*ware*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1995); program(s) used to solve structures: *SIR*92 (Altomare *et al.*, 1993); program(s) used to refine structures: *TEXSAN*; software used to prepare material for publication: *TEXSAN*.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: FR1071). Services for accessing these data are described at the back of the journal. Details of the synthesis and photochemistry are also available.

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# *N*-Benzyl-3-benzylideneisoindolin-1-one

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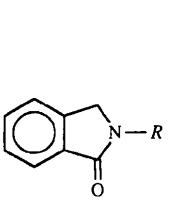
## Abstract

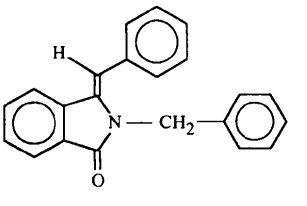
The title compound, $C_{22}H_{17}NO$, is formed by the palladium-catalyzed reaction between *N*-benzyl-*o*-iodobenzamide and phenylacetylene. The molecules contain three planar parts, namely the isoindolinone moiety (*A*) and the phenyl rings of the benzyl and benzylidene groups (*B* and *C*, respectively), and display the *Z* configuration. Rings *B* and *C* are inclined by 14.9 (1)° with respect to each other and are approximately orthogonal to the isoindolinone moiety *A*; the dihedral angles *A*/*B* and *A*/*C* are 98.23 (4) and 111.08 (3)°, respectively.

## Comment

Palladium-catalyzed heteroannulation has been found to be a useful synthetic tool for the formation of a variety of heterocyclic compounds (Chowdhury & Kundu, 1996; Spencer *et al.*, 1995; Kundu & Pal, 1993). However, efforts towards the synthesis of compounds containing the isoindolinone moiety, (1), through palladium-catalyzed reactions have been limited in nature (Cho *et al.*, 1996). Recently, we synthesized *N*-benzyl-3-benzylidene-1-isoindolinone, (2), by the palladium-catalyzed reaction between *N*-benzyl-*o*-iodobenzamide and phenylacetylene. The X-ray structural study of (2) was undertaken in order to establish the regio- and stereospecificities of the reaction.




(1)




(2)

The results of the present X-ray analysis are in agreement with those of analyses of corresponding substituted isoindolinone structures (Feeder & Jones, 1996; Barrett *et al.*, 1995; Barrett, Kahwa & Williams, 1996). The *Z* configuration of the molecule, which contains three essentially planar parts, is established by the torsion angles N—C15—C16—C17 −3.1 (2) and C15—N—C7—C6 −69.4 (2)°. The isoindolinone moiety (*A*: atoms N, C8–C15) is planar to within 0.012 (1) Å. The two phenyl rings (*B*: atoms C1–C6; *C*: atoms C17–C22), with a maximum deviation of 0.016 (2) Å for an in-plane atom (C20) from the corresponding least-squares plane

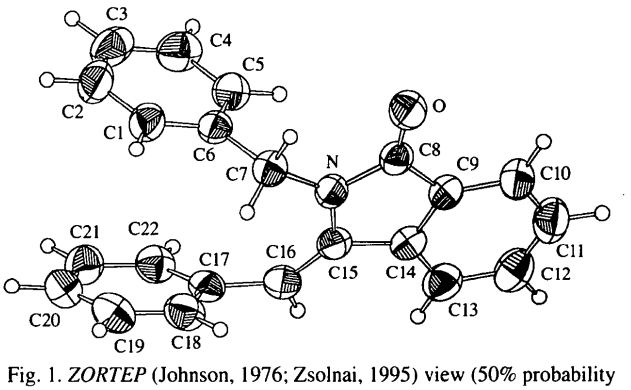



Fig. 1. *ZORTEP* (Johnson, 1976; Zsolnai, 1995) view (50% probability level) of the title molecule.

through the endocyclic atoms, are inclined by 14.9 (1)° with respect to each other. The dihedral angles *A*/*B* and *A*/*C* are 98.23 (4) and 111.08 (3)°, respectively. Interatomic distances and angles are within expected ranges. Weak C—H···O hydrogen bonds between the phenyl C atoms and the O atom of the isoindolinone group are indicated by the contacts C18—H18···O($-x+1$, $-y$, $-z+1$) 3.432 (2) and C19—H19···O($x-1$, $y$, $z$) 3.642 (2) Å.

