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3-[α-(4-Methoxyphenyl)-β-phenylvinyl]-2-methyl-1-phenylsulfonyl-1*H*-indole

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Key indicators

Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.003 Å
R factor = 0.048
wR factor = 0.142
Data-to-parameter ratio = 18.1

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

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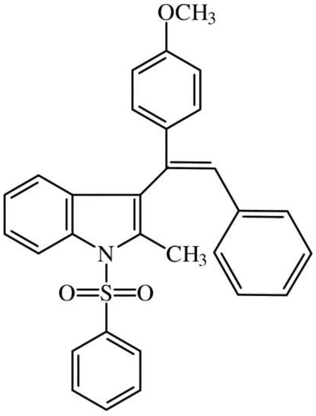
In the title compound, $C_{30}H_{25}NO_3S$, the phenylsulfonyl and methoxyphenyl groups are almost perpendicular to the indole unit, whereas the other phenyl ring is inclined at an angle of 68.9 (1)° to it. The benzene ring of the phenylsulfonyl substituent makes a dihedral angle of 68.0 (1)° with the benzene ring of the methoxyphenyl substituent. The molecular packing in the crystal is stabilized by weak intra- and intermolecular C—H···O interactions.

Comment

The indole unit is observed in 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. The wide range of biological activities of indole and its derivatives prompted us to undertake this structural study of the title compound, (I).



(I)

The S—O, S—C and S—N bond distances are in good agreement with the reported values of 1.435 (5), 1.767 (7) and 1.685 (5) Å, respectively (Govindasamy *et al.*, 1998). The larger values of the C—N distances in the indole unit [C5—N1 = 1.409 (2) Å and C2—N1 = 1.422 (2) Å] are due to the electron-withdrawing character of the phenylsulfonyl group, and this phenomenon is observed in similar reported structures (Rodriguez *et al.*, 1995; Govindasamy *et al.*, 1997, 1998).

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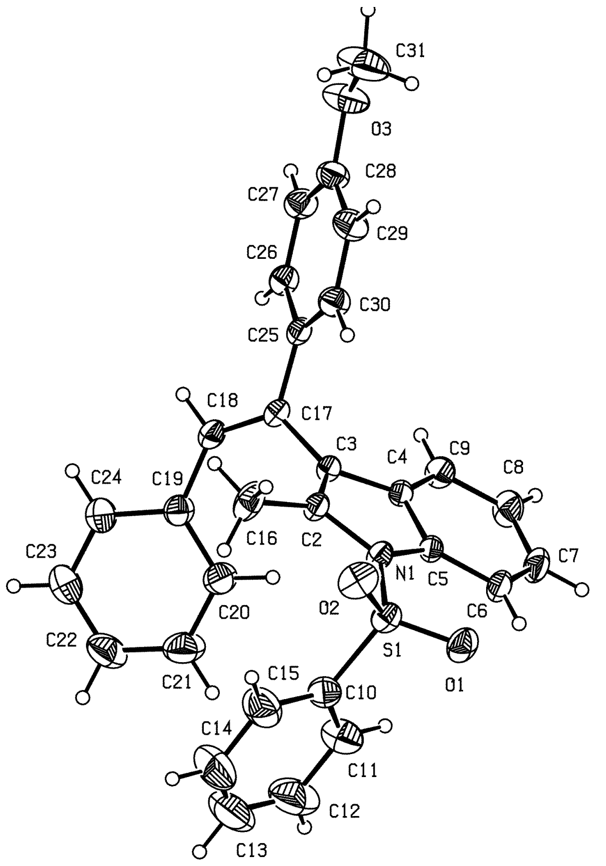

Figure 1
The molecular structure of the title compound, showing 30% probability displacement ellipsoids.

The sum of the angles around N1 (359.7°) shows the sp^2-hybridized character.

As normally observed in anisoles (Domiano *et al.*, 1979), the methoxy group atoms (O3 and C31) tend to be coplanar with the attached benzene ring but the exocyclic angles around C28 differ significantly [angle O3—C28—C29 is 9.31 (2)° larger than O3—C28—C27]. The benzene rings of the phenylsulfonyl and methoxyphenyl substituents make angles of 82.3 (1) and 82.7 (1)°, respectively, with the indole system. The angle between the other phenyl ring and the indole ring is 68.9 (1)°.

There are weak intra- and intermolecular C—H$\cdots$O interactions (Table 2 and Fig. 2).

