Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-(4-Methoxybenzyl)-3-methyl-1-phenylsulfonyl-1*H*-indole

M. Balasubramanian,[a] Pon. Sathya Moorthy,[a] V. Dhayalan,[b] A. K. Mohanakrishnan[b] and M. N. Ponnuswamy[a]*

[a]Centre of Advanced Study in Crystallography and Biophysics, University of Madras, Guindy Campus, Chennai 600 025, India, and [b]Department of Organic Chemistry, University of Madras, Guindy Campus, Chennai 600 025, India
Correspondence e-mail: mnpsy2004@yahoo.com

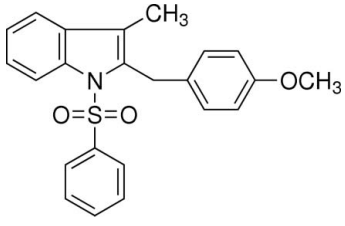
Received 11 September 2007; accepted 15 September 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.041; wR factor = 0.126; data-to-parameter ratio = 21.4.

In the title compound, $C_{23}H_{21}NO_3S$, the planar indole ring system is oriented at an angle of 77.7 (1)° to the sulfonyl-bound benzene ring and 80.1 (1)° to the methoxyphenyl group. The molecular structure is stabilized by intramolecular C—H···O interactions. In addition to van der Waals forces, the molecular packing is controlled by a weak C—H···π interaction.

Related literature

For related literature, see: Harris & Uhle (1960); Ho *et al.* (1986); Karali *et al.* (2007); Palani *et al.* (2006*a*,*b*); Ragno *et al.* (2006); Stevenson *et al.* (2000).



Experimental

Crystal data

$C_{23}H_{21}NO_3S$
M_r = 391.47
Triclinic, $P\overline{1}$
a = 8.2518 (3) Å
b = 10.0817 (4) Å
c = 12.8169 (5) Å
α = 97.244 (2)°
β = 97.876 (2)°
γ = 105.709 (2)°
V = 1001.76 (7) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.19 mm^{-1}
T = 293 (2) K
0.24 × 0.20 × 0.18 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: none
23750 measured reflections
5432 independent reflections
4234 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.126
S = 1.04
5432 reflections
254 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

Cg is the centroid of the C16–C21 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···O1	0.93	2.39	2.970 (2)	120
C15—H15*B*···O2	0.97	2.28	2.883 (2)	119
C21—H21···O2	0.93	2.56	3.127 (2)	120
C13—H13···Cg^{i}	0.93	2.77	3.527 (2)	139

Symmetry code: (i) $x+1, y, z$.

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: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PARST* (Nardelli, 1995).

MB thanks the University Grants Commision (UGC) for providing a Project Fellowship.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2208).

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  doi:10.1107/S1600536807045369

supplementary materials

Acta Cryst. (2007). E**63**, o4134 [**doi:10.1107/S1600536807045369**]

2-(4-Methoxybenzyl)-3-methyl-1-phenylsulfonyl-1*H*-indole

M. Balasubramanian, P. S. Moorthy, V. Dhayalan, A. K. Mohanakrishnan and M. N. Ponnuswamy

Comment

Indole compounds are used as bioactive drugs (Stevenson *et al.*, 2000). The indole derivatives exhibit antituberculosis (Karali *et al.*, 2007), anti-HIV (Ragno *et al.*, 2006), central nervous system depressant and muscle relaxant properties (Harris & Uhle, 1960; Ho *et al.*, 1986). Herein, we report the crystal structure of the title compound, (I).

In the molecule, the planar sulfonyl bound phenyl group subtends an angle of 77.7 (1)° with the planar indole moiety. The methyl atom is deviated from the indole ring by 0.075 (3) Å. The bond lengths and bond angles in the molecule are comparable with the values reported in literature (Palani *et al.*, 2006*a*,b). The methoxy group also lies in the plane of the benzyl ring. The methoxybenzyl group is oriented at angle of 80.1 (1)° with respect to the indole moiety. The geometry around S1 is distorted from tetrahedral values. The widening of the angle (O1—S1—O2=) 119.46 (8)° and narrowing of the angle (N1—S1—C9=) 105.19 (6)° are due to the electon withdrawing character of the phenyl sulfonyl group. The sum of the bond angle around N1 indicates that the atom is in an sp^2 hybridized state.

