Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-(1-Benzoyl-1-phenylethyl)-3-phenylsulfanyl-1-phenylsulfonyl-1*H*-indole

S. M. Malathy Sony,[a] K. Palani,[a] P. Charles,[a] M. N. Ponnuswamy,[a]* N. Sureshbabu,[b] P. C. Srinivasan[b] and M. Nethaji[c]

[a]Department of Crystallography and Biophysics, University of Madras, Guindy Campus, Chennai 600 025, India, [b]Department of Organic Chemistry, University of Madras, Guindy Campus, Chennai 600 025, India, and [c]Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore 560 012, India

Correspondence e-mail: mnpsy2004@yahoo.com

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.062
wR factor = 0.168
Data-to-parameter ratio = 15.9

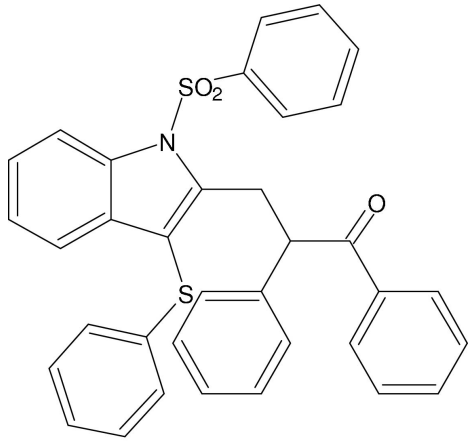
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 26 January 2005
Accepted 1 February 2005
Online 12 February 2005

In the title molecule, $C_{35}H_{27}NO_3S_2$, the indole system is approximately planar. The phenyl rings of the phenylsulfonyl and phenylsulfanyl groups are oriented at angles of 74.69 (7) and 88.35 (9)°, respectively, to the indole ring system. The dihedral angle between the two phenyl rings of the diphenylpropanone moiety is 74.25 (10)°. Inversion-related molecules form C—H···π interactions and C—H···O hydrogen bonds. The C—H···O intermolecular hydrogen bonds form a closed ring pattern in the crystal stucture.

Comment

Indole and its derivatives are found in many natural products as plant alkaloids which have antimicrobial (Gadaginamath & Patil, 1999), anti-inflammatory (Rodriguez *et al.*, 1985), antibacterial (Okabe & Adachi, 1998) and antidepressive activities. Many sulfur-containing compounds, such as sulfates, sulfones and sulfonamides, exhibit insecticidal, germicidal, antimicrobial and antibacterial activities (De-Benedetti *et al.*, 1985; Krishnaiah *et al.*, 1995) and certain phenyl sulfones show fungicidal properties (Wolf, 1999). In view of the many pharmacological activities of indole and sulfur-containing compounds, the crystal structure of the title compound, (I), was determined.



(I)

The angular disposition around atom S10 shows significant deviation from a regular tetrahedron, with the largest deviation in the O—S—O angle [119.0 (1)°]; this widening is presumably the result of the repulsive interactions between the short S═O bonds (Sankaranarayanan *et al.*, 2001; Govindasamy *et al.*, 1999; Rodriguez *et al.*, 1985). The sum of angles around atom N1 (351.6°) deviates significantly from 360° and this atom lies 0.253 (2) Å out of the plane of the

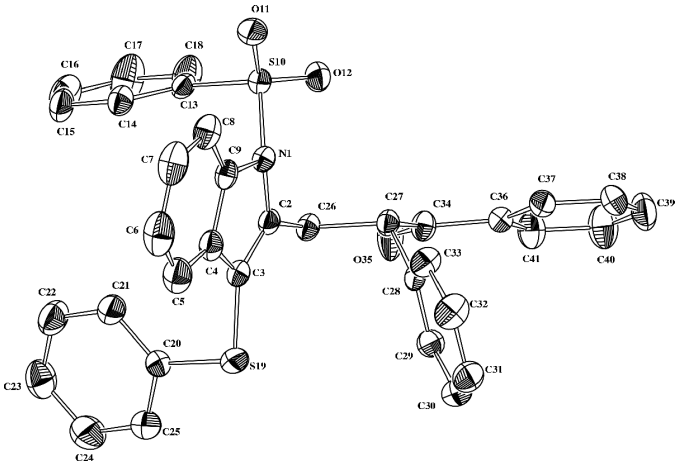


Figure 1
ZORTEP plot (Zsolnai, 1998) of the title molecule, showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity.

three atoms bonded to it (C2, C9 and S10). This slight pyramidalization is also observed in related indoles (Yokum & Fronczek, 1997; Sankaranarayanan *et al.*, 2001; Beddoes *et al.*, 1986).

The indole system is approximately planar. The phenyl ring of the phenylsulfonyl group is oriented at an angle of 74.69 (7)° to the indole system and the phenyl ring of the phenylsulfanyl group is oriented approximately perpendicular to the indole system, the dihedral angle being 88.35 (9)°. The two phenyl rings in the diphenylpropanone moiety are oriented at an angle of 74.25 (10)° and are positioned at angles of 48.72 (10) (ring C28–C33) and 69.98 (7)° (ring C36–C41) to the indole ring system. The O atom of the diphenylpropanone moiety is twisted by 120.9 (3)° with respect to ring C28–C33, as seen from the torsion angle C28—C27—C34—O35.

