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N-Butyl-*N*-*o*-tolylbenzenesulfonamide

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Key indicators

Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.004 Å
R factor = 0.061
wR factor = 0.179
Data-to-parameter ratio = 18.9

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

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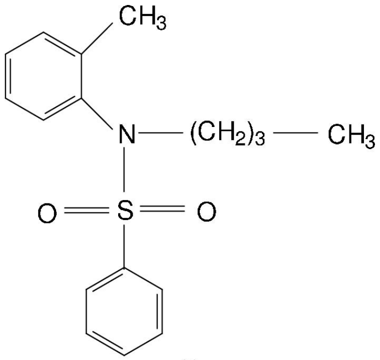
In the structure of *N*-butyl-*N*-*o*-tolylbenzenesulfonamide, $C_{17}H_{21}NO_2S$, the mean planes of the benzene rings are inclined to each other at 40.3 (1)°. The geometry around the S atom is considerably distorted from ideal tetrahedral geometry. Centrosymmetrically related pairs of molecules dimerize through C—H···O hydrogen bonds. The crystal packing is stabilized by intermolecular C—H···O hydrogen bonding.

Comment

Sulfonamides and their derivatives are well known antibacterial drugs and they are also observed to produce antimicrobial effects (Bock *et al.*, 1974). 4-Phthalimide-*N*-(1,3-thiazol-2-yl)benzene sulfonamide is used in the treatment of intestinal infections. A quinolyl sulfonamide has been used in industrial solvent-extraction processes to isolate copper(II) (Kordosky, 1976). The X-ray structural study of the title *N*-substituted sulfonamide, (I), has been carried out in order to obtain detailed structural information about the compound.



(I)

The hybridization of the N atom imposes restrictions on the relative orientations of the C—N—S and O=S=O planes. The angle between these planes is 89.8 (1)° for sp^3-hybridization [the sum of the angles around the N atom is 350.5°].

The geometry around the S atom is distorted tetrahedral, similar to that observed in other reported structures (Basak *et al.*, 1982, 1983; Basak, Mazumdar & Chaudhuri, 1984; Basak, Chaudhuri & Mazumdar, 1984). The maximum and minimum values of the angles around S are 119.9 (1) and 106.7 (1)°, respectively. This deviation can be attributed to the non-bonded interactions involving the two S—O bonds, resulting in structures with less steric interference (Cotton & Stokley, 1970) and the varied steric bulk of the substituents.

The S—N and S—C bond distances are comparable with the corresponding values in reported structures of substituted

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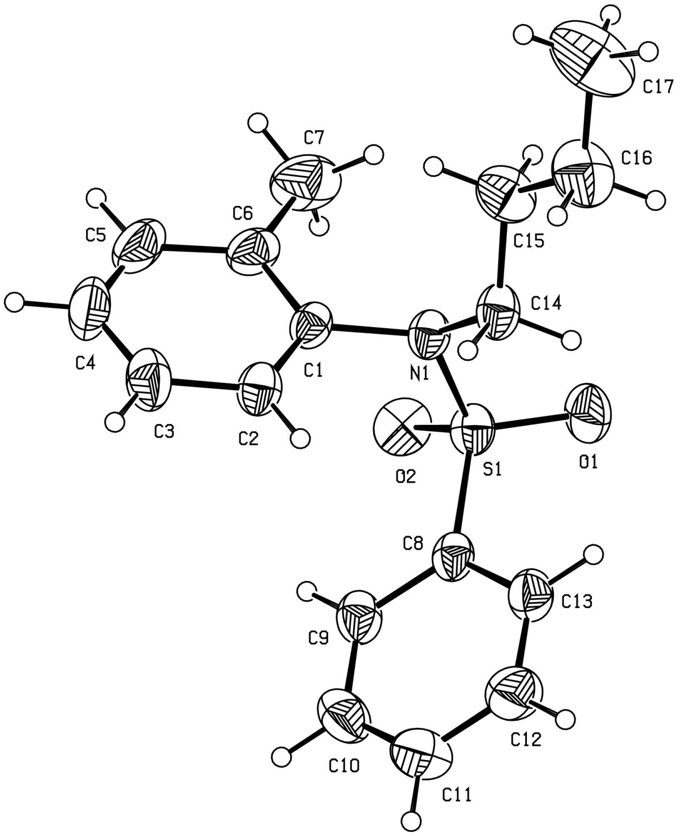

Figure 1
The molecular structure of the title compound, showing 30% probability displacement ellipsoids.

sulfonamides (Basak, Mazumdar & Chaudhuri, 1984; Germain *et al.*, 1983; Cotton *et al.*, 1970) but these distances are shorter than the corresponding single-bond distances. The shortening has been attributed to $d\pi$–$p\pi$ interaction between these atoms. The average S—O bond length is 1.426 (2) Å. The N1—C1 distance is slightly shorter than the Nsp^2—Csp^2 single-bond distance, whereas the N1—C14 distance is slightly greater.