A few C—H···O intramolecular interactions play the role to stabilize the molecules in addition to a C—H···π interaction (Table 1). The molecules in the unit cell are packed by van der Waals forces.

Experimental

1-Phenylsulfonyl-3-methyl-2-bromomethylindole (2 g, 5.49 mmol) was dissolved in dry CH_3CN (20 ml). To this anisole (0.89 ml, 8.23 mmol), $ZnBr_2$ (2.47 g, 10.96 mmol) were added and refluxed for 24 h. The reaction mixture was quenched with ice containing few drops of conc. HCl, extracted with $CHCl_3$ (3 × 5 ml) and dried Na_2SO_4. The solvent was removed under vacuo. Then crude was recrystallized from 5% ethyl acetate / hexane (5:95) to get the diffraction quality crystals.

Refinement

The H atoms were positioned geometrically and were treated as riding on their parent C atoms, with C—H distances of 0.93–0.98 Å, and with U_{iso}= 1.5U_{eq}(C) for methyl H and 1.2U_{eq}(C) for other H.

Figures

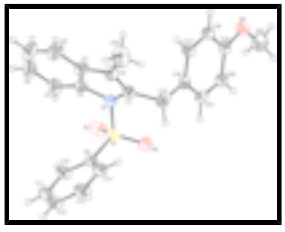

Fig. 1. The molecular structure of (I), with 30% probability displacement ellipsoids.

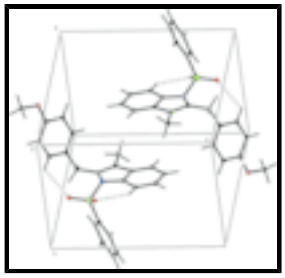

Fig. 2. The molecular packing of (I), viewed approximately along the *a* axis. Dashed lines indicate C—H···O hydrogen bonds.

2-(4-Methoxybenzyl)-3-methyl-1-phenylsulfonyl-1*H*-indole

Crystal data

$C_{23}H_{21}NO_3S$	$Z = 2$
$M_r = 391.47$	$F_{000} = 412$
Triclinic, $P\bar{1}$	$D_x = 1.298$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.2518$ (3) Å	Cell parameters from 14224 reflections
$b = 10.0817$ (4) Å	$\theta = 2.0$–27.5º
$c = 12.8169$ (5) Å	$\mu = 0.19$ mm^{-1}
$\alpha = 97.244$ (2)º	$T = 293$ (2) K
$\beta = 97.876$ (2)º	Needle, colourless
$\gamma = 105.709$ (2)º	0.24 × 0.20 × 0.18 mm
$V = 1001.76$ (7) Å^3	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	4234 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.024$
Monochromator: graphite	$\theta_{max} = 29.2$º
$T = 293(2)$ K	$\theta_{min} = 1.6$º
ω scans	$h = -11 \rightarrow 11$
Absorption correction: none	$k = -13 \rightarrow 13$
23750 measured reflections	$l = -17 \rightarrow 17$
5432 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.041$	H-atom parameters constrained
$wR(F^2) = 0.126$	$w = 1/[\sigma^2(F_o^2) + (0.0596P)^2 + 0.1977P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} < 0.001$

