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3,4-Dichlorobenzenesulfonamide

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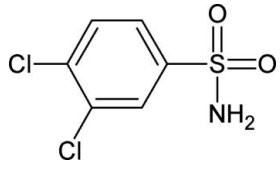
Key indicators: single-crystal X-ray study; T = 302 K; mean σ(C–C) = 0.003 Å; R factor = 0.031; wR factor = 0.089; data-to-parameter ratio = 15.4.

The structure of the title compound, $C_6H_5Cl_2NO_2S$, resembles those of other arylsulfonamides, with similar geometric parameters. The molecules in the title compound are packed into a layered structure parallel to the (100) plane *via* N—H···O hydrogen bonds.

Related literature

For related literature, see: Gowda *et al.* (2002, 2003); Gowda, Nayak, Kožíšek *et al.* (2007); Gowda, Nayak, Foro *et al.* (2007); Gowda, Srilatha *et al.* (2007); Jones & Weinkauf (1993); Kumar *et al.* (1992).



Experimental

Crystal data

$C_6H_5Cl_2NO_2S$
M_r = 226.07
Monoclinic, $P2_1/c$
a = 11.353 (2) Å
b = 5.9629 (7) Å
c = 13.452 (2) Å
β = 106.26 (1)°
V = 874.2 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.94 mm^{-1}
T = 302 (2) K
0.40 × 0.40 × 0.08 mm

Data collection

Oxford Diffraction Xcalibur diffractometer with Sapphire CCD detector
Absorption correction: analytical (*CrysAlis RED*; Oxford Diffraction, 2006) (Clark & Reid, 1995)
T_{min} = 0.706, T_{max} = 0.929
5809 measured reflections
1774 independent reflections
1297 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.089
S = 1.06
1774 reflections
115 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1^{i}	0.79 (3)	2.21 (3)	2.970 (3)	161 (3)
N1—H1B···O2^{ii}	0.82 (3)	2.13 (3)	2.945 (3)	174 (3)

Symmetry codes: (i) $-x+1, -y, -z+2$; (ii) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$.

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 for Windows* (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: DN2195).

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supplementary materials

Acta Cryst. (2007). E**63**, o3245 [**doi:10.1107/S1600536807028802**]

3,4-Dichlorobenzenesulfonamide

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Comment

Several arylsulfonamides and their N-halo compounds exhibit distinct physical, chemical and biological properties. Thus these compounds are of interest in synthetic, mechanistic, analytical and biological chemistry. In the present work, the structure of 3,4-dichlorobenzenesulfonamde (34DCBSA) has been determined to study the effect of substituents on the solid state structures of sulfonamides and N-halo arylsulfonamides (Gowda *et al.*, 2003; Gowda, Nayak, Kožíšek *et al.*, 2007; Gowda, Nayak, Foro *et al.*, 2007; Gowda, Srilatha *et al.*, 2007). The structure of 34DCBSA (Fig. 1) resembles those of other arylsulfonamides (Gowda *et al.*, 2003, Gowda, Nayak, Kožíšek *et al.*, 2007; Gowda, Nayak, Foro *et al.*, 2007; Gowda, Srilatha *et al.*, 2007); Jones & Weinkauf, 1993; Kumar *et al.*, 1992).

The bond parameters in 34DCBSA are similar to those in other arylsulfonamides. The molecules in the title compound are packed into layered structure developping parallel to the (1 0 0) plane *via* N—H···O hydrogen bonds (Table 1, Fig. 2).

Experimental

The title compound was prepared according to the literature method (Gowda *et al.*, 2002). The purity of the compound was checked by determining its melting point. It was characterized by recording its infrared and NMR spectra (Gowda *et al.*, 2002). Single crystals of the title compound were obtained from a slow evaporation of its ethanolic solution and used for X-ray diffraction studies at room temperature.

Figures

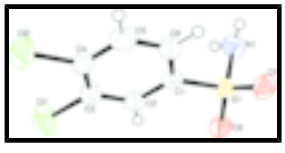

Fig. 1. Molecular structure of the title compound showing the atom labeling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii.

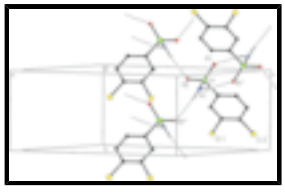

Fig. 2. Partial packing view showing the formation of the layered structure through N—H···O hydrogen bonds. H bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted for clarity. [Symmetry codes: (i) $1-x, -y, 2-z$; (ii) $1-x, 1/2+y, 3/2-z$].

