Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3-Phenylsulfanyl-1-phenylsulfonyl-1*H*-indole-2-carbaldehyde

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.037
wR factor = 0.113
Data-to-parameter ratio = 13.4

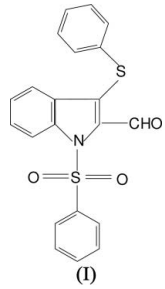
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 9 February 2006
Accepted 23 February 2006

In the title compound, $C_{21}H_{15}NO_3S_2$, the phenyl ring of the phenylsulfonyl substituent makes a dihedral angle of 73.6 (1)° with the mean plane of the indole ring system, whereas the phenyl ring of the phenylsulfanyl group forms a dihedral angle of 73.9 (1)° with the mean plane of the indole ring system. The crystal packing is stabilized by C—H···O 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 (Papenstasion & Newmeyer, 1972), antimicrobial (El-Sayed *et al.*, 1986; Gadaginamath & Patil, 1999) and anti-inflammatory activities (Rodriguez *et al.*, 1985; Polletto *et al.*, 1974). The *in vitro* antibacterial and antifungal activities of a series of pyridazinoindolonic acids-II against some selected fungi and Gram-positive and Gram-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). 2,3-Substituted indoles have been used as bidendate synthons 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). Indoles also intercalate with DNA (Sivaraman *et al.*, 1996), and this intercalation between the base pairs in DNA has been implicated for their medicinal activities. The indole ring system occurs in plants (Nigović *et al.*, 2000); for example, indole-3-acetic acid is a naturally occurring plant growth hormone that controls several plant growth activities (Moore, 1989; Fargasova, 1994). Indoles have also been proven to display high aldose reductose inhibitory activity (Rajeswaran *et al.*, 1999). In order to obtain detailed information on the molecular conformation in the solid state, an X-ray crystallographic study of the title indole derivative, (I), has been carried out.



(I)

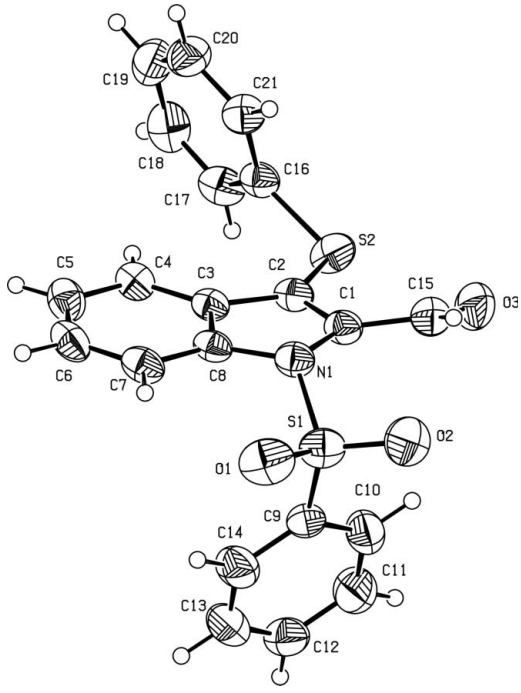


Figure 1
The molecular structure, showing 35% probability displacement ellipsoids and the atom-numbering scheme; H atoms are shown as small spheres of arbitrary radii.

The bond lengths do not show unusual values. Atom N1 is not planar but pyramidal. Slight pyramidalization is also observed in related indoles (Yokum & Fronczek, 1997; Beddoes *et al.*, 1986; Sethu Sankar *et al.*, 2002). The dihedral angle between the planes of the phenyl ring of the phenylsulfonyl residue and the indole system is 73.6 (1)°, as observed in similar structures (Yokum & Fronczek, 1997; Sankaranarayanan *et al.*, 2000; Sethu Sankar *et al.*, 2002). The dihedral angle formed by the mean plane through the indole system and the phenyl ring of the thiophenyl group is 73.9 (1)°. In addition to van der Waals interactions the molecular structure and the crystal packing are stabilized by C—H···O hydrogen bonds (Table 2).

Experimental

To a solution of 1-phenylsulfonyl-2-bromomethyl 3-phenylthioindole (5 mmol) in dry chloroform (60 ml) bis(tetra-*n*-butylammonium) dichromate (5.0 mmol) was added. The resulting solution was refluxed for 6–8 h. Evaporation of the organic solvents followed by chromatographic purification using hexane and ethyl acetate (7:3) afforded (I) in 70% yield.

Crystal data

$C_{21}H_{15}NO_3S_2$
M_r = 393.46
Monoclinic, $P2_1/c$
a = 10.003 (4) Å
b = 16.001 (6) Å
c = 11.750 (5) Å
β = 97.80 (3)°
V = 1863.3 (13) Å^3
Z = 4
D_x = 1.403 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 4.4–18.0°
μ = 0.31 mm^{-1}
T = 293 (2) K
Block, colourless
0.32 × 0.23 × 0.18 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
3729 measured reflections
3267 independent reflections
2080 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 25.0°
$h = 0 \rightarrow 11$
$k = -1 \rightarrow 19$
$l = -13 \rightarrow 13$
3 standard reflections
every 100 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.113
S = 1.06
3267 reflections
244 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0627P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—O1	1.419 (2)	S1—C9	1.754 (3)
S1—O2	1.426 (2)	N1—C8	1.414 (3)
S1—N1	1.690 (2)	N1—C1	1.426 (3)
O1—S1—N1—C8	−50.1 (2)	O1—S1—C9—C14	14.5 (3)
S1—N1—C8—C7	42.5 (3)	S1—C9—C10—C11	178.1 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···O3^{i}	0.93	2.48	3.387 (4)	164
C7—H7···O1	0.93	2.39	2.961 (4)	119
C15—H15···O2	0.93	2.41	2.807 (4)	106

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

All H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H distances of 0.93 Å and U_{iso}(H) = 1.2U_{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) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PARST* (Nardelli, 1995).

The authors thank Professor P. C. Srinivasan for providing the sample for X-ray study.

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