5432 reflections	$\Delta\rho_{max} = 0.26$ e Å^{-3}
254 parameters	$\Delta\rho_{min} = -0.26$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.36424 (4)	0.91092 (4)	0.76283 (3)	0.05054 (12)
N1	0.37371 (14)	0.75504 (11)	0.70911 (9)	0.0427 (2)
O1	0.46782 (14)	1.00993 (11)	0.71146 (12)	0.0716 (4)
O2	0.40232 (17)	0.92234 (13)	0.87515 (10)	0.0754 (4)
O3	1.06112 (15)	0.70612 (13)	1.03001 (10)	0.0685 (3)
C1	0.32438 (17)	0.63013 (14)	0.75472 (11)	0.0463 (3)
C2	0.2657 (2)	0.51995 (16)	0.67479 (14)	0.0604 (4)
C3	0.2704 (2)	0.56945 (17)	0.57476 (13)	0.0593 (4)
C4	0.33517 (17)	0.71415 (15)	0.59622 (11)	0.0469 (3)
C5	0.3562 (2)	0.7930 (2)	0.51567 (14)	0.0644 (4)
H5	0.3989	0.8900	0.5307	0.077*
C6	0.3111 (3)	0.7213 (3)	0.41179 (16)	0.0882 (7)
H6	0.3242	0.7712	0.3557	0.106*
C7	0.2472 (4)	0.5779 (3)	0.38937 (17)	0.1049 (8)
H7	0.2180	0.5329	0.3186	0.126*
C8	0.2258 (3)	0.5004 (2)	0.46920 (17)	0.0933 (7)
H8	0.1823	0.4035	0.4534	0.112*
C9	0.15053 (16)	0.90762 (13)	0.72524 (11)	0.0431 (3)
C10	0.1117 (2)	0.99273 (17)	0.65585 (14)	0.0581 (4)
H10	0.1972	1.0499	0.6275	0.070*
C11	−0.0566 (2)	0.9916 (2)	0.62901 (15)	0.0691 (5)
H11	−0.0848	1.0496	0.5831	0.083*
C12	−0.1822 (2)	0.9055 (2)	0.66976 (15)	0.0659 (4)
H12	−0.2955	0.9041	0.6504	0.079*
C13	−0.1415 (2)	0.8215 (2)	0.73890 (16)	0.0681 (5)
H13	−0.2274	0.7637	0.7666	0.082*
C14	0.0248 (2)	0.82196 (18)	0.76742 (14)	0.0585 (4)
H14	0.0526	0.7653	0.8146	0.070*

