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(*Z*)-[2-(1-Methyl-1*H*-indol-3-yl)methylidene]-cyclohexanone

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Key indicators

Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.003 Å
R factor = 0.052
wR factor = 0.141
Data-to-parameter ratio = 13.0

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

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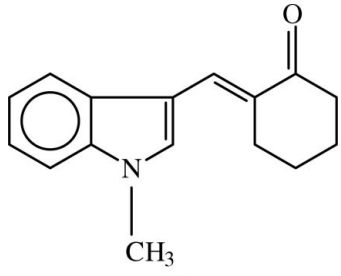
In the title compound, $C_{16}H_{17}NO$, the cyclohexanone ring adopts an envelope conformation.

Comment

Indole derivatives, widely distributed in living cells as tryptophan metabolites, have important biological functions. Various indole derivatives occur in many pharmacologically and biologically active compounds (Zhang *et al.*, 2000). They are present in a number of natural products, many of which are found to possess antihypertensive (Merk, 1971), anti-inflammatory (Rodriguez *et al.*, 1985) and antimalarial (El-Sayed *et al.*, 1986) activities. Indoles have been proved to display high aldose reductase inhibitory activity (Rajeswaran *et al.*, 1999). As a result of the biological and pharmacological potential of the title compound, (I), the present study was undertaken in order to obtain its three-dimensional structure (Fig. 1).



(I)

The Csp^2-Csp^2 single-bond distance [C7—C10 1.443 (3) Å] and the Csp^2-Csp^2 double-bond distance [C10═C11 1.342 (3) Å] are comparable with the corresponding mean values of 1.455 (11) and 1.330 (14) Å, respectively (Allen *et al.*, 1987).

The cyclohexanone ring adopts an envelope conformation, with an asymmetry parameter ΔC_s(C11) = 0.068 (1) (Nardelli, 1983). Atom C14 is displaced by 0.556 (3) Å from the C11–C13/C15/C16 least-squares plane.

In the absence of hydrogen-bond-donating groups, the molecules of (I) are held together by normal van der Waals interactions. In the crystal packing, the molecules show a herring-bone pattern (Fig. 2).

Experimental

In order to obtain crystals suitable for X-ray studies, the title compound (procured from Regional Research Laboratory, Jorhat, India) was dissolved in a methanol–water solution (90:10) and the solution was allowed to evaporate slowly.

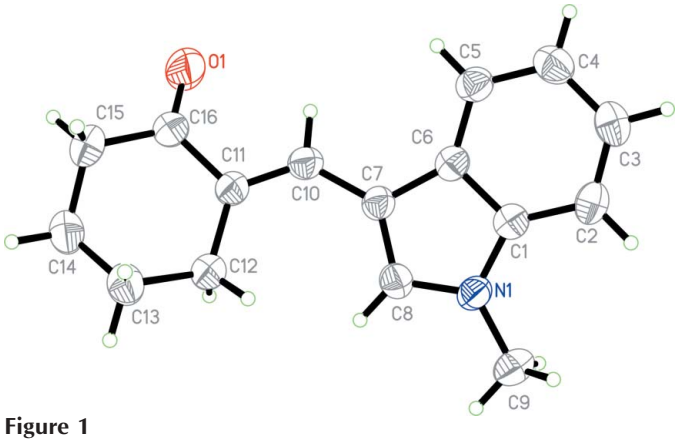


Figure 1
A view of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

Crystal data

$C_{16}H_{17}NO$
M_r = 239.31
Orthorhombic, *Pbca*
a = 7.9154 (9) Å
b = 13.7376 (14) Å
c = 22.980 (3) Å
V = 2498.8 (5) Å^3
Z = 8
D_x = 1.272 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2714 reflections
θ = 3.1–22.8°
μ = 0.08 mm^{-1}
T = 273 (2) K
Block, colourless
0.19 × 0.11 × 0.09 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
ω scans
Absorption correction: none
11800 measured reflections
2126 independent reflections
1770 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 25.0°
$h = -9 \rightarrow 9$
$k = -15 \rightarrow 14$
$l = -27 \rightarrow 25$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.141
S = 1.10
2126 reflections
164 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0709P)^2 + 0.755P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C16	1.210 (3)	N1—C1	1.374 (2)
N1—C8	1.359 (2)	N1—C9	1.456 (2)
C8—N1—C1	108.70 (16)	N1—C8—C7	111.12 (19)
C8—N1—C9	125.38 (17)	O1—C16—C11	121.8 (2)
C1—N1—C9	125.38 (17)	O1—C16—C15	119.70 (18)
N1—C1—C6	107.67 (16)		

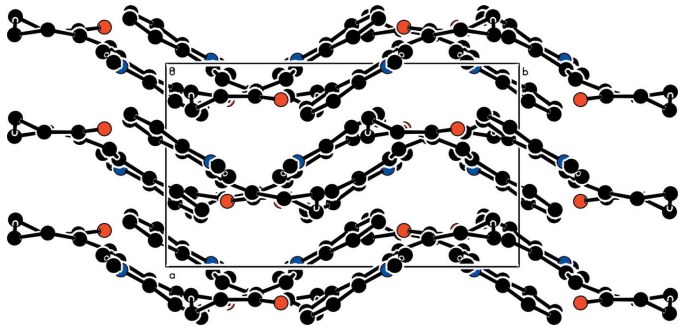


Figure 2
A packing diagram for (I), viewed down the c axis. H atoms have been omitted for clarity.

H atoms were included in calculated positions, with C—H = 0.93–0.98 Å, and refined as riding, with U_{iso}(H) set to 1.2 or 1.5 (CH_3) times U_{eq} of the parent atom. In addition, the methyl group was allowed to rotate but not to tip.

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: *SHELXTL/PC* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

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