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# (*E*)-1-(4-Methoxy-3-propoxybenzylidene)-2-(4-nitrophenyl)hydrazine

**Jun Shi‡**

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

**Key indicators**

Single-crystal X-ray study
*T* = 294 K
Mean σ(C–C) = 0.006 Å
*R* factor = 0.053
*wR* factor = 0.176
Data-to-parameter ratio = 13.5

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



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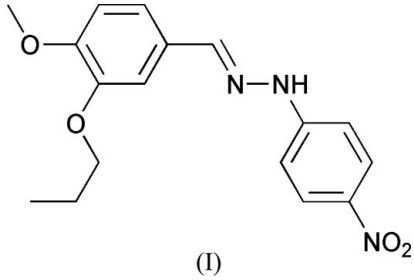
The molecule of the title compound, $C_{17}H_{19}N_3O_4$, is not planar. The isovanillin group makes a dihedral angle of 3.23 (14)° with the phenylhydrazine residue. The nitro group and its attached aromatic ring are not coplanar, the dihedral angle between them being 3.18 (6)°. Intermolecular N—H···O and C—H···O hydrogen bonds link adjacent molecules, forming infinite chains.

## Comment

Metal complexes based on Schiff bases have attracted much attention in biology and chemistry (Kahwa *et al.*, 1986). Consequently, numerous derivatives of Schiff bases have been developed for applications such as protein and enzyme mimics (Santos *et al.*, 2001). Structural investigations provide useful information on the coordination properties of Schiff bases functioning as ligands. In the present study, we report the synthesis and molecular structure of a nitrophenylhydrazine Schiff base derivative, (I) (Fig. 1 and Table 1).




(I)

In (I), the isovanillin group (C1–C6/C10/C11/O1/O2) is planar, with an r.m.s. deviation for the fitted atoms of 0.0230 Å. The phenylhydrazine residue (C12–C17/N1/N2) is

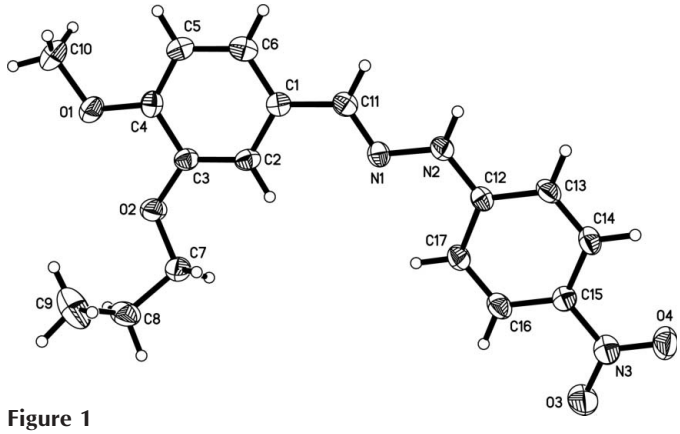



**Figure 1**
The structure of (I), with displacement ellipsoids for non-H atoms drawn at the 30% probability level.

also planar, the r.m.s. deviation being 0.0129 Å; the dihedral angle between these two planes is 3.23 (14)°. The nitro group (O3/N3/O4) and its attached aromatic ring are not coplanar, the dihedral angle being 3.18 (6)°. All bond lengths and angles (Table 1) are within normal ranges (Allen *et al.*, 1987). The packing is stabilized by intermolecular N2—H2···O3 hydrogen bonds, which form infinite chains along the *b* axis, together with weak non-classical intermolecular C13—H13···O3 hydrogen bonds (Fig. 2 and Table 2).

## Experimental

An anhydrous ethanol solution of 4-methoxy-3-propoxybenzaldehyde (1.94 g, 10 mmol) was added to an anhydrous ethanol solution of 1-(4-nitrophenyl)hydrazine (1.53 g, 10 mmol), and the mixture stirred at 350 K for 5 h under nitrogen. A red product precipitated and this was isolated, recrystallized from ethanol and dried in a vacuum to give the pure compound in 85% yield. Red single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an acetonitrile solution.

