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# *trans*-2-Benzoyl-1-phenylindan

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The title compound, $C_{22}H_{18}O$, was obtained as a single product from a stereoselective reaction. The five-membered ring adopts an envelope conformation. Two intramolecular C—H···O interactions stabilize the molecular conformation. An intermolecular C—H···O interaction generates chains of molecules running along the *b* axis.

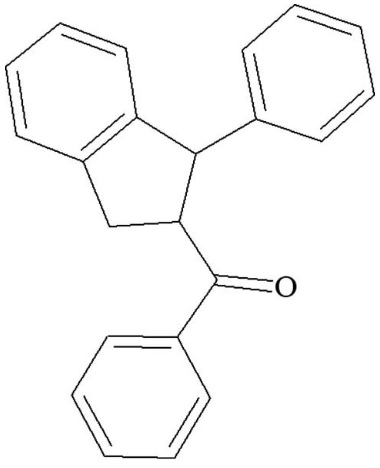
**Key indicators**

Single-crystal X-ray study
$T$ = 293 K
Mean $\sigma$(C–C) = 0.005 Å
$R$ factor = 0.048
$wR$ factor = 0.101
Data-to-parameter ratio = 14.5

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

## Comment

We have been performing extensive research on the synthesis and configurational effects of substitution in the five-membered ring of indan derivatives (Aguirre *et al.*, 1998; Aguirre *et al.*, 1999; Alesso *et al.*, 2002; Alesso *et al.*, 2003). In particular, we have been seeking alternative routes through stereoselective synthesis for indan and tetranilic derivatives *via* condensation of aryl ketones. As part of these results, the compound 2-benzoyl-1-phenylindan, (I), could be synthesized in acid solution and isolated as a single product. The *trans* configuration was assigned by NMR studies in $CDCl_3$ solution (Mufato *et al.*, 2002).



(I)

More recently, Rendy *et al.* (2004) indicated that this compound was obtained as a product from a reaction catalysed by superacids, but no configuration was assigned. The aim of this work is to provide experimental information about the configuration and conformation of (I) by X-ray crystallography and thus to confirm the *trans* configuration previously assigned by NMR studies.

Selected bond distances and angles are given in Table 1. The molecule (Fig. 1) has three planar benzene rings. The five-membered ring can be described as an envelope with C8 as the flap atom, which is displaced 0.488 (5) Å from the C1/C6/C7/

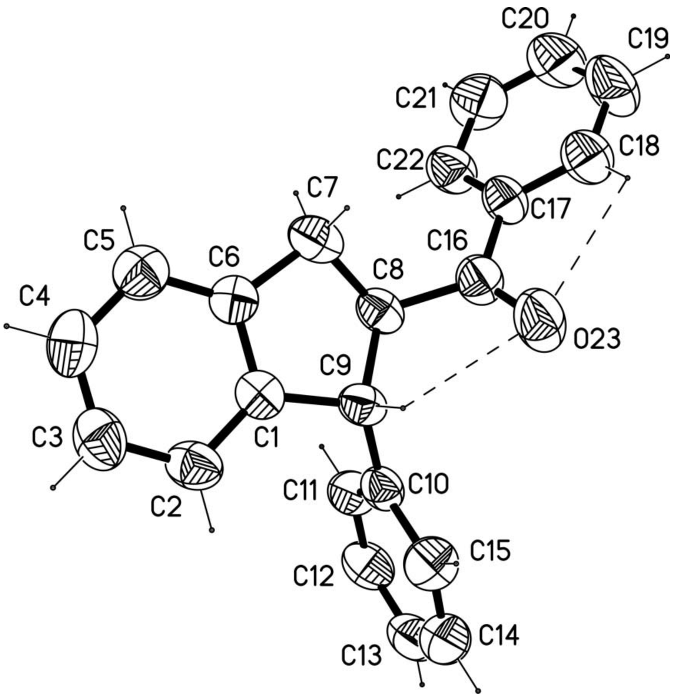


**Figure 1**
View of (I), showing the numbering scheme and displacement ellipsoids drawn at the 50% probability level. Intramolecular hydrogen bonds are shown as dashed lines.

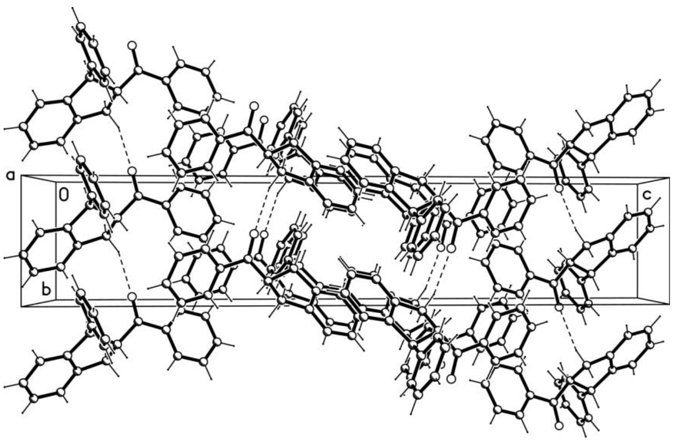


**Figure 2**
Packing diagram, showing the intermolecular hydrogen-bonding scheme (dashed lines).

C9 mean plane. The ring puckering parameters are $q_2$ = 0.312 (4) Å and $\varphi_2$ = 108.0 (7)° (Cremer & Pople, 1975). The proposed *trans* configuration in solution is also observed in this crystal structure, where the C10—C9—C8—C16 torsion angle has a value of −82.8 (4)°. Moreover, one conformation had been proposed as most probable, with a low value of the C9—C8—C16—O23 torsion angle; this torsion angle in the present crystal structure has a value of −7.9 (5)°.

