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N-Benzhydrylformamide

Chao Hua,* Xin-Gang Li and Shi-Min Xu

National Peiyang Distillation Technology Engineering Limited Company, Tianjin 300072, People's Republic of China, and, School of Chemical Engineering and Technology, Tianjin University, Tianjin 300072, People's Republic of China

Correspondence e-mail:
huacao1978@yahoo.com.cn

Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.044
wR factor = 0.148
Data-to-parameter ratio = 14.2

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

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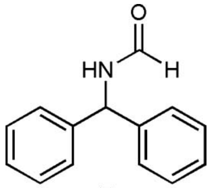
In the title compound, $C_{14}H_{13}ON$, the angle between the two phenyl rings is 100.7 (8)°. The amide group is planar and the phenyl rings subtend angles of 79.4 (9) and 52.3 (1)° to this plane. In the crystal structure, molecules are linked *via* intermolecular N—H···O interactions.

Comment

α-Aminophosphonic acid derivatives show activity as enzyme inhibitors, antibiotics, herbicides, fungicides or plant-growth regulators (Yang *et al.*, 2004). Benzhydrylamine (Haak, *et al.*, 2002), which is used as a starting material for the synthesis of α-aminophosphonic acid, can be easily prepared by hydrolysis of the title compound, *N*-benzhydrylformamide, (I) (Leuckart & Bach, 1886), whose structure is reported here (Fig. 1).



(I)

In (I), the angle between the two phenyl rings (C2–C7 and C8–C13) is 100.7 (8)°. The amide group (C1/N1/C14/O14) is planar; the maximum deviation from the mean plane is 0.005 (4) Å for atom C14. The aromatic rings C2–C7 and C8–C13 subtend angles of 79.4 (9) and 52.3 (1)°, respectively, to

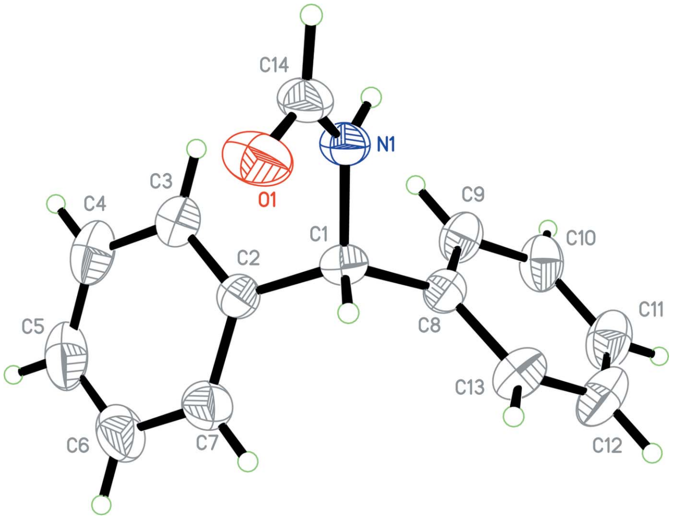


Figure 1
The molecular structure of (I), shown with 30% probability displacement ellipsoids (arbitrary spheres for H atoms).

this plane. In the crystal structure, N—H⋯O hydrogen bonds link the molecules into chains along the *b* axis (Fig. 2 and Table 1).

Experimental

The title compound, (I), was synthesized according to the procedure of Webers & Bruce (1948). Crystals suitable for X-ray analysis were grown by slow evaporation of a solution in absolute ethanol at room temperature over a period of 10 d.

Crystal data

$C_{14}H_{13}NO$
$M_r = 211.25$
Orthorhombic, *Pbca*
$a = 16.131$ (3) Å
$b = 8.2721$ (18) Å
$c = 17.602$ (4) Å
$V = 2348.7$ (9) Å^3

$Z = 8$
$D_x = 1.195$ Mg m^{-3}
Mo *Kα* radiation
$\mu = 0.08$ mm^{-1}
$T = 294$ (2) K
Block, colourless
0.22 × 0.14 × 0.10 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
$T_{\min} = 0.984$, $T_{\max} = 0.993$

10973 measured reflections
2068 independent reflections
1148 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.063$
$\theta_{\max} = 25.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.148$
$S = 1.03$
2068 reflections
146 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0628P)^2 + 0.5126P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.15$ e Å^{-3}
$\Delta\rho_{\min} = -0.18$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.028 (2)

Table 1
Hydrogen-bond geometry (Å, °).

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N1—H1⋯O1$^{\rm i}$	0.86	1.97	2.804 (3)	162

Symmetry code: (i) $-x + \frac{1}{2}, y - \frac{1}{2}, z$.

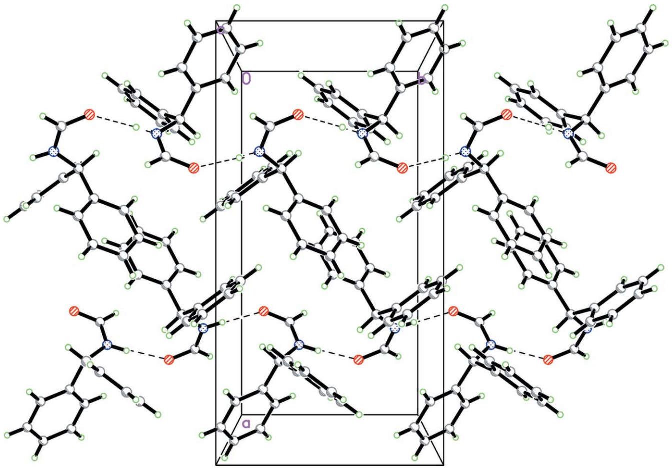


Figure 2
Part of the crystal structure of (I), with hydrogen bonds shown as dashed lines.

All H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 Å and $U_{\rm iso}(H) = 1.2U_{\rm eq}(C)$ for aromatic, C—H = 0.98 Å and $U_{\rm iso}(H) = 1.2U_{\rm eq}(C)$ for CH, and N—H = 0.86 Å and $U_{\rm iso}(H) = 1.2U_{\rm eq}(N)$ for the amide H 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*.

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