Table 2. *Selected geometric parameters* (Å, °)

Br—C18	1.904 (5)	C6—C12	1.508 (7)
O1—C14	1.187 (6)	C7—C8	1.555 (7)
O2—C11	1.458 (5)	C8—C9	1.520 (7)
O2—C14	1.356 (6)	C8—C11	1.543 (7)
C1—C2	1.550 (7)	C9—C10	1.321 (8)
C1—C10	1.516 (7)	C12—C13	1.342 (7)
C1—C11	1.544 (7)	C14—C15	1.495 (7)
C2—C3	1.552 (7)	C15—C16	1.376 (7)
C2—C7	1.569 (7)	C15—C20	1.395 (7)
C3—C4	1.547 (7)	C16—C17	1.382 (7)
C3—C12	1.506 (7)	C17—C18	1.373 (7)
C4—C5	1.562 (8)	C18—C19	1.356 (7)
C5—C6	1.550 (8)	C19—C20	1.390 (7)
C6—C7	1.540 (7)		
C11—O2—C14	114.4 (4)	C8—C9—C10	108.8 (5)
C2—C1—C10	109.1 (4)	C1—C10—C9	107.7 (4)
C2—C1—C11	100.9 (4)	O2—C11—C1	109.7 (4)
C10—C1—C11	96.4 (4)	O2—C11—C8	114.8 (4)
C1—C2—C3	119.7 (4)	C1—C11—C8	94.8 (4)
C1—C2—C7	103.6 (4)	C3—C12—C6	98.2 (4)
C3—C2—C7	103.0 (4)	C3—C12—C13	130.9 (6)
C2—C3—C4	106.2 (4)	C6—C12—C13	129.9 (6)
C2—C3—C12	103.6 (4)	O1—C14—O2	123.5 (5)
C4—C3—C12	97.8 (4)	O1—C14—C15	125.4 (5)
C3—C4—C5	103.8 (4)	O2—C14—C15	111.2 (5)
C4—C5—C6	102.9 (4)	C14—C15—C16	122.8 (5)
C5—C6—C7	106.4 (4)	C14—C15—C20	117.4 (5)
C5—C6—C12	98.6 (4)	C16—C15—C20	119.8 (5)
C7—C6—C12	103.3 (4)	C15—C16—C17	120.0 (5)
C2—C7—C6	103.5 (4)	C16—C17—C18	119.0 (5)
C2—C7—C8	102.6 (4)	Br—C18—C17	118.4 (4)
C6—C7—C8	119.8 (4)	Br—C18—C19	118.9 (4)
C7—C8—C9	109.6 (4)	C17—C18—C19	122.7 (5)
C7—C8—C11	100.7 (4)	C18—C19—C20	118.3 (5)
C9—C8—C11	95.9 (4)	C15—C20—C19	120.2 (5)

The structure was solved and refined using the direct-methods package *SDP* (Frenz, 1978).

We thank the University Research Committee of the University of Utah for supporting this work.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates, least-squares-planes data, torsion angles and cell-packing diagram have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71466 (25 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: HH1064]

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2-[1-Phenylsulfonyl-2-(3,4,5-trimethoxyphenyl)vinyl]-3-(phenylthio)indole

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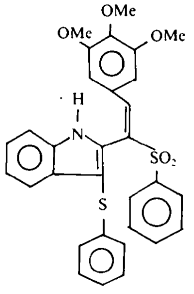
Abstract

The title molecule, $C_{31}H_{27}NO_5S_2$, consists of an indole ring with phenylthio, phenylsulfonyl and 3,4,5-methoxyphenyl groups as exocyclic substituents. All the ring systems are planar. The indole ring is slightly folded along the C(8)—C(9) bond.

Two of the three methoxy groups on the 2-(3,4,5-methoxyphenyl)vinyl substituent are slightly twisted from the molecular plane by 2.5 (9) and 13.9 (9)°, respectively, while the third occupies an equatorial position [79.3 (7)°]. Crystal cohesion is based on numerous van der Waals interactions.

Comment

The title compound (I) was chosen for X-ray study as part of our investigations of the stereochemistry of substituted indoles, many of which show interesting chemical and biological activities. Pharmacological studies of numerous indole derivatives have shown that most of them display anti-inflammatory (Rodriguez, Temprano, Estebancalderon, Martinez-Ripoll & Garciablanco, 1985) and antimicrobial (El-Sayed, Barnhart, Ammon & Wassel, 1986) properties.