C15	0.35876 (19)	0.62830 (19)	0.87222 (12)	0.0560 (4)
H15A	0.2936	0.5385	0.8858	0.067*
H15B	0.3190	0.6998	0.9095	0.067*
C16	0.54654 (18)	0.65305 (16)	0.91723 (10)	0.0475 (3)
C17	0.6286 (2)	0.55505 (15)	0.88721 (12)	0.0515 (3)
H17	0.5673	0.4739	0.8394	0.062*
C18	0.7990 (2)	0.57510 (15)	0.92664 (12)	0.0534 (3)
H18	0.8513	0.5078	0.9053	0.064*
C19	0.89245 (19)	0.69517 (15)	0.99790 (11)	0.0491 (3)
C20	0.8126 (2)	0.79269 (17)	1.03037 (12)	0.0586 (4)
H20	0.8734	0.8730	1.0792	0.070*
C21	0.6407 (2)	0.77048 (18)	0.98990 (12)	0.0586 (4)
H21	0.5876	0.8367	1.0125	0.070*
C22	1.1655 (3)	0.8269 (2)	1.10098 (18)	0.0878 (6)
H22A	1.2799	0.8202	1.1164	0.132*
H22B	1.1209	0.8347	1.1661	0.132*
H22C	1.1667	0.9080	1.0687	0.132*
C23	0.2103 (4)	0.3676 (2)	0.6834 (2)	0.1025 (8)
H23A	0.2918	0.3238	0.6598	0.154*
H23B	0.0999	0.3233	0.6395	0.154*
H23C	0.2038	0.3582	0.7565	0.154*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.04216 (18)	0.04139 (19)	0.0631 (2)	0.01361 (14)	−0.00070 (15)	−0.00118 (15)
N1	0.0429 (5)	0.0413 (6)	0.0453 (6)	0.0153 (4)	0.0078 (4)	0.0064 (4)
O1	0.0431 (5)	0.0430 (6)	0.1228 (11)	0.0036 (4)	0.0136 (6)	0.0136 (6)
O2	0.0846 (8)	0.0748 (8)	0.0606 (7)	0.0414 (7)	−0.0173 (6)	−0.0175 (6)
O3	0.0590 (6)	0.0716 (8)	0.0720 (7)	0.0274 (6)	−0.0035 (5)	0.0002 (6)
C1	0.0425 (6)	0.0470 (7)	0.0518 (7)	0.0139 (6)	0.0107 (5)	0.0135 (6)
C2	0.0661 (9)	0.0444 (8)	0.0640 (9)	0.0080 (7)	0.0052 (7)	0.0098 (7)
C3	0.0663 (9)	0.0534 (9)	0.0530 (8)	0.0158 (7)	0.0042 (7)	0.0011 (7)
C4	0.0427 (6)	0.0529 (8)	0.0463 (7)	0.0164 (6)	0.0079 (5)	0.0086 (6)
C5	0.0602 (9)	0.0751 (11)	0.0613 (9)	0.0189 (8)	0.0116 (7)	0.0257 (8)
C6	0.0914 (14)	0.125 (2)	0.0543 (10)	0.0340 (14)	0.0154 (10)	0.0323 (12)
C7	0.135 (2)	0.124 (2)	0.0474 (10)	0.0387 (18)	0.0052 (12)	−0.0045 (12)
C8	0.126 (2)	0.0763 (13)	0.0622 (11)	0.0247 (13)	−0.0018 (12)	−0.0128 (10)
C9	0.0411 (6)	0.0407 (6)	0.0489 (7)	0.0153 (5)	0.0091 (5)	0.0052 (5)
C10	0.0521 (8)	0.0566 (9)	0.0760 (10)	0.0221 (7)	0.0195 (7)	0.0271 (8)
C11	0.0643 (10)	0.0824 (12)	0.0777 (11)	0.0404 (9)	0.0148 (8)	0.0316 (10)
C12	0.0450 (8)	0.0816 (12)	0.0772 (11)	0.0286 (8)	0.0134 (7)	0.0108 (9)
C13	0.0506 (8)	0.0762 (11)	0.0874 (13)	0.0206 (8)	0.0307 (8)	0.0260 (10)
C14	0.0575 (8)	0.0640 (9)	0.0662 (9)	0.0255 (7)	0.0231 (7)	0.0261 (8)
C15	0.0530 (8)	0.0702 (10)	0.0513 (8)	0.0207 (7)	0.0167 (6)	0.0205 (7)
C16	0.0545 (7)	0.0562 (8)	0.0395 (6)	0.0218 (6)	0.0143 (6)	0.0173 (6)
C17	0.0616 (8)	0.0437 (7)	0.0499 (7)	0.0166 (6)	0.0080 (6)	0.0101 (6)
C18	0.0655 (9)	0.0476 (7)	0.0538 (8)	0.0277 (7)	0.0092 (7)	0.0102 (6)

C19	0.0566 (8)	0.0526 (8)	0.0424 (7)	0.0226 (6)	0.0066 (6)	0.0126 (6)
C20	0.0703 (10)	0.0580 (9)	0.0466 (7)	0.0276 (8)	−0.0002 (7)	−0.0024 (6)
C21	0.0705 (10)	0.0664 (10)	0.0467 (7)	0.0372 (8)	0.0092 (7)	0.0012 (7)
C22	0.0695 (12)	0.0920 (15)	0.0846 (13)	0.0189 (11)	−0.0098 (10)	−0.0116 (11)
C23	0.130 (2)	0.0469 (10)	0.1088 (18)	−0.0001 (11)	−0.0013 (15)	0.0169 (11)

Geometric parameters (Å, °)

