Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

2-Amino-5-(*p*-nitrophenylsulfonyl)-1,3-thiazole

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.003 Å
R factor = 0.041
wR factor = 0.105
Data-to-parameter ratio = 18.5

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

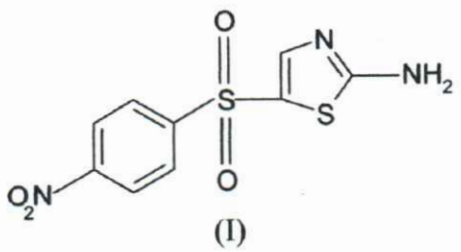
In the molecule of the title compound, $C_9H_7N_3O_4S_2$, the thiazole ring is oriented with respect to the benzene ring at a dihedral angle of 67.85 (5)°. Molecules are linked by intermolecular N—H···O and N—H···N hydrogen bonds between the amino H atoms and O and N atoms of the sulfonyl group and thiazole ring, respectively, forming infinite sheets.

Received 17 May 2006
Accepted 29 May 2006

Comment

Sulfathiazole derivatives are used as bacteriostatic drugs and are of importance in the treatment of certain infections. Sulfathiazole is widely used in veterinary practice for the treatment of various bacterial infections, *e.g.* in diseases of honey bees. In studies of aminophenyl sulfone derivatives, it was concluded that some of them have chemotherapeutic efficacy against tuberculosis *in vitro* and some modifications of the derivatives should afford drugs suitable for clinical applications (Bambas, 1945*a*).

The 1,3-thiazole ring has been identified as a central structural element of a number of biologically active natural products (Zabriskie *et al.*, 1988; Hara *et al.*, 1988; Crews *et al.*, 1988) and of pharmacologically active compounds (Metzger, 1979, 1984). The bioactivity of thiazoles is mainly due to their structural similarities with the imidazolyl entities of proteins (Kornis, 1984), as well as their biological, structural, electronic and spectroscopic properties (Comba, 1993; Brown & Lee, 1993). Their existence may modify the bioactive and pharmaceutical characteristics of the adducts (Chohan *et al.*, 2002; Nakamura *et al.*, 1995; Boden & Pattanden, 1994). We present here the crystal structure of the title compound, (I).



(I)

Compound (I) (Fig. 1) is a derivative of 2-aminothiazole, (II) (Caranoni & Capella, 1982), containing a nitrophenylsulfonyl group as substituent. The bond lengths and angles are in normal ranges (Allen *et al.*, 1987).

Comparing (I) with 2-amino-4-(4-methoxyphenyl)-1,3-thiazole, (III) (Hökelek *et al.*, 2006), reveals that all bond lengths and angles of the thiazole ring in (I) are nearly the same. The C2—S1—C5 [88.26 (7)°] bond angle in (I) is smaller than the corresponding one in 2-amino-4-phenylthiazole

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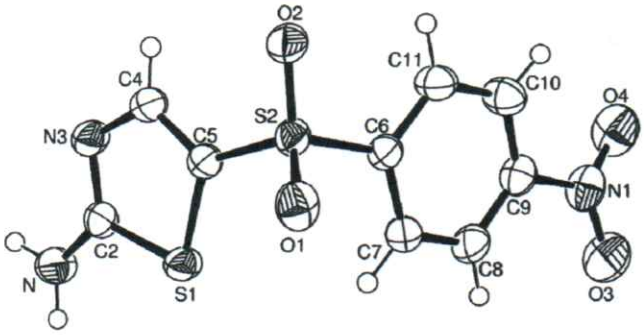


Figure 1
The molecular structure, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