The conformation of the molecule can be described by the torsion angles about the C8—S1, S1—N1, N1—C1 and N1—C14 central bonds; all lie well within the clustering range of $|\varepsilon|$ = 70–120° (Kálmán *et al.*, 1981). Sulfonyl atoms O1 and O2 are oriented +antiperiplanar and +synclinal, respectively, with respect to C1. The butyl and the tolyl groups are *trans* to one another and are symmetrically oriented with the sulfonyl group. The C14—C15—C16—C17 torsion angle shows a −antiperiplanar disposition.

In sulfonamides, generally the two planar rings are orthogonal to each other, but in the present study, the dihedral angle between the two rings is 40.3 (1)°, showing that the orientation of these rings is mainly determined by crystal forces and packing requirements. The planes of the butyl C atoms and tolyl C atoms make dihedral angles of 37.8 (2) and 39.8 (1)°, respectively, with the sulfonyl group.

In the crystal packing, the molecules form dimers through centrosymmetric pairs of C13—H13⋯O1 hydrogen bonds. The crystal packing is also stabilized by C—H⋯O interactions through C10 and O2 atoms (Table 2).

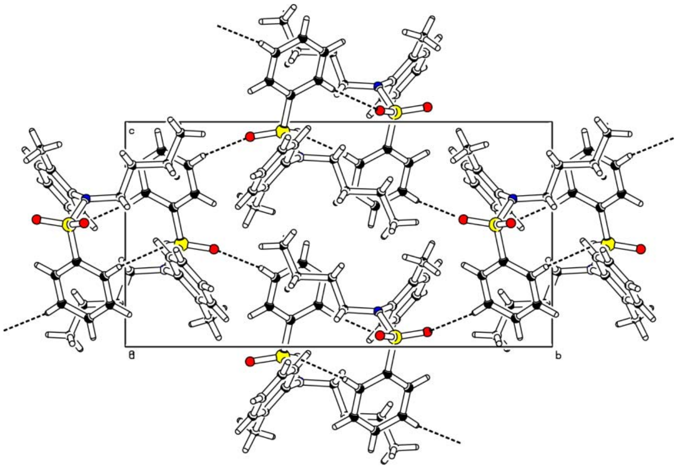

Figure 2
Packing of the molecules, viewed down the *a* axis. Hydrogen bonds are shown as dashed lines.

Experimental

A well ground mixture of *N*-phenylsulfonyl-*o*-toluidine (1 mmol), butyl bromide (1.2 mmol), a catalytic amount of tetra-*n*-butylammonium bromide and potassium carbonate (4 mmol) was heated in a domestic microwave oven in a conical flask for 3 min. After cooling, the reaction mixture was extracted with dichloromethane and washed with water. The extract was then dried with anhydrous sodium sulfate, filtered and the solvent evaporated to dryness. The crude product was purified by chromatographic separation on a silica-gel column (100–200 mesh) and eluted successively with hexane and ethyl acetate (9:1), giving the desired *N*-alkylated product in good yield. The crude product was recrystallized from ethyl acetate.

Crystal data

$C_{17}H_{21}NO_2S$
M_r = 303.41
Monoclinic, $P2_1/n$
a = 9.2614 (9) Å
b = 18.4306 (19) Å
c = 9.8602 (10) Å
β = 99.382 (2)°
V = 1660.6 (3) Å^3
Z = 4

D_x = 1.214 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2765 reflections
θ = 2.2–28°
μ = 0.20 mm^{-1}
T = 273 (2) K
Block, white
0.23 × 0.21 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: none
9999 measured reflections
3635 independent reflections

2765 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.021
$\theta_{\rm max}$ = 28.0°
$h = -9 \rightarrow 11$
$k = -24 \rightarrow 23$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.179
S = 1.06
3635 reflections
192 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.1P)^2 + 0.3505P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max}$ = 0.48 e Å^{-3}
$\Delta\rho_{\rm min}$ = −0.22 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—O2	1.423 (2)	N1—C1	1.454 (3)
S1—O1	1.429 (2)	N1—C14	1.482 (3)
S1—N1	1.636 (2)	C6—C7	1.477 (5)
S1—C8	1.755 (3)	C15—C16	1.531 (4)
O2—S1—O1	119.9 (1)	N1—S1—C8	107.5 (1)
O2—S1—N1	106.9 (1)	C1—N1—C14	116.8 (2)
O1—S1—N1	106.7 (1)	C1—N1—S1	116.8 (1)
O2—S1—C8	107.4 (1)	C14—N1—S1	116.9 (1)
O1—S1—C8	107.8 (1)		
C8—S1—N1—C14	72.7 (2)	N1—S1—C8—C13	−83.2 (2)
N1—S1—C8—C9	95.3 (2)	C14—C15—C16—C17	−178.2 (3)

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

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
C10—H10⋯O2^{i}	0.93	2.55	3.466 (3)	168
C13—H13⋯O1^{ii}	0.93	2.57	3.484 (3)	169

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

H atoms were positioned geometrically and were treated as riding on their parent C atoms, with aromatic C—H distances of 0.93 Å, methyl C—H distances of 0.96 Å and methylene C—H distances of 0.97 Å, and with $U_{\rm iso}$ = $1.5U_{\rm eq}$(C) for methyl H and $1.2U_{\rm eq}$(C) for other H atoms. The methyl groups were allowed to rotate, but not to tip.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PARST* (Nardelli, 1995).

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