels mm^{-1}	θ_{max} = 26.3º
T = 303(2) K	θ_{min} = 3.3º
Rotation method data acquisition using ω and φ scans	h = −7→7
Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2006)	k = −8→8
T_{min} = 0.623, T_{max} = 0.932	l = −12→12
6343 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.037	H-atom parameters constrained
$wR(F^2)$ = 0.098	$w = 1/[\sigma^2(F_o^2) + (0.0419P)^2 + 0.7009P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.09	$(\Delta/\sigma)_{max}$ = 0.003
912 reflections	$\Delta\rho_{max}$ = 0.55 e Å^{-3}
73 parameters	$\Delta\rho_{min}$ = −0.53 e Å^{-3}
Primary atom site location: structure-invariant direct methods	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 $F^2 > 2\text{sigma}(F^2)$ 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}	Occ. (<1)
K1	0.79613 (14)	0.2500	1.00401 (9)	0.0328 (3)	
Cl1	0.27258 (19)	0.2500	0.84491 (10)	0.0466 (3)	
S1	0.29017 (16)	0.2500	0.20716 (9)	0.0281 (3)	
O1	0.1741 (4)	0.4253 (3)	0.15569 (19)	0.0422 (5)	
O3	0.5178 (5)	0.2500	0.1871 (3)	0.0492 (9)	
C1	0.2845 (4)	0.2500	0.38707 (19)	0.0262 (8)	
C2	0.4690 (4)	0.1982 (4)	0.4761 (3)	0.0287 (15)	0.50
H2	0.5946	0.1567	0.4411	0.034*	0.50
C3	0.4658 (4)	0.2084 (7)	0.6175 (2)	0.034 (2)	0.50
H3	0.5892	0.1737	0.6770	0.041*	0.50
C4	0.2781 (5)	0.2704 (8)	0.6697 (2)	0.0252 (11)	0.50
C5	0.0935 (4)	0.3223 (7)	0.5807 (3)	0.0343 (13)	0.50
H5	−0.0321	0.3638	0.6157	0.041*	0.50
C6	0.0968 (4)	0.3120 (4)	0.4394 (3)	0.0304 (12)	0.50
H6	−0.0267	0.3467	0.3798	0.037*	0.50

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
K1	0.0309 (5)	0.0356 (5)	0.0326 (5)	0.000	0.0069 (3)	0.000
Cl1	0.0505 (6)	0.0685 (8)	0.0223 (5)	0.000	0.0102 (4)	0.000
S1	0.0327 (5)	0.0315 (5)	0.0200 (4)	0.000	0.0031 (3)	0.000
