

1-Benzenesulfonyl-2,3-dimethyl-1*H*-indoleK. Palani,<sup>a</sup> M. N. Ponnuswamy,<sup>a\*</sup>  
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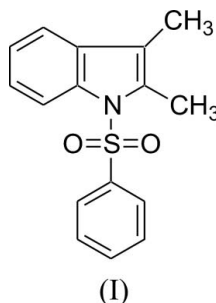
## Key indicators

Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å  
 $R$  factor = 0.052  
 $wR$  factor = 0.145  
Data-to-parameter ratio = 17.9For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

In the title compound,  $\text{C}_{16}\text{H}_{15}\text{NO}_2\text{S}$ , the indole group is planar and approximately perpendicular to the sulfonyl-bound phenyl ring; the dihedral angle between the planes is  $86.80(6)^\circ$ . The molecules form centrosymmetric dimers *via*  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonds.

## Comment

Indole compounds can be used as bioactive drugs (Stevenson *et al.*, 2000). Indole derivatives exhibit anti-allergic, central nervous system depressant and muscle relaxant properties (Harris & Uhle, 1960; Ho *et al.*, 1986). Indoles have also been proved to display high aldose reductase inhibitory activity (Rajeswaran *et al.*, 1999). In view of this biological importance, an X-ray study of the title compound, (I), was carried out.



A *ZORTEP* (Zsolnai, 1997) plot of the molecule is shown in Fig. 1. The relatively long  $\text{C}-\text{N}$  distances in the indole system are due to the electron-withdrawing character of the phenylsulfonyl group (Govindasamy *et al.*, 1997, 1998). The widening of the  $\text{O}-\text{S}-\text{O}$  and the resultant narrowing of the  $\text{N}-\text{S}-\text{C}$  angles (Table 1) from the ideal tetrahedral value are attributed to the Thorpe–Ingold effect (Bassindale, 1984). The dihedral angle between the  $\text{C}10-\text{C}15$  phenyl ring and the indole ring system is  $86.80(6)^\circ$ .

In the crystal structure, the molecules form centrosymmetric dimers *via*  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonds (Table 2 and Fig. 2). In addition, a  $\pi-\pi$  stacking interaction involving the pyrrole ring (centroid  $\text{Cg}1$ ), with a  $\text{Cg}1\cdots\text{Cg}1(1-x, 1-y, -z)$  distance of  $3.594(2)$  Å, is observed.

## Experimental

A solution of 2-methyl-3-methylindole (4 mmol) in dry tetrahydrofuran (THF, 10 ml) was added slowly to a stirred suspension of 50% sodium hydride (0.24 g, 10 mmol) in dry THF (4 ml) under nitrogen atmosphere at room temperature. The reaction mixture was refluxed for 3 h and cooled to 268 K. A solution of phenylsulfonyl chloride (0.86 ml, 6 mmol) in dry THF (8.0 ml) was then added slowly. The

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reaction mixture was stirred at 268 K for 6 h. The solution was then treated with saturated ammonium chloride solution (20 ml) and the organic layer was separated. The aqueous layer was extracted with chloroform (4 × 15 ml), and the combined organic layers were dried over anhydrous Na<sub>2</sub>SO<sub>4</sub> and concentrated under reduced pressure to give a white oil. This was crystallized from ethyl acetate and hexane (2:8) to give a white crystalline solid (yield 81%, m.p. 413 K). IR (KBr): 1380, 1140 cm<sup>-1</sup>.

Crystal data

C<sub>16</sub>H<sub>15</sub>NO<sub>2</sub>S                      Z = 2  
M<sub>r</sub> = 285.35                              D<sub>x</sub> = 1.346 Mg m<sup>-3</sup>  
Triclinic, P1̄                              Mo Kα radiation  
a = 7.8800 (13) Å                      Cell parameters from 2540  
b = 9.6020 (16) Å                      reflections  
c = 9.9864 (17) Å                      θ = 2.1–28.0°  
α = 82.210 (3)°                          μ = 0.23 mm<sup>-1</sup>  
β = 81.487 (3)°                          T = 293 (2) K  
γ = 71.087 (3)°                          Block, colourless  
V = 703.8 (2) Å<sup>3</sup>                        0.23 × 0.21 × 0.19 mm

