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3-[β-(4-Chlorophenyl)-α-(4-methoxyphenyl)vinyl]-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) = 0.006 Å
R factor = 0.085
wR factor = 0.277
Data-to-parameter ratio = 16.9

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

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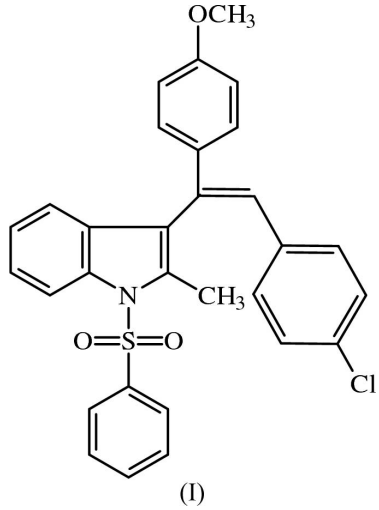
In the title compound, $C_{30}H_{24}ClNO_3S$, the phenylsulfonyl, chlorophenyl and methoxyphenyl rings are each almost perpendicular to the indole ring system. The crystal packing shows centrosymmetrically related pairs of molecules. Intermolecular C—H···O interactions are present.

Comment

Indoles and their various substituted products have long been known for their chemical and biological activites. Compounds of the 2-vinyl indole class are observed to exhibit anti-microbial (El-Sayed *et al.*, 1986) and anti-inflammatory activities (Rodriguez *et al.*, 1985). The *in vitro* antibacterial and antifungal activities of a series of pyridazinoindolonic acids-II against some selected fungi and Gram-positive and -negative bacteria have been investigated (Palluotto *et al.*, 1999). A series of 2-aryl indoles with affinity for the human neurokinin-1 (hNK1) receptor have been reported (Cooper *et al.*, 2001). Recently, 2,3-substituted indoles have been used as a bidendate synthon for the synthesis of various medicinally important carbazole alkaloids. Indoles with hallucinogenic properties act as agonists at the serotonin receptors in the brain (Mann, 1992). The indole derivative sumatriptan has been introduced into medicine as a drug for the treatment of migraine (Oxford, 1995). The crystal and molecular structures of the title compound, (I), was investigated in order to determine the stereochemistry of the substituents with respect to the indole ring system.



(I)

In the indole ring system of (I), the endocyclic angles at C6 and C9 are contracted to 117.2 (4) and 118.4 (3)°, respectively,

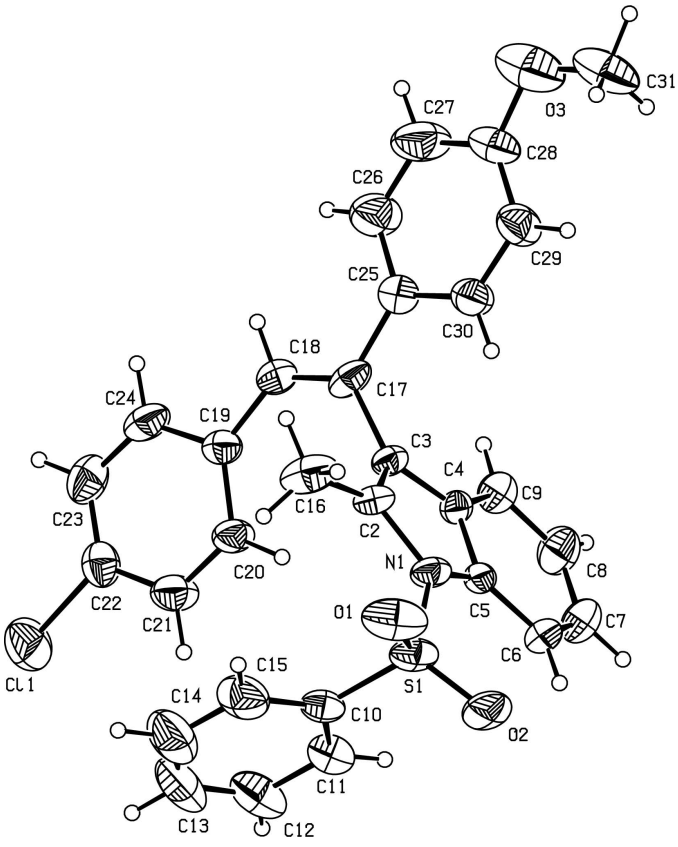


Figure 1
The molecular structure of (I), showing the atom-numbering scheme and 30% probability displacement ellipsoids.

