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2-Chlorobenzenesulfonamide

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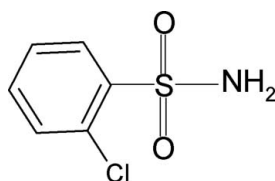
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Key indicators: single-crystal X-ray study; $T = 299$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.022; wR factor = 0.060; data-to-parameter ratio = 9.7.

In the crystal of the title compound, $\text{C}_6\text{H}_6\text{ClNO}_2\text{S}$, $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds pack the molecules into sheets parallel to the ac plane.

Related literature

For our studies of the effect of substituents on the solid state structures of sulfonamides and N -halo arylsulfonamides, see: Gowda *et al.* (2003); Gowda, Babitha *et al.* (2007); Gowda, Nayak *et al.* (2007); Gowda, Srilatha *et al.* (2007). For the parent benzenesulfonamide, see: Gowda, Nayak *et al.* (2007). For other aryl sulfonamides, see: Gowda, Babitha *et al.* (2007); Gowda, Srilatha *et al.* (2007); Jones & Weinkauff (1993); Kumar *et al.* (1992); O'Connor & Maslen (1965).



Experimental

Crystal data

 $\text{C}_6\text{H}_6\text{ClNO}_2\text{S}$ $M_r = 191.63$ Monoclinic, Cc $a = 6.955$ (1) Å $b = 14.848$ (3) Å $c = 7.751$ (1) Å $\beta = 91.51$ (1)° $V = 800.2$ (2) Å³ $Z = 4$ Mo $K\alpha$ radiation $\mu = 0.68$ mm⁻¹ $T = 299$ K $0.48 \times 0.48 \times 0.26$ mm

Data collection

Oxford Diffraction Xcalibur diffractometer with a Sapphire CCD detector

Absorption correction: multi-scan (*CrysAlis RED*; Oxford)

Diffraction, 2009)

 $T_{\min} = 0.735$, $T_{\max} = 0.842$

1598 measured reflections

1031 independent reflections

1004 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.008$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.022$ $wR(F^2) = 0.060$ $S = 1.03$

1031 reflections

106 parameters

4 restraints

H atoms treated by a mixture of independent and constrained refinement

 $\Delta\rho_{\max} = 0.14$ e Å⁻³ $\Delta\rho_{\min} = -0.21$ e Å⁻³

Absolute structure: Flack (1983), 215 Friedel pairs

Flack parameter: 0.04 (8)

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1}-\text{H11}\cdots\text{O1}^{\text{i}}$	0.857 (19)	2.12 (2)	2.908 (3)	152 (3)
$\text{N1}-\text{H12}\cdots\text{O2}^{\text{ii}}$	0.835 (18)	2.12 (2)	2.941 (3)	166 (3)

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

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: BT5028).

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supporting information

Acta Cryst. (2009). E65, o2144 [doi:10.1107/S1600536809031511]

2-Chlorobenzenesulfonamide

B. Thimme Gowda, Sabine Foro, K. Shakuntala and Hartmut Fues

S1. Comment

The chemistry of sulfonamides is of interest as they show distinct physical, chemical and biological properties. Many arylsulfonamides and their N-halo compounds exhibit pharmacological, fungicidal and herbicidal activities due to their oxidizing action in aqueous, partial aqueous and non-aqueous media. In the present work, the structure of 2-chlorobenzenesulfonamide has been determined to explore the substituent effects on the solid state structures of sulfonamides and N-halo arylsulfonamides (Gowda *et al.*, 2003; Gowda, Babitha *et al.* 2007; Gowda, Nayak *et al.* 2007; Gowda, Srilatha *et al.* 2007). The structure of the title compound (Fig. 1) closely resembles those of the parent benzenesulfonamide (Gowda, Nayak *et al.*, 2007) and other aryl sulfonamides (Gowda, Babitha *et al.*, 2007; Gowda, Srilatha *et al.*, 2007; Jones & Weinkauf, 1993; Kumar *et al.*, 1992; O'Connor & Maslen, 1965). The title compound crystallizes in monoclinic space group *Cc* in contrast to the monoclinic *Pc* space group observed with the parent sulfonamide (Gowda *et al.*, 2007b) and orthorhombic *Pbca* space group with 4-fluorobenzenesulfonamide (Jones & Weinkauf, 1993) and 4-aminobenzenesulfonamide (O'Connor & Maslen, 1965) and monoclinic $P2_1/n$ space group with 4-chlorobenzene-sulfonamide and 4-bromobenzenesulfonamide (Gowda *et al.*, 2003), and 4-methylbenzenesulfonamide (Kumar *et al.*, 1992). The molecules in the title compound are packed into infinite 3-D molecular network through N1—H11 \cdots O1 and N1—H12 \cdots O2 hydrogen bonding (Table 1 & Fig.2).

