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(*E*)-1-[4-(Benzyloxy)benzylidene]-2-(4-nitrophenyl)-hydrazine

Shi Jun‡

Department of Basic Course, Tianjin Agricultural College, Tianjin 300384, People's Republic of China

‡ Current address: School of Chemical Engineering and Technology, Tianjin University, Tianjin 300072, People's Republic of China.

Correspondence e-mail: shi_jun99@163.com

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Key indicators

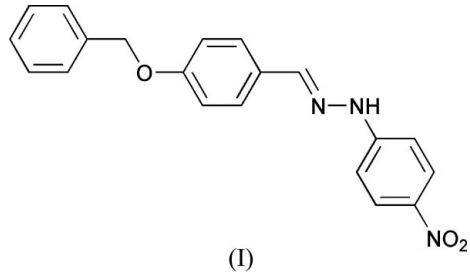
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.050
wR factor = 0.127
Data-to-parameter ratio = 15.5

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

The title compound, $C_{20}H_{17}N_3O_3$, was prepared by the reaction of 4-(benzyloxy)benzaldehyde and 1-(4-nitrophenyl)hydrazine. In the crystal structure, the central benzene ring makes dihedral angles of 3.16 (12) and 64.87 (6)° with the *p*-nitrophenyl and phenyl rings, respectively. The crystal packing is stabilized by intermolecular N—H···O hydrogen bonds.

Comment

In continuation of our search for new Schiff bases functioning as ligands (Jun, 2005), we present the crystal structure of the title compound, (I).



(I)

In (I) (Fig. 1), the bond lengths and angles (Table 1) are normal. The benzene ring (C8–C13) makes dihedral angles of 64.87 (6) and 3.16 (12)° with the phenyl (C1–C6) and benzene (C15–C20) rings, respectively. The crystal packing (Fig. 2) is stabilized by the intermolecular N—H···O hydrogen bonds (Table 2).

Experimental

An anhydrous ethanol solution of 4-(benzyloxy)benzaldehyde (2.12 g,10 mmol) was added to an anhydrous ethanol solution of 1-(4-nitrophenyl)hydrazine (1.53 g, 10 mmol), and the mixture was stirred at 350 K for 5 h under nitrogen. A yellow precipitate was isolated, recrystallized from ethanol, and then dried *in vacuo* to give the pure compound in 87% yield. Yellow single crystals suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution of (I).

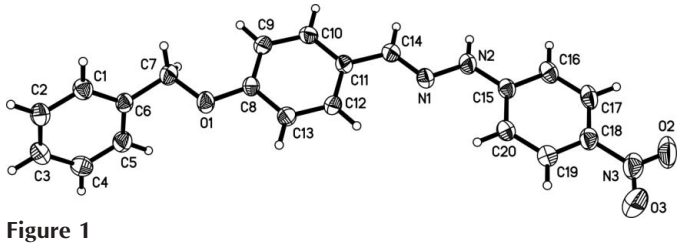


Figure 1
The structure of (I), with displacement ellipsoids for non-H atoms drawn at the 30% probability level.

Crystal data

$C_{20}H_{17}N_3O_3$
M_r = 347.37
Monoclinic, $P2_1/c$
a = 6.148 (3) Å
b = 36.651 (15) Å
c = 7.938 (3) Å
β = 93.551 (7)°
V = 1785.2 (13) Å^3
Z = 4
D_x = 1.292 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1822 reflections
θ = 2.6–22.7°
μ = 0.09 mm^{-1}
T = 294 (2) K
Block, yellow
0.40 × 0.34 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.958, T_{max} = 0.982
10028 measured reflections
3643 independent reflections
1738 reflections with $I > 2\sigma(I)$
R_{int} = 0.051
θ_{max} = 26.5°
$h = -7 \rightarrow 7$
$k = -18 \rightarrow 45$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.127
S = 1.00
3643 reflections
235 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0516P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C8	1.374 (2)	N1—C14	1.284 (2)
O1—C7	1.433 (2)	N1—N2	1.368 (2)
O2—N3	1.238 (3)	N2—C15	1.368 (3)
O3—N3	1.227 (3)	N3—C18	1.453 (3)
C8—O1—C7	117.79 (16)	O3—N3—O2	123.5 (3)
C14—N1—N2	117.18 (19)	O3—N3—C18	119.1 (3)
C15—N2—N1	120.48 (19)	O2—N3—C18	117.4 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O2^{i}	0.86	2.06	2.912 (3)	170

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

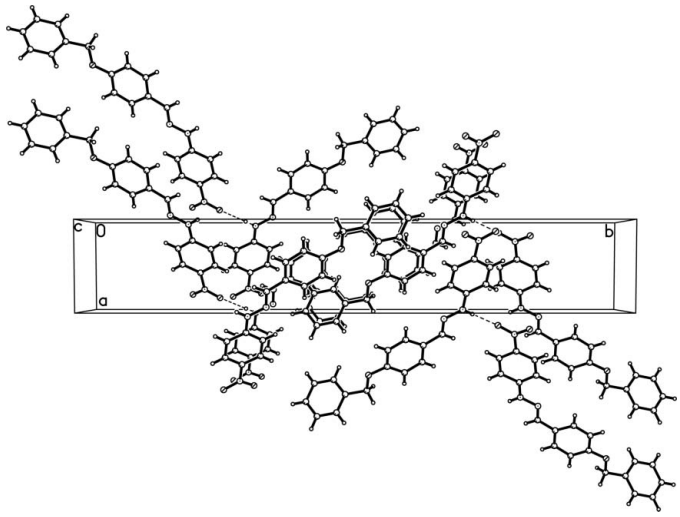


Figure 2
View of the crystal packing, with the intermolecular N—H···O hydrogen bonds shown by dashed lines.

All H atoms were included in calculated positions and refined using a riding-model approximation, with C—H = 0.93–0.97 Å, N—H = 0.86 Å and U_{iso}(H) = 1.2U_{eq}(C,N).

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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