S1—O2	1.4139 (13)	C11—C12	1.370 (3)
S1—O1	1.4208 (13)	C11—H11	0.9300
S1—N1	1.6607 (11)	C12—C13	1.370 (3)
S1—C9	1.7534 (13)	C12—H12	0.9300
N1—C4	1.4202 (17)	C13—C14	1.370 (2)
N1—C1	1.4376 (17)	C13—H13	0.9300
O3—C19	1.3664 (18)	C14—H14	0.9300
O3—C22	1.411 (2)	C15—C16	1.518 (2)
C1—C2	1.343 (2)	C15—H15A	0.9700
C1—C15	1.497 (2)	C15—H15B	0.9700
C2—C3	1.435 (2)	C16—C21	1.378 (2)
C2—C23	1.502 (2)	C16—C17	1.386 (2)
C3—C4	1.388 (2)	C17—C18	1.378 (2)
C3—C8	1.392 (2)	C17—H17	0.9300
C4—C5	1.382 (2)	C18—C19	1.384 (2)
C5—C6	1.382 (3)	C18—H18	0.9300
C5—H5	0.9300	C19—C20	1.378 (2)
C6—C7	1.375 (4)	C20—C21	1.389 (2)
C6—H6	0.9300	C20—H20	0.9300
C7—C8	1.366 (3)	C21—H21	0.9300
C7—H7	0.9300	C22—H22A	0.9600
C8—H8	0.9300	C22—H22B	0.9600
C9—C10	1.376 (2)	C22—H22C	0.9600
C9—C14	1.378 (2)	C23—H23A	0.9600
C10—C11	1.381 (2)	C23—H23B	0.9600
C10—H10	0.9300	C23—H23C	0.9600
O2—S1—O1	119.46 (8)	C11—C12—H12	119.9
O2—S1—N1	107.52 (7)	C13—C12—H12	119.9
O1—S1—N1	106.30 (7)	C14—C13—C12	120.39 (15)
O2—S1—C9	109.12 (7)	C14—C13—H13	119.8
O1—S1—C9	108.34 (7)	C12—C13—H13	119.8
N1—S1—C9	105.19 (6)	C13—C14—C9	119.12 (14)
C4—N1—C1	107.26 (11)	C13—C14—H14	120.4
C4—N1—S1	119.34 (9)	C9—C14—H14	120.4
C1—N1—S1	124.73 (9)	C1—C15—C16	113.44 (12)
C19—O3—C22	118.68 (14)	C1—C15—H15A	108.9
C2—C1—N1	108.44 (12)	C16—C15—H15A	108.9
C2—C1—C15	127.66 (14)	C1—C15—H15B	108.9
N1—C1—C15	123.39 (13)	C16—C15—H15B	108.9
C1—C2—C3	108.85 (14)	H15A—C15—H15B	107.7
C1—C2—C23	127.78 (17)	C21—C16—C17	117.55 (14)