S2. Experimental

The purity of the commercial sample (TCI, Tokyo) was checked and characterized by its infrared spectra. The single crystals used in X-ray diffraction studies were grown in ethanol solution by a slow evaporation of the solvent at room temperature.

S3. Refinement

The H atoms of the NH₂ group were located in difference map and refined with restrained geometry to 0.86 (2) Å. The other H atoms were positioned with idealized geometry using a riding model [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).

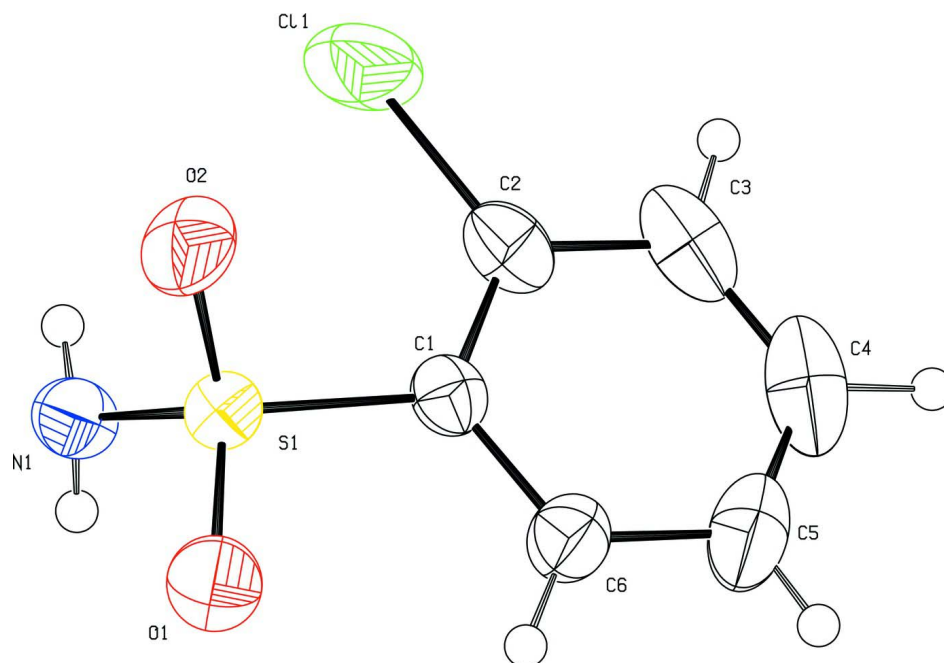


Figure 1

Molecular structure of (I), showing the atom labelling scheme and displacement ellipsoids are drawn at the 50% probability level.

