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2-(1*H*-Indol-3-ylmethylene)indane-1-one

G. Vasuki,[a] V. Parthasarathi,[a]* K. Ramamurthi,[a] S. Mohane Coumar[b] and D. P. Jindal[b]†

[a]Department of Physics, Bharathidasan University, Tiruchirappalli 620 024, India, and [b]University Institute of Pharmaceutical Sciences, Panjab University, Chandigarh 160 014, India

† Deceased

Correspondence e-mail: sarati@yahoo.com

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
R factor = 0.043
wR factor = 0.099
Data-to-parameter ratio = 6.8

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

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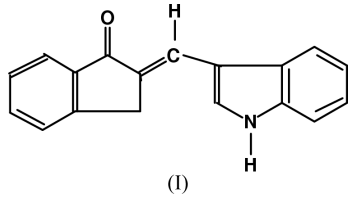
The indole and indane moieties of the title molecule, $C_{18}H_{13}NO$, form a dihedral angle of 10.2 (2)°. In the crystal structure, symmetry-related molecules are linked by intermolecular N—H···O and C—H···O hydrogen bonds to form infinite one-dimensional chains along the *b* axis. This chain structure is further stabilized by π–π and C—H···π interactions.

Comment

The X-ray structure determination of the title compound, (I), was undertaken to study the stereochemistry of the molecule and the nature of the hydrogen bonding. In (I), the indole ring is planar within 0.028 (4) Å and the indane ring system is also planar, with C19 deviating by a maximum of 0.027 (4) Å. The dihedral angle between the indole and indane moieties is 10.2 (2)°. The widening of the exocyclic angle C3—C10—C19 [130.0 (4)°] from 120° may be due to the steric repulsion between atoms H2 and H18*A* (H2···H18*A* = 2.40 Å). The dihedral angle of 7.68° between the O11/C11/C19/C10 and C10/C3/C2/N1 planes indicates that there is possibile delocalization of electrons from O11 to N1 (O11═C11—C19═C10—C3═C2—N1). As a result of this conjugation, the C10—C3 [1.437 (6) Å] bond distance is shortened from the normal value of 1.478 (14) Å (Allen *et al.*, 1987). The N atom is sp^2-hybridized.



(I)

In the crystal structure, glide-related molecules are linked by intermolecular N—H···O and C—H···O hydrogen bonds (Table 1) to form infinite one-dimensional chains along the *b* axis. Within a chain, molecules related by translation symmetry are stacked with significant π–π interactions and intermolecular C—H···π interactions involving atom C18 and the C12–C17 aromatic ring [H18*B*···*Cg* = 2.69 Å, C18···*Cg* = 3.567 (6) Å and C18—H18*B*···*Cg* = 150°, where *Cg* is the centroid of the C12–C17 ring at (*x*, *y* − 1, *z*)].

Experimental

Indol-3-carboxaldehyde (0.25 g, 1.72 mmol) was added to a solution of 1-indanone (0.2 g, 1.51 mmol) in methanol (25 ml) and the solution was stirred manually for 15 min. Sodium hydroxide (0.4 g, 10 mmol) was then added and the solution was stirred for 30 min and refluxed for 8 h. The completion of reaction was monitored with thin-layer

chromatography. The reaction mixture was then concentrated to about 5 ml and crushed ice was added. It was allowed to stand overnight and was then filtered. The product was crystallized from methanol and needle-shaped crystals of (I) were obtained (yield 0.076 g, 21%, m.p. 526–528 K).

Crystal data

$C_{18}H_{13}NO$
M_r = 259.29
Orthorhombic, $Pca2_1$
a = 12.3964 (17) Å
b = 4.961 (4) Å
c = 21.330 (4) Å
V = 1311.7 (10) Å^3
Z = 4
D_x = 1.313 Mg m^{-3}
Mo Kα radiation
Cell parameters from 25 reflections
θ = 10–15°
μ = 0.08 mm^{-1}
T = 293 (2) K
Needle, brown
0.40 × 0.20 × 0.05 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.968, T_{max} = 0.996
1686 measured reflections
1244 independent reflections
848 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 25.0°
$h = -1 \rightarrow 14$
$k = -1 \rightarrow 5$
$l = -25 \rightarrow 1$
2 standard reflections
frequency: 120 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.099
S = 1.19
1244 reflections
182 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0239P)^2 + 0.4636P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0077 (13)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O11^{i}	0.86	2.16	2.829 (5)	134
C18—H18A···O11^{ii}	0.97	2.42	3.371 (6)	168

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

All H atoms were fixed geometrically and allowed to ride on the parent non-H atoms, with aromatic N—H = 0.86 Å, C—H = 0.93 Å and methylene C—H = 0.97 Å. The displacement parameters U_{iso}(H) were set equal to 1.2U_{eq}. The Friedel opposites were not merged during the refinement.

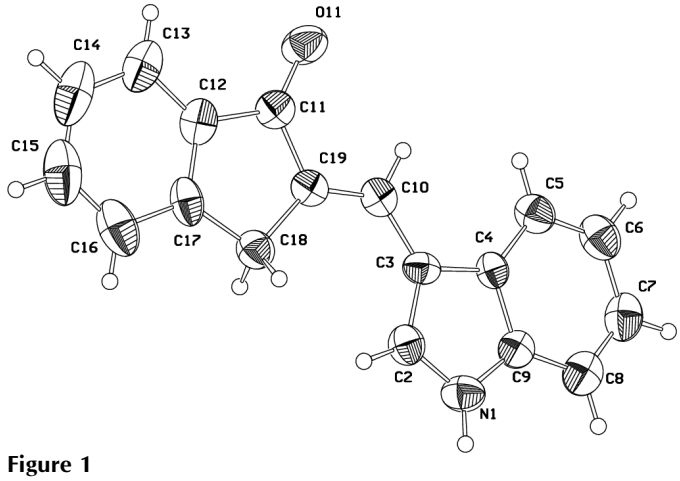


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

Data collection: *CAD*-4 *EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD*-4 *EXPRESS*; data reduction: *MolEN* (Fair, 1990); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ZORTEP* (Zsolnai, 1997); software used to prepare material for publication: *SHELXL*97.

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