C3—C2—C23	123.32 (17)	C21—C16—C15	122.13 (13)
C4—C3—C8	119.54 (17)	C17—C16—C15	120.31 (14)
C4—C3—C2	108.13 (14)	C18—C17—C16	121.48 (14)
C8—C3—C2	132.33 (18)	C18—C17—H17	119.3
C5—C4—C3	122.00 (15)	C16—C17—H17	119.3
C5—C4—N1	130.70 (15)	C17—C18—C19	120.15 (13)
C3—C4—N1	107.29 (12)	C17—C18—H18	119.9
C4—C5—C6	117.04 (19)	C19—C18—H18	119.9
C4—C5—H5	121.5	O3—C19—C20	125.29 (14)
C6—C5—H5	121.5	O3—C19—C18	115.38 (13)
C7—C6—C5	121.58 (19)	C20—C19—C18	119.33 (14)
C7—C6—H6	119.2	C19—C20—C21	119.66 (14)
C5—C6—H6	119.2	C19—C20—H20	120.2
C8—C7—C6	121.2 (2)	C21—C20—H20	120.2
C8—C7—H7	119.4	C16—C21—C20	121.81 (14)
C6—C7—H7	119.4	C16—C21—H21	119.1
C7—C8—C3	118.6 (2)	C20—C21—H21	119.1
C7—C8—H8	120.7	O3—C22—H22A	109.5
C3—C8—H8	120.7	O3—C22—H22B	109.5
C10—C9—C14	121.16 (13)	H22A—C22—H22B	109.5
C10—C9—S1	119.39 (11)	O3—C22—H22C	109.5
C14—C9—S1	119.44 (11)	H22A—C22—H22C	109.5
C9—C10—C11	118.78 (15)	H22B—C22—H22C	109.5
C9—C10—H10	120.6	C2—C23—H23A	109.5
C11—C10—H10	120.6	C2—C23—H23B	109.5
C12—C11—C10	120.27 (15)	H23A—C23—H23B	109.5
C12—C11—H11	119.9	C2—C23—H23C	109.5
C10—C11—H11	119.9	H23A—C23—H23C	109.5
C11—C12—C13	120.28 (15)	H23B—C23—H23C	109.5
O2—S1—N1—C4	178.01 (11)	C2—C3—C8—C7	−179.2 (2)
O1—S1—N1—C4	−52.97 (12)	O2—S1—C9—C10	132.11 (13)
C9—S1—N1—C4	61.81 (11)	O1—S1—C9—C10	0.56 (15)
O2—S1—N1—C1	34.54 (13)	N1—S1—C9—C10	−112.79 (13)
O1—S1—N1—C1	163.56 (11)	O2—S1—C9—C14	−46.57 (14)
C9—S1—N1—C1	−81.67 (11)	O1—S1—C9—C14	−178.11 (12)
C4—N1—C1—C2	2.16 (15)	N1—S1—C9—C14	68.54 (13)
S1—N1—C1—C2	149.25 (12)	C14—C9—C10—C11	0.2 (2)
C4—N1—C1—C15	174.49 (12)	S1—C9—C10—C11	−178.41 (13)
S1—N1—C1—C15	−38.42 (17)	C9—C10—C11—C12	−1.0 (3)
N1—C1—C2—C3	−1.54 (18)	C10—C11—C12—C13	1.1 (3)
C15—C1—C2—C3	−173.45 (14)	C11—C12—C13—C14	−0.4 (3)
N1—C1—C2—C23	175.7 (2)	C12—C13—C14—C9	−0.3 (3)
C15—C1—C2—C23	3.8 (3)	C10—C9—C14—C13	0.4 (2)
C1—C2—C3—C4	0.3 (2)	S1—C9—C14—C13	179.05 (13)
C23—C2—C3—C4	−177.07 (19)	C2—C1—C15—C16	99.95 (19)
C1—C2—C3—C8	179.5 (2)	N1—C1—C15—C16	−70.85 (18)
C23—C2—C3—C8	2.1 (3)	C1—C15—C16—C21	114.27 (16)
C8—C3—C4—C5	0.4 (3)	C1—C15—C16—C17	−66.92 (18)
C2—C3—C4—C5	179.70 (15)	C21—C16—C17—C18	−1.3 (2)