O1	0.0594 (13)	0.0351 (12)	0.0305 (10)	0.0043 (10)	0.0001 (9)	0.0074 (9)
O3	0.0364 (16)	0.083 (3)	0.0302 (15)	0.000	0.0105 (13)	0.000
C1	0.0314 (19)	0.0275 (19)	0.0198 (17)	0.000	0.0031 (14)	0.000
C2	0.027 (2)	0.033 (4)	0.027 (2)	0.0067 (18)	0.0070 (18)	−0.0005 (18)
C3	0.033 (2)	0.040 (7)	0.029 (2)	0.008 (2)	−0.0001 (18)	0.003 (2)
C4	0.035 (2)	0.019 (3)	0.0221 (18)	0.005 (3)	0.0055 (15)	0.006 (3)
C5	0.030 (2)	0.043 (3)	0.030 (3)	0.002 (2)	0.006 (2)	−0.001 (2)
C6	0.028 (2)	0.030 (3)	0.032 (3)	0.0013 (18)	0.001 (2)	−0.0009 (19)

Geometric parameters (Å, °)

K1—O3^{i}	2.636 (3)	O1—K1^{xiii}	2.864 (2)
K1—O1^{ii}	2.730 (2)	O3—K1^{xiv}	2.636 (3)
K1—O1^{iii}	2.730 (2)	C1—C2	1.3900
K1—O1^{iv}	2.864 (2)	C1—C2^{xi}	1.3900 (15)
K1—O1^{v}	2.864 (2)	C1—C6^{xi}	1.3900 (18)
K1—Cl1	3.4051 (14)	C1—C6	1.3900
K1—S1^{iv}	3.4243 (13)	C2—C3	1.3900
K1—Cl1^{vi}	3.4967 (14)	C2—C3^{xi}	1.527 (4)
K1—Cl1^{vii}	3.7598 (7)	C2—H2	0.9300
K1—Cl1^{viii}	3.7598 (7)	C3—C4^{xi}	1.3320 (12)
K1—K1^{ix}	4.2411 (11)	C3—C4	1.3900
K1—K1^{x}	4.2411 (11)	C3—C2^{xi}	1.527 (3)
Cl1—C4^{xi}	1.728 (2)	C3—H3	0.9300
Cl1—C4	1.728 (2)	C4—C3^{xi}	1.3320 (11)
Cl1—K1^{xii}	3.4967 (14)	C4—C5	1.3900
Cl1—K1^{vii}	3.7598 (7)	C4—C5^{xi}	1.485 (4)
Cl1—K1^{viii}	3.7598 (7)	C5—C6	1.3900
S1—O3	1.442 (3)	C5—C4^{xi}	1.485 (4)
S1—O1^{xi}	1.450 (2)	C5—C6^{xi}	1.663 (3)
S1—O1	1.450 (2)	C5—H5	0.9300
S1—C1	1.769 (2)	C6—C5^{xi}	1.663 (5)
S1—K1^{xiii}	3.4243 (13)	C6—H6	0.9300
O1—K1^{iii}	2.730 (2)		
O3^{i}—K1—O1^{ii}	119.17 (6)	O1^{xi}—S1—C1	106.03 (10)
O3^{i}—K1—O1^{iii}	119.17 (5)	O1—S1—C1	106.03 (10)
O1^{ii}—K1—O1^{iii}	108.27 (9)	O3—S1—K1^{xiii}	137.00 (13)
O3^{i}—K1—O1^{iv}	101.76 (8)	O1^{xi}—S1—K1^{xiii}	55.48 (9)
