Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-Methyl-*N*-(3-nitrophenyl)benzenesulfonamide

Jun-De Xing,[a]* Guo-Yi Bai,[b] Tao Zeng[a] and Jiang-Sheng Li[a]

[a]College of Pharmaceuticals and Biotechnology, Tianjin University, Tianjin 300072, People's Republic of China, and [b]College of Chemistry and Environmental Science, Hebei University, Hebei 071002, People's Republic of China

Correspondence e-mail: xing_junde@126.com

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.043
wR factor = 0.147
Data-to-parameter ratio = 16.6

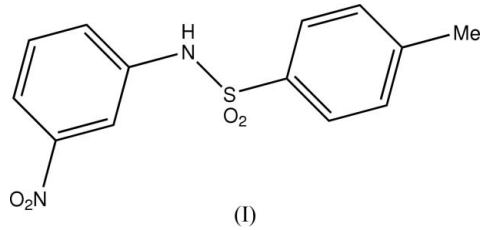
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 30 September 2005
Accepted 28 November 2005
Online 7 December 2005

In the molecule of the title compound, *m*-$(O_2N)C_6H_4NHSO_2$-C_6H_4-*p*-Me or $C_{13}H_{12}N_2O_4S$, the planes of two benzene rings are orthogonal to each other [dihedral angle 92.4 (1)°].

Comment

The title molecule represents an important synthon for the preparation of a variety of sulfonamide drugs (Thakur *et al.*, 2005). The planes of the two benzene rings are orthogonal to each other [dihedral angle 92.4 (1)°; the C—N—S—C torsion angle in the central part of the molecule is −67.82 (17)°]. An N—H···O bond links the molecules into infinite chains running along the diagonal of the *ac* plane of the crystal structure.



(I)

Experimental

The title compound was prepared according to the method of Sprague & Miller (1952). To a solution of 3-nitroaniline (27.6 g) in pyridine (100 ml) was added 4-tosyl chloride (41.8 g); the mixture was heated for 0.5 h at 373 K, then cooled to room temperature and poured into 500 ml of dilute HCl, yielding 4-methyl-*N*-(3-nitrophenyl)benzenesulfonamide in quantitative yield. X-ray quality crystals of the title compound (m.p. 405–407 K) were obtained by slow evaporation of an ethanol solution.

Crystal data

$C_{13}H_{12}N_2O_4S$
M_r = 292.31
Monoclinic, $P2_1/n$
a = 12.766 (3) Å
b = 7.7327 (15) Å
c = 13.550 (3) Å
β = 101.66 (3)°
V = 1310.0 (5) Å^3
Z = 4
D_x = 1.482 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 10604 reflections
θ = 3.0–27.5°
μ = 0.26 mm^{-1}
T = 293 (2) K
Block, light yellow
0.29 × 0.15 × 0.07 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Oscillation scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.928, T_{max} = 0.981
12545 measured reflections
2997 independent reflections
2519 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 27.5°
h = −16 → 16
k = −10 → 9
l = −17 → 16

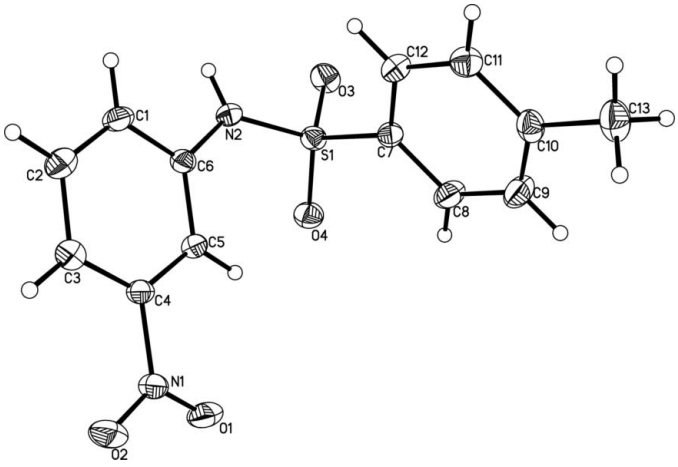


Figure 1
Molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level; H atoms are shown as small spheres of arbitrary radii.

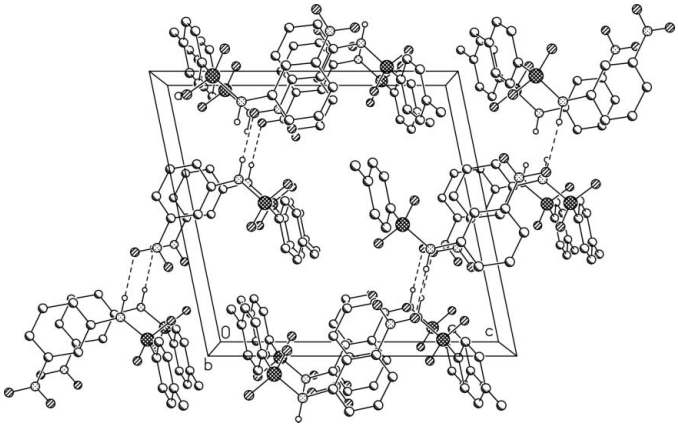


Figure 2
The packing of the title compound, projected on to the *ac* plane; the N—H···O bonds are shown as dashed lines. H atoms attached to C atoms have been omitted.

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.1119P)^2 + 0.1885P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.043$	$(\Delta/\sigma)_{max} = 0.005$
$wR(F^2) = 0.147$	$\Delta\rho_{max} = 0.39$ e Å^{-3}
$S = 1.01$	$\Delta\rho_{min} = -0.44$ e Å^{-3}
2997 reflections	
181 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

S1—O4	1.4277 (14)	N1—O1	1.213 (2)
S1—O3	1.4341 (14)	N1—O2	1.227 (2)
S1—N2	1.6316 (16)	N1—C4	1.468 (2)
S1—C7	1.7628 (17)	N2—C6	1.416 (2)
O4—S1—O3	119.37 (9)	O3—S1—C7	109.24 (8)
O4—S1—N2	108.83 (8)	N2—S1—C7	106.61 (8)
O3—S1—N2	104.23 (9)	O1—N1—O2	122.59 (16)
O4—S1—C7	107.87 (9)		
C7—S1—N2—C6	−67.82 (17)	O3—S1—C7—C12	67.70 (17)
S1—N2—C6—C1	161.38 (14)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O2^{i}	0.86	2.23	3.058 (2)	162

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

All H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 and 0.96 Å, N—H = 0.86 Å and $U_{iso}(H) = 1.2U_{eq}(C_{aromatic},N)$ and $1.5U_{eq}(C_{Me})$.

Data collection: *RAPID-AUTO* (Rigaku, 1997); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; 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: *SHELXL97*.

The authors thank the Research Center of Pharmaceutical Crystallization Engineering (Tianjin University, the State Pharmaceutical Administration of China) for help with the X-ray diffraction experiment.

References

Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Rigaku (1997). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (1997*a*). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sprague, J. M. & Miller, C. S. (1952). US Patent No. 2 608 506.
Thakur, M., Thakur, A., Khadikar, P. V. & Supuran, C. T. (2005). *Bioorg. Med. Chem. Lett.* **15**, 203–209.