## Experimental

Compound (2) [m.p. 395 (1) K] was synthesized by heating a mixture of *N*-benzyl-*o*-iodobenzamide and phenylacetylene in the presence of bis(triphenylphosphine)palladium(II) chloride (5 mol%), cuprous iodide (8 mol%) and triethylamine (4 equivalents) in dimethylformamide at 353 K for 16 h, followed by refluxing with sodium ethoxide in ethanol for 4 h. Single crystals suitable for X-ray analysis were obtained by slow crystallization from a dilute solution of (2) in $CCl_4$.

*Crystal data*

$C_{22}H_{17}NO$
$M_r$ = 311.37
Triclinic
$P\bar{1}$
$a$ = 8.545 (1) Å
$b$ = 9.643 (1) Å
$c$ = 10.807 (1) Å
$\alpha$ = 88.80 (1)°
$\beta$ = 67.61 (1)°
$\gamma$ = 82.98 (1)°
$V$ = 816.9 (2) Å$^3$
$Z$ = 2
$D_x$ = 1.266 Mg m$^{-3}$
$D_m$ not measured

Cu $K\alpha$ radiation
$\lambda$ = 1.5418 Å
Cell parameters from 25 reflections
$\theta$ = 10–20°
$\mu$ = 0.604 mm$^{-1}$
$T$ = 293 (2) K
Prism
0.50 × 0.40 × 0.32 mm
Colourless

*Data collection*

Enraf–Nonius CAD-4 diffractometer
$\omega$–2$\theta$ scans
Absorption correction: $\psi$ scan (North, Phillips & Mathews, 1968)
$T_{min}$ = 0.768, $T_{max}$ = 0.824
3473 measured reflections
3242 independent reflections

3009 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.012
$\theta_{max}$ = 75.75°
$h = 0 \rightarrow 10$
$k = -12 \rightarrow 12$
$l = -12 \rightarrow 13$
3 standard reflections
every 50 reflections
intensity decay: <2%

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.118
$S$ = 1.137
3242 reflections
285 parameters
H atoms refined isotropically
$w = 1/[\sigma^2(F_o^2) + (0.0668P)^2 + 0.0932P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = −0.001
$\Delta\rho_{max}$ = 0.158 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.235 e Å$^{-3}$
Extinction correction: none
Scattering factors from *International Tables for Crystallography* (Vol. C)

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

| | | | |
|---|---|---|---|
| O—C8 | 1.2217 (14) | C8—C9 | 1.469 (2) |
| N—C8 | 1.3839 (14) | C9—C14 | 1.385 (2) |
| N—C15 | 1.4119 (14) | C14—C15 | 1.475 (2) |
| N—C7 | 1.4511 (15) | C15—C16 | 1.337 (2) |
| C6—C7 | 1.510 (2) | C16—C17 | 1.478 (2) |
| C8—N—C15 | 111.70 (10) | N—C8—C9 | 106.38 (10) |
| C8—N—C7 | 120.44 (9) | C14—C9—C8 | 108.18 (10) |
| C15—N—C7 | 127.78 (9) | C9—C14—C15 | 108.60 (10) |
| N—C7—C6 | 115.17 (10) | N—C15—C14 | 105.11 (9) |
| O—C8—N | 125.02 (11) | C15—C16—C17 | 129.60 (12) |
| O—C8—C9 | 128.60 (11) | | |
| C7—N—C15—C16 | 1.1 (2) | N—C8—C9—C14 | 1.3 (1) |
| C8—N—C15—C14 | 1.4 (1) | C8—C9—C14—C15 | −0.4 (1) |
| C15—N—C7—C6 | −69.4 (2) | C9—C14—C15—N | −0.6 (1) |
| C15—N—C8—C9 | −1.7 (1) | N—C15—C16—C17 | −3.1 (2) |

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989). Cell refinement: *CAD-4 Software*. Data reduction: *CAD-4 Software*. Program(s) used to solve structure: *MULTAN88* (Debaerdemaeker *et al.*, 1988). Program(s) used to refine structure: *SHELXL93* (Sheldrick, 1993). Molecular graphics: *ZORTEP* (Zsolnai, 1995; Johnson, 1976). Software used to prepare material for publication: *SHELXL93*.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: HA1197). Services for accessing these data are described at the back of the journal.

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