

3-Benzyl-2-methyl-1-phenylsulfonyl-1*H*-indole

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## Key indicators

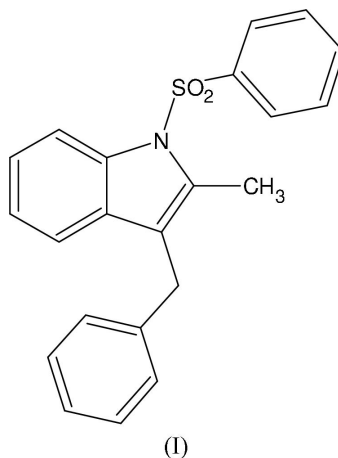
Single-crystal X-ray study  
T = 293 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.003 \text{ \AA}$   
R factor = 0.045  
wR factor = 0.143  
Data-to-parameter ratio = 16.5

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

In the title compound,  $\text{C}_{22}\text{H}_{19}\text{NO}_2\text{S}$ , the two phenyl rings adopt a *trans* conformation with respect to the indole moiety. The indole system deviates slightly from planarity. The aromatic ring of the phenylsulfonyl group is almost perpendicular to the indole ring, while the benzyl ring is oriented at an angle of  $77.01 (1)^\circ$ . A zigzag  $\text{C}-\text{H}\cdots\text{O}$  intermolecular hydrogen bond along the *b* axis and  $\text{C}-\text{H}\cdots\pi$  interactions stabilize the crystal packing.

## Comment

Indole and its derivatives have antimicrobial (Gadaginamath & Patil, 1999), anti-inflammatory (Rodriguez *et al.*, 1985), antibacterial (Okabe & Adachi, 1998) and antidepressive activities. Sulfates, sulfones and sulfonamides exhibit insecticidal, germicidal, antimicrobial and antibacterial activities (De-Benedetti *et al.*, 1985; Krishnaiah *et al.*, 1995), and certain phenyl sulfones show fungicidal properties (Wolf, 1999). In view of the above-mentioned pharmacological activities, the crystal structure of the title compound, (I), has been determined.

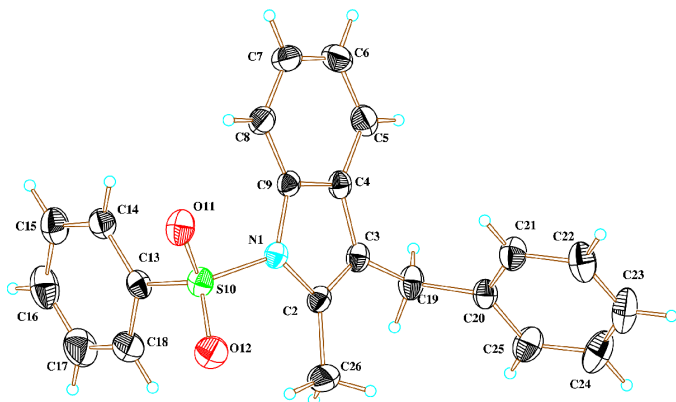


The two phenyl rings in (I) adopts a *trans* conformation with respect to the indole moiety. The angles around atom S10 show significant deviation from regular tetrahedral, the largest deviation being found for the  $\text{O}-\text{S}-\text{O}$  angle [ $119.73 (9)^\circ$ ]. This widening is presumably the result of the repulsive interactions between the short  $\text{S}=\text{O}$  bonds (Sankaranarayanan, *et al.*, 2001; Govindasamy *et al.*, 1999; Rodriguez *et al.*, 1985). The sum of the angles ( $353.9^\circ$ ) around N15 and the value of the out-of-plane distance [ $0.191 (1) \text{ \AA}$ ] with respect to the plane of the bonded atoms shows a slight pyramidalization, as observed in related indoles (Yokum & Fronczek, 1997; Sankaranar-

