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*.

We thank the Natural Sciences and Engineering Research Council of Canada for financial support.

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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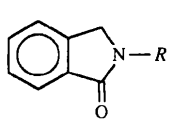
(*Received 23 June 1997; accepted 9 September 1997*)

Abstract

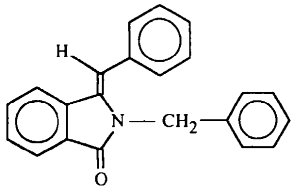
The title compound, $C_{22}H_{17}NO$, is formed by the palladium-catalyzed reaction between *N*-benzyl-*o*-iodobenzamide and phenylacetylene. The molecules contain three planar parts, namely the isoindolinone moiety (*A*) and the phenyl rings of the benzyl and benzylidene groups (*B* and *C*, respectively), 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

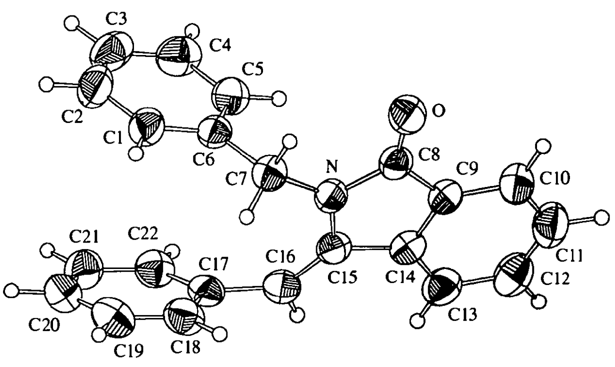


Fig. 1. *ZORTEP* (Johnson, 1976; Zsolnai, 1995) view (50% probability level) of the title molecule.

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
ω–2θ scans
Absorption correction: ψ scan (North, Phillips & Mathews, 1968)
$T_{\min} = 0.768$, $T_{\max} = 0.824$
3473 measured reflections
3242 independent reflections

3009 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.012$
$\theta_{\max} = 75.75°$
$h = 0 \rightarrow 10$
$k = -12 \rightarrow 12$
$l = -12 \rightarrow 13$
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: *MULTAN*88 (Debaerdemaeker *et al.*, 1988). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *ZORTEP* (Zsolnai, 1995; Johnson, 1976). Software used to prepare material for publication: *SHELXL*93.

The authors wish to acknowledge the use of the National Single Crystal X-ray Diffractometer Facility at the All India Institute of Medical Sciences, New Delhi, India. Financial support from the Council of Scientific and Industrial Research [grant No. 01 (1385)/95/EMR-II to NGK], New Delhi, India, is gratefully acknowledged.

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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