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3-[2-(2,4-Dichlorophenyl)vinyl]-2-methyl-1-phenylsulfonyl-1*H*-indole

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Key indicators

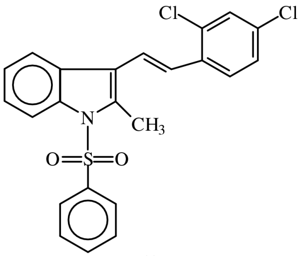
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.043
wR factor = 0.121
Data-to-parameter ratio = 18.5

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

The title compound, $C_{23}H_{17}Cl_2NO_2S$, crystallizes with $Z' = 2$ in space group $P\overline{1}$. The dihedral angle between the indole moiety and the aromatic rings of the phenylsulfonyl and dichlorophenyl groups are 76.2 (1) and 7.6 (1)° in molecule *A*, and 75.6 (1) and 11.6 (1)° in molecule *B*. The dihedral angle between the two aromatic rings is 79.7 (1)° in molecule *A* and 81.6 (1)° in molecule *B*. The molecular structure and molecular packing in the crystal are stabilized by C—H···O weak interactions.

Comment

The indole ring system is present in a number of natural products, many of which are found to possess antibacterial (Okabe & Adachi, 1998), antitumour (Schollmeyer *et al.*, 1995), antidepressant (Grinev *et al.*, 1984), antimicrobial (El-Sayed *et al.*, 1986; Gadaginamath & Patil, 1999) and anti-inflammatory (Rodriguez *et al.*, 1985) activities. Sivaraman *et al.* (1996) have studied the interaction of phenylsulfonyl indoles with calf-thymus DNA, by spectroscopic methods. Indoles have been proved to display high aldose reductose inhibitory activity (Rajeswaran *et al.*, 1999). The structure determination of the title compound, (I), was undertaken as part of our studies on indole derivatives.



(I)

The asymmetric unit contains two molecules, *A* and *B*; the corresponding bond lengths and angles of these two molecules agree with each other and no conformational changes are observed. Bond lengths and angles in the indole moiety are comparable with those observed in related *N*-phenylsulfonyl indole derivatives (Sankaranarayanan *et al.*, 2000; Sankaranarayanan, Yogavel, Velmurugan, Sekar, Babu et al., 2003; Sankaranarayanan, Yogavel, Velmurugan, Sekar, Srinivasan *et al.*, 2003; SethuSankar *et al.*, 2002; Govindasamy *et al.*, 1998). The lengthening of C—N bonds in the indole moiety is due to the electron-withdrawing character of the phenylsulfonyl group. The S1—N1 and S1—C10 bond distances are compar-

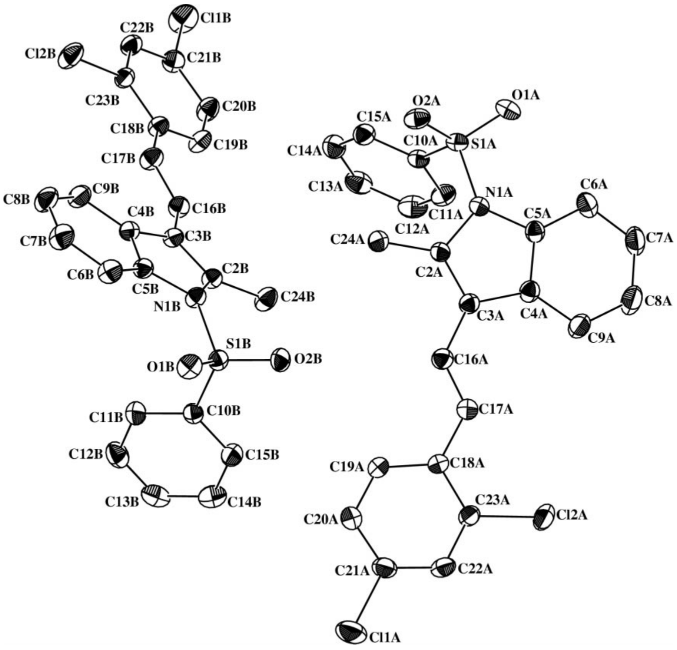


Figure 1
The asymmetric unit of the title compound, showing 35% probability displacement ellipsoids and the atom-numbering scheme.

