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3-(1,2-Diphenylvinyl)-2-methyl-1-phenylsulfonyl-1*H*-indole

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.052
wR factor = 0.137
Data-to-parameter ratio = 9.7

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

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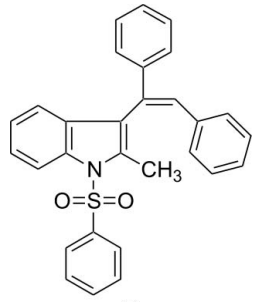
In the title compound, $C_{29}H_{23}NO_2S$, the bond angles around the S atom indicate a distorted tetrahedral configuration. The crystal structure is stabilized by weak C—H···O and C—H···π hydrogen bonds.

Comment

The indole unit is observed in many plants (Nigović *et al.*, 2000). Indole-3-acetic acid is a naturally occurring plant growth hormone that controls a number of plant-growth activities (Fargasova, 1994). Many indole-containing natural products are found to exhibit psychotropic (Grinev *et al.*, 1978) and hypertensive (Merk, 1971) properties. A large number of biologically active compounds, mostly those affecting the central nervous system (Zhang & Liebeskind, 1996), contain indolines and their oxidized counterparts as important pharmacophores. Some of the indole derivatives possess antitumour (Schollmeyer *et al.*, 1995) and antibacterial (Okabe & Adachi, 1998) activities. In view of this importance, the crystal structure of the title compound, (I), has been determined and the results are presented here.



(I)

A *ZORTEP* (Zsolnai, 1997) plot of the molecule is shown in Fig.1. The S—O, S—C and S—N bond distances are comparable with the previously reported values of 1.435 (5), 1.767 (7) and 1.685 (5) Å, respectively (Govindasamy *et al.*, 1998). As observed in other phenylsulfonylindoles (Rodriguez *et al.*, 1995; Govindasamy *et al.*, 1997, 1998), the C—N distances in the indole ring system are longer due to the electron-withdrawing character of the phenylsulfonyl group. The widening of the O1—S1—O2 angle to 119.4 (2)°, and the concomitant narrowing of the N1—S1—C10 angle to 104.5 (1)°, from the ideal tetrahedral value, are attributed to the Thorpe–Ingold effect (Bassindale, 1984). The C10–C15, C18–C23 and C25–C30 phenyl rings are oriented at angles of 75.1 (1), 81.3 (1), 59.9 (1)°, respectively, with respect to the indole ring system.

C—H···O-type hydrogen bonds are observed in the molecular structure. The crystal structure is stabilized by intermolecular C—H···O and C—H···π hydrogen bonds (Table 2 and Fig. 2).

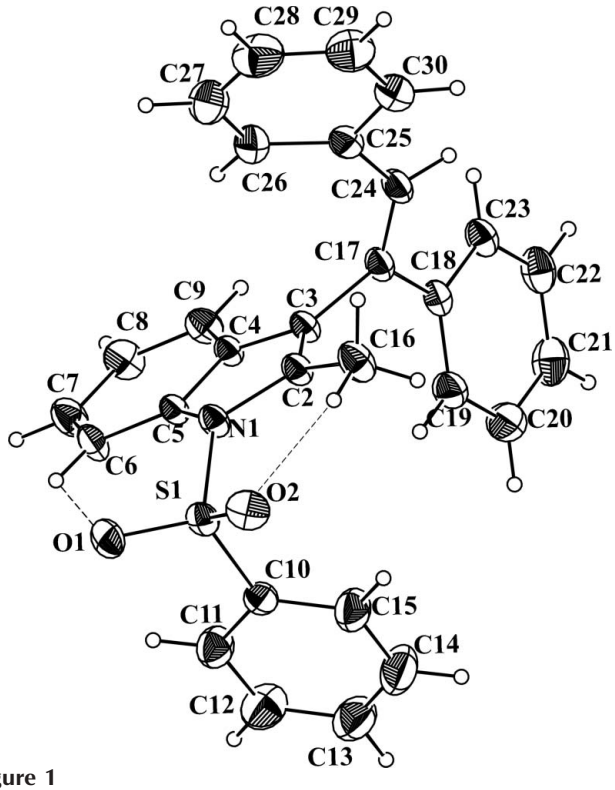


Figure 1
The structure of (I), showing 30% probability displacement ellipsoids and the atom-labelling scheme. Dashed lines indicate C—H···O hydrogen bonds.