(I)

The compound was synthesized by one of the authors (EVS) by the reductive condensation method (Sadanandan, Rajan, Seetharaman, Srinivasan & Usha, 1993). The crystals were grown from an aqueous solution of ethyl acetate by slow evaporation.

Fig. 1 shows a view of the molecular geometry and the numbering scheme adopted. The mean C_{sp^2}—C_{sp^2} bond length of 1.394 (5) Å agrees well with that observed in related compounds (Reimers, Guth & Wang, 1984; Chakraborty & Talapatra, 1986). The bond angles in all the six-membered rings have an average value of 120.1 (4)° but there are significant deviations among the individual values. In the indole ring system, the angles at C(7) and C(4) are contracted to 116.9 (5) and 117.2 (4)°, respectively, while those at C(8) and C(5) are expanded to 121.6 (4) and 121.9 (4)°, respectively. This would appear to be a real effect caused by the fusion of a smaller pyrrole ring to the six-membered phenyl ring system, the strain being taken up by angular distortion rather than by bond-length distortion (Allen & Trotter, 1970). Both the six-membered and the five-membered (pyrrole) parts of the indole ring are quite planar, and make a dihedral angle of 3.5 (1)° with each other, indicating that the indole ring is slightly folded along the C(8)—C(9) bond. The methoxy groups at C(3*b*) and C(5*b*) are slightly twisted from planarity with C(2*b*)—C(3*b*)—O(14)—C(17) = 2.5 (9)° and C(6*b*)—C(5*b*)—O(16)—C(19) = 13.9 (9)°, whereas the methoxy group at C(4*b*) occupies an equatorial position [C(3*b*)—C(4*b*)—O(15)—C(18) = 79.3 (7)°]. The dihedral angles between the indole ring system and the mean planes of the phenylthio, 3,4,5-trimethoxyphenyl and phenylsulfonyl rings are 108.4 (1), 97.5 (2) and 70.0 (1)°, respectively. The phenylthio and phenylsulfonyl rings are nearly parallel to each other, the dihedral angle between them being 6.9 (2)°. The packing gives rise to four significant intramolecular short contacts, indicative of possible C—H···O interactions. A stereoview of the molecular packing is shown in Fig. 2.

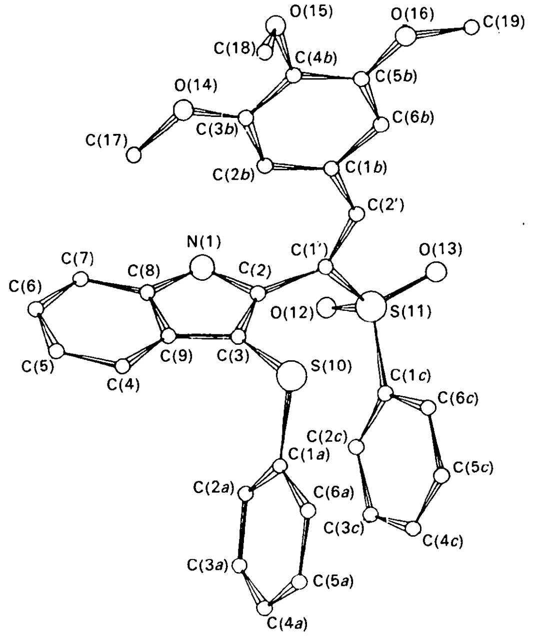


Fig. 1. *PLUTO* plot (Motherwell, 1976) of the molecular geometry and the numbering scheme adopted.

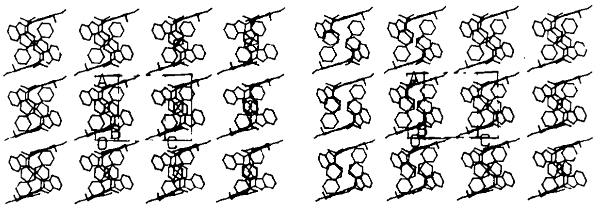


Fig. 2. Stereoview (Motherwell, 1976) of the molecular packing.