C8—C3—C4—N1	−178.30 (17)	C15—C16—C17—C18	179.83 (13)
C2—C3—C4—N1	1.01 (17)	C16—C17—C18—C19	0.0 (2)
C1—N1—C4—C5	179.56 (15)	C22—O3—C19—C20	−1.0 (2)
S1—N1—C4—C5	30.4 (2)	C22—O3—C19—C18	178.76 (17)
C1—N1—C4—C3	−1.91 (15)	C17—C18—C19—O3	−178.49 (13)
S1—N1—C4—C3	−151.10 (11)	C17—C18—C19—C20	1.3 (2)
C3—C4—C5—C6	−0.5 (2)	O3—C19—C20—C21	178.59 (14)
N1—C4—C5—C6	177.85 (16)	C18—C19—C20—C21	−1.1 (2)
C4—C5—C6—C7	0.3 (3)	C17—C16—C21—C20	1.4 (2)
C5—C6—C7—C8	0.0 (4)	C15—C16—C21—C20	−179.72 (14)
C6—C7—C8—C3	−0.1 (4)	C19—C20—C21—C16	−0.2 (2)
C4—C3—C8—C7	−0.1 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O1	0.93	2.39	2.970 (2)	120
C15—H15B···O2	0.97	2.28	2.883 (2)	119
C21—H21···O2	0.93	2.56	3.127 (2)	120
C13—H13···Cg^{i}	0.93	2.77	3.527 (2)	139

Symmetry codes: (i) *x*+1, *y*, *z*.

Fig. 1

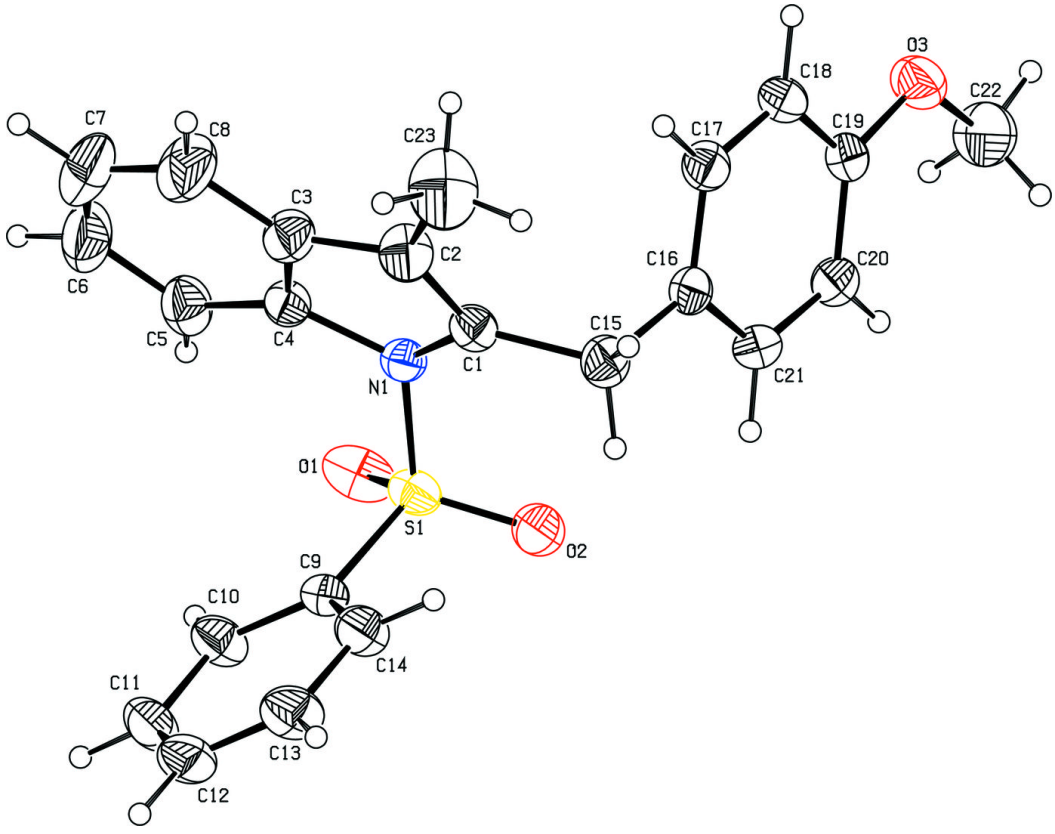
O3
C18
C22
C7
C8
C23
C17
C19
C3
C2
C16
C20
C6
C15
C5
C4
C1
C21
N1
O1
S1
O2
C9
C10
C14
C11
C13
C12

Fig. 2