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N-(2-Chlorophenyl)benzenesulfonamide

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In the crystal structure of the title compound, $C_{12}H_{10}ClNO_2S$, molecules form chains *via* hydrogen bonds, which create infinite helices along the *c* axis. The hydrogen-bond network can be described by graph set *C*(4) (an infinite chain with four atoms in the repeat pattern).

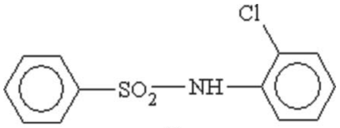
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.035
wR factor = 0.100
Data-to-parameter ratio = 10.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

Sulfanyls and sulfonamides are drugs used for the treatment of infections, some fungi and certain protozoa. Other therapeutic applications of the compounds are as diuretic and hypoglycaemic agents. On the other hand, the compounds are very interesting from a fundamental point of view, *e.g.* for studying the relationship between van der Waals interactions and hydrogen-bond topology in the formation of a crystal structure. This communication is a continuation of our work devoted to studying the crystal structures of sulfanyls and sulfonamides (Perlovich *et al.*, 2006).



(I)

A view of the title compound, (I), with the atomic numbering is presented in Fig. 1. The conformational state of the molecule in the crystal structure can be characterized and compared with the analogous parameters of *N*-(4-chlorophenyl)benzenesulfonamide, (II) (Perlovich *et al.*, 2006) (in square brackets), in the following way. The torsion angle O1—S—C1—C2, which describes the arrangement between the SO_2 group and the benzene ring Ph1 (C1–C6), is 5.83 (19)° [30.7 (4)°]. The benzene fragments are rotated relative to each other by 49.14 (9)° [54.39 (15)°]. The torsion angle N1—S—C1—C2, which describes the position of the NH group relative

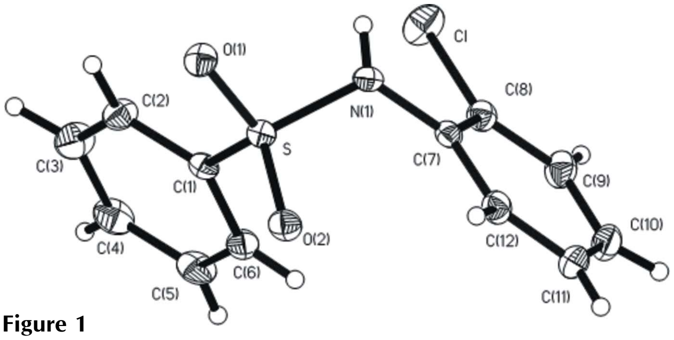


Figure 1
A view of (I) with the atomic numbering scheme. Displacement ellipsoids are drawn at the 20% probability level.

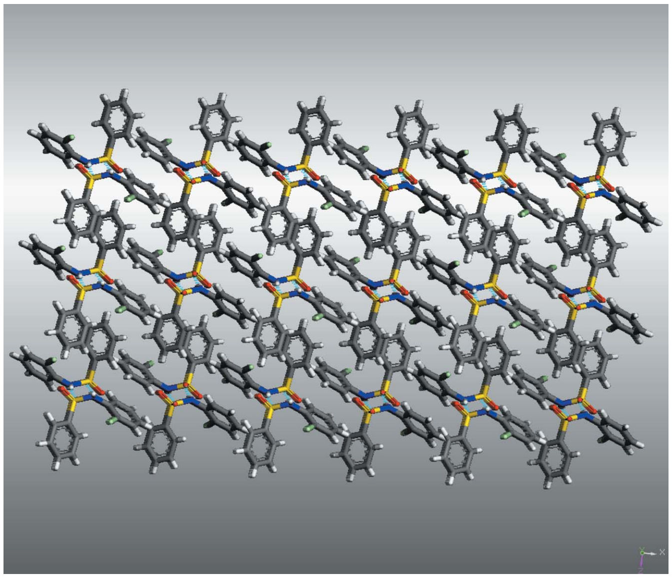


Figure 2
Projection of the crystal packing of (I) along the *b* axis.