Two weak intramolecular C—H···O hydrogen bonds C8···O11 and C27···O12 stabilize the molecular structure. Inversion-related molecules are packed such that they form the maximum possible C—H···π interactions and C—H···O hydrogen bonds. An interesting feature in the packing is that a closed ring of C—H···O intermolecular interactions is found, involving atoms C6 and C38 with O12. Atom O12 forms intermolecular C—H···O interactions with C6($1 + x, y, z$) and atom C38 of this latter molecule in turn interacts with O12($2 - x, 2 - y, 1 - z$). Again, O12($2 - x, 2 - y, 1 - z$) interacts with C6($1 - x, 2 - y, 1 - z$) and O12 of this molecule interacts with C38(x, y, z). These form a closed ring of C—H···O interactions, as shown in Fig. 3. Atoms C23 and C32 are involved in C—H···π interactions with the inversion-related benzene ring (centroid *Cg*1) of the indole systems at ($-1 - x, 1 - y, -z$) and ($-x, 2 - y, 1 - z$), respectively. Also, atoms C15 and C17 are involved in similar interactions with the phenyl ring (centroid *Cg*2) of the phenylsulfanyl groups at ($-1 - x, 1 - y, -z$) and ($-x, 1 - y, -z$), respectively, and atom C25 interacts with the C36–C41 phenyl ring (centroid *Cg*3) of the diphenylpropanone moiety at ($-x, 1 - y, 1 - z$) (Table 1).

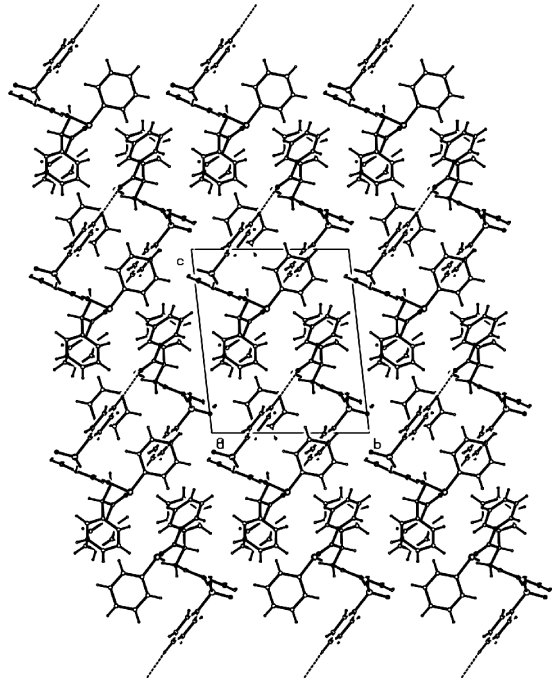


Figure 2
The crystal structure of the title compound, viewed down the *a* axis. Dashed lines represent hydrogen bonds.

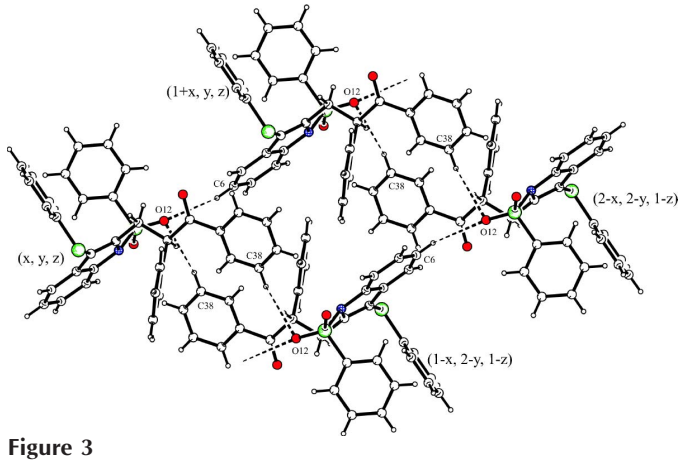


Figure 3
Intermolecular C—H···O interactions forming a closed ring.

Experimental

To a stirred suspension of sodium hydride (0.24 g, 10 mmol) in dry dimethylformamide (DMF, 10 ml), a solution of benzyl phenyl ketone (5 mmol) in the same solvent (15 ml) was added dropwise under nitrogen at room temperature. The intense yellow reaction mixture indicated the formation of a carbanion. After stirring for 30 min, the bromomethyl indole (1-phenylsulfonyl-2-bromomethyl-3-phenylthioindole) (2.29 g, 5 mmol) in dry DMF (25 ml) was added dropwise slowly. The reaction mixture was then stirred for 3 h at room temperature and poured over crushed ice containing hydrochloric acid (5 ml). The precipitated white solid was filtered off and dried over calcium chloride. Recrystallization of the solid from hexane and ethyl acetate (7:3) afforded the pure crystalline alkylated product.