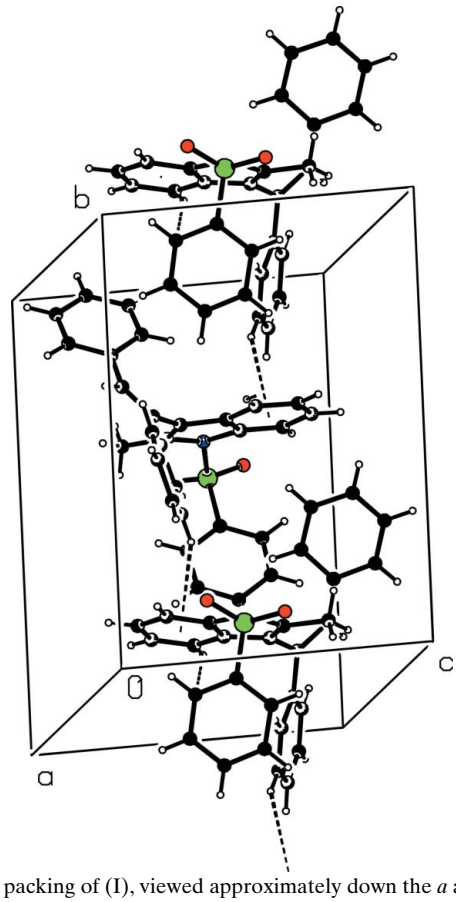


Figure 2
The crystal packing of (I), viewed approximately down the *a* axis. Dashed lines indicate C—H···π interactions.

Experimental

A solution of 3-(1,2-diarylvinyl)-2-methyl-1*H*-indole (5 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 a nitrogen atmosphere at room temperature. The reaction mixture was refluxed for 3 h and cooled to 268 K. A solution of phenylsulfonyl chloride (1.15 ml, 8 mmol) in dry THF (10 ml) was then added slowly. The solution was then treated with saturated aqueous ammonium chloride solution (50 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_2SO_4 and concentrated under reduced pressure to give a white oil. This was crystallized from ethyl acetate and hexane (1:4) to give a crystalline solid (yield 1.59 g (71%), m.p. 427 K). ^{1}H NMR (400 MHz, $CDCl_3$): *d* = 2.24 (*s*, 3H, CH_3), 6.93–7.58 (*m*, 18H, Ar—H and 1H vinylic), 8.23–8.25 (*d*, 1H, *J* = 8.0 Hz, indole-7H). Mass (*m*/*z* %): 449(M^+, 75.6), 308 (77.2), 293 (39.1), 230 (100), 217 (10.8), 77 (34.2), 57(10.3).

Crystal data

$C_{29}H_{23}NO_2S$
M_r = 449.54
Monoclinic, $P2_1$
a = 9.029 (3) Å
b = 14.891 (7) Å
c = 9.8459 (17) Å
β = 117.588 (18)°
V = 1173.3 (7) Å^3
Z = 2
D_x = 1.272 Mg m^{-3}
Mo *K*α radiation
Cell parameters from 25 reflections
θ = 2.3–28.0°
μ = 0.16 mm^{-1}
T = 293 (2) K
Block, yellow
0.36 × 0.28 × 0.18 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω scans
Absorption correction: none
3078 measured reflections
2905 independent reflections
2520 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 28.0°
$h = 0 \rightarrow 11$
$k = 0 \rightarrow 19$
$l = -12 \rightarrow 11$
3 standard reflections
frequency: 60 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.137
S = 1.06
2905 reflections
299 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1042P)^2 + 0.0294P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}
Absolute structure: Flack (1983), 0 Friedel pairs
Flack parameter: 0.37 (10)

Table 1
Selected geometric parameters (Å, °).

S1—O1	1.423 (2)	S1—C10	1.759 (4)
S1—O2	1.423 (2)	N1—C5	1.417 (3)
S1—N1	1.667 (2)	N1—C2	1.436 (3)
O1—S1—N1—C5	−50.4 (3)	C10—S1—N1—C5	65.3 (3)
O2—S1—N1—C5	−178.8 (2)	O1—S1—N1—C2	168.7 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···O1	0.93	2.37	2.948 (5)	120
C9—H9···O2^{i}	0.93	2.49	3.344 (5)	153
C16—H16B···O2	0.96	2.40	2.858 (5)	109
C20—H20···Cg^{ii}	0.93	2.83	3.658 (5)	148

Symmetry codes: (i) $x+1, y, z$; (ii) $-x+1, y-\frac{1}{2}, -z+1$. Cg denotes the centroid of the C4–C9 benzene ring.

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_{iso}(H) = 1.2–1.5U_{eq}(C).

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); 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: *PLATON* (Spek, 2003).

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