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1-Phenylsulfonyl-1*H*-1,2,4-triazole

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.004 Å
R factor = 0.045
wR factor = 0.125
Data-to-parameter ratio = 12.0

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

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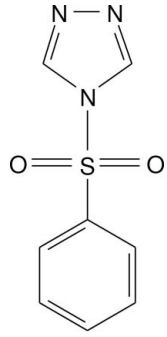
In the title compound, $C_8H_7N_3O_2S$, the dihedral angle between the 1,2,4-triazole ring and the phenyl ring is 82.17 (14)°. The geometry around the S atom is distorted tetrahedral. The molecules are linked by intermolecular C—H···N and C—H···O hydrogen bonds.

Comment

1,2,4-Triazoles have attracted considerable attention in the fields of medicine and agrochemical research and also in materials science due to their unique structures and properties. Fluconazole, which contains two 1,2,4-triazole residues, is a powerful antifungal agent (Al-Soud *et al.*, 2004). Substituted 1,2,4-triazoles have been found to exhibit anti-inflamatory, insecticidal, antifungal and antimicrobial activities (Boschelli *et al.*, 1993). Sulfonamides are among the most widely used antibacterial agents in the world, chiefly because of their low cost, low toxicity and excellent activity against common bacterial diseases. In the light of the above information, the title compound, (I), was synthesized and we report here its crystal structure.



(I)

The molecular structure and the atom-numbering scheme of (I) are shown in Fig. 1. In (I), the dihedral angle between the

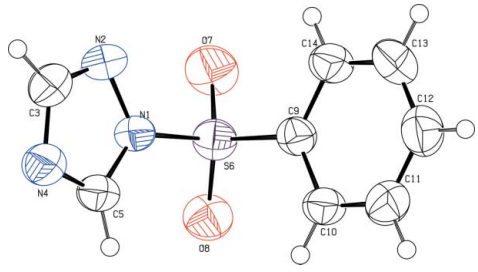


Figure 1
The molecular structure of (I), shown with 50% probability displacement ellipsoids.

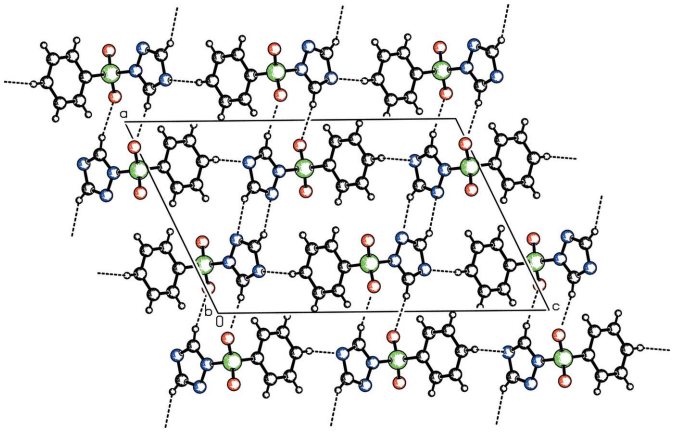


Figure 2
The packing of (I), viewed down the *b* axis. Dashed lines indicate intermolecular hydrogen bonds.

1,2,4-triazole ring and the phenyl ring is 82.17 (14)°. The geometry around the S atom is distorted tetrahedral, with the largest deviations being observed for the O—S—O and O—S—N angles (Table 1). The O—S—O widening may be due to the repulsive interaction betwen the two short S=O bonds. The S—N bond distances lie within the expected range of 1.63–1.69 Å. The reduction of the N1—S6—C9 angle to 103.86 (10)° from the ideal tetrahedral value is attributed to the Thorpe–Ingold effect (Bassindale *et al.*, 1984).

The crystal packing is stabilized by C—H···N and C—H···O hydrogen bonds (Table 2). These hydrogen bonds links the molecules into chains (Fig. 2).

Experimental

1-Benzenesulfonyl-1*H*-1,2,4-triazole was obtained by the condensation of 1,2,4-triazole with benzenesulfonyl chloride in the presence of triethylamine as the base. First, 1,2,4-triazole (1 g, 14.4 mmol) was dissolved in dichloromethane (10 ml) and cooled to 273–278 K in an ice bath. Triethylamine (4.37 g, 43.2 mmol) was then added to the cold reaction mixture and the resulting solution was stirred for 10 min. Benzenesulfonyl chloride (2.44 g, 14.4 mmol) was added to the reaction mixture which was then allowed to cool to room temperature and stirred for 5 h. The reaction mass was monitored by thin-layer chromatography. On completion of the reaction, the solvent was removed under reduced pressure and the residue was taken up in water and extracted with ethyl acetate. Finally, the organic layer was washed with water and dried over anhydrous sodium sulfate. The product was a white crystalline solid (yield 2.25 g, 89%), which was dissolved in ethyl acetate–methanol (3:1) and kept for 4 d. Upon slow evaporation of the solvent, white crystals of (I) developed (m.p. 442.15 K).

Crystal data

$C_8H_7N_3O_2S$
M_r = 209.23
Monoclinic, $P2_1/c$
a = 11.395 (14) Å
b = 5.045 (3) Å
c = 17.698 (19) Å
β = 115.445 (3)°
V = 918.7 (16) Å^3
Z = 4
D_x = 1.513 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.33 mm^{-1}
T = 295 (2) K
Block, white
0.25 × 0.20 × 0.20 mm

Data collection

MacScience DIPLabo 32001 diffractometer
ω scans
Absorption correction: none
2728 measured reflections
1535 independent reflections
1284 reflections with $I > 2\sigma(I)$
R_{int} = 0.018
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.125
S = 1.06
1535 reflections
128 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0688P)^2 + 0.33P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.038 (5)

Table 1
Selected geometric parameters (Å, °).

S6—O7	1.413 (3)	N1—C5	1.346 (4)
S6—O8	1.422 (3)	N2—C3	1.307 (4)
S6—N1	1.699 (3)	N4—C3	1.347 (5)
S6—C9	1.741 (3)	N4—C5	1.299 (4)
N1—N2	1.361 (3)		
O7—S6—O8	121.63 (11)	N2—N1—C5	109.50 (19)
O7—S6—N1	105.74 (11)	N1—N2—C3	101.2 (2)
O7—S6—C9	110.69 (12)	C3—N4—C5	102.6 (2)
O8—S6—N1	103.42 (11)	N2—C3—N4	116.3 (3)
O8—S6—C9	109.69 (11)	N1—C5—N4	110.4 (2)
N1—S6—C9	103.85 (10)	S6—C9—C10	119.12 (19)
S6—N1—N2	122.01 (17)	S6—C9—C14	119.47 (18)
S6—N1—C5	128.08 (17)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···N2^{i}	0.93	2.55	3.425 (6)	157
C5—H5···O8^{ii}	0.93	2.38	3.296 (5)	169
C12—H12···N4^{iii}	0.93	2.57	3.490 (6)	169

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

H atoms were placed at idealized positions and allowed to ride on their parent atoms, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(carrier atom).

Data collection: *XPRESS* (MacScience, 2002); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003) and *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *PLATON*.

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