Experimental

To a stirred solution of sodium hydride (1.5 mmol) in dry tetrahydrofuran (THF, 5 ml) under an N_2 atmosphere at reflux temperature (333 K) was added a solution of 3-[α-(4-methoxyphenyl)-β-phenylvinyl]-2-methyl-1*H*-indole (1 mmol) in dry THF (5 ml). After 1 h, the reaction mixture was cooled to room temperature. Phenylsulfonyl chloride (1.1 mmol) was added to the same solvent (5 ml) and stirred for 4 h. The solution was then poured over crushed ice and treated with a saturated solution of ammonium chloride, extracted with chloroform, concentrated, and passed through a chromatography column to give a pure white product. Diffraction-quality crystals were obtained from an ethyl acetate solution.

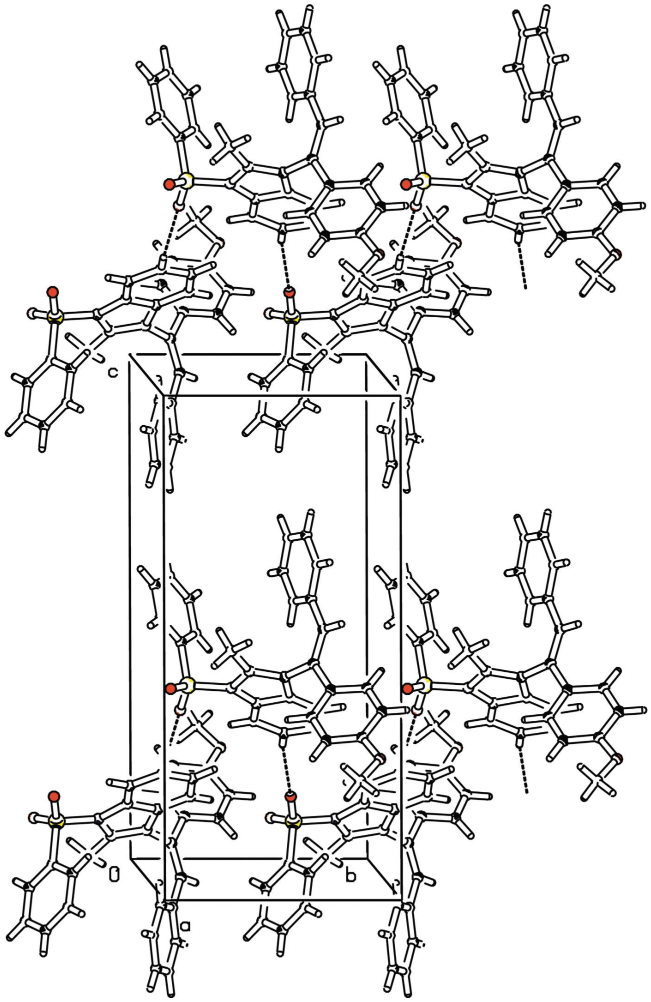

Figure 2
The molecular packing of the title compound. Dashed lines indicate hydrogen bonds.

Crystal data

$C_{30}H_{25}NO_3S$
M_r = 479.57
Monoclinic, $P2_1/c$
a = 14.8973 (11) Å
b = 8.9581 (7) Å
c = 18.9941 (14) Å
β = 97.658 (1)°
V = 2512.2 (3) Å^3
Z = 4
D_x = 1.268 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4749 reflections
θ = 2.2–27.2°
μ = 0.16 mm^{-1}
T = 273 (2) K
Block, colourless
0.22 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: none
14866 measured reflections
5748 independent reflections
4309 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.024
$\theta_{\rm max}$ = 28.0°
$h = -19 \rightarrow 19$
$k = -11 \rightarrow 11$
$l = -24 \rightarrow 20$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.143$
S = 1.01
5748 reflections
318 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0809P)^2 + 0.396P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max}$ = 0.28 e Å^{-3}
$\Delta\rho_{\rm min}$ = −0.33 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—O2	1.416 (1)	O3—C28	1.368 (2)
S1—O1	1.417 (1)	O3—C31	1.395 (3)
S1—N1	1.666 (1)	N1—C5	1.409 (2)
S1—C10	1.750 (2)	N1—C2	1.422 (2)
O2—S1—O1	119.3 (1)	O2—S1—C10	109.2 (1)
O2—S1—N1	107.4 (1)	O1—S1—C10	109.0 (1)
O1—S1—N1	106.2 (1)	N1—S1—C10	104.8 (1)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···O1	0.93	2.32	2.893 (2)	120
C7—H7···O1^{i}	0.93	2.53	3.397 (2)	155

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

The H atoms were positioned geometrically and were treated as riding on their parent C atoms, with aromatic C—H = 0.93 Å, methyl C—H = 0.96 Å and methylene C—H = 0.97 Å, and with N—H = 0.86 Å, and with $U_{\rm iso} = 1.5U_{\rm eq}$(C) for methyl H and $1.2U_{\rm eq}$(N,C) for the remaining H atoms.

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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