Experimental

Crystal data

$C_{31}H_{27}NO_5S_2$ D_x = 1.339 Mg m^{-3}
M_r = 557 D_m = 1.321 Mg m^{-3}

Triclinic
$P\bar{1}$
$a = 10.849$ (2) Å
$b = 11.311$ (2) Å
$c = 12.013$ (2) Å
$\alpha = 71.09$ (2)°
$\beta = 89.87$ (2)°
$\gamma = 82.28$ (2)°
$V = 1380.61$ Å^3
$Z = 2$

Cu $K\alpha$ radiation
$\lambda = 1.5418$ Å
Cell parameters from 20 reflections
$\theta = 20$–$30°$
$\mu = 1.94$ mm^{-1}
$T = 293$ K
Rectangular blocks
0.35 × 0.3 × 0.25 mm
Pale yellow

Data collection

Enraf-Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: empirical
$T_{\min} = 0.710$, $T_{\max} = 0.821$
4887 measured reflections
4624 independent reflections
4394 observed reflections [$I > 3\sigma(I)$]

$R_{\rm int} = 0.0073$
$\theta_{\max} = 65°$
$h = -12 \rightarrow 12$
$k = -12 \rightarrow 13$
$l = 0 \rightarrow 14$
2 standard reflections monitored every 100 reflections
intensity variation: <2%

Refinement

Refinement on F
$R = 0.046$
$wR = 0.065$
$S = 1.03$
4394 reflections
460 parameters
All H-atom parameters refined

$w = 1/[\sigma^2(F) + 0.011683F^2]$
$(\Delta/\sigma)_{\max} = 0.092$
$\Delta\rho_{\max} = 0.29$ e Å^{-3}
$\Delta\rho_{\min} = -0.38$ e Å^{-3}
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$$B_{\rm eq} = (8\pi^2/3)\Sigma_i\Sigma_jU_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$B_{\rm eq}$
N(1)	0.1929 (1)	1.2535 (1)	0.2765 (1)	3.50 (4)
C(2)	0.2632 (2)	1.1918 (2)	0.2100 (1)	3.21 (5)
C(3)	0.3785 (2)	1.2299 (2)	0.1982 (2)	3.46 (4)
C(4)	0.4672 (2)	1.4003 (2)	0.2642 (2)	5.07 (6)
C(5)	0.4330 (3)	1.4871 (2)	0.3210 (3)	6.15 (9)
C(6)	0.3174 (3)	1.4969 (2)	0.3698 (2)	6.04 (8)
C(7)	0.2299 (2)	1.4221 (2)	0.3631 (2)	5.02 (7)
C(8)	0.2617 (2)	1.3353 (2)	0.3031 (2)	3.84 (5)
C(9)	0.3787 (2)	1.3231 (2)	0.2550 (2)	3.78 (5)
S(10)	0.4951 (1)	1.1879 (1)	0.1120 (1)	4.38 (2)
S(11)	0.2019 (1)	0.9537 (1)	0.2316 (1)	3.41 (1)
O(12)	0.1441 (1)	0.8989 (1)	0.1562 (1)	4.66 (4)
O(13)	0.1475 (1)	0.9493 (1)	0.3416 (1)	4.72 (4)
O(14)	0.1466 (1)	1.6227 (1)	−0.0884 (1)	4.72 (5)
O(15)	0.0707 (1)	1.6388 (1)	−0.3067 (1)	3.84 (3)
O(16)	0.0515 (1)	1.4321 (1)	−0.3620 (1)	4.16 (4)
C(17)	0.1876 (3)	1.6182 (2)	0.0260 (2)	5.65 (7)
C(18)	0.1761 (2)	1.6955 (2)	−0.3581 (2)	4.94 (6)
C(19)	0.0086 (2)	1.3290 (2)	−0.3868 (2)	4.97 (7)
C(1′)	0.2081 (1)	1.1157 (2)	0.1498 (1)	3.16 (5)
C(2′)	0.1590 (2)	1.1575 (2)	0.0396 (2)	3.39 (4)
C(1*a*)	0.6188 (2)	1.1066 (2)	0.2158 (2)	4.10 (6)
C(2*a*)	0.6074 (2)	1.0678 (2)	0.3373 (2)	4.52 (6)
C(3*a*)	0.7119 (2)	1.0048 (2)	0.4110 (2)	5.75 (8)
C(4*a*)	0.8245 (2)	0.9823 (3)	0.3672 (4)	7.21 (12)
C(5*a*)	0.8355 (2)	1.0176 (3)	0.2471 (4)	6.97 (12)
C(6*a*)	0.7340 (2)	1.0795 (2)	0.1699 (3)	5.52 (8)
C(1*b*)	0.1423 (2)	1.2858 (2)	−0.0462 (1)	3.43 (5)
C(2*b*)	0.1594 (2)	1.3944 (2)	−0.0194 (2)	3.70 (5)
C(3*b*)	0.1366 (2)	1.5126 (2)	−0.1066 (2)	3.56 (5)
C(4*b*)	0.1000 (2)	1.5222 (2)	−0.2210 (1)	3.32 (5)
C(5*b*)	0.0849 (1)	1.4135 (2)	−0.2477 (1)	3.25 (5)
C(6*b*)	0.1043 (2)	1.2957 (2)	−0.1608 (2)	3.42 (1)
C(1*c*)	0.3583 (2)	0.8826 (2)	0.2617 (1)	3.31 (1)
C(2*c*)	0.4034 (2)	0.8324 (2)	0.3775 (2)	3.96 (5)
C(3*c*)	0.5254 (2)	0.7714 (2)	0.4011 (2)	4.78 (6)
C(4*c*)	0.5997 (2)	0.7620 (2)	0.3097 (2)	5.01 (7)
C(5*c*)	0.5539 (2)	0.8110 (2)	0.1957 (2)	5.44 (8)
C(6*c*)	0.4327 (2)	0.8730 (2)	0.1697 (2)	4.72 (6)

