Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1,1-Dibenzyl-6-methoxy-3,4-dihydro-1*H*-naphthalen-2-one

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.004 Å
R factor = 0.052
wR factor = 0.174
Data-to-parameter ratio = 14.0

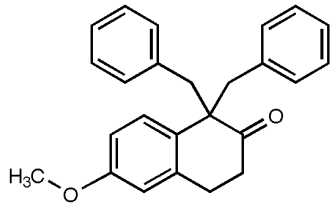
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 9 January 2002
Accepted 14 January 2002
Online 25 January 2002

The structure of the title compound, $C_{25}H_{24}O_2$, has been determined as part of an ongoing investigation into the biological activity of compounds based on the β-tetralone core. The conformational structure of (I) is stabilized by C—H$\cdots\pi$ interactions between the aliphatic ring H atoms and the π-electron systems of the benzyl subunits.

Comment

The bond lengths and angles in (I) are in accord with conventional values (Allen *et al.*, 1987). The molecule adopts a 'bat-like' conformational structure. The methoxy group and the tetralone group are approximately coplanar. The cyclohexanone ring adopts a half-chair conformation such that the axial H atoms on C3 and C4 are able to interact with the π system of the benzyl units, with C—H$\cdots\pi$ distances in the range 3.2–3.4 Å. The methylene C atoms on the benzyl groups are eclipsed as a consequence of these interactions.



(I)

Experimental

6-Methoxy-3,4-dihydro-1*H*-naphthalen-2-one (1.0 g, 5.7 mmol), dissolved in tetrahydrofuran (thf, 20 ml), was cooled to 228 K under an N_2 atmosphere. *n*-BuLi (3.8 ml of a 1.6 *M* solution in hexane, 6.1 mmol) was added dropwise *via* syringe. The reaction mixture was left to stir for 30 min at 228 K. Benzyl bromide (1.21 g, 7.1 mmol) was added *via* syringe and the reaction left to stir whilst warming to room temperature for another 30 min before quenching with water. The solvent was removed *in vacuo*. Purification of the product was achieved by column chromatography (1:1 hexane/ether). Crystals for X-ray diffraction studies were obtained by slow evaporation of a hexane solution [m.p. 408–410 K].

Crystal data

$C_{25}H_{24}O_2$
M_r = 356.44
Monoclinic, $P2_1/a$
a = 14.766 (5) Å
b = 11.214 (4) Å
c = 12.089 (4) Å
β = 102.51 (3)°
V = 1954.2 (12) Å^3
Z = 4
D_x = 1.212 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 17.1–19.7°
μ = 0.08 mm^{-1}
T = 295 K
Prism, colorless
0.50 × 0.40 × 0.25 mm

 DOI: 10.1107/S1600536802000715

Data collection

Rigaku AFC-7*R* diffractometer	$h = -17 \rightarrow 8$
$\omega/2\theta$ scans	$k = 0 \rightarrow 13$
3985 measured reflections	$l = -14 \rightarrow 14$
3440 independent reflections	3 standard reflections
2037 reflections with $I > 2\sigma(I)$	every 150 reflections
$R_{int} = 0.029$	intensity decay: 0.2%
$\theta_{max} = 25.0^\circ$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0825P)^2 + 0.4084P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.052$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.174$	$\Delta\rho_{max} = 0.50$ e Å^{-3}
$S = 1.03$	$\Delta\rho_{min} = -0.31$ e Å^{-3}
3440 reflections	Extinction correction: *SHELXL*97
245 parameters	Extinction coefficient: 0.0071 (18)
H-atom parameters constrained	

H atoms were included at calculated positions, with C—H set to 0.95 Å. Due to a large fraction of weak data at higher angles, the 2θ maximum was limited to 50°.

Data collection: *MSC/AFC-7 Diffractometer Control Software* (Molecular Structure Corporation, 1999); cell refinement: *MSC/AFC-7 Diffractometer Control Software*; data reduction: *TEXSAN for Windows* (Molecular Structure Corporation, 1997–2001); program(s) used to solve structure: *TEXSAN for Windows*; program(s) used to refine structure: *TEXSAN for Windows* and *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *TEXSAN for Windows* and *PLATON* (Spek, 2001).

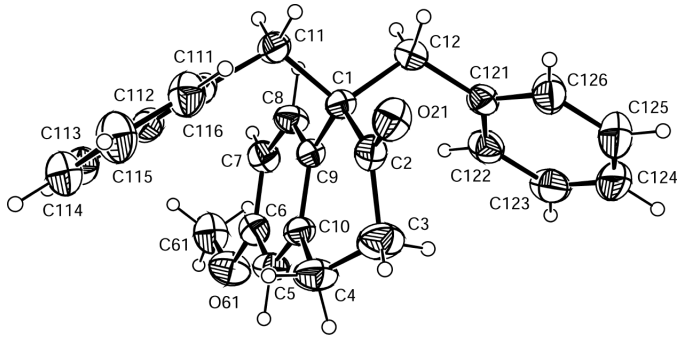


Figure 1
ORTEP-3 (Farrugia, 1997) plot showing the atomic numbering scheme for (I). Displacement ellipsoids are drawn at the 30% probability level for non-H atoms.

Financial support from the Australian Research Council is gratefully acknowledged.

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