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2-Methyl-1-phenylsulfonyl-1*H*-indole-3-carbaldehyde

C. Ramathilagam,[a] V. Saravanan,[b] A. K. Mohanakrishnan,[b] P. R. Umarani[c] and V. Manivannan[d]*

[a]Department of Physics, AMET University, Kanathur, Chennai 603 112, India, [b]Department of Organic Chemistry, University of Madras, Guindy Campus, Chennai 600 025, India, [c]Department of Physics, Presidency College (Autonomous), Chennai 600 005, India, and [d]Department of Research and Development, PRIST University, Vallam, Thanjavur 613 403, Tamil Nadu, India
Correspondence e-mail: crystallography2010@gmail.com

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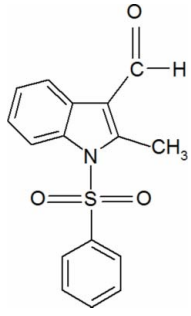
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.002 Å; R factor = 0.041; wR factor = 0.116; data-to-parameter ratio = 22.2.

In the title compound, $C_{16}H_{13}NO_3S$, the sulfonyl-bound phenyl ring forms a dihedral angle of 84.17 (6)° with the indole ring system. An intramolecular C—H···O hydrogen bond generates an S(6) ring motif. The crystal structure exhibits weak intermolecular C—H···O hydrogen bonds and π–π interactions between the five- and six-membered rings of the indole group [centroid–centroid distance = 3.6871 (9) Å].

Related literature

For the biological activities of indole compounds, see: Chai *et al.* (2006); Singh *et al.* (2000); Andreani *et al.* (2001). For related structures, see: Chakkaravarthi *et al.* (2007, 2008); Ramathilagam *et al.* (2011). For graph-set notation, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{16}H_{13}NO_3S$ M_r = 299.33
Monoclinic, $P2_1/c$
a = 11.6305 (5) Å
b = 8.4039 (4) Å
c = 14.3128 (8) Å
β = 93.126 (1)°
V = 1396.87 (12) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 295 K
0.22 × 0.20 × 0.18 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.949, T_{max} = 0.958
18442 measured reflections
4242 independent reflections
3212 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.116
S = 1.06
4242 reflections
191 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···O1	0.93	2.28	2.8723 (19)	121
C12—H12···O3^{i}	0.93	2.48	3.1664 (19)	131
C16—H16···O2^{ii}	0.93	2.48	3.388 (2)	167

Symmetry codes: (i) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x, -y+2, -z$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI5199).

References

Andreani, A., Granaiola, M., Leoni, A., Locatelli, A., Morigi, R., Rambaldi, M., Giorgi, G., Salvini, L. & Garaliene, V. (2001). *Anti-Cancer Drug Des.* **16**, 167–174.
Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Bruker (2004). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Chai, H., Zhao, C. & Gong, P. (2006). *Bioorg. Med. Chem.* **14**, 911–917.
Chakkaravarthi, G., Dhayalan, V., Mohanakrishnan, A. K. & Manivannan, V. (2008). *Acta Cryst.* E**64**, o749.
Chakkaravarthi, G., Ramesh, N., Mohanakrishnan, A. K. & Manivannan, V. (2007). *Acta Cryst.* E**63**, o3564.
Ramathilagam, C., Saravanan, V., Mohanakrishnan, A. K., Chakkaravarthi, G., Umarani, P. R. & Manivannan, V. (2011). *Acta Cryst.* E**67**, o632.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Singh, U. P., Sarma, B. K., Mishra, P. K. & Ray, A. B. (2000). *Folia Microbiol. (Prague)*, **45**, 173–176.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

supplementary materials

Acta Cryst. (2011). E**67**, o2614 [**doi:10.1107/S1600536811035665**]

2-Methyl-1-phenylsulfonyl-1*H*-indole-3-carbaldehyde

C. Ramathilagam, V. Saravanan, A. K. Mohanakrishnan, P. R. Umarani and V. Manivannan

Comment

Indole derivatives are found in many natural products and these derivatives exhibit antibacterial, antifungal (Singh *et al.*, 2000) and antitumour activities (Andreani *et al.*, 2001). In addition, certain indole derivatives exhibit anti-hepatitis B virus (Chai *et al.*, 2006) activity.

