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2-(2,5-Dimethylbenzyl)-3-phenylsulfanyl-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 = 0.049
wR factor = 0.143
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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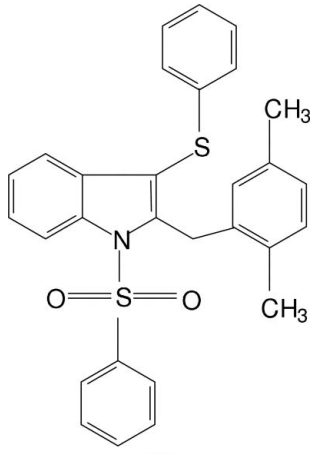
In the title compound, $C_{29}H_{25}NO_2S_2$, the benzene rings of the phenylsulfonyl and the dimethylbenzyl substituents are almost perpendicular to the indole unit, whereas the dihedral angle between the phenyl rings of the phenylsulfanyl and phenylsulfonyl groups is 71.2 (1)°. The molecules in the crystal structure are held together by van der Waals, C—H···O and C—H···S interactions.

Comment

Indoles and their derivatives have been of interest for many years, since a large number of natural products contain indole systems, and they are found in a number of pharmaceutical products, fragrances and dyes (Padwa *et al.*, 1999). Spiroindole derivatives exhibit antibacterial and antifungal properties (Sehgal *et al.*, 1994). The sulfonamide-containing drugs inhibit the growth of bacterial organisms and are also used for treating urinary and gastrointestinal infections. The wide range of biological activities of indole and its derivatives prompted us to undertake the crystal structure analysis of the title compound, (I).



(I)

The S—O, S—C and S—N bond distances are in good agreement with the related reported values of 1.435 (5), 1.767 (7) and 1.685 (5) Å, respectively (Govindasamy *et al.*, 1998). The electron-withdrawing character of the phenylsulfonyl group affects the C—N distances in the indole ring system [C5—N1 = 1.417 (2) Å and C2—N1 = 1.416 (2) Å] and this is observed in similar reported structures (Rodriguez *et al.*, 1995; Govindasamy *et al.*, 1999). The sum of the angles around atom N1 (358.4°) indicates sp^2 hybridization. In the dimethylphenyl ring, the endocyclic angles at C19 and C22 are 117.4 (2) and 117.6 (2)°, respectively, and this decrease can be

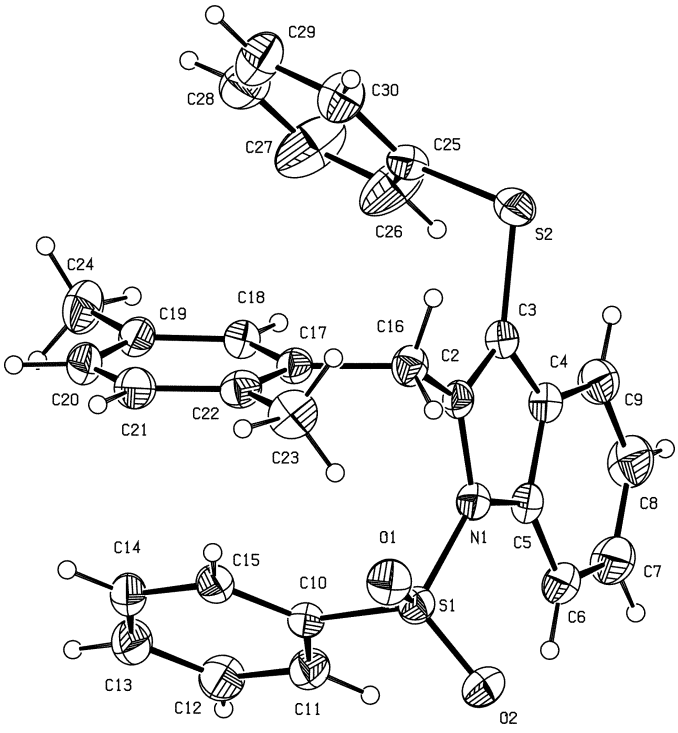


Figure 1
The molecular structure of the title compound, showing 30% probability displacement ellipsoids.

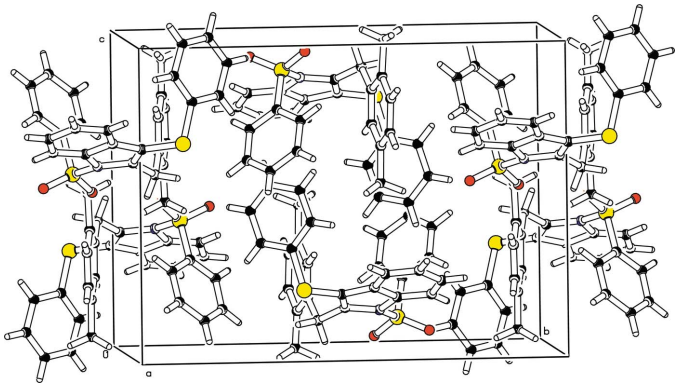


Figure 2
The molecular packing of (I), viewed approximately down the *c* axis.

attributed to the steric hindrance caused by the methyl groups. The bond angle C2—C16—C17 [115.5 (2)°] is widened.