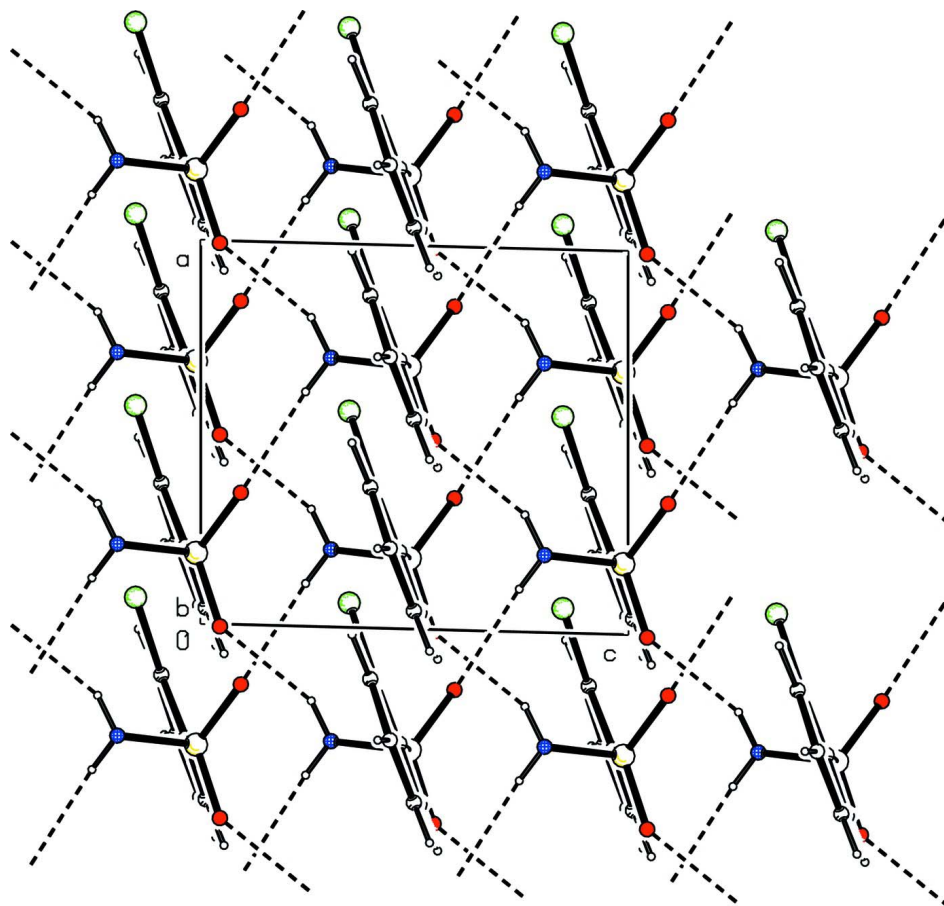


Figure 2

Molecular packing of (I) with hydrogen bonding shown as dashed lines.

2-Chlorobenzenesulfonamide

Crystal data

$C_6H_6ClNO_2S$

$M_r = 191.63$

Monoclinic, Cc

Hall symbol: C -2yc

$a = 6.955$ (1) Å

$b = 14.848$ (3) Å

$c = 7.751$ (1) Å

$\beta = 91.51$ (1)°

$V = 800.2$ (2) Å³

$Z = 4$

$F(000) = 392$

$D_x = 1.591$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 1188 reflections

$\theta = 2.6$ – 27.8 °

$\mu = 0.68$ mm⁻¹

$T = 299$ K

Prism, colourless

$0.48 \times 0.48 \times 0.26$ 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 ω and ϕ scans.

Absorption correction: multi-scan

(*CrysAlis RED*; Oxford Diffraction, 2009)

$T_{\min} = 0.735$, $T_{\max} = 0.842$

1598 measured reflections

1031 independent reflections

1004 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.008$

$\theta_{\max} = 26.4^\circ$, $\theta_{\min} = 2.7^\circ$
 $h = -8 \rightarrow 4$

$k = -18 \rightarrow 15$
 $l = -9 \rightarrow 9$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.022$
 $wR(F^2) = 0.060$
 $S = 1.03$
 1031 reflections
 106 parameters
 4 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
 $w = 1/[\sigma^2(F_o^2) + (0.0417P)^2 + 0.2306P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.041$
 $\Delta\rho_{\max} = 0.14 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.21 \text{ e } \text{\AA}^{-3}$
 Absolute structure: Flack (1983), 215 Friedel
 pairs
 Absolute structure parameter: 0.04 (8)

