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Potassium *N*,2-dichlorobenzenesulfonamidate sesquihydrate

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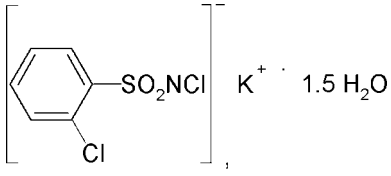
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.042; wR factor = 0.105; data-to-parameter ratio = 16.2.

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, 2011*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

$K^+\cdot C_6H_4Cl_2NO_2S^-\cdot 1.5H_2O$
M_r = 291.19
Monoclinic, $C2/c$
a = 12.301 (2) Å
b = 6.8277 (6) Å
c = 27.965 (3) Å
β = 106.28 (1)°
V = 2254.5 (5) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.12 mm^{-1}
T = 293 K
0.44 × 0.44 × 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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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ5159).

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