

N-Methyl-*N*-(1-phenylsulfonylindol-2-ylmethyl)aniline

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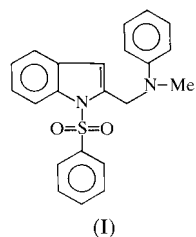
Received 9 October 2000

Accepted 11 January 2001

In the title compound, 2-[(methylphenylamino)methyl]-1-(phenylsulfonyl)indole, C₂₂H₂₀N₂O₂S, the indole system is not strictly planar and the dihedral angle between the fused rings is 2.7 (1)°. The angles around the S atom of the sulfonyl substituent deviate significantly from the ideal value for tetrahedral geometry. The pyramidalization at the indole N atom is very small. Of the two C—H···O interactions, one influences the orientation of indole with respect to the sulfonyl group and the other determines the orientation of the phenyl bound to sulfonyl. The phenyl ring of the sulfonyl substituent makes a dihedral angle of 89.6 (1)° with the best plane of the indole. The molecular packing is stabilized by C—H···π and C—H···O hydrogen bonds.

Comment

The biological activities of indoles and their derivatives have been known for a long time. The indole unit occurs naturally in a wide variety of structures. The indole ring system occurs in plants (Nigović *et al.*, 2000). Indolines and their oxidized counterparts are important pharmacophores that appear in



numerous biologically active compounds, most notably those affecting the central nervous system (Zhang & Liebeskind, 1996). Certain indole derivatives possess antidepressive (Papenstasion & Newmeyer, 1972), anti-inflammatory (Rodriguez *et al.*, 1985; Polletto *et al.*, 1974), antimicrobial (El-Sayed *et al.*, 1986; Gadaginamath & Patil, 1999), antitumor

(Schollmeyer *et al.*, 1995) and antibacterial (Okabe & Adachi, 1998) activities. They have been proven to display high aldose reductase inhibitory activity (Rajeswaran *et al.*, 1999). Because of the wide range of biological activities of indole derivatives, we have undertaken X-ray studies on an indole derivative, (I), in order to study its conformation in the solid state.

The indole system is not strictly planar and the dihedral angle formed by the pyrrole and benzo planes is 2.7 (1)°. Atom N1 deviates by −0.104 (2) Å from the mean plane passing through S1, C1 and C4. This slight pyramidalization behaviour is also observed in related indoles (Yokum & Fronczek, 1997; Beddoes *et al.*, 1986). The torsion angles O2—S1—N1—C4 of 152.0 (2)° and O2—S1—C9—C14 of 175.5 (2)° describe the conformation of the phenylsulfonyl group with respect to the indole system which causes the best planes of the indole and phenyl rings to form a dihedral angle of 89.6 (1)°, as observed in similar structures (Yokum & Fronczek, 1997).

In the benzene ring of the indole system, the endocyclic angles at C8 and C5 are contracted to 117.3 (2) and 119.2 (2)° while those at C7 and C4 are expanded to 122.4 (2) and 121.5 (2)°, respectively. This would appear to be a real effect caused by the fusion of the smaller pyrrole ring to the six-membered benzene ring. A similar effect has also been observed by Sivaraman *et al.* (1994*a,b*, 1996), Govindasamy *et al.* (1999) and Sankaranarayanan *et al.* (2000).

The phenyl ring attached to N16 is inclined at an angle of 83.1 (1)° to the indole mean plane and 66.0 (1)° to the phenyl ring of the sulfonyl group. The sum of the angles around N16 [359.1 (4)°] is indicative of *sp*²-hybridized character. The orientation of the indole substituent is influenced by a weak C8—H8···O1 interaction quantitatively defined by the torsion angles C8—C4—N1—S1 [−9.6 (3)°] and C4—N1—S1—C9 [−93.6 (2)°], while the orientation of the phenyl bound to the sulfonyl group is governed by the C10—H10···O2 interaction (Table 2) quantitatively defined by the torsion angle O2—S1—C9—C10 [−4.2 (2)°].

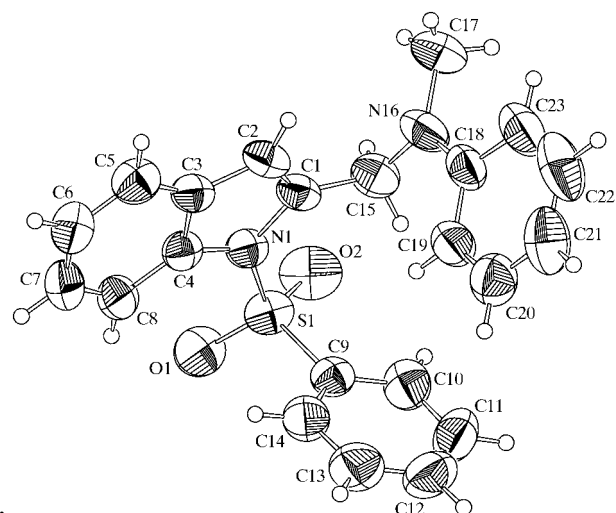


Figure 1

The molecular structure of (I) showing 50% probability displacement ellipsoids and the atom-numbering scheme.

The angular disposition of the bonds about the S atom shows significant deviation from that of a regular tetrahedron, with the largest deviation being in the O—S—O angle. The widening of the O1—S1—O2 angle [120.4 (1)°] from the ideal tetrahedral value is presumably the result of repulsive interactions between the short S=O bonds similar to that observed in related structures (Govindasamy *et al.*, 1999; Rodriguez *et al.*, 1985; Beddoes *et al.*, 1986). The S—N and S—C bond distances agree well with the literature values of 1.64 (2) and 1.758 (13) Å, respectively (Allen *et al.*, 1987).

