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6,7-Dimethyl-3a,8a-dihydro-3*H*-8-oxacyclopenta[*a*]inden-5-yl benzoate

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The title compound, $C_{20}H_{18}O_3$, was prepared in a one-step synthesis by intramolecular cyclization following the sigmatropic rearrangement of the allyl aryl ether intermediate. The room-temperature crystal structure determination reveals a *cis* conformation of the ring annellation.

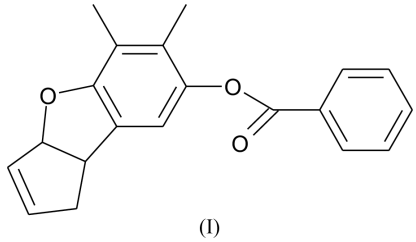
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.052
wR factor = 0.158
Data-to-parameter ratio = 28.0

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

Comment

In the title compound, (I), the cyclopentyl and phenyl groups form angles of 65.85 (5) and 52.78 (4)° to the indene moiety, respectively. Two molecules form a centrosymmetrically related pair, with an interplanar distance of 3.60 Å between the indene units. A distorted herring-bone arrangement of the indene rings characterizes the packing.



(I)

Experimental

The preparation of the title compound is described in detail by Novák *et al.* (1997).

Crystal data

$C_{20}H_{18}O_3$
M_r = 306.34
Monoclinic, $P2_1/a$
a = 7.9964 (10) Å
b = 18.6031 (10) Å
c = 10.9254 (10) Å
β = 101.274 (5)°
V = 1593.9 (2) Å^3
Z = 4
D_x = 1.277 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 10.0–20.9°
μ = 0.09 mm^{-1}
T = 293 (2) K
Needle, colourless
0.50 × 0.50 × 0.17 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
Absorption correction: ψ scan (*MolEN*; Enraf–Nonius, 1990)
T_{min} = 0.959, T_{max} = 0.986
6538 measured reflections
6020 independent reflections
3130 reflections with $I > 2\sigma(I)$
R_{int} = 0.017
θ_{max} = 33.0°
$h = 0 \rightarrow 12$
$k = -28 \rightarrow 0$
$l = -16 \rightarrow 16$
3 standard reflections
frequency: 60 min
intensity decay: 2%

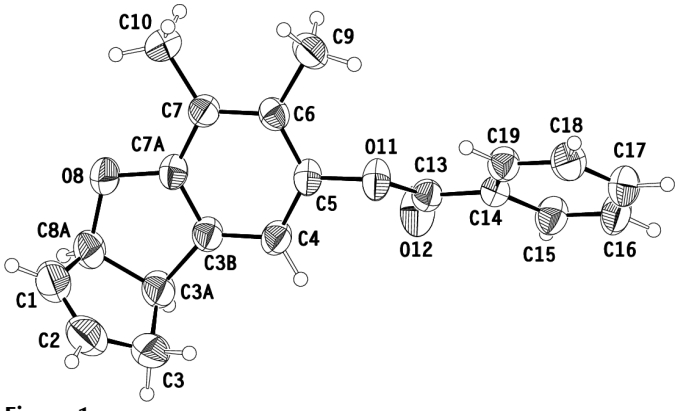


Figure 1
The molecular structure of (I) with 50% probability ellipsoids.

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.052$	$w = 1/[\sigma^2(F_o^2) + (0.0815P)^2 + 0.0559P]$ $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.158$	$(\Delta/\sigma)_{max} = 0.009$
$S = 0.97$	$\Delta\rho_{max} = 0.30$ e Å^{-3}
6020 reflections	$\Delta\rho_{min} = -0.22$ e Å^{-3}
215 parameters	

Table 1
Selected geometric parameters (Å, °).

C1—C2	1.324 (2)	C7a—O8	1.3762 (13)
C2—C3	1.478 (3)	O8—C8a	1.4597 (17)
C3a—C8a	1.548 (2)	O11—C13	1.3459 (14)
C3b—C7a	1.3804 (17)	O12—C13	1.1986 (14)
C5—O11	1.4151 (14)		
C1—C2—C3	112.64 (17)	O8—C7a—C7	122.61 (11)
C3b—C3a—C3	114.75 (12)	O8—C8a—C1	112.05 (12)
C4—C3b—C3a	131.12 (12)	C13—O11—C5	120.04 (9)
O8—C7a—C3b	113.38 (11)	O12—C13—O11	123.69 (11)

Data collection: *CAD*-4 *EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD*-4 *EXPRESS*; data reduction: *XCAD*4 (Harms, 1996); program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1985); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ZORTEP* (Zsolnai & Pritzkow, 1994); software used to prepare material for publication: *SHELXL*97.

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