Table 2. *Selected geometric parameters* (Å, °)

N(1)—C(2)	1.387 (3)	O(16)—C(5*b*)	1.362 (2)
N(1)—C(8)	1.376 (3)	C(1′)—C(2′)	1.338 (3)
C(2)—C(3)	1.369 (4)	C(2′)—C(1*b*)	1.470 (3)
C(2)—C(1′)	1.471 (3)	C(1*a*)—C(2*a*)	1.392 (3)
C(3)—C(9)	1.430 (4)	C(1*a*)—C(6*a*)	1.401 (4)
C(3)—S(10)	1.746 (3)	C(2*a*)—C(3*a*)	1.398 (4)
C(4)—C(5)	1.379 (4)	C(3*a*)—C(4*a*)	1.354 (4)
C(4)—C(9)	1.409 (4)	C(4*a*)—C(5*a*)	1.376 (7)
C(5)—C(6)	1.389 (5)	C(5*a*)—C(6*a*)	1.393 (4)
C(6)—C(7)	1.373 (4)	C(1*b*)—C(2*b*)	1.402 (4)
C(7)—C(8)	1.403 (4)	C(1*b*)—C(6*b*)	1.403 (3)
C(8)—C(9)	1.402 (3)	C(2*b*)—C(3*b*)	1.397 (3)
S(10)—C(1*a*)	1.770 (3)	C(3*b*)—C(4*b*)	1.397 (3)
S(11)—O(12)	1.438 (2)	C(4*b*)—C(5*b*)	1.397 (3)
S(11)—O(13)	1.435 (1)	C(5*b*)—C(6*b*)	1.391 (3)
S(11)—C(1′)	1.787 (2)	C(1*c*)—C(2*c*)	1.383 (3)
S(11)—C(1*c*)	1.762 (3)	C(1*c*)—C(6*c*)	1.391 (3)
O(14)—C(17)	1.428 (3)	C(2*c*)—C(3*c*)	1.392 (4)
O(14)—C(3*b*)	1.350 (3)	C(3*c*)—C(4*c*)	1.384 (3)
O(15)—C(18)	1.427 (3)	C(4*c*)—C(5*c*)	1.366 (3)
O(15)—C(4*b*)	1.382 (2)	C(5*c*)—C(6*c*)	1.389 (4)
O(16)—C(19)	1.427 (3)		
C(8)—N(1)—C(2)	109.0 (4)	C(4*a*)—C(5*a*)—C(6*a*)	121.3 (6)
N(1)—C(2)—C(3)	108.8 (2)	C(1*a*)—C(6*a*)—C(5*a*)	119.2 (4)
C(2)—C(3)—C(9)	107.4 (5)	C(2*b*)—C(1*b*)—C(6*b*)	120.1 (2)
C(5)—C(4)—C(9)	117.2 (4)	C(1*b*)—C(2*b*)—C(3*b*)	119.8 (2)
C(4)—C(5)—C(6)	121.9 (4)	C(2*b*)—C(3*b*)—C(4*b*)	120.1 (3)
C(5)—C(6)—C(7)	122.1 (3)	C(3*b*)—C(4*b*)—C(5*b*)	119.9 (2)
C(6)—C(7)—C(8)	116.9 (5)	C(4*b*)—C(5*b*)—C(6*b*)	120.5 (2)
C(7)—C(8)—C(9)	121.6 (4)	C(1*b*)—C(6*b*)—C(5*b*)	119.7 (2)
C(4)—C(9)—C(8)	120.3 (3)	C(2*c*)—C(1*c*)—C(6*c*)	121.1 (3)
C(3)—C(9)—C(8)	106.9 (4)	C(1*c*)—C(2*c*)—C(3*c*)	118.8 (3)
C(3)—C(9)—C(4)	132.7 (4)	C(2*c*)—C(3*c*)—C(4*c*)	120.2 (3)
C(2*a*)—C(1*a*)—C(6*a*)	119.4 (4)	C(3*c*)—C(4*c*)—C(5*c*)	120.5 (4)
C(1*a*)—C(2*a*)—C(3*a*)	119.2 (4)	C(4*c*)—C(5*c*)—C(6*c*)	120.5 (3)
C(2*a*)—C(3*a*)—C(4*a*)	121.7 (3)	C(1*c*)—C(6*c*)—C(5*c*)	118.9 (2)
C(3*a*)—C(4*a*)—C(5*a*)	119.3 (6)		