The geometric parameters of the title molecule (Fig. 1) agree well with those observed in related structures (Chakkaravarthi *et al.*, 2007, 2008; Ramathilagam *et al.*, 2011). The dihedral angle between the benzene (C1–C6) and phenyl rings (C11–C16) is 83.81 (7)°. The sum of bond angles around N1 [359.9°] indicates sp^2 hybridization.

The molecular structure is stabilized by a weak intramolecular C—H···O hydrogen bond and the crystal packing is stabilized by weak intermolecular C—H···O hydrogen bonds. The intramolecular C5—H5···O1 hydrogen bond generates an S(6) ring (Bernstein *et al.*, 1995).

Experimental

2-Methylindole-3-carboxaldehyde (5 g, 31.4 mmol) was dissolved in distilled benzene (100 ml). To this benzenesulfonylchloride (6.6 g, 4.8 ml, 37.7 mmol) and 60% aqueous NAOH (32g in 53ml) were added along with tetrabutyl ammonium hydrogensulfate (1.0 g). This two phase system was stirred at room temperature for 2h. It was then diluted with water (200 ml) and the organic layer was separated. The aqueous layer was extracted with benzene (2× 30 ml) and the combined organic extracts were dried (Na_2SO_4). The solvent was removed completely and the crude product was recrystallized from methanol (m.p 431–433 K).

Refinement

H atoms were positioned geometrically and refined using riding model, with d(C–H) = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic C–H and d(C–H) = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for methyl C–H.

Figures

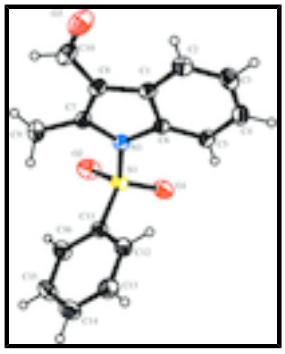

Fig. 1. The molecular structure of the title compound, with atom labels and 30% probability displacement ellipsoids for non-H atoms.

2-Methyl-1-phenylsulfonyl-1*H*-indole-3-carbaldehyde

Crystal data

$C_{16}H_{13}NO_3S$	$F(000) = 624$
$M_r = 299.33$	$D_x = 1.423$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2Ybc	Cell parameters from 4242 reflections
$a = 11.6305$ (5) Å	$\theta = 2.8$–$30.5°$
$b = 8.4039$ (4) Å	$\mu = 0.24$ mm^{-1}
$c = 14.3128$ (8) Å	$T = 295$ K
$\beta = 93.126$ (1)°	Block, colourless
$V = 1396.87$ (12) Å^3	0.22 × 0.20 × 0.18 mm
$Z = 4$	

Data collection

Bruker Kappa APEXII CCD diffractometer	4242 independent reflections
Radiation source: fine-focus sealed tube	3212 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.024$
ω and φ scans	$\theta_{max} = 30.5°$, $\theta_{min} = 2.8°$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$h = -8 \rightarrow 16$
$T_{min} = 0.949$, $T_{max} = 0.958$	$k = -11 \rightarrow 11$
18442 measured reflections	$l = -20 \rightarrow 20$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.041$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.116$	H-atom parameters constrained

$S = 1.06$	$w = 1/[\sigma^2(F_o^2) + (0.051P)^2 + 0.3293P]$ where $P = (F_o^2 + 2F_c^2)/3$
4242 reflections	$(\Delta/\sigma)_{max} = 0.001$
191 parameters	$\Delta\rho_{max} = 0.31$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.27$ e Å^{-3}

