organic papers

4-Amino-N-(2,3-dichlorophenyl)benzenesulfonamide

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In the crystal structure of the title compound, $C_{12}H_{10}Cl_2N_2O_2S$, there are two independent molecules in the asymmetric unit. Hydrogen bonds between NH_2 and SO_2 groups link molecules into layers, which interact with each other only by van der Waals forces

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 sulfonamides (Perlovich et al., 2006a,b; Tkachev et al., 2006).

In the title compound, (I), there are two independent molecules (A and B) in the asymmetric unit (Figs. 1 and 2). The torsion angle C2—C1—S1—O1 of molecule A, which characterizes the relationship between the SO_2 group and the aminobenzene ring (C1–C6), is 47.30 (16)°. The analogous angle for molecule B, C22—C21—S21—O21, is 37.43 (17)°. It is interesting to compare this parameter with the corresponding angle in N-(2,3-dichlorophenyl)benzenesulfonamide, (II) (Tkachev et al., 2006), which is 7.4 (4)°. The benzene rings are rotated relative to each other by 81.56 (6)° for A, 79.11 (7)° for B and 54.8 (2)° for (II). Thus, introducing an additional NH_2 group in (I), which creates hydrogen bonds, leads to an increase in the angle between the benzene rings. The torsion angles C2—C1—S1—N1 (in A) and C22—C21—S21—N21 (in B), which describe the position of the NH group relative to the aminobenzene ring, are −64.82 (16) and
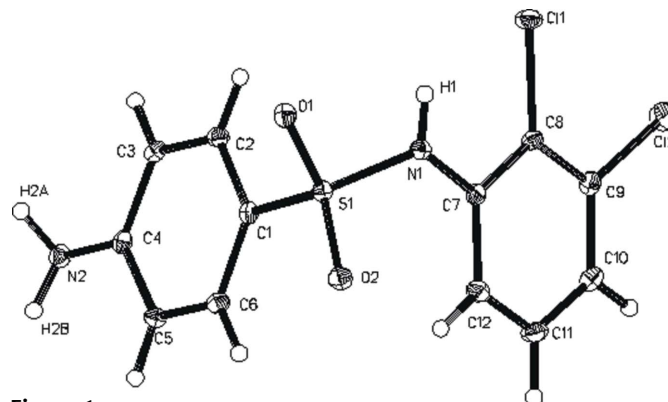
Figure 1
The structure of molecule A with the atomic numbering scheme. Displacement ellipsoids are drawn at the 20% probability level.
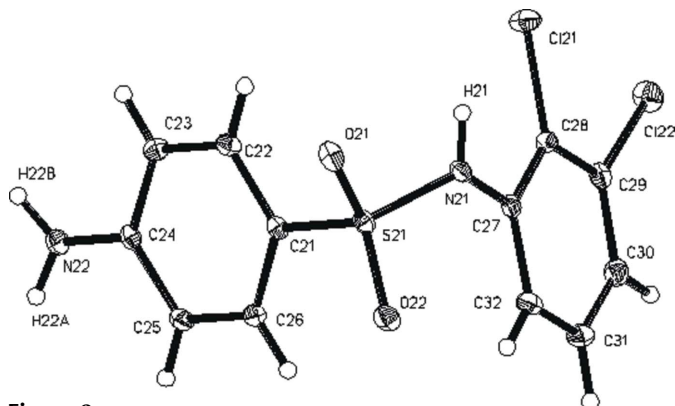
Figure 2
The structure of molecule *B* with the atomic numbering scheme. Displacement ellipsoids are drawn at the 20% probability level.
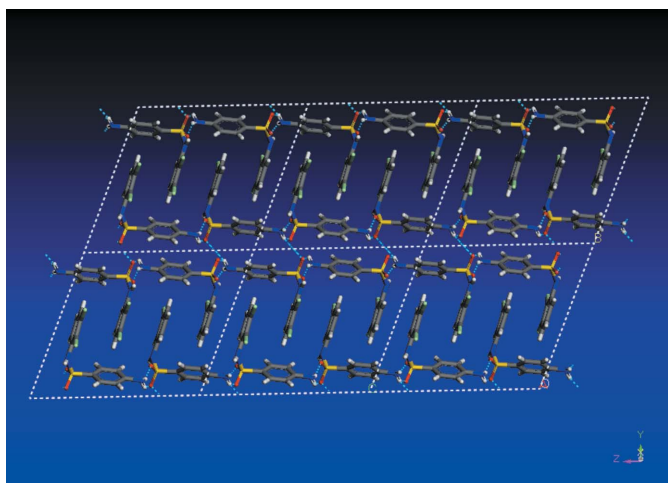

Figure 3
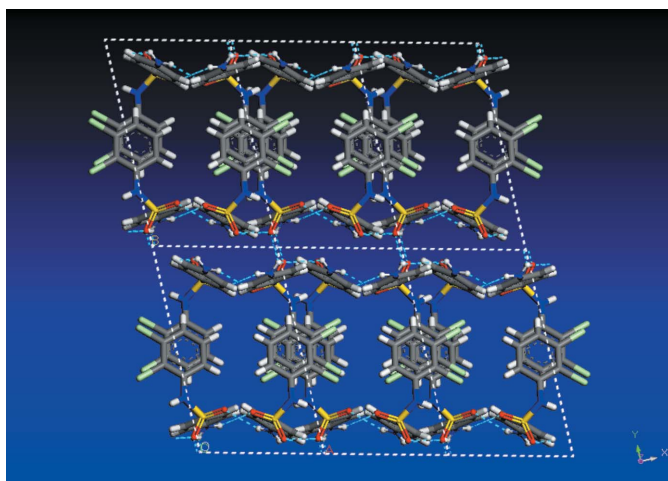Projection of the molecular packing of (I) along the *a* axis.

