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N-(2,3-Dichlorophenyl)benzenesulfonamide

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
R factor = 0.049
wR factor = 0.103
Data-to-parameter ratio = 12.1

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

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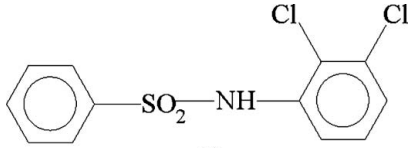
In the crystal structure of the title compound, $C_{12}H_9Cl_2NO_2S$, the dihedral angle between the two benzene rings is 54.8 (2)°. Intermolecular N—H···O hydrogen bonds lead to infinite helices along the *b* axis.

Comment

Sulfanyls and sulfonamides are drugs used for the treatment of infections, some fungal and some protozoal. Other therapeutic applications are as diuretic and hypoglycaemic agents. Furthermore, 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 crystal structures.



(I)

A view of the title compound, (I), with the atomic numbering is presented in Fig. 1. The conformation can be characterized in the following way. The torsion angle O1—S1—C1—C2, defining the orientation of the SO_2 group relative to ring Ph1 (atoms C1–C6), is 7.4 (4)°. The benzene rings are rotated relative to each other by 54.8 (2)°. The torsion angle N1—S1—C1—C2 is −106.8 (3)°, whereas the torsion angle S1—N1—C7—C12, defining the orientation of the SO_2 group with respect to ring Ph2 (C7–C12), is −63.8 (4)°.

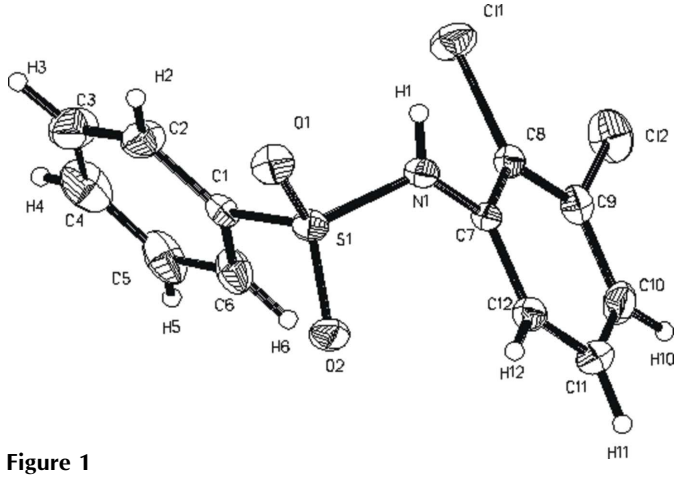


Figure 1
A view of the molecular structure, showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 20% probability level.

Intermolecular N—H···O hydrogen bonds (dashed lines in Fig. 2) result in infinite helices along the *b* axis. Numeric details are given in Table 1. The hydrogen-bond network can be described by the graph-set *C*4 (Etter, 1990). The packing of molecules in the crystal structure is also illustrated in Fig. 3.

Experimental

The chemical synthesis of the compound has been performed by analogy with procedures described in papers by Crosley *et al.* (1940), Anderson *et al.* (1942) and Gutsche *et al.* (1974), by reaction of a substituted aromatic amine (here 2,3-dichloroaniline) 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. Single crystals of the title compound were grown from a water–ethanol solution (20:1) by vapour diffusion. (Guillory, 1999).

Crystal data

$C_{12}H_9Cl_2NO_2S$
M_r = 302.16
Monoclinic, $P2_1/c$
a = 8.466 (1) Å
b = 9.805 (1) Å
c = 15.876 (2) Å
β = 92.10 (1)°
V = 1317.0 (3) Å^3
Z = 4
D_x = 1.524 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.64 mm^{-1}
T = 293 (2) K
Prism, colourless
0.28 × 0.2 × 0.11 mm

Data collection

Bruker P4 diffractometer
ω–2θ scans
Absorption correction: none
2824 measured reflections
2022 independent reflections
1152 reflections with $I > 2\sigma(I)$
R_{int} = 0.042
θ_{max} = 25.0°
3 standard reflections
frequency: 120 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.103
S = 1.00
2022 reflections
167 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.034P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0030 (9)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2^{i}	0.76 (4)	2.30 (4)	3.039 (4)	166 (4)

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

C-bound H atoms were positioned geometrically and refined as riding, with C—H = 0.93 Å; U_{iso}(H) values were set equal to $1.2U_{eq}$(C). The coordinates of the N-bound H atom were determined by an optimization procedure and refined freely [N—H = 0.76 (4) Å]

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

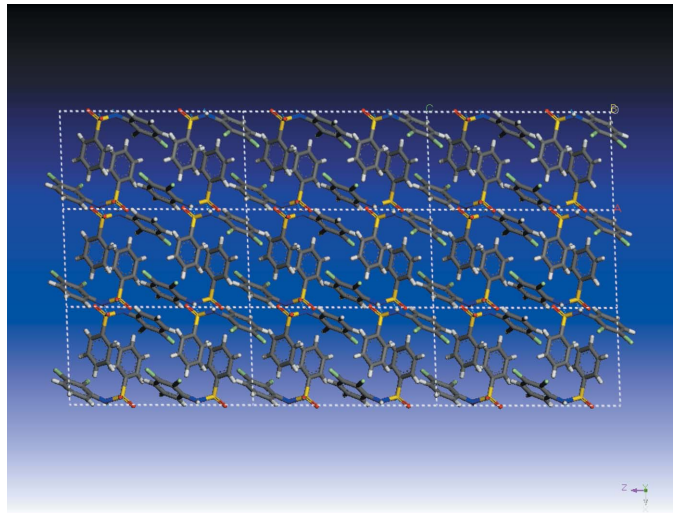


Figure 2
Projection of the molecular packing along the *a* axis. Hydrogen bonds are indicated by dashed lines.

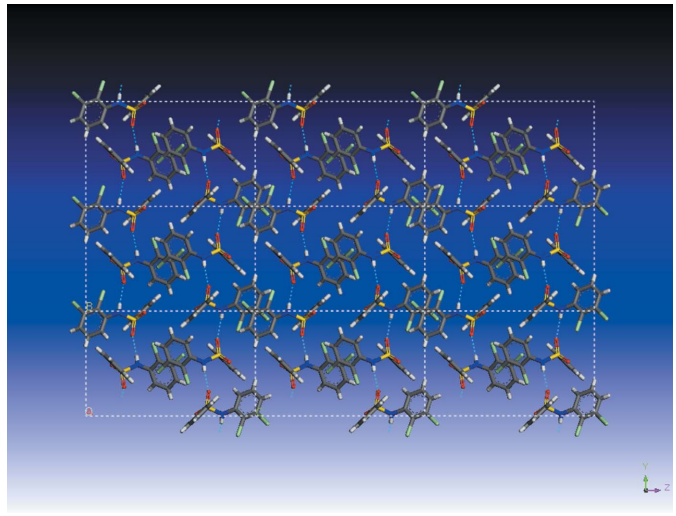


Figure 3
Projection of the molecular packing along the *b* axis.

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