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C11	0.56409 (10)	0.10747 (7)	0.84733 (11)	0.0700 (3)
S1	0.18379 (8)	0.20974 (3)	0.98884 (8)	0.03276 (14)
O1	-0.0067 (3)	0.22742 (12)	1.0448 (3)	0.0486 (5)
O2	0.3434 (3)	0.23916 (13)	1.0939 (2)	0.0535 (5)
N1	0.2010 (4)	0.25747 (15)	0.8048 (3)	0.0396 (5)
H11	0.309 (3)	0.251 (2)	0.755 (4)	0.048*
H12	0.105 (4)	0.249 (2)	0.740 (3)	0.048*
C1	0.1995 (4)	0.09052 (15)	0.9649 (3)	0.0335 (5)
C2	0.3626 (4)	0.04740 (18)	0.9082 (4)	0.0443 (6)
C3	0.3663 (6)	-0.0459 (2)	0.8966 (4)	0.0588 (8)
H3	0.4755	-0.0751	0.8582	0.071*
C4	0.2078 (7)	-0.0951 (2)	0.9421 (4)	0.0674 (10)
H4	0.2106	-0.1576	0.9341	0.081*
C5	0.0464 (6)	-0.05329 (19)	0.9990 (4)	0.0590 (8)
H5	-0.0600	-0.0872	1.0292	0.071*
C6	0.0415 (4)	0.04025 (18)	1.0117 (4)	0.0432 (6)
H6	-0.0677	0.0689	1.0515	0.052*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0380 (4)	0.0856 (6)	0.0871 (6)	0.0153 (4)	0.0158 (4)	0.0148 (5)
S1	0.0338 (3)	0.0335 (2)	0.0310 (2)	-0.0015 (3)	0.00213 (18)	-0.0023 (2)
O1	0.0468 (11)	0.0480 (9)	0.0520 (11)	0.0068 (9)	0.0205 (9)	-0.0043 (9)
O2	0.0590 (14)	0.0501 (11)	0.0506 (11)	-0.0152 (10)	-0.0172 (10)	-0.0031 (9)
N1	0.0364 (11)	0.0449 (11)	0.0375 (11)	0.0035 (10)	0.0025 (8)	0.0055 (9)
C1	0.0381 (12)	0.0343 (10)	0.0280 (11)	0.0023 (11)	-0.0025 (9)	0.0013 (8)
C2	0.0478 (16)	0.0476 (13)	0.0374 (13)	0.0118 (13)	-0.0008 (12)	0.0047 (11)
C3	0.078 (2)	0.0498 (15)	0.0485 (15)	0.0276 (17)	-0.0026 (15)	0.0016 (13)
C4	0.116 (3)	0.0360 (14)	0.0497 (18)	0.0069 (19)	-0.0055 (19)	0.0025 (12)
C5	0.079 (2)	0.0399 (14)	0.0574 (18)	-0.0158 (15)	-0.0058 (17)	0.0052 (13)
C6	0.0445 (16)	0.0412 (12)	0.0436 (14)	-0.0049 (12)	-0.0026 (12)	0.0022 (11)

Geometric parameters (\AA , $^\circ$)

Cl1—C2	1.737 (3)	C2—C3	1.389 (4)
S1—O1	1.429 (2)	C3—C4	1.376 (5)
S1—O2	1.4275 (19)	C3—H3	0.9300
S1—N1	1.600 (2)	C4—C5	1.366 (5)
S1—C1	1.784 (2)	C4—H4	0.9300
N1—H11	0.857 (19)	C5—C6	1.393 (4)
N1—H12	0.835 (18)	C5—H5	0.9300
C1—C6	1.385 (4)	C6—H6	0.9300
C1—C2	1.384 (4)		
O1—S1—O2	118.92 (13)	C3—C2—Cl1	118.6 (2)
O1—S1—N1	106.32 (13)	C4—C3—C2	119.8 (3)
O2—S1—N1	107.32 (12)	C4—C3—H3	120.1
O1—S1—C1	105.88 (12)	C2—C3—H3	120.1
O2—S1—C1	108.31 (12)	C5—C4—C3	120.8 (3)
N1—S1—C1	109.91 (11)	C5—C4—H4	119.6
S1—N1—H11	116 (2)	C3—C4—H4	119.6
S1—N1—H12	113 (2)	C4—C5—C6	119.8 (3)
H11—N1—H12	114 (3)	C4—C5—H5	120.1
C6—C1—C2	119.8 (2)	C6—C5—H5	120.1
C6—C1—S1	117.2 (2)	C1—C6—C5	119.9 (3)
C2—C1—S1	123.0 (2)	C1—C6—H6	120.1
C1—C2—C3	119.9 (3)	C5—C6—H6	120.1
C1—C2—Cl1	121.5 (2)		
O1—S1—C1—C6	-3.7 (2)	S1—C1—C2—Cl1	-2.5 (3)
O2—S1—C1—C6	124.8 (2)	C1—C2—C3—C4	-0.2 (4)
N1—S1—C1—C6	-118.19 (19)	Cl1—C2—C3—C4	-179.3 (2)
O1—S1—C1—C2	178.5 (2)	C2—C3—C4—C5	-0.1 (4)
O2—S1—C1—C2	-52.9 (2)	C3—C4—C5—C6	-0.1 (5)
N1—S1—C1—C2	64.0 (2)	C2—C1—C6—C5	-1.0 (4)

C6—C1—C2—C3	0.7 (4)	S1—C1—C6—C5	-178.8 (2)
S1—C1—C2—C3	178.4 (2)	C4—C5—C6—C1	0.7 (4)
C6—C1—C2—C11	179.77 (19)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
N1—H11 \cdots O1 ⁱ	0.86 (2)	2.12 (2)	2.908 (3)	152 (3)
N1—H12 \cdots O2 ⁱⁱ	0.84 (2)	2.12 (2)	2.941 (3)	166 (3)

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