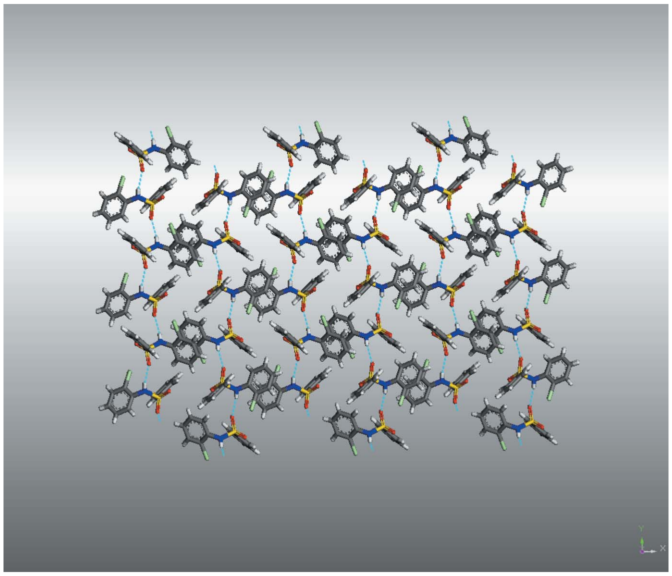


Figure 3
Projection of the crystal packing of (I) along the *c* axis.

to Ph1, is −108.50 (17)° [−83.5 (3)°]; the torsion angle S—N1—C7—C12, which characterizes the location of the SO_2 group with respect to benzene fragment Ph2 (C7–C12), is −68.3 (2)° [−71.1 (4)°]. One molecule of the title crystal structure has two equivalent hydrogen bonds: N1—H1···O2^{i} and O2···(H1—N1)^{i}; the values of the hydrogen-bond geometric parameters for (I) and (II) are summarized in Table 1.

The molecular packing architecture is shown in Figs. 2 and 3. The molecules of (I) form chains with adjacent molecules by means of the hydrogen bonds described above. The hydrogen bonds create infinite helices along the *c* axis. The hydrogen-bond network can be described by the graph set assignment introduced by Etter (1990) as *C*(4) (an infinite chain with four involved atoms). In turn, the chains of molecules interact with adjacent chains by van der Waals forces between parallel chlorophenyl fragments. It should be mentioned that the Ph1 benzene rings are arranged parallel to each other.

Experimental

The chemical synthesis of the title compound has been performed with reference to procedures described previously (Crosley *et al.*, 1940; Anderson *et al.*, 1942; Gutsche *et al.*, 1974) by reaction of a substituted aromatic amine (chloroaniline) with benzenesulfonyl chloride in dry pyridine, followed by precipitation of the end product by pouring the reaction mixture into water and by acidification to pH 5. Generally, the compounds have been recrystallized from ethanol/water. Single crystals of (I) were grown by vapour diffusion between water and an ethanol solution.

Crystal data

$C_{12}H_{10}ClNO_2S$
$M_r = 267.72$
Monoclinic, $P2_1/a$
$a = 14.821$ (3) Å
$b = 9.656$ (2) Å
$c = 8.365$ (2) Å
$\beta = 92.46$ (3)°
$V = 1196.0$ (4) Å^3
$Z = 4$
$D_x = 1.487$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 26 reflections
$\theta = 5$–10°
$\mu = 0.48$ mm^{-1}
$T = 293$ (2) K
Prism, colourless
0.4 × 0.3 × 0.2 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
Absorption correction: none
2262 measured reflections
2108 independent reflections
1727 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.027$
$\theta_{\rm max} = 25.1$°
$h = -17 \rightarrow 17$
$k = 0 \rightarrow 11$
$l = 0 \rightarrow 9$
3 standard reflections
frequency: 120 min
intensity decay: 2%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.100$
$S = 1.05$
2108 reflections
194 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0669P)^2 + 0.0406P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} = 0.001$
$\Delta\rho_{\rm max} = 0.33$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.26$ e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °) in (I) and (II).

	D—H···A	D—H	H···A	D···A	D—H···A
(I)	N1—H1···O2A^{i}	0.75 (2)	2.26 (2)	2.994 (2)	167 (2)
(II)	N1—H1···O2A^{ii}	0.78 (3)	2.21 (3)	2.993 (4)	175 (4)

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

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CELDIM* in *CAD-4 Software*; data reduction: *CAD-4 Software*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XPW* in *SHELXTL* (Sheldrick, 2000); software used to prepare material for publication: *CIFTAB* (Sheldrick, 1997).

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