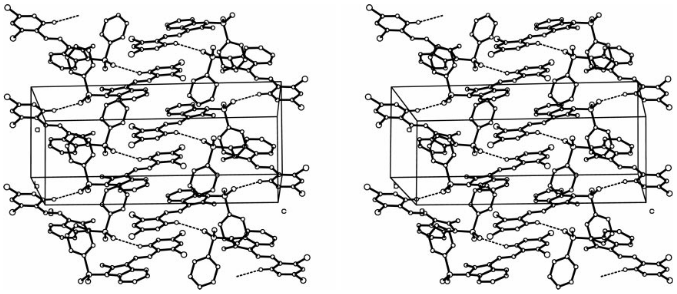


Figure 2
A stereoview of the molecular packing in the title compound, showing two anti-parallel helices along the **a** direction. For clarity, H atoms not involved in hydrogen bonding have been omitted.

able with the respective mean values of 1.642 (24) and 1.758 (18) Å (Allen *et al.*, 1987). In both molecules, the angular disposition of the bonds about the S atoms shows significant deviation from that of a regular tetrahedron, with the largest deviation being in the O—S—O angles. As previously reported, the widening of the O—S—O angle is presumably the result of repulsive interaction between the S═O bonds (Rodriguez *et al.* 1985; Beddoes *et al.*, 1986; Govindasamy *et al.*, 1998; Sankaranarayanan *et al.*, 2000, 2001; SethuSankar *et al.*, 2002).

In both molecules, the dichlorophenyl ring is nearly coplanar with the indole ring system, with a dihedral angle of 7.6 (1)° in molecule *A* and 11.6 (1)° in molecule *B*. The dihedral angle between the indole ring system and the sulfonyl-bound phenyl ring is 76.2 (1)° in molecule *A* and 75.6 (1)° in molecule *B*. The sulfonylphenyl and dichlorophenyl rings are nearly orthogonal [dihedral angles 79.7 (1) and 81.5 (1)°]. Atom N1 deviates from the plane passing through C2, C5 and S1 by 0.186 (2) Å in molecule *A* and 0.179 (2) Å in molecule *B*, and the sum of the angles around N1 is 355.4 (1)° in molecule *A* and 355.7 (1)° in molecule *B*. This slight pyramidalization is also observed in related indole derivatives (Sankaranarayanan *et al.*, 2000; Sankaranarayanan, Yogavel, Velmurugan, Sekar, Babu *et al.*, 2003; Sankaranarayanan, Yogavel, Velmurugan, Sekar, Srinivasan *et al.*, 2003; SethuSankar *et al.*, 2002).

Both the molecular and crystal structures are stabilized by weak C—H···O interactions. In the molecular structure, the orientations of the indole and phenyl subtituents with respect to the sulfonyl group are influenced by C6—H6···O1 and C15—H15···O2 weak interactions (Table 2). In the crystal structure, the C19*A*—H19*A*···O2*B* and C19*B*—H19*B*···O2*A*$(1 + x, y, z)$ interactions link the molecules to form helices along the **a** direction (Fig. 2).

Experimental

To a suspension of NaH (0.15 g, 6 mmol) in dry tetrahydrofuran (THF, 20 ml) at room temperature was slowly added the 2,4-dichlorobenzyl phosphonium bromide (6 mmol) in dry THF (40 ml) under N_2 and stirred for 1 h. A solution of 1-phenylsulfonyl-2-methylindole-3-carbaldehyde (1 equivalent, 6 mmol) in dry THF (20 ml) was then added. Stirring was continued for another 2 h. The red–brown solution was poured over ice (200 g) containing saturated NH_4Cl solution. Then it was extracted with dichloromethane and the organic extract was washed with water (3 × 25 ml), dried over $MgSO_4$ and filtered. Removal of solvent and chromatographic separation on a silica-gel column by elution with hexane–ethyl acetate (9:1) afforded the title compound.

Crystal data

$C_{23}H_{17}Cl_2NO_2S$
$M_r = 442.34$
Triclinic, $P\bar{1}$
$a = 8.0083$ (1) Å
$b = 11.7242$ (2) Å
$c = 21.9150$ (4) Å
$\alpha = 86.474$ (1)°
$\beta = 89.831$ (1)°
$\gamma = 81.037$ (1)°
$V = 2028.60$ (6) Å^3
$Z = 4$
$D_x = 1.448$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5639 reflections
$\theta = 0.9$–28.3°
$\mu = 0.44$ mm^{-1}
$T = 293$ (2) K
Parallelepiped, yellow
0.48 × 0.42 × 0.36 mm

Data collection

Siemens SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.815$, $T_{\max} = 0.857$
16575 measured reflections
9692 independent reflections
7077 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.038$
$\theta_{\max} = 28.3°$
$h = -10 \rightarrow 10$
$k = -14 \rightarrow 15$
$l = -29 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.121$
$S = 1.04$
9692 reflections
525 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0553P)^2 + 0.042P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.29$ e Å^{-3}
$\Delta\rho_{\min} = -0.42$ e Å^{-3}

o704 V. K. Ganesh *et al.* • $C_{23}H_{17}Cl_2NO_2S$ *Acta Cryst.* (2003). E**59**, o703–o705

Table 1
Selected geometric parameters (Å, °).