Crystal data

$C_{35}H_{27}NO_3S_2$	$Z = 2$
$M_r = 573.70$	$D_x = 1.299$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 10.0183$ (8) Å	Cell parameters from 9003 reflections
$b = 12.1239$ (10) Å	$\theta = 1.6$–$28.0°$
$c = 13.4174$ (11) Å	$\mu = 0.22$ mm^{-1}
$\alpha = 91.415$ (2)°	$T = 293$ (2) K
$\beta = 101.451$ (2)°	Block, colourless
$\gamma = 112.473$ (1)°	0.25 × 0.22 × 0.20 mm
$V = 1466.8$ (2) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	4293 reflections with $I > 2\sigma(I)$
	$R_{int} = 0.019$
ω scans	$\theta_{max} = 28.0°$
Absorption correction: none	$h = -13 \rightarrow 12$
9003 measured reflections	$k = -15 \rightarrow 15$
5883 independent reflections	$l = -14 \rightarrow 16$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0947P)^2 + 0.1442P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.062$	
$wR(F^2) = 0.168$	
$S = 1.02$	$(\Delta/\sigma)_{max} = 0.001$
5883 reflections	$\Delta\rho_{max} = 0.34$ e Å^{-3}
370 parameters	$\Delta\rho_{min} = -0.20$ e Å^{-3}
H-atom parameters constrained	

Table 1
Hydrogen-bonding geometry (Å, °) for (I).

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8···O11	0.93	2.33	2.896 (4)	119
C27—H27···O12	0.98	2.49	3.128 (3)	123
C6—H6···O12^{i}	0.93	2.59	3.502 (5)	167
C14—H14···O11^{ii}	0.93	2.68	3.152 (4)	112
C16—H16···O35^{iii}	0.93	2.37	3.297 (4)	174
C38—H38···O12^{iv}	0.93	2.69	3.573 (3)	159
C23—H23···*Cg*1^{v}	0.93	3.05	3.864 (4)	147
C32—H32···*Cg*1^{vi}	0.93	3.19	3.771 (4)	122
C15—H15···*Cg*2^{v}	0.93	3.07	3.893 (5)	149
C17—H17···*Cg*2^{iii}	0.93	3.17	3.904 (6)	137
C25—H25···*Cg*3^{vii}	0.93	2.78	3.567 (4)	144

Symmetry codes: (i) $x-1, y, z$; (ii) $-x, 2-y, -z$; (iii) $-x, 1-y, -z$; (iv) $1-x, 2-y, 1-z$; (v) $-1-x, 1-y, -z$; (vi) $-x, 2-y, 1-z$; (vii) $-x, 1-y, 1-z$.

All H atoms were positioned geometrically (C—H = 0.93–0.98 Å) and allowed to ride on their parent atoms, with U_{iso}(H) = $1.2U_{eq}$(parent atom).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003), *ORTEP-3* (Farrugia, 1997) and *ZORTEP* (Zsolnai, 1998); software used to prepare material for publication: *SHELXL97* and *PLATON*.

SMMS acknowledges the Council of Scientific and Industrial Research for financial support.

References

Beddoes, R. L., Dalton, L., Joule, J. A., Mills, O. S., Street, J. D. & Watt, C. I. F. (1986). *J. Chem. Soc. Perkin Trans.* 2, pp. 787–797.

De-Benedetti, P. G., Folli, U., Iarossi, D. & Frassineti, C. (1985). *J. Chem. Soc. Perkin Trans.* 2, pp. 1527–1532.

Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.

Gadaginamath, G. S. & Patil, S. A. (1999). *Ind. J. Chem. Sect. B*, **38**, 1070–1074.

Govindasamy, L., Velmurugan, D., Shanmuga Sundara Raj, S. & Fun, H.-K. (1999). *Acta Cryst.* C**55**, 1315–1317.

Krishnaiah, M., Narayana Raju, K. V., Lu, I.-L., Chen, Y.-S. & Narasinga Rao, S. (1995). *Acta Cryst.* C**51**, 2429–2430.

Okabe, N. & Adachi, Y. (1998). *Acta Cryst.* C**54**, 386–387.

Rodriguez, J. G., Temprano, F., Esteban-Calderon, C., Martinez-Ripoll, M. & Garcia-Blanco, S. (1985). *Tetrahedron*, **41**, 3813–3823.

Sankaranarayanan, R., Velmurugan, D., Raj, S. S. S., Fun, H.-K., Rao, S. N., Kannadasan, S. & Srinivasan, P. C. (2001). *Acta Cryst.* C**57**, 569–571.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

Siemens (1996). *SAINT* (Version 4) and *SMART*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

Wolf, W. M. (1999). *Acta Cryst.* C**55**, 469–472.

Yokum, T. S. & Fronczek, F. R. (1997). *Acta Cryst.* C**53**, 362–363.

Zsolnai, L. (1998). *ZORTEP*. University of Heidelberg, Germany.