

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

2-Chlorobenzenesulfonamide

B. Thimme Gowda,^{a*} Sabine Foro,^b K. Shakuntala^a and Hartmut Fuess^b

^aDepartment of Chemistry, Mangalore University, Mangalagangotri 574 199, Mangalore, India, and ^bInstitute of Materials Science, Darmstadt University of Technology, Petersenstrasse 23, D-64287 Darmstadt, Germany
Correspondence e-mail: gowdabt@yahoo.com

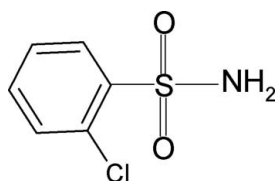
Received 8 August 2009; accepted 10 August 2009

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*.

BTG thanks the Alexander von Humboldt Foundation, Bonn, Germany, for an extension of his research fellowship.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5028).

References

- Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.
 Gowda, B. T., Babitha, K. S., Svoboda, I. & Fuess, H. (2007). *Acta Cryst.* **E63**, o3245.
 Gowda, B. T., Jyothi, K., Kozisek, J. & Fuess, H. (2003). *Z. Naturforsch. Teil A*, **58**, 656–660.
 Gowda, B. T., Nayak, R., Kožiček, J., Tokarčík, M. & Fuess, H. (2007). *Acta Cryst.* **E63**, o2967.
 Gowda, B. T., Srilatha, Foro, S., Kozisek, J. & Fuess, H. (2007). *Z. Naturforsch. Teil A*, **62**, 417–424.
 Jones, P. G. & Weinkauff, A. (1993). *Z. Kristallogr.* **208**, 128–129.
 Kumar, S. V., Senadhi, S. E. & Rao, L. M. (1992). *Z. Kristallogr.* **202**, 1–6.
 O'Connor, B. H. & Maslen, E. N. (1965). *Acta Cryst.* **18**, 363–366.
 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.

supplementary materials

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

2-Chlorobenzenesulfonamide

B. T. Gowda, S. Foro, K. Shakuntala and H. Fuess

Comment

The chemistry of sulfonamides is of interest as they show distinct physical, chemical and biological properties. Many aryl-sulfonamides 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 & Weinkauff, 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 & Weinkauff, 1993) and 4-aminobenzenesulfonamide (O'Connor & Maslen, 1965) and monoclinic $P2_1/n$ space group with 4-chlorobenzenesulfonamide 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...O1 and N1—H12...O2 hydrogen bonding (Table 1 & Fig.2).

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.

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).

Figures

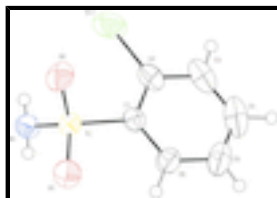


Fig. 1. Molecular structure of (I), showing the atom labelling scheme and displacement ellipsoids are drawn at the 50% probability level.

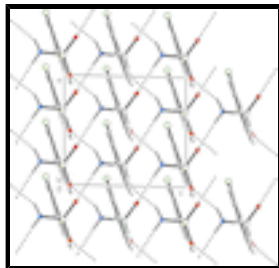


Fig. 2. Molecular packing of (I) with hydrogen bonding shown as dashed lines.

2-Chlorobenzenesulfonamide

Crystal data

$C_6H_6ClNO_2S$

$M_r = 191.63$

Monoclinic, *Cc*

Hall symbol: C -2yc

$a = 6.955 (1) \text{ \AA}$

$b = 14.848 (3) \text{ \AA}$

$c = 7.751 (1) \text{ \AA}$

$\beta = 91.51 (1)^\circ$

$V = 800.2 (2) \text{ \AA}^3$

$Z = 4$

$F_{000} = 392$

$D_x = 1.591 \text{ Mg m}^{-3}$

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

Cell parameters from 1188 reflections

$\theta = 2.6\text{--}27.8^\circ$

$\mu = 0.68 \text{ mm}^{-1}$

$T = 299 \text{ K}$

Prism, colourless

$0.48 \times 0.48 \times 0.26 \text{ mm}$

Data collection

Oxford Diffraction Xcalibur diffractometer with a Sapphire CCD detector

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 299 \text{ K}$

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

$R[F^2 > 2\sigma(F^2)] = 0.022$

$wR(F^2) = 0.060$

$S = 1.03$

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 $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.041$

$\Delta\rho_{\max} = 0.14 \text{ e \AA}^{-3}$

1031 reflections	$\Delta\rho_{\min} = -0.21 \text{ e } \text{\AA}^{-3}$
106 parameters	Extinction correction: none
4 restraints	Absolute structure: Flack (1983), 215 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.04 (8)
Secondary atom site location: difference Fourier map	

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}
C11	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)

supplementary materials

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 (Å, °)

C11—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—C11	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—C11	121.5 (2)		
O1—S1—C1—C6	-3.7 (2)	S1—C1—C2—C11	-2.5 (3)
O2—S1—C1—C6	124.8 (2)	C1—C2—C3—C4	-0.2 (4)
N1—S1—C1—C6	-118.19 (19)	C11—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	0.857 (19)	2.12 (2)	2.908 (3)	152 (3)

N1—H12...O2ⁱⁱ 0.835 (18) 2.12 (2) 2.941 (3) 166 (3)
 Symmetry codes: (i) $x+1/2, -y+1/2, z-1/2$; (ii) $x-1/2, -y+1/2, z-1/2$.

Fig. 1

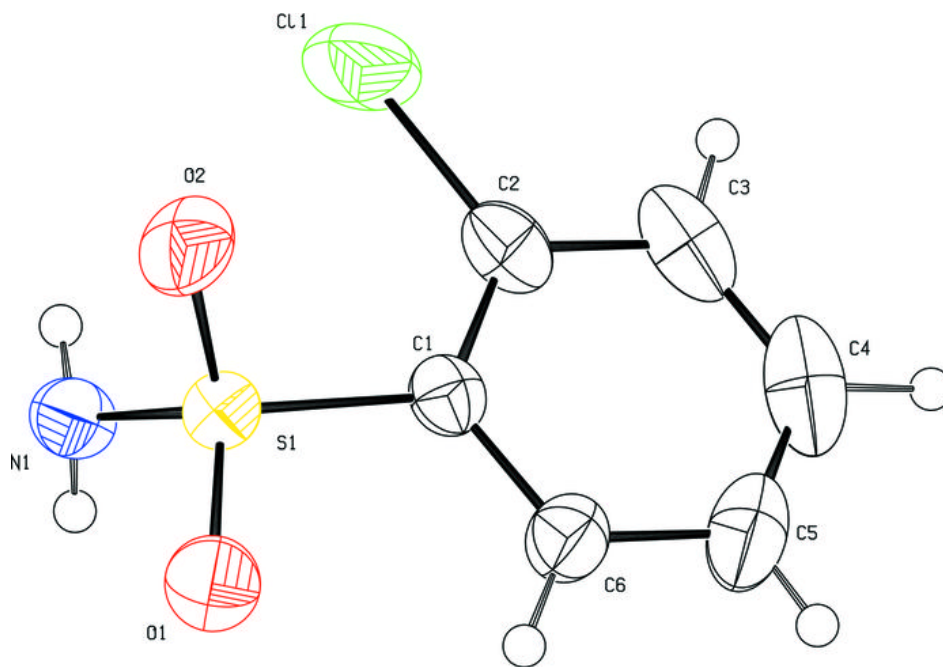


Fig. 2