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.51033 (11)	1.03657 (16)	0.11957 (9)	0.0372 (3)
C2	0.62740 (13)	1.0134 (2)	0.14228 (11)	0.0488 (3)
H2	0.6794	1.0968	0.1382	0.059*
C3	0.66431 (13)	0.8654 (2)	0.17072 (12)	0.0541 (4)
H3	0.7420	0.8486	0.1863	0.065*
C4	0.58737 (14)	0.7403 (2)	0.17652 (11)	0.0509 (4)
H4	0.6148	0.6412	0.1961	0.061*
C5	0.47145 (13)	0.75842 (17)	0.15415 (10)	0.0442 (3)
H5	0.4203	0.6739	0.1581	0.053*
C6	0.43434 (11)	0.90840 (16)	0.12546 (9)	0.0356 (3)
C7	0.33085 (13)	1.12984 (17)	0.07792 (10)	0.0429 (3)
C8	0.44359 (12)	1.17348 (17)	0.08955 (9)	0.0412 (3)
C9	0.22868 (16)	1.2312 (2)	0.05301 (14)	0.0655 (5)
H9A	0.2527	1.3399	0.0472	0.098*
H9B	0.1747	1.2233	0.1012	0.098*
H9C	0.1929	1.1958	−0.0053	0.098*
C10	0.48781 (17)	1.3321 (2)	0.07368 (12)	0.0559 (4)
H10	0.4355	1.4109	0.0545	0.067*
C11	0.13200 (11)	0.92243 (17)	0.19354 (9)	0.0395 (3)
C12	0.18938 (12)	0.90248 (19)	0.27999 (10)	0.0457 (3)
H12	0.2640	0.8624	0.2845	0.055*
C13	0.13415 (16)	0.9431 (2)	0.35933 (11)	0.0569 (4)
H13	0.1717	0.9313	0.4180	0.068*
C14	0.02338 (16)	1.0010 (2)	0.35188 (13)	0.0624 (4)
H14	−0.0138	1.0270	0.4058	0.075*
C15	−0.03304 (14)	1.0211 (2)	0.26584 (13)	0.0613 (4)
H15	−0.1078	1.0608	0.2618	0.074*
C16	0.02108 (12)	0.9824 (2)	0.18524 (11)	0.0516 (4)
H16	−0.0163	0.9964	0.1267	0.062*
N1	0.32271 (9)	0.96653 (14)	0.09734 (8)	0.0411 (3)
O1	0.23308 (10)	0.69878 (14)	0.10309 (9)	0.0575 (3)

O2	0.13304 (10)	0.91043 (19)	0.01249 (8)	0.0667 (4)
O3	0.58819 (13)	1.36833 (15)	0.08380 (10)	0.0742 (4)
S1	0.20015 (3)	0.86138 (5)	0.09314 (2)	0.04468 (12)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0448 (6)	0.0379 (7)	0.0289 (6)	−0.0030 (5)	0.0030 (5)	−0.0032 (5)
C2	0.0440 (7)	0.0547 (9)	0.0472 (8)	−0.0074 (6)	−0.0017 (6)	−0.0046 (7)
C3	0.0436 (7)	0.0656 (11)	0.0522 (9)	0.0079 (7)	−0.0060 (6)	−0.0027 (8)
C4	0.0571 (8)	0.0483 (9)	0.0471 (8)	0.0133 (7)	0.0004 (6)	0.0037 (7)
C5	0.0496 (7)	0.0387 (7)	0.0446 (7)	0.0006 (6)	0.0056 (6)	0.0048 (6)
C6	0.0385 (6)	0.0379 (7)	0.0307 (6)	0.0009 (5)	0.0045 (5)	0.0004 (5)
C7	0.0510 (7)	0.0415 (7)	0.0364 (7)	0.0070 (6)	0.0045 (6)	0.0049 (6)
C8	0.0537 (8)	0.0364 (7)	0.0336 (6)	−0.0022 (6)	0.0026 (5)	−0.0003 (5)
C9	0.0608 (10)	0.0607 (11)	0.0750 (12)	0.0181 (8)	0.0052 (9)	0.0158 (9)
C10	0.0760 (11)	0.0397 (8)	0.0511 (9)	−0.0074 (7)	−0.0044 (8)	0.0027 (7)
C11	0.0338 (6)	0.0439 (7)	0.0407 (7)	−0.0018 (5)	0.0020 (5)	0.0007 (6)
C12	0.0411 (7)	0.0510 (8)	0.0445 (8)	0.0027 (6)	−0.0011 (6)	0.0027 (6)
C13	0.0653 (10)	0.0651 (11)	0.0400 (8)	0.0036 (8)	0.0012 (7)	0.0007 (7)
C14	0.0630 (10)	0.0713 (12)	0.0545 (10)	0.0056 (9)	0.0169 (8)	−0.0067 (9)
C15	0.0439 (8)	0.0717 (12)	0.0690 (11)	0.0132 (8)	0.0091 (7)	−0.0060 (9)
C16	0.0385 (7)	0.0648 (10)	0.0508 (8)	0.0050 (6)	−0.0042 (6)	0.0012 (7)
N1	0.0372 (5)	0.0421 (7)	0.0442 (6)	−0.0003 (4)	0.0050 (4)	0.0063 (5)
O1	0.0532 (6)	0.0470 (6)	0.0737 (8)	−0.0101 (5)	0.0156 (5)	−0.0129 (6)
O2	0.0536 (6)	0.1042 (11)	0.0411 (6)	−0.0050 (7)	−0.0075 (5)	−0.0038 (6)
O3	0.0809 (9)	0.0546 (8)	0.0847 (10)	−0.0268 (7)	−0.0179 (7)	0.0078 (7)
S1	0.03861 (17)	0.0548 (2)	0.0407 (2)	−0.00535 (14)	0.00263 (13)	−0.00445 (15)