Cl1*A*—C21*A*	1.738 (2)	Cl1*B*—C21*B*	1.739 (2)
Cl2*A*—C23*A*	1.737 (2)	Cl2*B*—C23*B*	1.738 (2)
S1*A*—O1*A*	1.426 (1)	S1*B*—O2*B*	1.428 (1)
S1*A*—O2*A*	1.429 (1)	S1*B*—O1*B*	1.429 (1)
S1*A*—N1*A*	1.665 (2)	S1*B*—N1*B*	1.668 (2)
S1*A*—C10*A*	1.760 (2)	S1*B*—C10*B*	1.761 (2)
N1*A*—C2*A*	1.415 (2)	N1*B*—C2*B*	1.419 (2)
N1*A*—C5*A*	1.430 (2)	N1*B*—C5*B*	1.424 (2)
C3*A*—C16*A*	1.445 (3)	C3*B*—C16*B*	1.444 (3)
C16*A*—C17*A*	1.310 (3)	C16*B*—C17*B*	1.314 (3)
C17*A*—C18*A*	1.459 (3)	C17*B*—C18*B*	1.460 (3)
O1*A*—S1*A*—O2*A*	119.03 (8)	O2*B*—S1*B*—O1*B*	118.9 (1)
O1*A*—S1*A*—N1*A*	107.11 (8)	O2*B*—S1*B*—N1*B*	107.5 (1)
O2*A*—S1*A*—N1*A*	107.58 (8)	O1*B*—S1*B*—N1*B*	107.1 (1)
O1*A*—S1*A*—C10*A*	109.81 (9)	O2*B*—S1*B*—C10*B*	108.3 (1)
O2*A*—S1*A*—C10*A*	108.00 (8)	O1*B*—S1*B*—C10*B*	109.8 (1)
N1*A*—S1*A*—C10*A*	104.33 (8)	N1*B*—S1*B*—C10*B*	104.3 (1)
C2*A*—N1*A*—C5*A*	107.8 (1)	C2*B*—N1*B*—C5*B*	107.9 (1)
C2*A*—N1*A*—S1*A*	122.8 (1)	C2*B*—N1*B*—S1*B*	122.8 (1)
C5*A*—N1*A*—S1*A*	124.8 (1)	C5*B*—N1*B*—S1*B*	125.0 (1)
C3*A*—C2*A*—C24*A*	128.0 (2)	C3*B*—C2*B*—C24*B*	127.9 (2)
N1*A*—C2*A*—C24*A*	122.2 (2)	N1*B*—C2*B*—C24*B*	122.5 (2)
C2*A*—C3*A*—C16*A*	123.8 (2)	C2*B*—C3*B*—C16*B*	124.4 (2)
C16*A*—C3*A*—C4*A*	128.8 (2)	C16*B*—C3*B*—C4*B*	128.4 (2)
C17*A*—C16*A*—C3*A*	128.9 (2)	C17*B*—C16*B*—C3*B*	127.8 (2)
C16*A*—C17*A*—C18*A*	126.9 (2)	C16*B*—C17*B*—C18*B*	127.7 (2)
C10*A*—S1*A*—N1*A*—C5*A*	95.3 (2)	C10*B*—S1*B*—N1*B*—C5*B*	95.0 (2)
S1*A*—N1*A*—C5*A*—C6*A*	24.2 (3)	S1*B*—N1*B*—C5*B*—C6*B*	23.1 (3)
O2*A*—S1*A*—C10*A*—C15*A*	17.5 (2)	O2*B*—S1*B*—C10*B*—C15*B*	15.7 (2)

Table 2
Short-contact geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6*A*—H6*A*···O1*A*	0.93	2.28	2.866 (3)	120
C6*B*—H6*B*···O1*B*	0.93	2.29	2.878 (2)	121
C15*A*—H15*A*···O2*A*	0.93	2.53	2.901 (3)	104
C15*B*—H15*B*···O2*B*	0.93	2.54	2.907 (2)	104
C17*A*—H17*A*···Cl2*A*	0.93	2.61	3.052 (2)	110
C17*B*—H17*B*···Cl2*B*	0.93	2.60	3.047 (2)	110
C19*A*—H19*A*···O2*B*	0.93	2.61	3.513 (2)	163
C19*B*—H19*B*···O2*A*$^{\rm i}$	0.93	2.59	3.487 (2)	163

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

The H atoms were fixed geometrically and treated as riding atoms on the parent C atoms, with aromatic C—H = 0.93 Å and methyl C—H = 0.96 Å. Rotating group refinement was used for the methyl groups.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ZORTEP* (Zsolnai, 1997) and *PLATON* (Spek, 1990); software used to prepare material for publication: *SHELXL*97 and *PARST* (Nardelli, 1995).

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Acta Cryst. (2003). E**59**, o703–o705 V. K. Ganesh *et al.* • $C_{23}H_{17}Cl_2NO_2S$ **o705**