O1^{ii}—K1—O1^{iv}	121.78 (5)	O1—S1—K1^{xiii}	55.48 (9)
O1^{iii}—K1—O1^{iv}	81.41 (6)	C1—S1—K1^{xiii}	116.88 (10)
O3^{i}—K1—O1^{v}	101.76 (8)	S1—O1—K1^{iii}	143.24 (13)
O1^{ii}—K1—O1^{v}	81.41 (6)	S1—O1—K1^{xiii}	99.86 (11)
O1^{iii}—K1—O1^{v}	121.78 (5)	K1^{iii}—O1—K1^{xiii}	98.59 (6)
O1^{iv}—K1—O1^{v}	49.30 (9)	S1—O3—K1^{xiv}	145.25 (18)
O3^{i}—K1—Cl1	69.54 (7)	C2—C1—C2^{xi}	29.4 (2)
O1^{ii}—K1—Cl1	82.28 (5)	C2—C1—C6^{xi}	110.21 (9)
O1^{iii}—K1—Cl1	82.28 (5)	C2^{xi}—C1—C6^{xi}	120.00 (7)
O1^{iv}—K1—Cl1	154.30 (5)	C2—C1—C6	120.0
O1^{v}—K1—Cl1	154.30 (5)	C2^{xi}—C1—C6	110.21 (10)

O3^{i}—K1—S1^{iv}	102.25 (7)	C6^{xi}—C1—C6	35.4 (2)
O1^{ii}—K1—S1^{iv}	102.38 (5)	C2—C1—S1	120.59 (16)
O1^{iii}—K1—S1^{iv}	102.38 (5)	C2^{xi}—C1—S1	120.59 (16)
O1^{iv}—K1—S1^{iv}	24.66 (4)	C6^{xi}—C1—S1	119.33 (16)
O1^{v}—K1—S1^{iv}	24.66 (4)	C6—C1—S1	119.33 (15)
Cl1—K1—S1^{iv}	171.79 (4)	C2^{xi}—C2—C1	75.3
O3^{i}—K1—Cl1^{vi}	163.75 (8)	C2^{xi}—C2—C3	87.1
O1^{ii}—K1—Cl1^{vi}	67.86 (5)	C1—C2—C3	120.0
O1^{iii}—K1—Cl1^{vi}	67.86 (5)	C2^{xi}—C2—C3^{xi}	65.4 (3)
O1^{iv}—K1—Cl1^{vi}	63.67 (5)	C1—C2—C3^{xi}	111.15 (16)
O1^{v}—K1—Cl1^{vi}	63.67 (5)	C3—C2—C3^{xi}	21.8 (3)
Cl1—K1—Cl1^{vi}	126.71 (4)	C2^{xi}—C2—H2	107.7
S1^{iv}—K1—Cl1^{vi}	61.51 (3)	C1—C2—H2	120.0
O3^{i}—K1—Cl1^{vii}	67.43 (2)	C3—C2—H2	120.0
O1^{ii}—K1—Cl1^{vii}	168.32 (5)	C3^{xi}—C2—H2	124.6
O1^{iii}—K1—Cl1^{vii}	60.71 (5)	C3^{xi}—C3—C4^{xi}	83.8 (5)
O1^{iv}—K1—Cl1^{vii}	62.77 (5)	C3^{xi}—C3—C4	72.3
O1^{v}—K1—Cl1^{vii}	107.35 (5)	C4^{xi}—C3—C4	11.5 (5)
Cl1—K1—Cl1^{vii}	91.89 (2)	C3^{xi}—C3—C2	92.9
S1^{iv}—K1—Cl1^{vii}	84.67 (2)	C4^{xi}—C3—C2	120.8
Cl1^{vi}—K1—Cl1^{vii}	108.57 (2)	C4—C3—C2	120.0