3,4-Dichlorobenzenesulfonamide

Crystal data

$C_6H_5Cl_2NO_2S$	$F_{000} = 456$
$M_r = 226.07$	$D_x = 1.718$ Mg m^{-3}

Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 2408 reflections
$a = 11.353$ (2) Å	$\theta = 3.1–25.8°$
$b = 5.9629$ (7) Å	$\mu = 0.94$ mm^{-1}
$c = 13.452$ (2) Å	$T = 302$ (2) K
$\beta = 106.26$ (1)°	Prism, colourless
$V = 874.2$ (2) Å^3	0.40 × 0.40 × 0.08 mm
$Z = 4$	

Data collection

Oxford Diffraction Xcalibur diffractometer with Sapphire CCD detector	1774 independent reflections
Radiation source: Enhance (Mo) X-ray Source	1297 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.020$
$T = 302(2)$ K	$\theta_{max} = 26.4°$
Rotation method data acquisition using ω and phi scans.	$\theta_{min} = 3.2°$
Absorption correction: analytical (CrysAlis RED; Oxford Diffraction, 2006) (Clark & Reid, 1995)	$h = -11\rightarrow14$
$T_{min} = 0.706$, $T_{max} = 0.929$	$k = -7\rightarrow6$
5809 measured reflections	$l = -16\rightarrow16$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.031$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.089$	$w = 1/[\sigma^2(F_o^2) + (0.0437P)^2 + 0.2808P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} = 0.001$
1774 reflections	$\Delta\rho_{max} = 0.24$ e Å^{-3}
115 parameters	$\Delta\rho_{min} = -0.22$ 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 $F^2 > 2$sigma(F^2) is used only for calculat-

ing *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	0.3139 (2)	0.3022 (4)	0.86230 (15)	0.0351 (5)
C2	0.2565 (2)	0.4551 (4)	0.78694 (15)	0.0387 (5)
H2	0.2722	0.4538	0.7227	0.046*
C3	0.1767 (2)	0.6082 (4)	0.80752 (16)	0.0380 (5)
C4	0.1528 (2)	0.6091 (4)	0.90318 (17)	0.0411 (5)
C5	0.2108 (2)	0.4574 (5)	0.97803 (17)	0.0485 (6)
H5	0.1955	0.4597	1.0424	0.058*
C6	0.2913 (2)	0.3024 (4)	0.95846 (17)	0.0437 (6)
H6	0.3299	0.1992	1.0089	0.052*
N1	0.5551 (2)	0.2049 (4)	0.88648 (17)	0.0451 (5)
H1A	0.573 (2)	0.202 (4)	0.948 (2)	0.054*
H1B	0.568 (2)	0.321 (5)	0.858 (2)	0.054*
O1	0.41096 (15)	−0.0934 (3)	0.89211 (12)	0.0458 (4)
O2	0.40003 (16)	0.1024 (3)	0.72771 (11)	0.0488 (4)
S1	0.41992 (5)	0.10901 (9)	0.83756 (4)	0.03697 (18)
Cl1	0.10759 (7)	0.80068 (14)	0.71418 (5)	0.0653 (2)
Cl2	0.05152 (7)	0.79949 (14)	0.92960 (6)	0.0701 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0384 (12)	0.0349 (12)	0.0322 (10)	−0.0044 (11)	0.0104 (9)	−0.0055 (9)
C2	0.0435 (13)	0.0429 (14)	0.0307 (10)	−0.0046 (11)	0.0121 (9)	−0.0018 (10)
C3	0.0375 (12)	0.0368 (13)	0.0383 (11)	−0.0018 (11)	0.0084 (9)	0.0009 (10)
C4	0.0377 (12)	0.0456 (14)	0.0408 (12)	−0.0008 (11)	0.0125 (9)	−0.0088 (11)
C5	0.0548 (15)	0.0610 (17)	0.0336 (11)	0.0009 (13)	0.0187 (10)	−0.0027 (11)
C6	0.0532 (15)	0.0466 (14)	0.0329 (11)	0.0064 (13)	0.0150 (10)	0.0042 (10)
N1	0.0483 (13)	0.0456 (13)	0.0422 (11)	−0.0059 (11)	0.0143 (9)	0.0090 (10)
O1	0.0580 (11)	0.0332 (9)	0.0467 (9)	−0.0045 (8)	0.0157 (8)	0.0015 (7)
O2	0.0675 (11)	0.0475 (10)	0.0329 (8)	0.0081 (9)	0.0164 (7)	−0.0042 (7)
S1	0.0467 (3)	0.0338 (3)	0.0318 (3)	−0.0009 (3)	0.0132 (2)	−0.0016 (2)
Cl1	0.0719 (5)	0.0671 (5)	0.0566 (4)	0.0228 (4)	0.0173 (3)	0.0205 (3)
Cl2	0.0712 (5)	0.0779 (6)	0.0666 (4)	0.0264 (4)	0.0282 (4)	−0.0060 (4)

Geometric parameters (Å, °)