Geometric parameters (Å, °)

C1—C2	1.3962 (19)	C9—H9C	0.96
C1—C6	1.3988 (18)	C10—O3	1.207 (2)
C1—C8	1.4404 (19)	C10—H10	0.93
C2—C3	1.370 (2)	C11—C12	1.3835 (19)
C2—H2	0.93	C11—C16	1.3841 (19)
C3—C4	1.386 (2)	C11—S1	1.7552 (14)
C3—H3	0.93	C12—C13	1.378 (2)
C4—C5	1.377 (2)	C12—H12	0.93
C4—H4	0.93	C13—C14	1.376 (2)
C5—C6	1.3871 (19)	C13—H13	0.93
C5—H5	0.93	C14—C15	1.374 (3)
C6—N1	1.4246 (16)	C14—H14	0.93
C7—C8	1.363 (2)	C15—C16	1.383 (2)
C7—N1	1.4046 (19)	C15—H15	0.93
C7—C9	1.490 (2)	C16—H16	0.93
C8—C10	1.451 (2)	N1—S1	1.6753 (12)
C9—H9A	0.96	O1—S1	1.4242 (13)
C9—H9B	0.96	O2—S1	1.4190 (12)

C2—C1—C6	119.32 (13)	O3—C10—C8	124.15 (17)
C2—C1—C8	133.15 (13)	O3—C10—H10	117.9
C6—C1—C8	107.53 (12)	C8—C10—H10	117.9
C3—C2—C1	118.80 (14)	C12—C11—C16	121.52 (13)
C3—C2—H2	120.6	C12—C11—S1	118.64 (10)
C1—C2—H2	120.6	C16—C11—S1	119.77 (11)
C2—C3—C4	120.88 (14)	C13—C12—C11	118.90 (14)
C2—C3—H3	119.6	C13—C12—H12	120.6
C4—C3—H3	119.6	C11—C12—H12	120.6
C5—C4—C3	121.96 (15)	C14—C13—C12	120.02 (15)
C5—C4—H4	119.0	C14—C13—H13	120.0
C3—C4—H4	119.0	C12—C13—H13	120.0
C4—C5—C6	117.02 (14)	C15—C14—C13	120.82 (15)
C4—C5—H5	121.5	C15—C14—H14	119.6
C6—C5—H5	121.5	C13—C14—H14	119.6
C5—C6—C1	122.02 (12)	C14—C15—C16	120.14 (15)
C5—C6—N1	131.25 (12)	C14—C15—H15	119.9
C1—C6—N1	106.74 (12)	C16—C15—H15	119.9
C8—C7—N1	108.28 (12)	C15—C16—C11	118.59 (14)
C8—C7—C9	128.68 (14)	C15—C16—H16	120.7
N1—C7—C9	123.01 (14)	C11—C16—H16	120.7
C7—C8—C1	108.71 (12)	C7—N1—C6	108.71 (11)
C7—C8—C10	125.09 (14)	C7—N1—S1	125.08 (10)
C1—C8—C10	126.20 (14)	C6—N1—S1	126.14 (10)
C7—C9—H9A	109.5	O2—S1—O1	119.54 (8)