O3^{i}—K1—Cl1^{viii}	67.43 (2)	C3^{xi}—C3—C2^{xi}	65.4 (2)
O1^{ii}—K1—Cl1^{viii}	60.71 (5)	C4^{xi}—C3—C2^{xi}	114.5 (3)
O1^{iii}—K1—Cl1^{viii}	168.32 (5)	C4—C3—C2^{xi}	108.33 (10)
O1^{iv}—K1—Cl1^{viii}	107.35 (5)	C2—C3—C2^{xi}	27.5 (2)
O1^{v}—K1—Cl1^{viii}	62.77 (5)	C3^{xi}—C3—H3	104.7
Cl1—K1—Cl1^{viii}	91.89 (2)	C4^{xi}—C3—H3	117.9
S1^{iv}—K1—Cl1^{viii}	84.67 (2)	C4—C3—H3	120.0
Cl1^{vi}—K1—Cl1^{viii}	108.57 (2)	C2—C3—H3	120.0
Cl1^{vii}—K1—Cl1^{viii}	129.93 (4)	C2^{xi}—C3—H3	124.9
O3^{i}—K1—K1^{ix}	116.83 (4)	C4^{xi}—C4—C3^{xi}	96.2 (4)
O1^{ii}—K1—K1^{ix}	123.87 (6)	C4^{xi}—C4—C5	104.7
O1^{iii}—K1—K1^{ix}	41.89 (5)	C3^{xi}—C4—C5	114.44 (14)
O1^{iv}—K1—K1^{ix}	39.52 (4)	C4^{xi}—C4—C3	72.3
O1^{v}—K1—K1^{ix}	84.18 (5)	C3^{xi}—C4—C3	23.9 (4)
Cl1—K1—K1^{ix}	121.47 (2)	C5—C4—C3	120.0
S1^{iv}—K1—K1^{ix}	61.60 (2)	C4^{xi}—C4—C5^{xi}	64.8 (3)
Cl1^{vi}—K1—K1^{ix}	57.17 (2)	C3^{xi}—C4—C5^{xi}	117.31 (19)
Cl1^{vii}—K1—K1^{ix}	51.400 (19)	C5—C4—C5^{xi}	39.9 (3)
Cl1^{viii}—K1—K1^{ix}	146.26 (4)	C3—C4—C5^{xi}	105.45 (15)
O3^{i}—K1—K1^{x}	116.83 (4)	C4^{xi}—C4—Cl1	85.4 (3)

O1^{ii}—K1—K1^{x}	41.89 (5)	C3^{xi}—C4—Cl1	121.20 (18)
O1^{iii}—K1—K1^{x}	123.87 (6)	C5—C4—Cl1	121.86 (18)
O1^{iv}—K1—K1^{x}	84.18 (5)	C3—C4—Cl1	117.62 (19)
O1^{v}—K1—K1^{x}	39.52 (4)	C5^{xi}—C4—Cl1	116.1 (3)
Cl1—K1—K1^{x}	121.47 (2)	C5^{xi}—C5—C4	75.3
S1^{iv}—K1—K1^{x}	61.60 (2)	C5^{xi}—C5—C6	87.1
Cl1^{vi}—K1—K1^{x}	57.17 (2)	C4—C5—C6	120.0
Cl1^{vii}—K1—K1^{x}	146.26 (4)	C5^{xi}—C5—C4^{xi}	64.8 (4)
Cl1^{viii}—K1—K1^{x}	51.400 (19)	C4—C5—C4^{xi}	10.5 (4)
K1^{ix}—K1—K1^{x}	106.88 (4)	C6—C5—C4^{xi}	117.29 (11)
C4^{xi}—Cl1—C4	9.3 (3)	C5^{xi}—C5—C6^{xi}	56.61 (17)
C4^{xi}—Cl1—K1	108.62 (11)	C4—C5—C6^{xi}	106.79 (9)