Figure 4
Projection of the molecular packing of (I) along the *c* axis.

−75.61 (17), respectively; the equivalent angle in (II) is −106.8 (3)°. The torsion angles S1—N1—C7—C12 (in *A*) and S21—N21—C27—C32 (*B*), which characterize the orientation of the SO_2-group with respect to the dichlorobenzene ring are −28.1 (2)° and −43.0 (2)°, respectively; the equivalent angle

in (II) is 63.8 (4)°. The values of the hydrogen-bond geometric parameters are summarized in Table 1. The molecular packing is shown in Figs. 3 and 4. The molecules of (I) form a complex layered structure in which the layers involve a hydrogen-bond network between NH_2 and SO_2 groups. The layers interact with each other by van der Waals forces (contacts between the dichlorophenyl fragments).

(I)

(II)
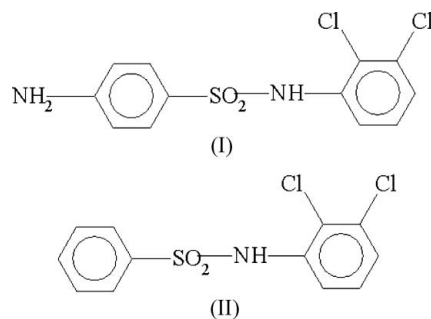
Experimental

The chemical synthesis of the title compound has been performed in two steps [in analogy to procedures described by Crosley *et al.* (1940) and Anderson *et al.* (1942)], by reaction of a substituted aromatic amine (here 2,3-dichloroaniline) with 4-acetylaminobenzenesulfonyl chloride in dry pyridine, followed by hydrolytic deacetylation in alkaline aqueous medium ($\sim$1 *M* NaOH) and precipitation of the end product by acidification ($\sim$1 *M* HCl) to pH 5. Single crystals of the title compound were grown from a water–ethanol solution (20:1) by vapour diffusion of ethanol vapour into an aqueous solution (Guillory, 1999).

Crystal data

$C_{12}H_{10}Cl_2N_2O_2S$	$V = 1343.6$ (2) Å^3
$M_r = 317.18$	$Z = 4$
Triclinic, $P\bar{1}$	$D_x = 1.568$ Mg m^{-3}
$a = 7.4700$ (8) Å	Mo $K\alpha$ radiation
$b = 13.613$ (1) Å	$\mu = 0.64$ mm^{-1}
$c = 14.548$ (1) Å	$T = 200$ (2) K
$\alpha = 110.91$ (1)°	Prism, colourless
$\beta = 90.51$ (1)°	$0.4 \times 0.2 \times 0.2$ mm
$\gamma = 102.42$ (1)°	

Data collection

Siemens P4 diffractometer	$R_{int} = 0.011$
ω–2θ scans	$\theta_{max} = 25.0°$
Absorption correction: none	3 standard reflections
5502 measured reflections	every 2 reflections
4499 independent reflections	intensity decay: none
4325 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0359P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.029$	$+ 0.8502P]$
$wR(F^2) = 0.080$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.10$	$(\Delta/\sigma)_{max} = 0.001$
4499 reflections	$\Delta\rho_{max} = 0.31$ e Å^{-3}
362 parameters	$\Delta\rho_{min} = -0.34$ e Å^{-3}
H atoms treated by a mixture of	Extinction correction: *SHELXL97*
independent and constrained	Extinction coefficient: 0.0131 (8)
refinement	

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

$D\mathrm{-H}\cdots A$	$D\mathrm{-H}$	$\mathrm{H}\cdots A$	$D\cdots A$	$D\mathrm{-H}\cdots A$
N1—H1···N22[i]	0.79 (2)	2.325 (25)	3.083 (2)	160 (2)
N2—H2A···O1[ii]	0.86 (3)	2.47 (2)	3.126 (2)	134 (2)
N2—H2A···O21[ii]	0.86 (3)	2.45 (2)	3.066 (2)	130 (2)
N2—H2B···O22[iii]	0.86 (2)	2.22 (3)	3.047 (2)	161 (2)
N21—H21···N2[ii]	0.82 (2)	2.245 (25)	3.034 (2)	160 (2)
N22—H22A···O2[iv]	0.83 (2)	2.41 (3)	3.190 (2)	156 (2)
N22—H22A···O21[iv]	0.83 (2)	2.94 (2)	3.401 (2)	117 (2)
N22—H22B···O1[i]	0.84 (2)	2.40 (2)	2.999 (2)	129 (2)

Symmetry codes: (i) $-x, -y, -z+1$; (ii) $-x, -y, -z$; (iii) $-x+1, -y, -z$; (iv) $-x+1, -y, -z+1$.

H-atom coordinates were determined by an independent optimization procedure.

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, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics: *XPW* in *SHELXTL* (Sheldrick, 1997b); software used to prepare material for publication: *CIFTAB* in *SHELXTL*.

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