Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-Methyl-*N*′-[(*E*)-4-methylbenzylidene]-benzenesulfonohydrazide

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Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.002 Å
R factor = 0.037
wR factor = 0.107
Data-to-parameter ratio = 29.2

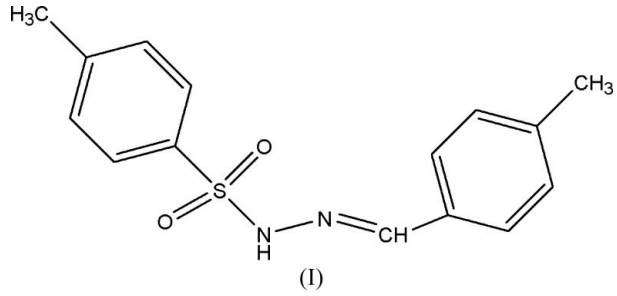
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 21 February 2007
Accepted 20 March 2007

Reaction of toluene-4-sulfonohydrazide with 4-methylbenzaldehyde resulted in the formation of the imine title compound, $C_{15}H_{16}N_2O_2S$. In the crystal structure, molecules are linked into chains through intermolecular N—H···O hydrogen-bond interactions.

Comment

Sulfonamides represent an important class of biologically active compounds (Supuran *et al.*, 1999). Aromatic sulfonamides are strong inhibitors of carbonic anhydrase (Maren, 1967) and are of pharmacological value because of their effects on various physiological reactions ultimately involving bicarbonate. Sulfonamides have also been useful in studies of the physical chemistry and the mechanism of action of carbonic anhydrase because of their highly specific interaction with the active site (King & Burgen, 1976). Moreover, sulfonamides containing different donor atoms find use in coordination chemistry (Culf *et al.*, 1997; Beloso *et al.*, 2004, 2005). In this communication, we report the synthesis and crystal structure of the title compound, (I), containing a sulfonamide and an imine functional group.



(I)

In the molecule of (I) (Fig. 1), the bond lengths and angles are unexceptional. The aromatic rings assume an almost perpendicular orientation, forming a dihedral angle of 81.90 (3)°. The molecular structure is stabilized by an intramolecular C—H···O hydrogen-bond interaction (Table 1). In the crystal packing (Fig. 2), molecules are linked into chains running parallel to the *a* axis by N—H···O hydrogen bonds (Table 1).

Experimental

A mixture of toluene-4-sulfonohydrazide (1.86 g, 10 mmol) in ethanol (20 ml) and 4-methylbenzaldehyde (1.8 ml, 15 mmol) was refluxed for 6 h at 373 K. The progress of the reaction was monitored by thin-layer chromatography. After completion of the reaction, the solid crude title compound was filtered off and washed with cold

ethanol (5 ml). The filtrate was dissolved in CH_2Cl_2 and kept at 277 K. Colourless crystals suitable for X-ray analysis were obtained after a few days on slow evaporation of the solvent.

Crystal data

$C_{15}H_{16}N_2O_2S$
M_r = 288.36
Monoclinic, $P2_1/n$
a = 5.3411 (2) Å
b = 15.8299 (7) Å
c = 17.4133 (8) Å
β = 98.0340 (10)°
V = 1457.83 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.23 mm^{-1}
T = 100 (2) K
0.20 × 0.10 × 0.10 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.957, T_{max} = 0.978
22219 measured reflections
5374 independent reflections
4457 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.107
S = 1.03
5374 reflections
184 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.54 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C14—H14A···O1	0.95	2.56	2.9233 (14)	103
N1—H1···O1^{i}	0.92	2.12	3.0308 (12)	170

Symmetry code: (i) $x+1, y, z$.

The H atom bound to the N atom was located in a difference Fourier map and refined as riding with an isotropic displacement parameter. All other H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.95–0.98 Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

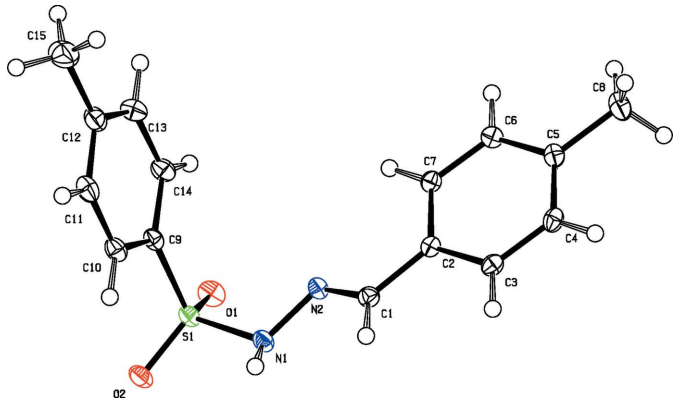


Figure 1
The molecular structure of (I). Displacement ellipsoids are drawn at the 50% probabiity level.

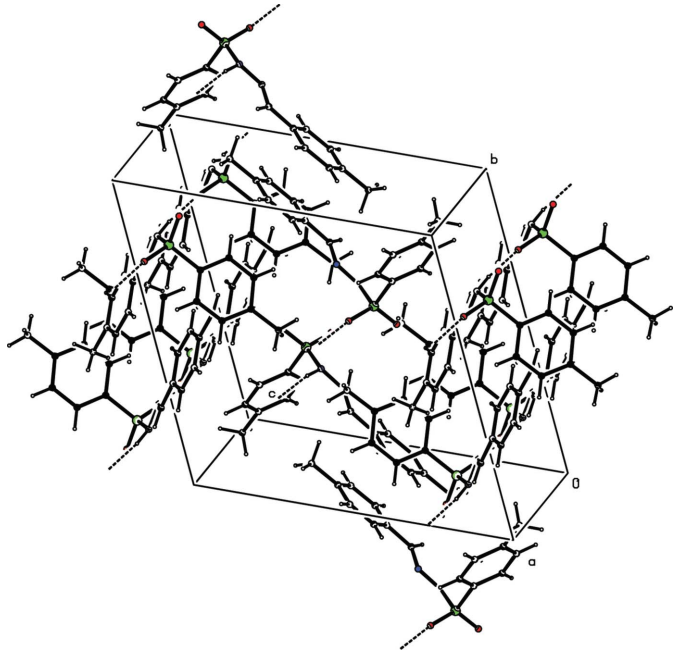


Figure 2
Packing diagram of (I), showing the intermolecular hydrogen bonds (dashed lines) linking the molecules along the *a*-axis direction.

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