

3-Phenylsulfinylmethyl-1-phenylsulfonyl-1*H*-indoleG. Senthil Kumar,^a
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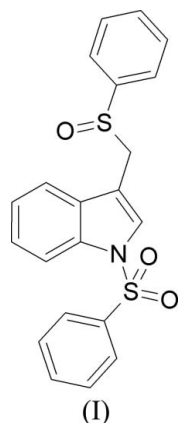
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In the title molecule, C₂₁H₁₇NO₃S₂, the sulfonyl-bound and sulfinyl-bound phenyl rings form dihedral angles of 82.04 (5) and 26.26 (8)°, respectively, with the indole ring system. In the crystal structure C—H···O, C—H···π and π–π interactions form a two-dimensional network.

Comment

Some substituted 3-aryl- and 3-(heteroaryl)indoles exhibit antibacterial activity (Al-Hiari *et al.*, 2006). 4-(2-Aminoethoxy)-*N*-(phenylsulfonyl)indoles exhibit high affinity towards the 5-HT₆ receptor (Zhou *et al.*, 2005). Substituted indole derivatives show antimalarial (Agarwal *et al.*, 2005), and weak anti-HIV and cytotoxic activities (Wang *et al.*, 2005). We report here the structure of the title compound, (I).



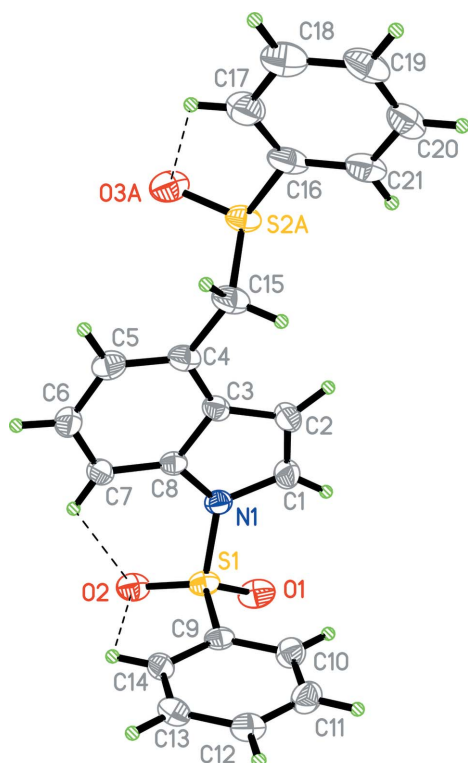
Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ (C–C) = 0.003 Å
Disorder in main residue
R factor = 0.045
wR factor = 0.119
Data-to-parameter ratio = 19.9For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

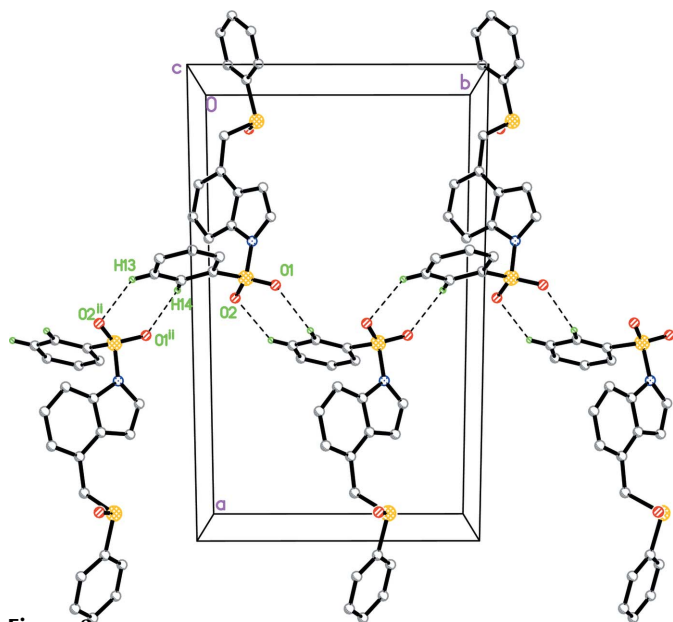
The molecular structure of compound (I) is illustrated in Fig. 1. Bond lengths and angles in the phenylsulfonyl unit of (I) are normal (Beddoes *et al.*, 1986; Ravishankar *et al.*, 2003*a,b*, 2005*a,b,c*). The indole ring system is planar with a maximum deviation of 0.027 (1) Å for atom C1. Atom N1 deviates by 0.191 (2) Å from the plane through atoms C1, C8 and S1, indicating a slight degree of pyramidalization.