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C(18)—H(18*c*)···O(14)	1.09 (3)	2.61 (3)	3.101 (3)	106
C(2′)—H(2′)···O(12)	1.03 (3)	2.34 (2)	2.831 (2)	106
C(2*c*)—H(2*c*)···O(13)	1.06 (3)	2.36 (2)	2.880 (5)	108
C(6*c*)—H(6*c*)···O(12)	1.06 (2)	2.77 (2)	3.105 (3)	97

Cell refinement and data reduction: *SDP* (Frenz, 1978). Program used to solve structure: *SHELXS*86 (Sheldrick, 1985). Program used to refine structure: *SHELX*76 (Sheldrick, 1976). Software used to prepare material for publication: *PARST* (Nardell, 1983) and *PLUTO* (Motherwell, 1976).

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and bond distances, bond angles and least-squares-planes data have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71653 (29 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: AB1073]

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[2-(3,4-Methylenedioxyphenyl)-1-(phenylsulfonyl)vinyl]-3-(phenylthio)indole

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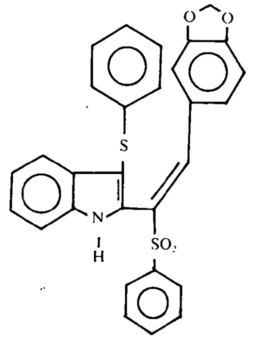
Abstract

The dioxole ring of the title compound, $C_{29}H_{21}NO_4S_2$, is inclined at an angle of 67.9 (2)° to the indole ring system. The phenyl rings of the phenylsulfonyl and phenylthio substituents are almost perpendicular to each other [73.3 (2)°], while the phenylthio and the phenyl ring of the methylenedioxyphenyl ring system are almost parallel to each other [8.2 (2)°]. The indole ring system is slightly folded along the central C—C bond (2.1°). All the rings are quite planar. The molecules are linked by N—H···O-type hydrogen bonds.

Comment

2-Vinylindole and its various substituted products have long been known for their interesting chemical and biological activities. Compounds of this class are reported to exhibit antimicrobial (El-Sayed, Barnhart, Ammon & Wassel, 1986) and anti-inflammatory activities (Rodriguez, Temprano, Estebancalderon, Martinez-Ripoll & Garciablanco, 1985). The present study constitutes part of a series of studies on the structure and conformation of substituted indoles, which has been undertaken in order to correlate chemical structure and biological activity.

The bond parameters of the title compound (I) have expected values. The bond angles in all the six-membered rings have an average value of 120.01 (1)° but there are significant deviations among the individual values. In the indole ring system, the angles at C(7) and C(4) are contracted to 117.7 (4) and 118.0 (4)°, respectively, while those at C(8) and C(5) are expanded to 121.9 (4) and 121.2 (4)°, respectively. This would appear to be a real effect caused by the fusion of a smaller pyrrole ring to the six-membered phenyl ring, the strain being taken up by angular distortion rather than bond-length distortion. This effect has been observed by Allen & Trotter (1970). The same effect is also observed in the methylenedioxyphenyl part of the molecule [angles at C(2*b*) and C(5*b*) are contracted to 117.0 (4) and 116.9 (4)°, respectively, whereas those at C(3*b*) and C(6*b*) are expanded to 122.9 (4) and 122.4 (4)°, respectively] because of the fusion of the phenyl ring with the dioxole ring. The sum of the angles around C(1′) is 359.6°. It has been found that the indole system is nearly planar ($\chi^2 = 12.6$°) (Chakraborty & Talapatra, 1986) with a maximum deviation for C(9) (0.025 Å) from the mean plane containing atoms N(1) and C(2)–C(9). The dihedral angles between the indole ring system and the mean planes of the phenylthio phenyl ring, the methylenedioxy phenyl



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