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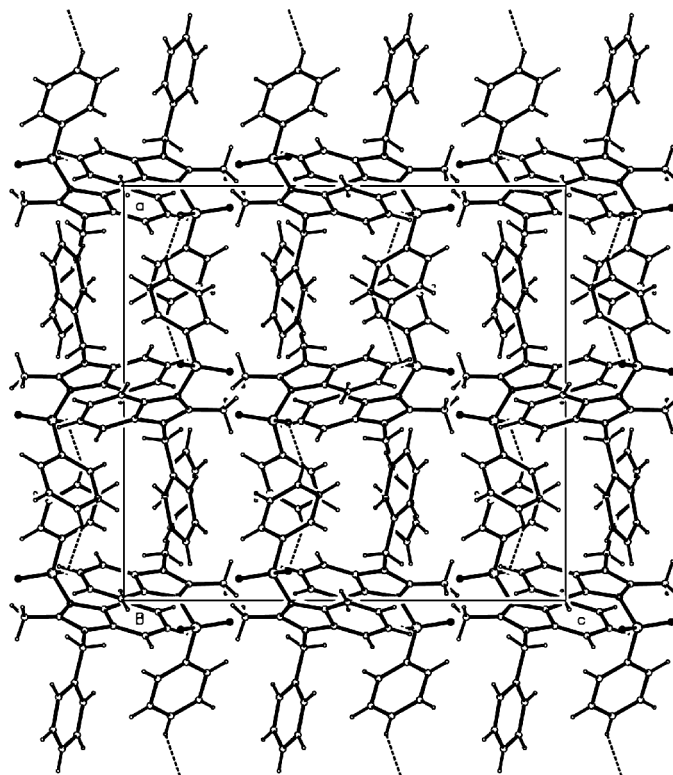
**Figure 1**  
A plot of the molecule of (I), with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

ayan, *et al.*, 2001; Beddoes *et al.*, 1986). The indole system deviates slightly from planarity, as indicated by the dihedral angle between the pyrrole and benzene ring planes [ $1.10(3)^\circ$ ]. In the phenylsulfonamide group, the phenyl ring is oriented almost perpendicular to the indole ring, at an angle of  $83.93(1)^\circ$ . The benzyl ring is found to be oriented at an angle of  $77.01(1)^\circ$  with respect to the indole ring. The methyl group at C2 is displaced significantly from the indole plane, by  $0.104(2) \text{ \AA}$ .

An intramolecular C—H $\cdots$ O hydrogen bond of pattern type *S*(6) between atoms C26 and O12 stabilizes the structure of (I) (Table 2). The molecules in the crystal structure form a zigzag chain along the *b* axis *via* intermolecular C—H $\cdots$ O hydrogen bonds of pattern type *C*(7) involving atoms C16 and O11( $\frac{1}{2} - x, y - \frac{1}{2}, z$ ). The pyrrole and benzene  $\pi$  systems of the centrosymmetric ( $-x, -y, 1 - z$ ) indole moieties are stacked over one another [dihedral angle  $1.19(6)^\circ$ ], the separation between their centroids being  $4.662(3) \text{ \AA}$ . The indole moiety interacts with the phenylsulfonamide ring of an inversion-related molecule at ( $-x, -y, 1 - z$ ) *via* a weak C—H $\cdots$  $\pi$  interaction involving atom C5, the separation between H5 and the centroid of the C13–C18 ring being  $3.09 \text{ \AA}$ . The phenylsulfonamide ring interacts with symmetry-related C20–C25 benzyl rings through weak C—H $\cdots$  $\pi$  interactions involving atoms C15 and C17, the distances between atoms H15 and H17 and the centroids of the rings at ( $-x, -y, 1 - z$ ) and ( $\frac{1}{2} + x, y, \frac{1}{2} - z$ ) being  $3.05$  and  $3.27 \text{ \AA}$ , respectively.

## Experimental

2-Methyl-3-benzylindole (5.52 g, 25 mM) in dry tetrahydrofuran (THF) (50 ml) was slowly added to a stirred suspension of sodium hydride (1.2 g, 50 mM) in dry THF (10 ml) under nitrogen at room temperature. The reaction mixture was refluxed for 3 h under nitrogen and then cooled to 278 K, followed by the slow addition of phenylsulfonamide (5 ml, 40 mM) in dry THF (25 ml). The reaction mixture was stirred at 273–278 K for 6 h, then treated with a saturated ammonium chloride solution (50 ml), and the layers were separated. The aqueous layer was extracted with dichloromethane



**Figure 2**  
A packing diagram of the crystal structure of (I), viewed down the *b* axis. Dashed lines represent hydrogen bonds.