C4—Cl1—K1	108.62 (11)	C6—C5—C6^{xi}	30.52 (17)
C4^{xi}—Cl1—K1^{xii}	124.49 (12)	C4^{xi}—C5—C6^{xi}	99.6 (3)
C4—Cl1—K1^{xii}	124.49 (11)	C5^{xi}—C5—H5	107.7
K1—Cl1—K1^{xii}	126.71 (4)	C4—C5—H5	120.0
C4^{xi}—Cl1—K1^{vii}	118.81 (18)	C6—C5—H5	120.0
C4—Cl1—K1^{vii}	109.62 (17)	C4^{xi}—C5—H5	121.7
K1—Cl1—K1^{vii}	88.11 (2)	C6^{xi}—C5—H5	124.9
K1^{xii}—Cl1—K1^{vii}	71.43 (2)	C6^{xi}—C6—C5	92.9
C4^{xi}—Cl1—K1^{viii}	109.62 (17)	C6^{xi}—C6—C1	72.3
C4—Cl1—K1^{viii}	118.81 (18)	C5—C6—C1	120.0
K1—Cl1—K1^{viii}	88.11 (2)	C6^{xi}—C6—C5^{xi}	56.6 (3)
K1^{xii}—Cl1—K1^{viii}	71.43 (2)	C5—C6—C5^{xi}	36.3 (3)
K1^{vii}—Cl1—K1^{viii}	129.93 (4)	C1—C6—C5^{xi}	103.76 (14)
O3—S1—O1^{xi}	113.52 (11)	C6^{xi}—C6—H6	104.7
O3—S1—O1	113.52 (11)	C5—C6—H6	120.0
O1^{xi}—S1—O1	110.91 (18)	C1—C6—H6	120.0
O3—S1—C1	106.12 (15)	C5^{xi}—C6—H6	124.6
O3^{i}—K1—Cl1—C4^{xi}	−175.12 (19)	S1—C1—C2—C3^{xi}	154.6 (2)
O1^{ii}—K1—Cl1—C4^{xi}	−49.98 (19)	C2^{xi}—C2—C3—C3^{xi}	0.0
O1^{iii}—K1—Cl1—C4^{xi}	59.75 (19)	C1—C2—C3—C3^{xi}	−71.2
O1^{iv}—K1—Cl1—C4^{xi}	110.8 (2)	C2^{xi}—C2—C3—C4^{xi}	84.5 (5)
O1^{v}—K1—Cl1—C4^{xi}	−101.0 (2)	C1—C2—C3—C4^{xi}	13.3 (5)
S1^{iv}—K1—Cl1—C4^{xi}	−175.12 (19)	C3^{xi}—C2—C3—C4^{xi}	84.5 (5)
Cl1^{vi}—K1—Cl1—C4^{xi}	4.88 (19)	C2^{xi}—C2—C3—C4	71.2
Cl1^{vii}—K1—Cl1—C4^{xi}	119.85 (19)	C1—C2—C3—C4	0.0
Cl1^{viii}—K1—Cl1—C4^{xi}	−110.09 (19)	C3^{xi}—C2—C3—C4	71.2
K1^{ix}—K1—Cl1—C4^{xi}	75.22 (19)	C1—C2—C3—C2^{xi}	−71.2
K1^{x}—K1—Cl1—C4^{xi}	−65.46 (19)	C3^{xi}—C2—C3—C2^{xi}	0.0
O3^{i}—K1—Cl1—C4	175.12 (18)	C3^{xi}—C3—C4—C4^{xi}	180.0

O1^{ii}—K1—Cl1—C4	−59.75 (19)	C2—C3—C4—C4^{xi}	97.1
O1^{iii}—K1—Cl1—C4	49.98 (19)	C2^{xi}—C3—C4—C4^{xi}	124.51 (19)
O1^{iv}—K1—Cl1—C4	101.0 (2)	C4^{xi}—C3—C4—C3^{xi}	180.0
