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N-(4-Chlorophenyl)benzenesulfonamide

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.038
wR factor = 0.127
Data-to-parameter ratio = 11.6

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

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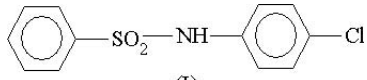
The crystal structure of the title compound, $C_{12}H_{10}ClNO_2S$, has been determined. The molecules of the substance form chains with adjacent molecules by means of hydrogen bonds, which create infinite helicoids along the *b* axis. The hydrogen-bond network can be described by the graph-set as *C*(4) (infinite chain with four atoms in the repeat pattern).

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, for studying the relationship between van der Waals interactions and hydrogen-bond topology forming a crystal structure architecture.



(I)

A view of the *N*-(4-chlorophenyl)benzenesulfonamide molecule, (I), with the atomic numbering is presented in Fig. 1. The conformational state of the molecule in the crystal structure can be characterized in the following way. The torsion angle O1—S—C1—C2, which characterizes the orientation of the SO_2 group and the phenyl ring Ph1 [C1–C6], is 30.7 (4) Å. The benzene rings are rotated relative to each other by 54.39 (15)°. The torsion angle N1—S—C1—C2, which describes the position of the NH group relative to the Ph1 ring, is −83.4 (3)°, whereas the torsion angle S—N1—C7—C12, which characterizes the location of the SO_2 group with respect to the Ph2 [C7–C12] ring, is −71.1 (4)°.

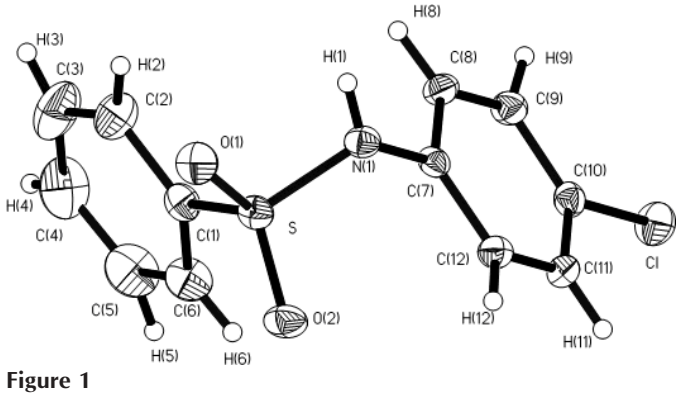


Figure 1
A view of (I), with the atomic numbering scheme. Displacement ellipsoids are drawn at the 20% probability level.

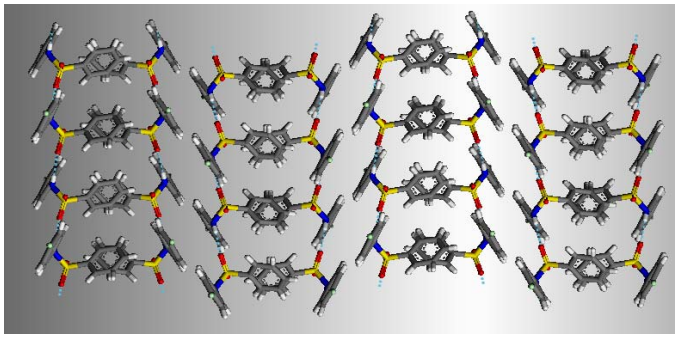


Figure 2
Projection of the molecular packing of (I) along the *a* axis.

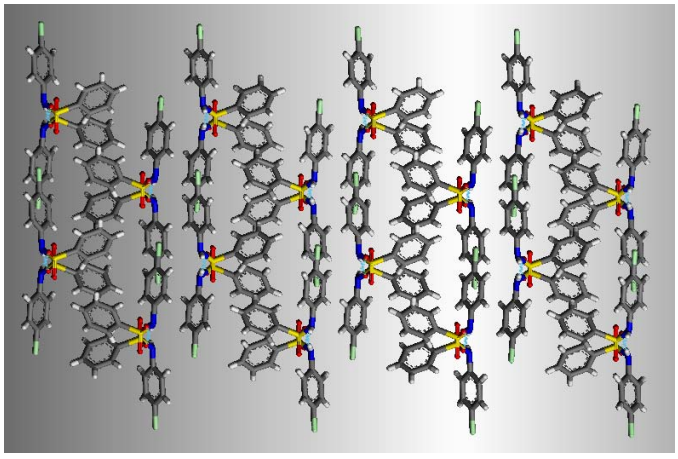


Figure 3
Projection of the molecular packing of (I) along the *b* axis.

The values of the hydrogen-bond geometric parameters 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 hydrogen bonds, which create infinite helicoids along the *b* axis. The hydrogen-bond network can be described by the graph-set assignment introduced by Etter (1990) as *C*(4) (infinite chain with four atoms in the repeat pattern). The chains form a complex layer structure which can be characterized as follows. The layer includes two types of chains which are situated in such a way that the periphery consists of the chlorophenyl groups, whereas the inner part consists of the unsubstituted phenyl rings. The chlorophenyl fragments of adjacent layers are parallel and interact with each other only by van der Waals forces. The unsubstituted phenyl rings also interact with each other by van der Waals forces, but because of the non-parallel arrangement the energy of these interactions is lower than the analogous one for the chlorophenyl fragments. These conclusions are confirmed by our data from sublimation experiments, which will be published in the near future.

Experimental

The chemical synthesis of the title compound was performed by analogy to procedures described previously (Crosley *et al.*, 1940; Anderson *et al.*, 1942; Gutsche *et al.*, 1974), by reaction of a substituted aromatic amine (here 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 were recrystallized from ethanol/water. Single crystals of *N*-(4-chlorophenyl)benzenesulfonamide were grown from a water–ethanol solution by vapour diffusion of water.

Crystal data

$C_{12}H_{10}ClNO_2S$
$M_r = 267.72$
Orthorhombic, *Pbca*
$a = 10.840\ (2)$ Å
$b = 9.740\ (1)$ Å
$c = 23.596\ (3)$ Å
$V = 2491.3\ (6)$ Å^3
$Z = 8$
$D_x = 1.428$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 35 reflections
$\theta = 5$–12°
$\mu = 0.46$ mm^{-1}
$T = 293\ (2)$ K
Prism, colourless
$0.5 \times 0.4 \times 0.1$ mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
1838 measured reflections
1838 independent reflections
1568 reflections with $I > 2\sigma(I)$
$\theta_{max} = 23.5^\circ$
$h = 0 \rightarrow 12$
$k = 0 \rightarrow 10$
$l = -26 \rightarrow 0$
3 standard reflections
frequency: 120 min
intensity decay: 2%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.127$
$S = 1.15$
1838 reflections
158 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.075P)^2 + 2.965P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.41$ e Å^{-3}
$\Delta\rho_{min} = -0.34$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0094 (9)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2^{i}	0.78 (3)	2.212 (34)	2.993 (4)	175 (4)

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

C-bound H atoms were positioned geometrically and refined as riding, with C—H = 0.93 Å. Coordinates of the N-bound H atom were determined by an optimization procedure (using a riding model), where U_{iso}(H) values were set at $1.2U_{eq}$(C,N).

Data collection: *CAD-4-PC Software* (Enraf–Nonius, 1989); cell refinement: *CELDIM* in *CAD-4-PC Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *CIFTAB* in *SHELXTL*.

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