*Crystal data*

$C_{17}H_{19}N_3O_4$
$M_r$ = 329.35
Monoclinic, $P2_1/n$
$a$ = 4.5854 (13) Å
$b$ = 14.953 (4) Å
$c$ = 24.363 (7) Å
$\beta$ = 92.475 (5)°
$V$ = 1668.9 (8) Å$^3$
$Z$ = 4
$D_x$ = 1.311 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 1175 reflections
$\theta$ = 2.9–23.1°
$\mu$ = 0.10 mm$^{-1}$
$T$ = 294 (2) K
Block, red
0.20 × 0.16 × 0.12 mm

*Data collection*

Bruker SMART APEX CCD area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.967, $T_{max}$ = 0.989
8289 measured reflections
2949 independent reflections
1219 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.090
$\theta_{max}$ = 25.0°
$h = -4 \rightarrow 5$
$k = -14 \rightarrow 17$
$l = -28 \rightarrow 28$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.176
$S$ = 0.99
2949 reflections
219 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0744P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.18 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.20 e Å$^{-3}$

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

| | | | |
|---|---|---|---|
| O1—C4 | 1.361 (4) | O4—N3 | 1.219 (4) |
| O1—C10 | 1.422 (4) | N1—C11 | 1.276 (4) |
| O2—C3 | 1.371 (4) | N1—N2 | 1.357 (4) |
| O2—C7 | 1.420 (4) | N2—C12 | 1.354 (4) |
| O3—N3 | 1.239 (4) | N3—C15 | 1.430 (5) |
| | | | |
| C4—O1—C10 | 118.5 (3) | O1—C4—C5 | 125.0 (4) |
| C3—O2—C7 | 118.2 (3) | O1—C4—C3 | 115.8 (4) |
| C11—N1—N2 | 116.7 (3) | O2—C7—C8 | 107.0 (3) |
| C12—N2—N1 | 121.3 (3) | N1—C11—C1 | 122.5 (4) |
| O4—N3—O3 | 121.5 (4) | N2—C12—C13 | 119.8 (3) |
| O4—N3—C15 | 120.4 (4) | N2—C12—C17 | 121.3 (3) |
| O3—N3—C15 | 118.1 (3) | C16—C15—N3 | 120.5 (4) |
| O2—C3—C4 | 114.3 (3) | C14—C15—N3 | 119.5 (4) |

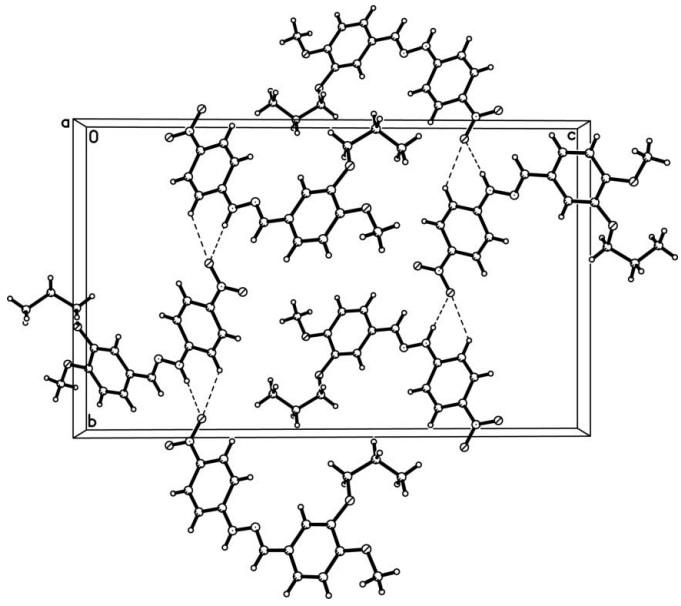



**Figure 2**
A packing diagram for (I), with hydrogen bonds shown as dashed lines.

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N2—H2···O3$^{i}$ | 0.86 | 2.19 | 2.968 (4) | 151 |
| C13—H13···O3$^{i}$ | 0.93 | 2.58 | 3.298 (5) | 135 |

Symmetry code: (i) $-x+\frac{5}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$.

H atoms were included in calculated positions and refined using a riding-model approximation. Constrained C—H and N—H bond lengths and isotropic $U$ parameters were as follows: 0.93 Å and $U_{iso}$(H) = 1.2$U_{eq}$(C) for aromatic; 0.97 Å and $U_{iso}$(H) = 1.2$U_{eq}$(C) for methylene; 0.96 Å and $U_{iso}$(H) = 1.5$U_{eq}$(C) for methyl; 0.86 Å and $U_{iso}$(H) = 1.2$U_{eq}$(N) for NH H atoms.

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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