O1^{v}—K1—Cl1—C4	−110.8 (2)	C2—C3—C4—C3^{xi}	−82.9
S1^{iv}—K1—Cl1—C4	175.12 (18)	C2^{xi}—C3—C4—C3^{xi}	−55.49 (19)
Cl1^{vi}—K1—Cl1—C4	−4.88 (18)	C3^{xi}—C3—C4—C5	82.9
Cl1^{vii}—K1—Cl1—C4	110.09 (18)	C4^{xi}—C3—C4—C5	−97.1
Cl1^{viii}—K1—Cl1—C4	−119.85 (18)	C2—C3—C4—C5	0.0
K1^{ix}—K1—Cl1—C4	65.46 (19)	C2^{xi}—C3—C4—C5	27.41 (19)
K1^{x}—K1—Cl1—C4	−75.22 (19)	C3^{xi}—C3—C4—C5^{xi}	123.5 (3)
O3^{i}—K1—Cl1—K1^{xii}	0.0	C4^{xi}—C3—C4—C5^{xi}	−56.5 (3)
O1^{ii}—K1—Cl1—K1^{xii}	125.13 (5)	C2—C3—C4—C5^{xi}	40.6 (3)
O1^{iii}—K1—Cl1—K1^{xii}	−125.13 (5)	C2^{xi}—C3—C4—C5^{xi}	68.0 (4)
O1^{iv}—K1—Cl1—K1^{xii}	−74.13 (12)	C3^{xi}—C3—C4—Cl1	−105.2 (3)
O1^{v}—K1—Cl1—K1^{xii}	74.13 (12)	C4^{xi}—C3—C4—Cl1	74.8 (3)
S1^{iv}—K1—Cl1—K1^{xii}	0.000 (1)	C2—C3—C4—Cl1	171.9 (3)
Cl1^{vi}—K1—Cl1—K1^{xii}	180.0	C2^{xi}—C3—C4—Cl1	−160.7 (4)
Cl1^{vii}—K1—Cl1—K1^{xii}	−65.031 (18)	K1—Cl1—C4—C4^{xi}	91.56 (15)
Cl1^{viii}—K1—Cl1—K1^{xii}	65.031 (18)	K1^{xii}—Cl1—C4—C4^{xi}	−93.19 (18)
K1^{ix}—K1—Cl1—K1^{xii}	−109.66 (3)	K1^{vii}—Cl1—C4—C4^{xi}	−173.67 (15)
K1^{x}—K1—Cl1—K1^{xii}	109.66 (3)	K1^{viii}—Cl1—C4—C4^{xi}	−6.81 (15)
O3^{i}—K1—Cl1—K1^{vii}	65.031 (18)	C4^{xi}—Cl1—C4—C3^{xi}	−94.5 (6)
O1^{ii}—K1—Cl1—K1^{vii}	−169.83 (5)	K1—Cl1—C4—C3^{xi}	−2.9 (6)
O1^{iii}—K1—Cl1—K1^{vii}	−60.10 (5)	K1^{xii}—Cl1—C4—C3^{xi}	172.3 (5)
O1^{iv}—K1—Cl1—K1^{vii}	−9.10 (11)	K1^{vii}—Cl1—C4—C3^{xi}	91.9 (6)
O1^{v}—K1—Cl1—K1^{vii}	139.16 (12)	K1^{viii}—Cl1—C4—C3^{xi}	−101.3 (6)
S1^{iv}—K1—Cl1—K1^{vii}	65.031 (19)	C4^{xi}—Cl1—C4—C5	104.46 (18)
Cl1^{vi}—K1—Cl1—K1^{vii}	−114.969 (18)	K1—Cl1—C4—C5	−163.98 (18)
Cl1^{vii}—K1—Cl1—K1^{vii}	0.0	K1^{xii}—Cl1—C4—C5	11.3 (3)
Cl1^{viii}—K1—Cl1—K1^{vii}	130.06 (4)	K1^{vii}—Cl1—C4—C5	−69.2 (2)
