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2,2′-(Oxydimethylene)bis[3-bromo-1-(phenylsulfonyl)-1*H*-indole]

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In the title compound, $C_{30}H_{22}Br_2N_2O_5S_2$, the sulfonyl-bound phenyl ring makes a dihedral angle of 84.28 (11)° with the indole ring system. A crystallographic twofold rotation axis passes through the central O atom. The molecules are linked into a chain along the *b* axis by π–π interactions.

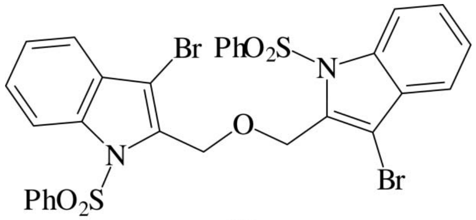
Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.005 Å
R factor = 0.054
wR factor = 0.155
Data-to-parameter ratio = 25.5

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

Comment

Polyhalogenated indole derivatives exhibit marked antimicrobial activities against Gram-positive and Gram-negative bacteria and fungi (Piscopo, Diurno, Mazzoni, Ciaccio & Veneruso, 1990; Piscopo, Diurno, Mazzoni & Ciaccio, 1990). The title compound, (I), exhibits a more potent activity against *Staphylococcus aureus*, *Bacillus subtilis*, *Escherichia coli* and *Salmonella typhi* pathogens; its activity is comparable with those observed for the antibiotics penicillin, bacitracin, streptomycin, vancomycin and rifampicin (Senthil Kumar, Chinnakali, Balagurunathan *et al.*, 2006). As part of our investigations of indole derivatives, we have undertaken the X-ray crystal structure analysis of the title compound, (I).



(I)

The molecule of (I) is located on a twofold rotation axis (Fig. 1), which passes through atom O3. The geometry of the phenylsulfonylindole system agrees with those reported for similar structures (Beddoes *et al.*, 1986; Ravishankar *et al.*, 2005; Senthil Kumar, Chinnakali, Ramesh *et al.*, 2006). The indole ring system is planar, with a maximum deviation of 0.022 (2) Å for atom C2. The dihedral angle between the sulfonyl-bound phenyl ring and the indole ring system is 84.28 (11)°. The two symmetry-related indole ring systems in the molecule form a dihedral angle of 57.30 (4)°. The plane of the C—O—C linkage is twisted by an angle of 83.61 (10)° with respect to the indole ring system.

Intramolecular C—H···O interactions (Table 1) involving the sulfonyl atoms O1 and O2 generate rings of graph-set motifs $S(5)$ and $S(6)$ (Bernstein *et al.*, 1995). In the crystal structure, molecules are linked into a chain along the *b* axis (Fig. 2) by π–π interactions between the benzene (centroid *Cg*1) and pyrrole (centroid *Cg*2) rings of the indole unit, with a

$Cg1\cdots Cg2^{ii}$ distance of 3.6047 (19) Å [symmetry code: (ii) $\frac{1}{2} - x, 1 - y, z$].

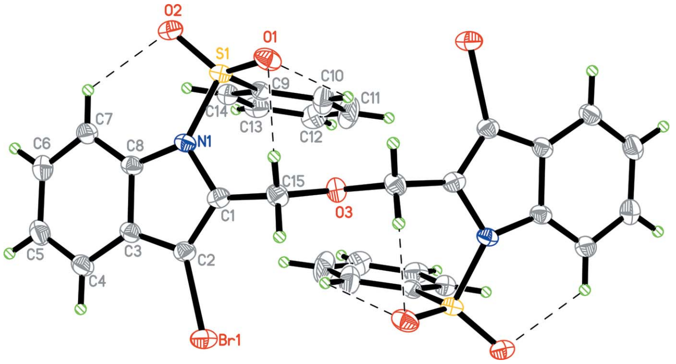


Figure 1
The molecular structure of (I). Displacement ellipsoids are drawn at the 80% probability level. Unlabelled atoms are related to labelled atoms by the symmetry operation ($x, \frac{1}{2} - y, \frac{1}{2} - z$). Hydrogen bonds are shown as dashed lines.