C7—C9—H9B	109.5	O2—S1—N1	107.77 (7)
H9A—C9—H9B	109.5	O1—S1—N1	106.19 (6)
C7—C9—H9C	109.5	O2—S1—C11	109.16 (7)
H9A—C9—H9C	109.5	O1—S1—C11	109.24 (7)
H9B—C9—H9C	109.5	N1—S1—C11	103.76 (6)
C6—C1—C2—C3	−0.7 (2)	C13—C14—C15—C16	0.2 (3)
C8—C1—C2—C3	178.78 (15)	C14—C15—C16—C11	0.5 (3)
C1—C2—C3—C4	0.3 (2)	C12—C11—C16—C15	−0.7 (2)
C2—C3—C4—C5	0.1 (2)	S1—C11—C16—C15	176.34 (13)
C3—C4—C5—C6	−0.1 (2)	C8—C7—N1—C6	2.23 (15)
C4—C5—C6—C1	−0.2 (2)	C9—C7—N1—C6	−175.57 (14)
C4—C5—C6—N1	179.63 (14)	C8—C7—N1—S1	179.33 (10)
C2—C1—C6—C5	0.6 (2)	C9—C7—N1—S1	1.5 (2)
C8—C1—C6—C5	−178.94 (12)	C5—C6—N1—C7	178.03 (14)
C2—C1—C6—N1	−179.26 (12)	C1—C6—N1—C7	−2.08 (14)
C8—C1—C6—N1	1.17 (14)	C5—C6—N1—S1	1.0 (2)
N1—C7—C8—C1	−1.48 (16)	C1—C6—N1—S1	−179.15 (9)
C9—C7—C8—C1	176.15 (15)	C7—N1—S1—O2	41.89 (14)
N1—C7—C8—C10	178.30 (13)	C6—N1—S1—O2	−141.51 (11)
C9—C7—C8—C10	−4.1 (3)	C7—N1—S1—O1	171.10 (11)
C2—C1—C8—C7	−179.31 (15)	C6—N1—S1—O1	−12.30 (13)
C6—C1—C8—C7	0.18 (15)	C7—N1—S1—C11	−73.79 (13)
C2—C1—C8—C10	0.9 (2)	C6—N1—S1—C11	102.82 (12)

C6—C1—C8—C10	−179.60 (13)	C12—C11—S1—O2	−172.81 (12)
C7—C8—C10—O3	−179.51 (16)	C16—C11—S1—O2	10.03 (16)
C1—C8—C10—O3	0.2 (3)	C12—C11—S1—O1	54.80 (13)
C16—C11—C12—C13	0.2 (2)	C16—C11—S1—O1	−122.36 (13)
S1—C11—C12—C13	−176.90 (13)	C12—C11—S1—N1	−58.13 (13)
C11—C12—C13—C14	0.6 (3)	C16—C11—S1—N1	124.72 (13)
C12—C13—C14—C15	−0.8 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O1	0.93	2.28	2.8723 (19)	121
C12—H12···O3^{i}	0.93	2.48	3.1664 (19)	131
C16—H16···O2^{ii}	0.93	2.48	3.388 (2)	167

Symmetry codes: (i) −*x*+1, *y*−1/2, −*z*+1/2; (ii) −*x*, −*y*+2, −*z*.

Fig. 1