In addition to van der Waals interactions, the molecular packing is stabilized by a C—H···O hydrogen bond and a C—H··· π interaction (Table 2).

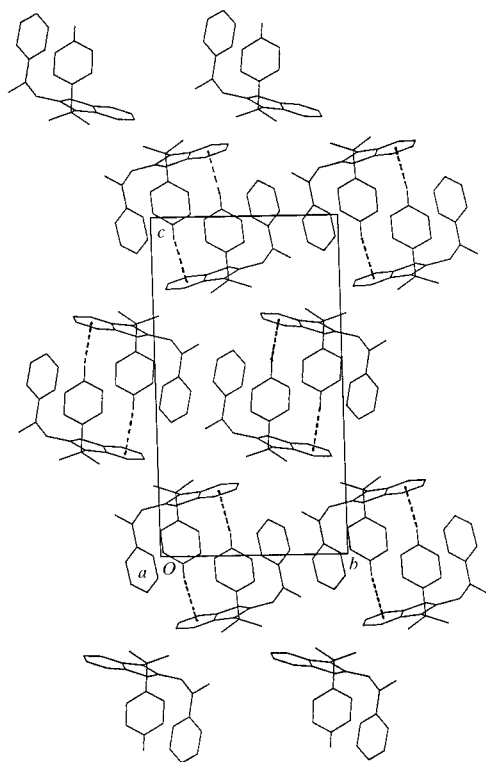


Figure 2
The packing of the molecule viewed down the *a* axis showing C—H··· π interactions.

Experimental

3-Bromo-(1-phenylsulfonylindol-2-ylmethyl)-*N*-methylaniline was treated with tetrakis(triphenylphosphine)palladium(0) in dimethylformamide at 353 K and gave the corresponding debrominated product of the title compound in 70% yield.

Crystal data

C₂₂H₂₀N₂O₂S
M_r = 376.46
 Orthorhombic, *P*2₁2₁2₁
a = 8.3162 (2) Å
b = 11.2384 (3) Å
c = 20.4080 (5) Å
V = 1907.35 (8) Å³
Z = 4
D_x = 1.311 Mg m⁻³

Mo *K* α radiation
 Cell parameters from 4762 reflections
 θ = 1.58–28.32°
 μ = 0.189 mm⁻¹
T = 293 (2) K
 Block, yellow
 0.44 × 0.42 × 0.24 mm

Data collection

Siemens SMART CCD area-detector diffractometer
 ω scans
 13 206 measured reflections
 4707 independent reflections
 3474 reflections with *I* > 2 σ (*I*)

*R*_{int} = 0.035
 θ_{\max} = 28.29°
h = -10 → 11
k = -14 → 10
l = -22 → 27

Refinement

Refinement on *F*²
R [*F*² > 2 σ (*F*²)] = 0.041
wR(*F*²) = 0.119
S = 0.910
 4707 reflections
 245 parameters
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0673P)^2 + 0.2417P]$
 where $P = (F_o^2 + 2F_c^2)/3$

(Δ/σ)_{max} < 0.001
 $\Delta\rho_{\max}$ = 0.17 e Å⁻³
 $\Delta\rho_{\min}$ = -0.19 e Å⁻³
 Extinction correction: *SHELXL97* (Sheldrick, 1997)
 Extinction coefficient: 0.0070 (12)
 Absolute structure: Flack (1983)
 Flack parameter = 0.06 (8)

Table 1

Selected geometric parameters (Å, °).

S1—O1	1.424 (2)	S1—C9	1.759 (2)
S1—O2	1.419 (2)	N1—C4	1.417 (3)
S1—N1	1.664 (2)	N1—C1	1.425 (3)
O1—S1—O2	120.4 (1)	C4—N1—C1	108.0 (2)
O1—S1—N1	106.6 (1)	C4—N1—S1	125.9 (1)
O2—S1—N1	106.3 (1)	C1—N1—S1	124.6 (2)
O1—S1—C9	109.6 (1)	C18—N16—C17	121.7 (2)
O2—S1—C9	108.4 (1)	C18—N16—C15	119.4 (2)
N1—S1—C9	104.3 (1)	C17—N16—C15	118.0 (3)
C1—C15—N16—C18	81.2 (3)	C1—C15—N16—C17	-109.3 (3)

Table 2

Hydrogen-bonding geometry (Å, °).

Cg1 is the ring centroid of the C3—C8 benzene ring.

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
C8—H8···O1	0.93	2.33	2.911 (3)	121
C10—H10···O2	0.93	2.53	2.904 (3)	104
C8—H8···O2 ⁱ	0.93	2.43	3.217 (3)	142
C12—H12···Cg1 ⁱⁱ	0.93	2.75	3.568 (5)	148

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

All H atoms were included in calculated positions and allowed to ride on their corresponding parent atoms (C—H = 0.93–0.96 Å).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ZORTEP* (Zsolnai, 1997); software used to prepare material for publication: *SHELXL97* and *PARST* (Nardelli, 1995).

RS thanks CSIR, India, for a Senior Research Fellowship and DV thanks DST, India, for a project. SSSR thanks Universiti Sains Malaysia for a visiting Postdoctoral Research Fellowship and HKF thanks the Malaysian Government and Universiti Sains Malaysia for research grant R&D No. 190-9609-2801.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: NA1496). Services for accessing these data are described at the back of the journal.

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