C1—C2	1.383 (3)	C5—C6	1.376 (3)
C1—C6	1.388 (3)	C5—H5	0.9300
C1—S1	1.764 (2)	C6—H6	0.9300
C2—C3	1.368 (3)	N1—S1	1.597 (2)
C2—H2	0.9300	N1—H1A	0.79 (3)
C3—C4	1.387 (3)	N1—H1B	0.82 (3)

C3—Cl1	1.720 (2)	O1—S1	1.4310 (16)
C4—C5	1.376 (3)	O2—S1	1.4315 (15)
C4—Cl2	1.722 (2)		
C2—C1—C6	120.7 (2)	C4—C5—H5	119.7
C2—C1—S1	119.88 (16)	C5—C6—C1	119.0 (2)
C6—C1—S1	119.38 (17)	C5—C6—H6	120.5
C3—C2—C1	119.60 (19)	C1—C6—H6	120.5
C3—C2—H2	120.2	S1—N1—H1A	111 (2)
C1—C2—H2	120.2	S1—N1—H1B	112.4 (18)
C2—C3—C4	120.2 (2)	H1A—N1—H1B	118 (3)
C2—C3—Cl1	119.35 (17)	O1—S1—O2	119.53 (9)
C4—C3—Cl1	120.46 (18)	O1—S1—N1	106.80 (11)
C5—C4—C3	119.9 (2)	O2—S1—N1	106.91 (11)
C5—C4—Cl2	119.51 (18)	O1—S1—C1	107.70 (10)
C3—C4—Cl2	120.60 (19)	O2—S1—C1	107.10 (10)
C6—C5—C4	120.6 (2)	N1—S1—C1	108.42 (11)
C6—C5—H5	119.7		
C6—C1—C2—C3	0.0 (3)	C4—C5—C6—C1	0.5 (4)
S1—C1—C2—C3	−178.39 (17)	C2—C1—C6—C5	−0.1 (4)
C1—C2—C3—C4	−0.4 (3)	S1—C1—C6—C5	178.35 (19)
C1—C2—C3—Cl1	178.96 (17)	C2—C1—S1—O1	−147.14 (18)
C2—C3—C4—C5	0.8 (4)	C6—C1—S1—O1	34.4 (2)
Cl1—C3—C4—C5	−178.54 (19)	C2—C1—S1—O2	−17.4 (2)
C2—C3—C4—Cl2	−179.46 (18)	C6—C1—S1—O2	164.16 (18)
Cl1—C3—C4—Cl2	1.2 (3)	C2—C1—S1—N1	97.6 (2)
C3—C4—C5—C6	−0.9 (4)	C6—C1—S1—N1	−80.8 (2)
Cl2—C4—C5—C6	179.4 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···O1^{i}	0.79 (3)	2.21 (3)	2.970 (3)	161 (3)
N1—H1B···O2^{ii}	0.82 (3)	2.13 (3)	2.945 (3)	174 (3)

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

Fig. 1

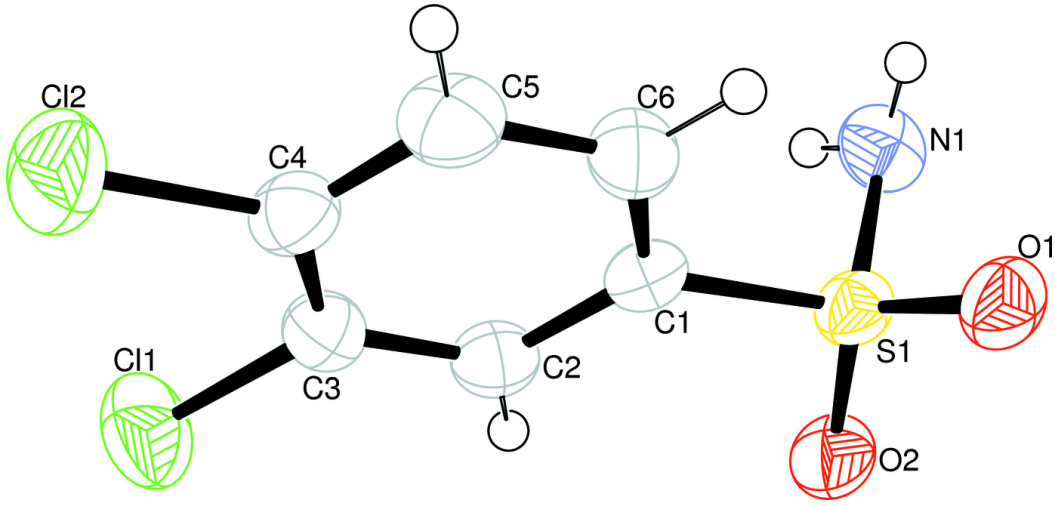

Fig. 2