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N-Phenylbenzimidic acid 2-allylphenyl ester

Yuping Guo,[a] Bing Zhao,[b] Chun-Bao Li,[a] Wei-Min Gao,[c] Jie Li[a] and Yang Li[b]*

[a]Department of Chemistry, Tianjin University, Tianjin 300072, People's Republic of China, [b]School of Chemical Engineering and Technology, Tianjin University, Tianjin 300072, People's Republic of China, and [c]Material Research Institute, Jiangxi Science and Technology Normal University, Nanchang 330013, People's Republic of China

Correspondence e-mail: yupguo@sohu.com

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.036
wR factor = 0.101
Data-to-parameter ratio = 13.9

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

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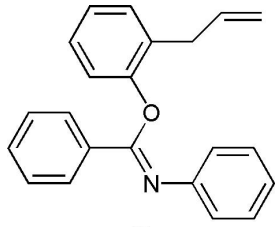
In the title compound, $C_{22}H_{19}NO$, the Csp^2 atom of the benzimido group reveals a distorted trigonal geometry, which results in the approximately overall trigonal shape of the molecule.

Comment

N-Phenylbenzimidic acid esters belong to an important class of intermediates in the Chapman rearrangement (Relles, 1968). A large number of substituted *N*-phenylbenzimidic acid ester analogues have been synthesized and investigated (Rowe, 1980). The title compound, (I), has been prepared by our group from the substrate of *N*-phenylbenzimidoyll chloride. The X-ray crystal structure determination of (I) was carried out and the results are presented here.



(I)

The molecular structure of (I) and the atom-numbering scheme are shown in Fig. 1. The C17—N1—C10—C11 torsion angle of 9.3 (3)° indicates that the two phenyl rings attached to atoms C10 (ring *A*) and N1 (ring *B*) are in a *cis*-configuration. The dihedral angle between these rings is 63.7°(4). Rings *A* and *B* make dihedral angles of 55.6 (3) and 78.6 (4)°, respectively, with ring *C* (attached to oxygen); rings *B* and *C* are thus close to be orthogonal. Atom C10 has a distorted trigonal geometry [N1—C10—C11 = 130.27 (13)°]. The conjugation of bonds involved explains the distortion from regular sp^2 hybridization.

Experimental

N-Phenylbenzimidoyl chloride (0.28 g,1.3 mmol) in dichloromethane (10 ml) was added to a rapidly stirred solution of 2-allylphenol (0.19 g, 1.4 mmol), sodium hydroxide (0.055 g, 1.4 mmol) and tetrabutylammonium bromide (0.010 g, 0.03 mmol) in water (10 ml). The mixture was stirred at room temperature for 3 h. The mixture was diluted with chloroform (20 ml), the organic layer separated, dried with anhydrous sodium sulfate, and evaporated to give the crude product which was recrystallized from ethanol; m.p. 323 K. IR (KBr, ν cm^{-1}): 1666, 1637, 1593, 1485, 1444, 1089; ^{1}H NMR ($CDCl_3$, δ, p.p.m.): 7.4–6.9 (*m*, 14H), 6.0 (*m*, 1H), 5.1 (*d*, 2H), 3.5 (*d*, 2H).

Crystal data

$C_{22}H_{19}NO$	$Z = 2$
$M_r = 313.38$	$D_x = 1.214$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo Kα radiation
$a = 9.6168$ (13) Å	Cell parameters from 1319 reflections
$b = 9.7218$ (13) Å	$\theta = 2.3$–22.7°
$c = 10.7494$ (15) Å	$\mu = 0.07$ mm^{-1}
$\alpha = 64.237$ (2)°	$T = 293$ (2) K
$\beta = 71.310$ (2)°	Block, colourless
$\gamma = 80.941$ (2)°	0.24 × 0.22 × 0.20 mm
$V = 857.2$ (2) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	2055 reflections with $I > 2\sigma(I)$
	$R_{int} = 0.014$
φ and ω scans	$\theta_{max} = 25.0^\circ$
Absorption correction: none	$h = -11 \rightarrow 11$
4715 measured reflections	$k = -11 \rightarrow 11$
3026 independent reflections	$l = -12 \rightarrow 12$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0501P)^2 + 0.0427P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.036$	
$wR(F^2) = 0.101$	
$S = 1.05$	$(\Delta/\sigma)_{max} < 0.001$
3026 reflections	$\Delta\rho_{max} = 0.24$ e Å^{-3}
217 parameters	$\Delta\rho_{min} = -0.16$ e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

N1—C10	1.2567 (17)	O1—C10	1.3685 (16)
N1—C17	1.4110 (18)	O1—C1	1.4101 (16)
C10—N1—C17	122.90 (12)	N1—C10—C11	130.27 (13)
C10—O1—C1	116.93 (10)	O1—C10—C11	110.12 (12)

H atoms were placed in calculated positions (C—H = 0.93–0.97 Å) and allowed to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(parent atom).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

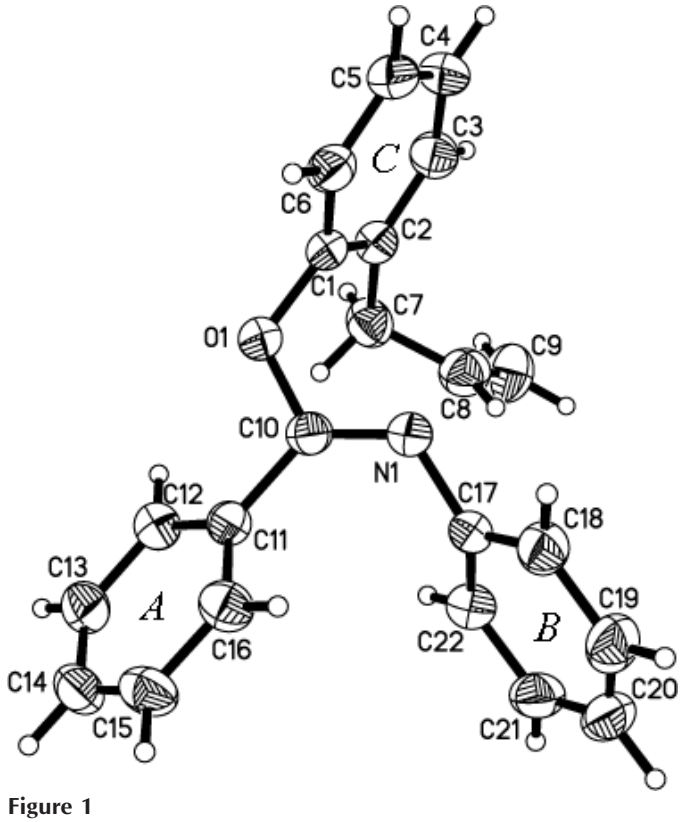


Figure 1
View of the molecule of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

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