(4  $\times$  15 ml) and the combined organic layer was dried ( $\text{Na}_2\text{SO}_4$ ) and concentrated *in vacuo* to give (I) as an oil, which was then crystallized from acetone.

### Crystal data

$\text{C}_{22}\text{H}_{19}\text{NO}_2\text{S}$   
 $M_r = 361.44$   
Orthorhombic, *Pbca*  
 $a = 17.160(9) \text{ \AA}$   
 $b = 11.680(6) \text{ \AA}$   
 $c = 18.274(10) \text{ \AA}$   
 $V = 3663(3) \text{ \AA}^3$   
 $Z = 8$   
 $D_x = 1.311 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation  
Cell parameters from 26 996 reflections  
 $\theta = 2.2\text{--}27.3^\circ$   
 $\mu = 0.19 \text{ mm}^{-1}$   
 $T = 293(2) \text{ K}$   
Block, colourless  
 $0.25 \times 0.22 \times 0.20 \text{ mm}$

### Data collection

Siemens SMART CCD area-detector diffractometer  
 $\omega$  scans  
Absorption correction: none  
26 996 measured reflections  
3882 independent reflections

3235 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.020$   
 $\theta_{\text{max}} = 27.3^\circ$   
 $h = -21 \rightarrow 21$   
 $k = -15 \rightarrow 15$   
 $l = -22 \rightarrow 23$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.045$   
 $wR(F^2) = 0.143$   
 $S = 1.02$   
3882 reflections  
235 parameters  
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0872P)^2 + 1.131P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.38 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.32 \text{ e \AA}^{-3}$   
Extinction correction: none

**Table 1**

Selected geometric parameters (Å, °).

N1–C9	1.424 (2)	S10–O11	1.4271 (16)
N1–C2	1.432 (2)	S10–O12	1.4275 (17)
N1–S10	1.6650 (15)	S10–C13	1.754 (2)
C9–N1–C2	107.81 (13)	O12–S10–N1	107.20 (8)
C9–N1–S10	122.63 (11)	O11–S10–C13	108.89 (9)
C2–N1–S10	123.53 (12)	O12–S10–C13	108.73 (10)
O11–S10–O12	119.73 (9)	N1–S10–C13	105.57 (8)
O11–S10–N1	105.81 (8)		
S10–N1–C2–C26	–30.4 (2)	O11–S10–C13–C14	27.27 (17)
S10–N1–C9–C8	28.1 (2)	N1–S10–C13–C14	–85.95 (16)
C9–N1–S10–O11	–39.92 (14)	O12–S10–C13–C18	–21.35 (19)
C2–N1–S10–O12	41.93 (16)	N1–S10–C13–C18	93.40 (18)
C9–N1–S10–C13	75.43 (14)	C2–C3–C19–C20	–86.5 (2)
C2–N1–S10–C13	–73.88 (15)	C3–C19–C20–C21	–31.7 (3)

**Table 2**

Hydrogen-bond geometry (Å, °).

$C_{g1}$  and  $C_{g2}$  are the centroids of the C13–C18 and C20–C25 phenyl rings, respectively.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C26–H26A $\cdots$ O12	0.96	2.07	2.862 (3)	139
C16–H16 $\cdots$ O11 <sup>i</sup>	0.93	2.56	3.399 (3)	151
C5–H5 $\cdots$ C <sub>g1</sub> <sup>ii</sup>	0.93	3.09	4.018 (4)	173
C15–H15 $\cdots$ C <sub>g2</sub> <sup>ii</sup>	0.93	3.05	3.701 (4)	129
C17–H17 $\cdots$ C <sub>g2</sub> <sup>iii</sup>	0.93	3.27	3.953 (4)	132

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

All H atoms were positioned geometrically (C–H = 0.93–0.98 Å) and allowed to ride on their parent atoms, with  $U_{iso}(H) = 1.2$  or 1.5 times  $U_{eq}$  (parent atom).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINTE* (Siemens, 1996); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003), *ORTEP3* (Farrugia, 1997) and *ZORTEP* (Zsolnai, 1998); software used to prepare material for publication: *PLATON*.

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