The conformation of the phenylsulfonyl group with respect to the indole unit is described by the torsion angles O1–S1–N1–C1 = –34.10 (16)°, O2–S1–N1–C8 = 44.03 (16)° and N1–S1–C9–C10 = –77.69 (15)°. This conformation is influenced by the C7–H7···O2 and C14–H14···O2 interactions (Table 1), involving sulfonyl atoms O1 and O2, which deviate by –0.176 (2) and 0.005 (2) Å, respectively, from the plane of the indole ring system. The dihedral angle between the sulfonyl-bound phenyl ring and the indole ring system is 82.04 (5)°.

The O3A–S2A–C16–C17 [15.0 (2)°] and O3B–S2B–C16–C17 [125.4 (6)°] torsion angles describe the relative

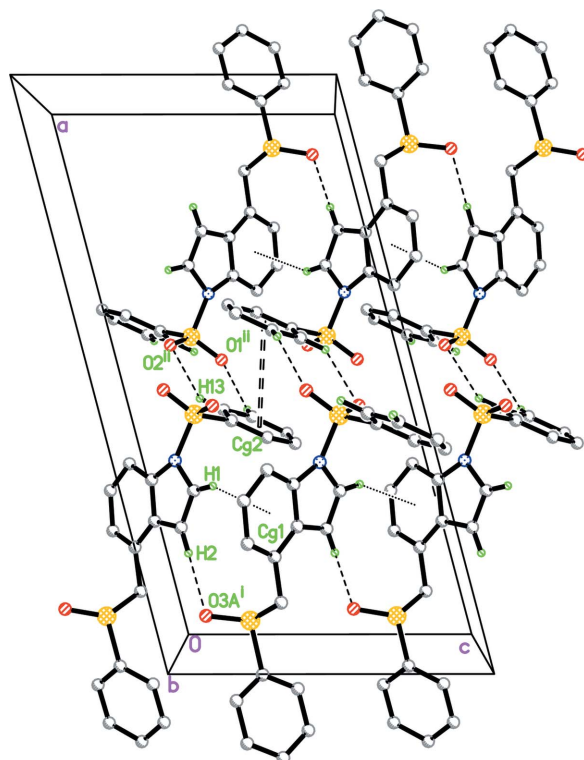
**Figure 1**

The molecular structure of (I). Displacement ellipsoids are drawn at the 80% probability level. Hydrogen bonds are shown as dashed lines. Only the major component (87%) of the disordered sulfanyl group is shown.

**Figure 2**

A view of a hydrogen-bonded (dashed lines) chain in the crystal structure of (I). For the sake of clarity, H atoms not involved in the interactions have been omitted. Symmetry codes are as given in Table 1. Only the major disorder component is shown.

orientations of the major and minor disorder components of the sulfanyl group in relation to the C16–C21 benzene ring. The O3A–S2A–C15–C4 and C16–S2A–C15–C4 torsion

**Figure 3**

Part of the two-dimensional network in the crystal structure of (I). Dashed, dotted and dashed-open lines indicate C–H...O, C–H... π and π – π interactions, respectively. For the sake of clarity, H atoms not involved in the interactions have been omitted. Symmetry codes are as given in Table 1. Only the major disorder component is shown.

angles are 62.67 (17) and 171.28 (16)°, respectively. The dihedral angle between the sulfanyl-bound phenyl ring and the indole ring system is 26.26 (8)°.