A search was made for indane derivatives substituted at C8 and C9 in the CSD (Version 5.27; Allen, 2002), the C9—C10 and C8—C16 bonds being excluded from ring formation. Five were found, all of them having an envelope conformation with C8 as the flap atom, and the *trans* configuration was observed, with the C10—C9—C8—C16 torsion angle spanning a wide range of values: −38.6° in FEVHIX (Troutman *et al.*, 1999), 85.9° in QICXAB (Dandekar *et al.*, 1999), 148.9° in YUPSEH (Yang *et al.*, 1995) and 101.4° and −146.6° in YUPSIL (Yang *et al.*, 1995).

Electrostatic interactions determine the way that the molecule is folded *via* two very weak intramolecular C—H···O interactions (Fig. 1 and Table 2). O23 is also involved in an intermolecular C—H···O interaction (Fig. 2 and Table 2), generating chains of molecules running along the *b* axis. Molecules also display $\pi$–$\pi$ interactions between the C1–C6 ring and its inversion-related partner (symmetry code $1 - x$, $1 - y$, $-z$), with a centroid–centroid distance of 3.969 (2) Å and a slip angle of 28.9°, providing further cohesion to the crystal packing.

## Experimental

The compound was synthesized by the method of Mufato *et al.* (2002). Crystals suitable for X-ray diffraction were obtained by slow evaporation of a methanol solution at room temperature.

### *Crystal data*

$C_{22}H_{18}O$
$M_r$ = 298.36
Monoclinic, $P2_1/n$
$a$ = 9.085 (1) Å
$b$ = 5.981 (1) Å
$c$ = 30.091 (6) Å
$\beta$ = 95.66 (3)°
$V$ = 1627.1 (6) Å$^3$
$Z$ = 4
$D_x$ = 1.218 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 20 reflections
$\theta$ = 14–25°
$\mu$ = 0.07 mm$^{-1}$
$T$ = 293 (2) K
Needle, colourless
0.5 × 0.2 × 0.1 mm

### *Data collection*

Rigaku AFC6 diffractometer
$\omega$ scans
Absorption correction: none
6911 measured reflections
3022 independent reflections
817 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.240
$\theta_{\rm max}$ = 25.5°
$h = -1 \rightarrow 11$
$k = -7 \rightarrow 7$
$l = -36 \rightarrow 36$
3 standard reflections every 147 reflections intensity decay: none

### *Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.101
$S$ = 0.85
3022 reflections
209 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0253P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max}$ = 0.16 e Å$^{-3}$
$\Delta\rho_{\rm min}$ = −0.15 e Å$^{-3}$
Extinction correction: *SHELXL*
Extinction coefficient: 0.0036 (5)

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| C1—C6 | 1.387 (4) | C8—C16 | 1.518 (4) |
| C1—C9 | 1.521 (4) | C8—C9 | 1.547 (4) |
| C6—C7 | 1.506 (4) | C16—O23 | 1.218 (3) |
| C7—C8 | 1.552 (4) | C16—C17 | 1.491 (4) |
| | | | |
| C6—C1—C9 | 110.5 (3) | C16—C8—C9 | 113.9 (3) |
| C1—C6—C7 | 110.8 (3) | C9—C8—C7 | 104.8 (2) |
| C6—C7—C8 | 102.2 (3) | C1—C9—C8 | 101.9 (3) |

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**Table 2**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C9—H9$A$···O23 | 0.98 | 2.45 | 2.800 (4) | 101 |
| C18—H18$A$···O23 | 0.93 | 2.47 | 2.769 (4) | 99 |
| C7—H7$B$···O23$^{\rm i}$ | 0.97 | 2.40 | 3.220 (4) | 142 |

Symmetry code: (i) $x, y + 1, z$.

The crystals were very weakly diffracting, particularly at high $\theta$ values, resulting in a high $R_{\rm int}$ value and a low proportion of 'observed' reflections. H atoms were positioned geometrically (C—H = 0.93–0.98Å) and refined using a riding model, with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C).

Data collection: *AFC6S Diffractometer Control Software* (Molecular Structure Corporation, 1993); cell refinement: *AFC6S Diffractometer Control Software*; data reduction: *AFC6S Diffractometer Control Software*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-PC* (Sheldrick, 1994); software used to prepare material for publication: *SHELXTL-PC*.

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