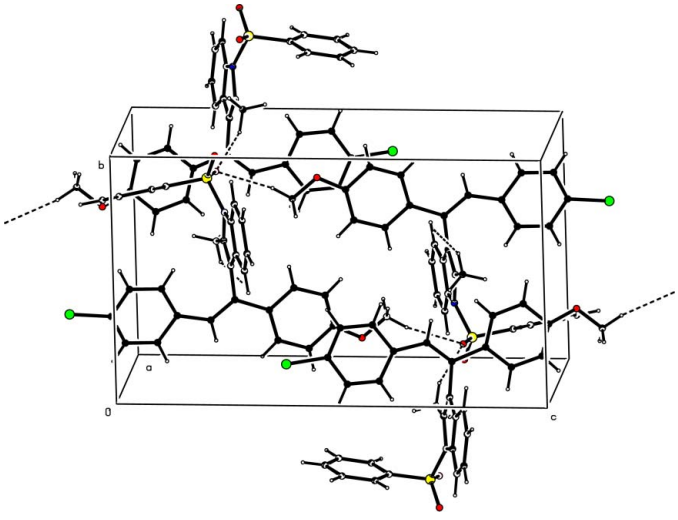


Figure 2
The packing of the molecules of (I), viewed approximately down the *a* axis. Dashed lines indicate hydrogen bonds.

whereas the angles at C5 and C8 are expanded to 121.4 (3) and 121.0 (4)°, respectively. This may be due to the angular distortion caused by the fusion of the five-membered pyrrole ring to the six-membered benzene ring. A similar effect is observed in related reported structures (Allen & Trotter 1970; Sivaraman *et al.*, 1994*a*,*b*; Sethu Sankar *et al.*, 2002).

The S—O, S—C and S—N bond distances of 1.417 (3), 1.738 (4) and 1.658 (2) Å, respectively, agree well with the corresponding bond distances in related structures (Beddoes *et al.*, 1994; Seetharaman & Rajan, 1995). The sum of the angles around N1 (355.9°) is in the same range as in similar structures (Govindasamy *et al.*, 1997, 1998).

The indole ring system is planar and this planarity is considered to be essential for intercalation with DNA (Neidle, 1979). The dihedral angles between the indole system and the phenylsulfonyl, chlorophenyl and methoxyphenyl rings are 86.2 (1), 86.8 (1) and 87.7 (1)°, respectively, indicating that the substituent rings are each almost perpendicular to the indole ring system. There is an asymmetry in the exocyclic angles at C22 and C28 [the Cl1—C22—C23 angle is 5.5 (2)° larger than the Cl1—C22—C21 angle, and the O3—C28—C29 angle is 16.1 (5)° larger than the O3—C28—C27 angle].

The molecular structure of (I) possesess a number of weak intramolecular C—H···O interactions. Centrosymmetrically related pairs of molecules form a dimer *via* C—H···O contacts (Table 2).

Experimental

To a stirred solution of sodium hydride (1.5 mmol) in dry tetrahydrofuran (THF, 5 ml), 2-methyl [3-(α-4-methoxyphenyl)-β-4-chlorophenyl]vinylindole (1 mmol) in dry THF (5 ml) was slowly added under N_2 at refluxing temperature. After 1 h, the reaction mixture was cooled to room temperature. Phenylsulfonyl chloride (1.5 mmol) was added to the same solvent 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. Crystals of (I) were obtained after dissolving this product in ethyl acetate and allowing slow evaporation.

Crystal data

$C_{30}H_{24}ClNO_3S$
M_r = 514.01
Monoclinic, $P2_1/c$
a = 13.6402 (9) Å
b = 10.4097 (6) Å
c = 18.4430 (11) Å
β = 99.756 (1)°
V = 2580.9 (3) Å^3
Z = 4
D_x = 1.323 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5225 reflections
θ = 2.3–25.6°
μ = 0.26 mm^{-1}
T = 273 (2) K
Block, colourless
0.24 × 0.22 × 0.19 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
ω scans
Absorption correction: none
15377 measured reflections
5533 independent reflections
4054 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 28.0°
$h = -17 \rightarrow 14$
$k = -13 \rightarrow 13$
$l = -23 \rightarrow 24$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.085
$wR(F^2)$ = 0.277
S = 1.05
5533 reflections
327 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1623P)^2 + 1.4648P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.98 e Å^{-3}
$\Delta\rho_{min}$ = −0.51 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—O1	1.407 (3)	O3—C31	1.353 (4)
S1—O2	1.426 (3)	N1—C5	1.421 (4)
S1—N1	1.658 (2)	N1—C2	1.429 (4)
S1—C10	1.738 (4)	C2—C16	1.485 (5)
Cl1—C22	1.773 (4)	C17—C25	1.544 (6)
O3—C28	1.340 (6)		
O1—S1—O2	119.7 (2)	N1—S1—C10	104.8 (1)
O1—S1—N1	107.2 (2)	C23—C22—Cl1	122.7 (3)
O2—S1—N1	105.9 (2)	C21—C22—Cl1	117.2 (3)
O1—S1—C10	109.4 (2)	O3—C28—C29	129.6 (5)
O2—S1—C10	108.9 (2)	O3—C28—C27	113.5 (5)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···O2	0.93	2.31	2.889 (5)	120
C16—H16*A*···O1^{i}	0.96	2.47	3.264 (5)	140
C31—H31*B*···O1^{ii}	0.96	2.59	3.531 (6)	168

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

The H atoms were positioned geometrically and were treated as riding on their parent C atoms, with aromatic C—H distances of 0.93 Å, methyl C—H distances of 0.96 Å and methylene C—H distances of 0.97 Å, and an N—H distance of 0.86 Å, and with U_{iso}(H) = 1.5U_{eq}(C) for methyl H and 1.2U_{eq}(N or C) for other H.

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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