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1-(4-Methoxybenzyl)-1*H*-indole-3-carbaldehyde

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Key indicators

Single-crystal X-ray study
T = 90 K
Mean σ(C–C) = 0.002 Å
R factor = 0.043
wR factor = 0.112
Data-to-parameter ratio = 16.5

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

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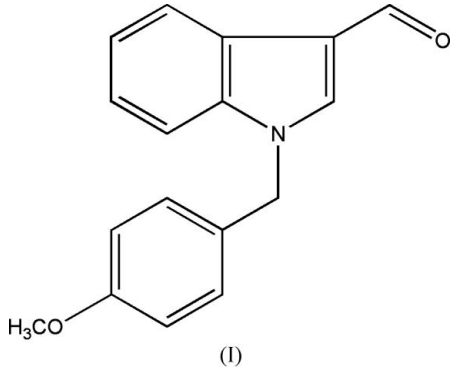
Crystals of the title compound, $C_{17}H_{15}NO_2$, were obtained by the reaction of indole-3-carbaldehyde with 4-methoxybenzyl chloride and recrystallization of the product from ethanol. The dihedral angle between the indole and the 4-methoxyphenyl ring systems is 70.18 (4)°. The crystal packing is stabilized by van der Waals forces.

Comment

The title compound is a synthetic intermediate in our ongoing synthesis of 2-(substituted benzylidene/heteroaryl-3-yl-methylene)-1-azabicylo[2.2.2]octan-3-ones. 1-Benzylindole-3-carbaldehyde readily undergoes base-catalyzed condensation with azabicylo[2.2.2]octan-3-one (Sonar *et al.*, 2003). However, 1-(4-methoxybenzyl)indole-3-carbaldehyde failed to undergo a similar condensation reaction. This prompted us to study the molecular conformation of the title compound, (I), which was prepared by the reaction of indole-3-carbaldehyde with 4-methoxybenzyl chloride in the presence of potassium carbonate and dimethylformamide under reflux, and recrystallization of the resultant product from ethanol. The present X-ray crystallographic determination was carried out in order to obtain more detailed information on the conformation of the molecule.



(I)

Fig. 1 shows a view of (I) and selected geometric parameters are presented in Table 1. The indole ring system is planar, with bond distances and angles comparable with those reported for other indole derivatives (Mason *et al.*, 2003). The plane of the indole ring system makes a dihedral angle of 70.18 (4)° with the plane of the 4-methoxyphenyl ring of the 4-methoxybenzyl group. The observed bond lengths, C15—O2 and C18—O2, are comparable with values for aromatic methoxy bonds, and there is an asymmetry of the exocyclic angles at C15 (Domiano *et al.*, 1979).

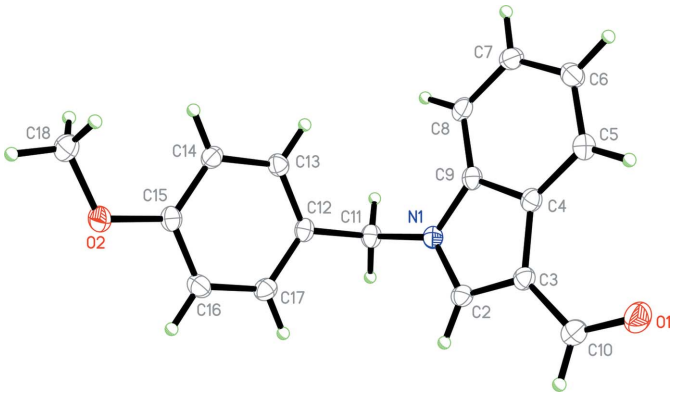


Figure 1
A view of the molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

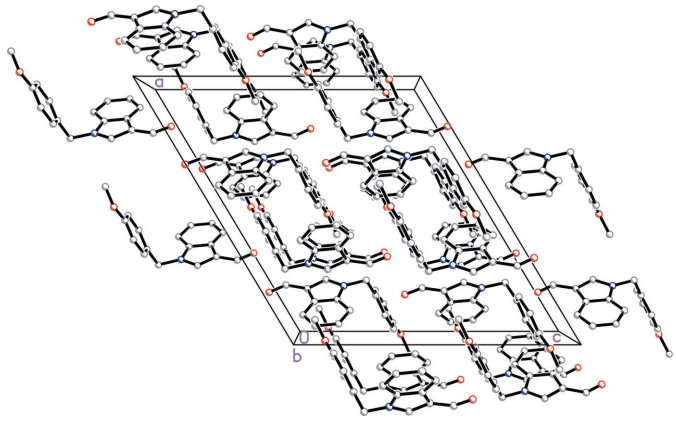


Figure 2
A packing diagram for (I), viewed down the *b* axis. H atoms have been omitted for clarity.

The mode of packing of (I), as viewed down the *b* axis, is illustrated in Fig. 2. In addition to non-bonded interactions, van der Waals forces contribute to the stabilization of the crystal structure.

Experimental

A mixture of indole-3-carbaldehyde (1.45 g, 10 mmol), 4-methoxybenzyl chloride (1.7 g, 10.85 mmol), anhydrous K_2CO_3 (1.4 g) and dimethylformamide (10 ml) was stirred vigorously and refluxed for 2 h. The cooled reaction mixture was poured into water (40 ml) and the precipitated solid was collected by filtration and air dried. Recrystallization from ethanol afforded pale-yellow crystals of (I).

Crystal data

$C_{17}H_{15}NO_2$
M_r = 265.30
Monoclinic, $C2/c$
a = 17.9743 (2) Å
b = 10.2389 (1) Å
c = 16.5413 (2) Å
β = 120.9154 (6)°
V = 2611.71 (5) Å^3
Z = 8
D_x = 1.349 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 90.0 (2) K
Irregular block, yellow
0.27 × 0.20 × 0.12 mm

Data collection

Nonius KappaCCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SCALEPACK*; Otwinowski & Minor, 1997)
T_{min} = 0.977, T_{max} = 0.989
5831 measured reflections
3003 independent reflections
2289 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.112
S = 1.06
3003 reflections
182 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0568P)^2 + 1.2723P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C2—N1	1.3567 (17)	C10—O1	1.2262 (17)
C2—C3	1.3840 (19)	C15—O2	1.3691 (16)
C3—C10	1.4405 (19)	C18—O2	1.4276 (17)
N1—C11—C12	112.72 (10)	O2—C15—C16	115.28 (12)
O2—C15—C14	124.52 (12)	C15—O2—C18	117.34 (11)
C2—C3—C10—O1	176.54 (13)	C14—C15—O2—C18	−2.07 (18)

H atoms were placed in idealized positions and were constrained with C—H distances of 0.99, 0.98 and 0.95 Å for CH_3, CH_2 and C_{ar} atoms, respectively, and $U_{iso}(H)$ = $1.2U_{eq}(CH_2$ or $C_{ar})$, or $1.5U_{eq}(CH_3)$.

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 1995); software used to prepare material for publication: *SHELXL97* and local procedures.

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References

Domiano, P., Nardelli, M., Balsamo, A., Macchia, B. & Macchia, F. (1979). *Acta Cryst.* B**35**, 1363–1372.
Mason, M. R., Barnard, T. S., Segla, M. F., Xie, B. & Kirschbaum, K. (2003). *J. Chem. Crystallogr.* **33**, 531–540.
Nonius (1999). *COLLECT*. Nonius, BV, Delft, The Netherlands.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
Sheldrick, G. M. (1995). *XP* in *SHELXTL*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sonar, V. N., Parkin, S. & Crooks, P. A. (2003). *Acta Cryst.* E**59**, o1478–o1480.