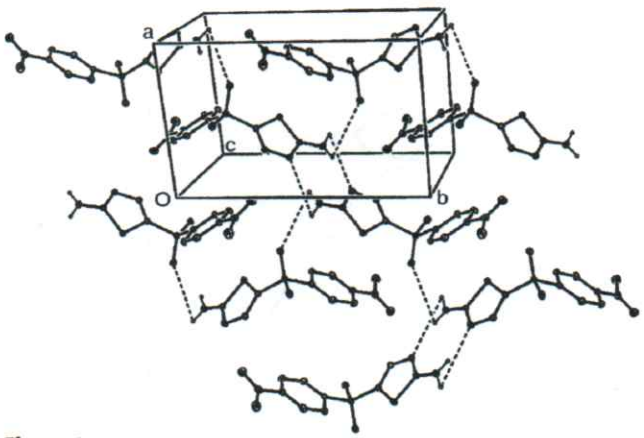


Figure 2
A packing diagram for (I). Intermolecular N—H···O and N—H···N hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted for clarity.

hydrobromide monohydrate, (IV) (90.17°; Form *et al.*, 1974), while it is nearly the same as that in (III) [88.4 (3)°].

An examination of the deviations from the least-squares planes through individual rings shows that the thiazole and phenyl rings *A* (S1/C2/N3/C4/C5) and *B* (C6–C11) are both planar. The dihedral angle between the two rings is 68.85 (5)°. Ring *A* has a pseudo-twofold axis running through atom C5 and the midpoint of the N3—C2 bond, as is evident from the torsion angles (Table 1).

The O2—S2—C6 [108.02 (6)°] angle is enlarged. It is well known that nitro substituents are very strong electron-withdrawing groups, so the endocyclic C8—C9—C10 [122.93 (16)°] angle is also enlarged. The electron-withdrawing character of the nitrophenylsulfonyl group affects the bond lengths C5—S2 [1.7231 (15) Å] and C6—S2 [1.7740 (16) Å]. On the other hand, the electron-withdrawing character of the nitro group has an influence on the C9—N1 [1.472 (2) Å] bond length, as in *N*-(*p*-nitrophenylsulfonyl)-1*H*-pyrrole (Gültekin *et al.*, 2004).

The crystal packing of (I) is stabilized by intermolecular N—H···N [H1···N3^{i} = 2.14 (2) Å, N···N3^{i} = 2.995 (2) Å and N—H1···N3^{i} = 170 (2)°] and N—H···O [H2···O1^{ii} = 2.36 (2) Å, N···O1^{ii} = 3.108 (2) Å and N—H2···O1^{ii} 142 (2)°] hydrogen bonds [symmetry codes: (i) $-x, -y, -z$; (ii) $1-x, y-\frac{1}{2}, \frac{1}{2}-z$], forming infinite sheets extending parallel to the (110) plane and stacked along the *c* axis (Fig. 2).

Experimental

The title compound was synthesized according to the literature method of Bambas (1945*b*) and crystallized from a solution in ethanol.

Crystal data

$C_9H_7N_3O_4S_2$
M_r = 285.30
Monoclinic, $P2_1/c$
a = 8.6310 (2) Å
b = 12.4943 (3) Å
c = 11.4911 (4) Å
β = 110.874 (2)°
V = 1157.85 (6) Å^3
Z = 4
D_x = 1.637 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.47 mm^{-1}
T = 296 (2) K
Block, yellow
0.20 × 0.20 × 0.20 mm

Data collection

Rigaku R-AXIS RAPID-S diffractometer
ω scans
Absorption correction: none
22950 measured reflections
3543 independent reflections
3314 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 30.6°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.106
S = 1.16
3543 reflections
191 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.042P)^2 + 0.3858P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}

Table 1
Selected torsion angles (°).

C2—S1—C5—C4	0.26 (13)	C4—N3—C2—S1	0.80 (18)
C5—S1—C2—N3	−0.62 (13)	S1—C5—C4—N3	0.1 (2)
C2—N3—C4—C5	−0.6 (2)		

H atoms were located in a difference synthesis and refined isotropically; refined values are in the ranges N—H = 0.87 (2)–0.883 (16) Å and U_{iso}(H) = 0.062 (7)–0.067 (7) Å^2, and C—H = 0.91 (2)–0.98 (2) Å and U_{iso}(H) = 0.037 (5)–0.070 (7) Å^2.

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors are indebted to the Department of Chemistry and Atatürk University, Erzurum, Turkey, for the use of the X-ray diffractometer purchased under grant No. 2003/219 of the University Research Fund.

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