K1^{ix}—K1—Cl1—K1^{vii}	−44.63 (3)	K1^{viii}—Cl1—C4—C5	97.7 (2)
K1^{x}—K1—Cl1—K1^{vii}	174.69 (4)	C4^{xi}—Cl1—C4—C3	−67.25 (16)
O3^{i}—K1—Cl1—K1^{viii}	−65.031 (18)	K1—Cl1—C4—C3	24.3 (2)
O1^{ii}—K1—Cl1—K1^{viii}	60.10 (5)	K1^{xii}—Cl1—C4—C3	−160.44 (14)
O1^{iii}—K1—Cl1—K1^{viii}	169.83 (5)	K1^{vii}—Cl1—C4—C3	119.08 (18)
O1^{iv}—K1—Cl1—K1^{viii}	−139.16 (12)	K1^{viii}—Cl1—C4—C3	−74.1 (2)
O1^{v}—K1—Cl1—K1^{viii}	9.10 (11)	C4^{xi}—Cl1—C4—C5^{xi}	59.0 (4)
S1^{iv}—K1—Cl1—K1^{viii}	−65.031 (19)	K1—Cl1—C4—C5^{xi}	150.6 (3)
Cl1^{vi}—K1—Cl1—K1^{viii}	114.969 (18)	K1^{xii}—Cl1—C4—C5^{xi}	−34.2 (5)
Cl1^{vii}—K1—Cl1—K1^{viii}	−130.06 (4)	K1^{vii}—Cl1—C4—C5^{xi}	−114.7 (4)
Cl1^{viii}—K1—Cl1—K1^{viii}	0.0	K1^{viii}—Cl1—C4—C5^{xi}	52.2 (4)

K1^{ix}—K1—Cl1—K1^{viii}	−174.69 (4)	C4^{xi}—C4—C5—C5^{xi}	0.0
K1^{x}—K1—Cl1—K1^{viii}	44.63 (3)	C3^{xi}—C4—C5—C5^{xi}	104.0 (4)
O3—S1—O1—K1^{iii}	12.9 (3)	C3—C4—C5—C5^{xi}	77.8
O1^{xi}—S1—O1—K1^{iii}	−116.33 (19)	Cl1—C4—C5—C5^{xi}	−93.7 (3)
C1—S1—O1—K1^{iii}	129.01 (19)	C4^{xi}—C4—C5—C6	−77.8
K1^{xiii}—S1—O1—K1^{iii}	−119.1 (2)	C3^{xi}—C4—C5—C6	26.2 (4)
O3—S1—O1—K1^{xiii}	131.96 (13)	C3—C4—C5—C6	0.0
O1^{xi}—S1—O1—K1^{xiii}	2.75 (18)	C5^{xi}—C4—C5—C6	−77.8
C1—S1—O1—K1^{xiii}	−111.92 (10)	Cl1—C4—C5—C6	−171.5 (3)
O1^{xi}—S1—O3—K1^{xiv}	63.94 (11)	C3^{xi}—C4—C5—C4^{xi}	104.0 (4)
O1—S1—O3—K1^{xiv}	−63.94 (11)	C3—C4—C5—C4^{xi}	77.8
C1—S1—O3—K1^{xiv}	180.0	C5^{xi}—C4—C5—C4^{xi}	0.0
K1^{xiii}—S1—O3—K1^{xiv}	0.0	Cl1—C4—C5—C4^{xi}	−93.7 (3)
O3—S1—C1—C2	−17.16 (15)	C4^{xi}—C4—C5—C6^{xi}	−47.66 (15)
O1^{xi}—S1—C1—C2	103.86 (19)	C3^{xi}—C4—C5—C6^{xi}	56.4 (5)
O1—S1—C1—C2	−138.18 (18)	C3—C4—C5—C6^{xi}	30.14 (15)