The dihedral angles between the indole ring system and the mean planes of the phenylsulfonyl, dimethylphenyl and the phenylsulfanyl rings are 85.1 (1), 82.6 (1) and 71.2 (1)°, respectively, and show that the substituent rings are almost perpendicular to the indole system.

The packing of the molecules in the unit cell is governed by van der Waals forces and the crystal structure is stabilized by C—H···O and C—H···S interactions.

Experimental

The title compound was prepared by the reaction of 2-hydroxymethyl-3-phenylsulfanyl-1-phenylsulfonyl-1*H*-indole with *p*-xylene in the presence of a catalytic amount of boron trifluoride etherate in boiling chloroform, following a published procedure (Rajeswaran & Srinivasan, 1992). The crude product was purified by silica-gel column chromatography, eluting with hexane–ethyl acetate (9:1). Diffraction quality crystals were obtained from a hexane/ethyl acetate (1:1) solution.

Crystal data

$C_{29}H_{25}NO_2S_2$
M_r = 483.62
Monoclinic, $P2_1/n$
a = 10.8372 (6) Å
b = 17.2384 (10) Å
c = 12.7220 (7) Å
β = 90.269 (1)°
V = 2376.6 (2) Å^3
Z = 4
D_x = 1.352 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5656 reflections
θ = 2.2–27.5°
μ = 0.25 mm^{-1}
T = 273 (2) K
Block, colourless
0.23 × 0.22 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: none
14279 measured reflections
5221 independent reflections
4227 reflections with $I > 2\sigma(I)$
R_{int} = 0.020
θ_{max} = 28.0°
$h = -14 \rightarrow 14$
$k = -22 \rightarrow 21$
$l = -14 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.143
S = 1.01
5221 reflections
309 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0882P)^2 + 0.5156P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—O1	1.414 (2)	N1—C5	1.417 (2)
S1—O2	1.422 (2)	N1—C2	1.416 (2)
S1—N1	1.682 (2)	C2—C16	1.496 (3)
S1—C10	1.760 (2)	C16—C17	1.522 (2)
S2—C3	1.759 (2)	C19—C24	1.499 (3)
S2—C25	1.780 (2)	C22—C23	1.501 (3)
O1—S1—O2	120.6 (1)	C3—S2—C25	103.0 (1)
O1—S1—N1	106.7 (1)	C5—N1—C2	108.5 (2)
O2—S1—N1	105.5 (1)	C5—N1—S1	122.1 (1)
O1—S1—C10	109.2 (1)	C2—N1—S1	127.8 (1)
O2—S1—C10	108.7 (1)	C2—C16—C17	115.5 (2)
N1—S1—C10	105.0 (1)		
O2—S1—C10—C15	149.7 (2)		

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	2.900 (3)	121
C15—H15···O1	0.93	2.55	2.914 (3)	104
C16—H16*A*···S2	0.97	2.83	3.294 (2)	110
C16—H16*B*···O1	0.97	2.38	2.881 (3)	112

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 $U_{iso} = 1.5U_{eq}$(C) for methyl H and $1.2U_{eq}$(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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References

Bruker (2001). *SAINT* (Version 6.28a) and *SMART* (Version 5.625). Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Govindasamy, L., Velmurugan, D., Ravikumar, K. & Mohanakrishnan, A. K. (1998). *Acta Cryst.* C**54**, 635–637.
Govindasamy, L., Velmurugan, D., Shanmuga Sundara Raj, S. & Fun, H. K. (1999). *Acta Cryst.* C**55**, 1315–1317.
Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
Padwa, A., Brodney, M. A.,Liu, B., Stake, K. & Wu, T. (1999). *J. Org. Chem.* **64**, 3595–3607.
Rajeswaran, W. G. & Srinivasan, P. C. (1992). *Ind. J. Heterocyclic Chem.* **2**, 89–90.
Rodriguez, J. G., del Valle, C., Calderon, C. E. & Ripoll, M. M. (1995). *J. Chem. Crystallogr.* **25**, 249–257.
Sehgal, V., Singh, P., Dandia, A. & Bohra, R. (1994). *Acta Cryst.* C**50**, 1156–1159.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.