Data collection

Bruker SMART APEX CCD area-                      3284 independent reflections  
detector diffractometer                      2540 reflections with I > 2σ(I)  
ω scans                                      R<sub>int</sub> = 0.017  
Absorption correction: multi-scan                      θ<sub>max</sub> = 28.0°  
(SADABS; Sheldrick, 1996)                      h = -10 → 10  
T<sub>min</sub> = 0.948, T<sub>max</sub> = 0.957                      k = -12 → 12  
8276 measured reflections                      l = -13 → 13

Refinement

Refinement on F<sup>2</sup>                              w = 1/[σ<sup>2</sup>(F<sub>o</sub><sup>2</sup>) + (0.0803P)<sup>2</sup>  
R[F<sup>2</sup> > 2σ(F<sup>2</sup>)] = 0.052                              + 0.1221P]  
wR(F<sup>2</sup>) = 0.145                              where P = (F<sub>o</sub><sup>2</sup> + 2F<sub>c</sub><sup>2</sup>)/3  
S = 1.04    (Δ/σ)<sub>max</sub> = 0.001  
3284 reflections                              Δρ<sub>max</sub> = 0.31 e Å<sup>-3</sup>  
183 parameters                              Δρ<sub>min</sub> = -0.19 e Å<sup>-3</sup>  
H-atom parameters constrained

Table 1 Selected geometric parameters (Å, °).

S1–O2	1.4166 (16)	S1–C10	1.760 (2)
S1–O1	1.4203 (16)	N1–C5	1.415 (2)
S1–N1	1.6577 (16)	N1–C2	1.436 (2)
O2–S1–O1	119.53 (10)	C5–C4–C9	119.3 (2)
N1–S1–C10	105.17 (8)	C6–C5–C4	121.7 (2)
C16–C2–C3–C4	178.6 (2)	C17–C3–C4–C5	178.2 (2)

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

D–H...A	D–H	H...A	D...A	D–H...A
C6–H6...O1	0.93	2.36	2.938 (3)	120
C6–H6...O1 <sup>i</sup>	0.93	2.54	3.317 (3)	141
C15–H15...O2	0.93	2.58	2.932 (3)	103

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

H atoms were placed in idealized positions and allowed to ride on their parent atoms, with C–H = 0.93 or 0.96 Å and U<sub>iso</sub>(H) = 1.2 or 1.5U<sub>eq</sub>(C).

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:

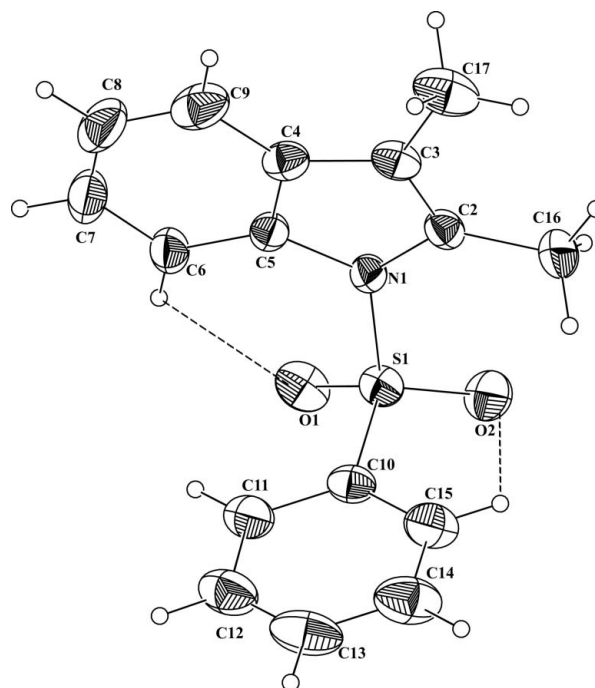


Figure 1 The structure of (I), showing 30% probability displacement ellipsoids and the atom-labelling scheme. Dashed lines indicate C–H...O hydrogen bonds.

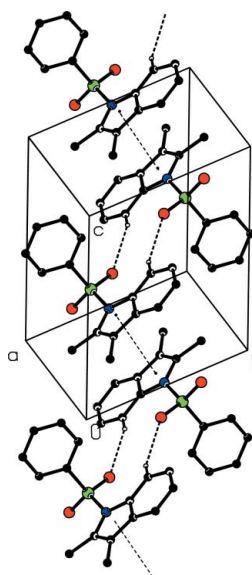


Figure 2 The crystal packing of (I), showing C–H...O hydrogen-bonded (dashed lines) dimers.

ZORTEP (Zsolnai, 1997); software used to prepare material for publication: PLATON (Spek, 2003).

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