Screw-related molecules are linked through C13–H13...O2ⁱⁱ and C14–H14...Oⁱⁱ hydrogen bonds, forming a chain along the *b* axis (Fig. 2). Glide-related molecules in the adjacent chains are cross-linked *via* C2–H2...O3Aⁱ and C1–H1...Cg1ⁱ interactions involving the C3–C8 benzene ring (centroid Cg1), forming a two-dimensional network parallel to the *bc* plane (Fig. 3). The network structure is further strengthened by π – π interactions between the sulfanyl-bound phenyl rings (centroid Cg2), with a Cg2...Cg2^{iv} distance of 3.7987 (11) Å and a perpendicular distance between the rings of 3.524 Å. C19–H19...Cg2ⁱⁱⁱ interactions link adjacent networks. [Symmetry codes (i) to (iii) are given in Table 1; additionally, (iv) 1 – *x*, –*y*, 1 – *z*.]

Experimental

To a solution of KF (2 mmol) in acetonitrile (8 ml) and water (2 ml), 70% *m*-CPBA (2 mmol) was added and stirred at 273 K for 30 min. To this, 1-phenylsulfanyl-4-phenylthiomethylindole (1.0 mmol) was added and the stirring was continued for an additional 30 min. The reaction mixture was then poured into a saturated aqueous NaHCO₃ solution, extracted with ethyl acetate (2 × 10 ml) and the extract dried (Na₂SO₄). Removal of the solvent followed by crystallization from ethyl acetate–hexane (1:5 v/v) afforded good quality crystals.

Crystal data

$C_{21}H_{17}NO_3S_2$	$Z = 4$
$M_r = 395.48$	$D_x = 1.416 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 18.3174 (3) \text{ \AA}$	$\mu = 0.31 \text{ mm}^{-1}$
$b = 10.8625 (2) \text{ \AA}$	$T = 100.0 (1) \text{ K}$
$c = 9.6364 (1) \text{ \AA}$	Plate, colourless
$\beta = 104.697 (1)^\circ$	$0.33 \times 0.27 \times 0.06 \text{ mm}$
$V = 1854.65 (5) \text{ \AA}^3$	

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer	27648 measured reflections
ω scans	5242 independent reflections
Absorption correction: multi-scan (SADABS; Bruker, 2005)	4215 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.864$, $T_{\max} = 0.982$	$R_{\text{int}} = 0.040$
	$\theta_{\max} = 29.7^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0519P)^2 + 0.9013P]$
$R[F^2 > 2\sigma(F^2)] = 0.046$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.120$	$(\Delta/\sigma)_{\max} = 0.001$
$S = 1.09$	$\Delta\rho_{\max} = 0.62 \text{ e \AA}^{-3}$
5242 reflections	$\Delta\rho_{\min} = -0.38 \text{ e \AA}^{-3}$
263 parameters	
H-atom parameters constrained	

Table 1

Hydrogen-bond geometry (\AA , $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C2-H2\cdots O3A^i$	0.95	2.34	3.286 (3)	176
$C7-H7\cdots O2$	0.95	2.47	3.051 (2)	119
$C13-H13\cdots O2^{ii}$	0.95	2.49	3.298 (2)	143
$C14-H14\cdots O2$	0.95	2.57	2.937 (2)	103
$C14-H14\cdots O1^{ii}$	0.95	2.58	3.385 (2)	143
$C17-H17\cdots O3A$	0.95	2.58	2.959 (3)	104
$C1-H1\cdots Cg1^i$	0.95	2.80	3.669 (2)	152
$C19-H19\cdots Cg2^{iii}$	0.95	2.89	3.689 (2)	142

Symmetry codes: (i) $x, -y + \frac{1}{2}, z + \frac{1}{2}$; (ii) $-x + 1, y - \frac{1}{2}, -z + \frac{1}{2}$; (iii) $-x, -y, -z$. Cg1 is the centroid of the C3–C8 benzene ring and Cg2 is the centroid of the sulfonyl-bound phenyl ring.

The sulfinyl group is disordered over two orientations (S2A/O3A and S2B/O3B) with occupancies of 0.869 (3) and 0.131 (3). The U^{ij}

components of atoms S2B and O2B were restrained to approximately isotropic behaviour. H atoms were positioned geometrically ($C-H = 0.95-0.99 \text{ \AA}$) and were treated as riding on their parent C atoms, with $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C)$.

Data collection: APEX2 (Bruker, 2005); cell refinement: APEX2; data reduction: SAINT (Bruker, 2005); program(s) used to solve structure: SHELXTL (Sheldrick, 1998); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL and PLATON (Spek, 2003).

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