K1^{xiii}—S1—C1—C2	162.84 (15)	C5^{xi}—C4—C5—C6^{xi}	−47.66 (15)
O3—S1—C1—C2^{xi}	17.16 (13)	Cl1—C4—C5—C6^{xi}	−141.4 (4)
O1^{xi}—S1—C1—C2^{xi}	138.18 (16)	C5^{xi}—C5—C6—C6^{xi}	0.0
O1—S1—C1—C2^{xi}	−103.86 (17)	C4—C5—C6—C6^{xi}	71.2
K1^{xiii}—S1—C1—C2^{xi}	−162.84 (13)	C4^{xi}—C5—C6—C6^{xi}	59.7 (4)
O3—S1—C1—C6^{xi}	−159.59 (12)	C5^{xi}—C5—C6—C1	−71.2
O1^{xi}—S1—C1—C6^{xi}	−38.57 (16)	C4—C5—C6—C1	0.0
O1—S1—C1—C6^{xi}	79.39 (15)	C4^{xi}—C5—C6—C1	−11.5 (4)
K1^{xiii}—S1—C1—C6^{xi}	20.41 (12)	C6^{xi}—C5—C6—C1	−71.2
O3—S1—C1—C6	159.59 (15)	C4—C5—C6—C5^{xi}	71.2
O1^{xi}—S1—C1—C6	−79.39 (17)	C4^{xi}—C5—C6—C5^{xi}	59.7 (4)
O1—S1—C1—C6	38.57 (18)	C6^{xi}—C5—C6—C5^{xi}	0.0
K1^{xiii}—S1—C1—C6	−20.41 (15)	C2—C1—C6—C6^{xi}	−82.9
C6^{xi}—C1—C2—C2^{xi}	−115.6 (2)	C2^{xi}—C1—C6—C6^{xi}	−113.7 (2)
C6—C1—C2—C2^{xi}	−77.8	S1—C1—C6—C6^{xi}	100.33 (14)
S1—C1—C2—C2^{xi}	98.93 (14)	C2—C1—C6—C5	0.0
C2^{xi}—C1—C2—C3	77.8	C2^{xi}—C1—C6—C5	−30.8 (2)
C6^{xi}—C1—C2—C3	−37.8 (2)	C6^{xi}—C1—C6—C5	82.9
C6—C1—C2—C3	0.0	S1—C1—C6—C5	−176.76 (14)
S1—C1—C2—C3	176.72 (14)	C2—C1—C6—C5^{xi}	−35.2 (2)
C2^{xi}—C1—C2—C3^{xi}	55.7 (3)	C2^{xi}—C1—C6—C5^{xi}	−66.0 (3)
C6^{xi}—C1—C2—C3^{xi}	−59.9 (4)	C6^{xi}—C1—C6—C5^{xi}	47.7 (2)
C6—C1—C2—C3^{xi}	−22.1 (3)	S1—C1—C6—C5^{xi}	148.04 (16)

Symmetry codes: (i) *x*, *y*, *z*+1; (ii) −*x*+1, *y*−1/2, −*z*+1; (iii) −*x*+1, −*y*+1, −*z*+1; (iv) *x*+1, *y*, *z*+1; (v) *x*+1, −*y*+1/2, *z*+1; (vi) *x*+1, *y*, *z*; (vii) −*x*+1, −*y*+1, −*z*+2; (viii) −*x*+1, −*y*, −*z*+2; (ix) −*x*+2, −*y*+1, −*z*+2; (x) −*x*+2, −*y*, −*z*+2; (xi) *x*, −*y*+1/2, *z*; (xii) *x*−1, *y*, *z*; (xiii) *x*−1, *y*, *z*−1; (xiv) *x*, *y*, *z*−1.

Fig. 1

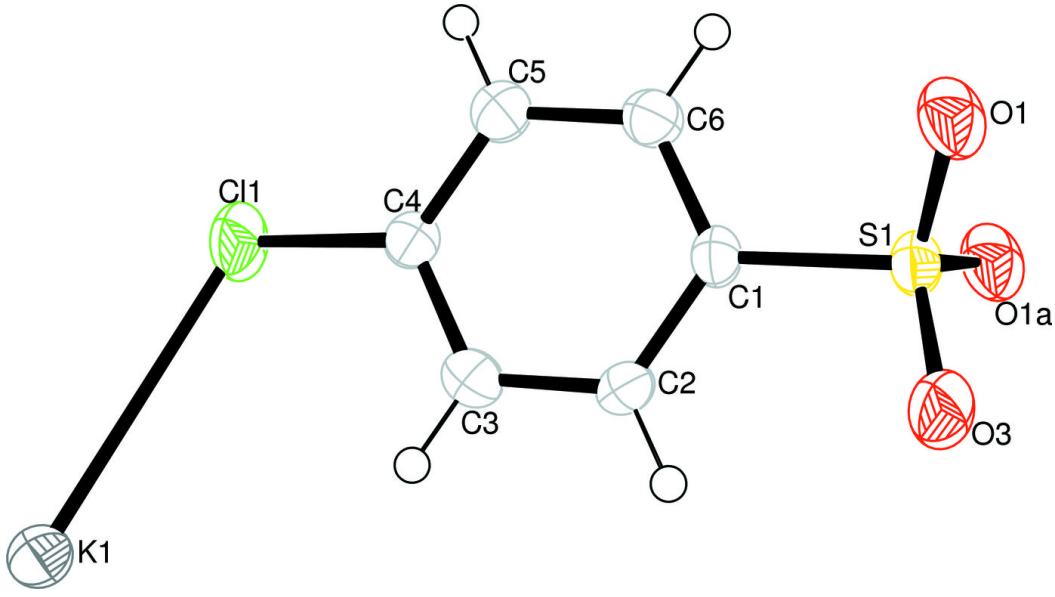

Fig. 2