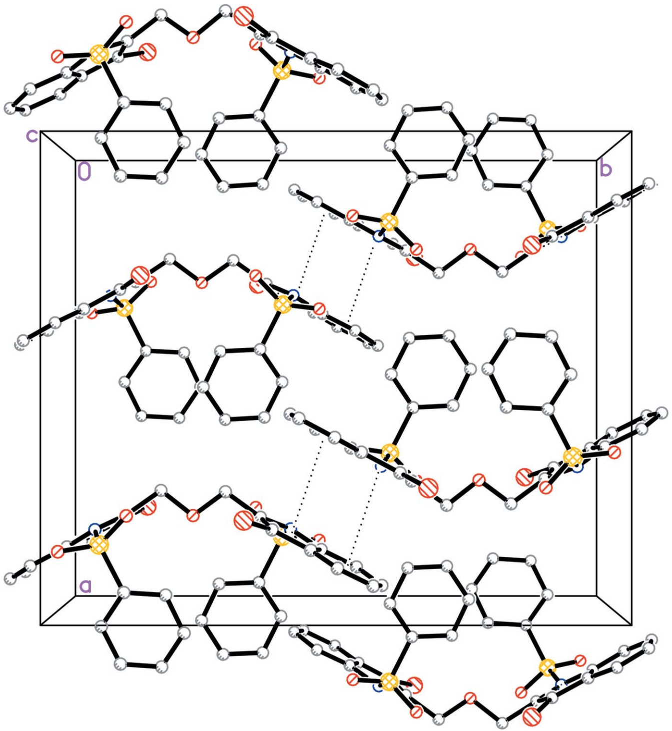


Figure 2
A packing diagram for (I), viewed down the *c* axis, showing the π–π interactions (dotted lines). H atoms have been omitted.

Experimental

1-Phenylsulfonyl-3-bromo-2-hydroxymethylindole (1.37 mmol), K_2CO_3 (3.42 mmol) and 1-phenylsulfonyl-3-bromo-2-bromomethylindole (1.37 mmol) in CH_3CN (20 ml) were refluxed for 2 h. The reaction mixture was then quenched with water containing HCl (1 ml) and extracted with ethyl acetate. The organic layer was washed with water (2 × 10 ml) and dried over Na_2SO_4. The crude product was purified by column chromatography with hexane–ethyl acetate (9:1 *v*/*v*) to give (I) as a white crystalline product. The compound was further recrystallized from a hexane–ethyl acetate (99:1 *v*/*v*) solution.

Crystal data

$C_{30}H_{22}Br_2N_2O_5S_2$
M_r = 714.44
Orthorhombic, *Pnna*
a = 16.0538 (2) Å
b = 19.2295 (2) Å
c = 9.0482 (1) Å
V = 2793.24 (5) Å^3
Z = 4
D_x = 1.699 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 3.10 mm^{-1}
T = 100.0 (1) K
Plate, colourless
0.33 × 0.21 × 0.05 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{\min}$ = 0.429, $T_{\max}$ = 0.866
54115 measured reflections
4751 independent reflections
3348 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.072
$\theta_{\max}$ = 31.7°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.155
S = 1.05
4751 reflections
186 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0728P)^2 + 7.3085P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max}$ = 0.001
$\Delta\rho_{\max}$ = 3.13 e Å^{-3}
$\Delta\rho_{\min}$ = −0.92 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C7—H7$\cdots$O2	0.95	2.33	2.926 (4)	120
C10—H10$\cdots$O1	0.95	2.55	2.923 (5)	103
C15—H15*A*$\cdots$O1	0.99	2.39	2.867 (4)	109

H atoms were positioned geometrically, with C—H = 0.95–0.99 Å, and treated as riding, with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C). The highest unassigned peak in the difference map is located 0.97 and 1.89 Å from atoms H6 and C6, respectively. Attempts to assign this peak as a partial-occupancy Br atom attached to C6 resulted in an occupancy of 0.04. Since this may not make chemical sense, the original model was retained.

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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