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# (*E*)-*N*′-[(*E*)-3-Phenylallylidene]benzohydrazide

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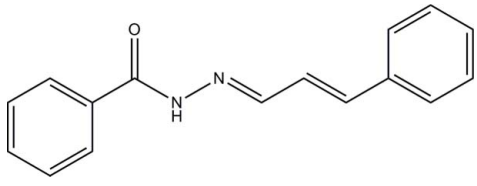
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.041; $wR$ factor = 0.096; data-to-parameter ratio = 10.0.

In the title molecule, $C_{16}H_{14}N_2O$, the dihedral angle between the two phenyl rings is 23.5 (6)°. In the crystal, N—H—O hydrogen bonds link molecules into chains running along the *a* axis.

## Related literature

For general background to the applications of Schiff bases in the pharmaceutical and agrochemical fields, see: Bernardino *et al.* (2006); Zhang *et al.* (2008). For related structures, see: Ji & Shi (2008); He & Liu (2005); Zhen & Han (2005); Zhang *et al.* (2007).



## Experimental

### *Crystal data*

$C_{16}H_{14}N_2O$
$M_r$ = 250.29
Orthorhombic, $Pna2_1$
$a$ = 8.427 (3) Å
$b$ = 10.439 (4) Å
$c$ = 15.724 (6) Å
$V$ = 1383.2 (9) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.08 mm$^{-1}$
$T$ = 296 K
0.16 × 0.13 × 0.10 mm

### *Data collection*

Bruker APEXII CCD diffractometer
6868 measured reflections
1761 independent reflections
1361 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.040

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.096
$S$ = 1.01
1761 reflections
176 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.09 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.12 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1$A$···O1$^{i}$ | 0.88 (2) | 2.05 (2) | 2.898 (3) | 161 (2) |

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2003); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

This work was supported by the National Natural Science Foundation of China (30940094) and the Science Foundation for Excellent Youth Scholars of the Education Commission of Hunan Province, China (10B077).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV5216).

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# supporting information

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## (*E*)-*N*′-[(*E*)-3-Phenylallylidene]benzohydrazide

**Gui-Ming Deng, Zhen Chen, Chao-Run Wang and He-Ming Zhang**

### S1. Comment

Schiff bases have attracted much attention due to their various activities in pharmaceutical and agrochemical fields (Bernardino *et al.*, 2006; Zhang *et al.*, 2008). We now report the synthesis and structure of the title compound, (I).

In (I) (Fig. 1), the Schiff base molecule adopts an *E* geometry with respect to the C=N bond. All bond lengths and angles are normal and comparable with those found in the related compounds (Ji *et al.*, 2008; He *et al.*., 2005; Zhen *et al.*, 2005; Zhang *et al.*., 2007). The dihedral angle between the two benzene rings is 23.5 (6)°.

In the crystal structure, intermolecular N—H—O hydrogen bonds (Table 1) link molecules into chains running along the *a* axis (Fig. 2).

### S2. Experimental

The title compound was synthesized by the reaction of benzoylhydrazine (1 mmol, 136.2 mg) with 3-phenyl-propenal (1 mmol, 132.2 mg) in ethanol (20 ml) under reflux conditions (348 K) for 6 h. The solvent was removed and the solid product recrystallized from tetrahydrofuran. After two days yellow crystals suitable for X-ray diffraction study were obtained. Yield, 222.7 mg, 83%. Analysis calculated for $C_{16}H_{14}N_2O$: C 76.78, H 5.64, N 11.19%; found: C 76.73, H 5.61, N 11.21%.

### S3. Refinement

The H1A atom bonded to N1 was located in a difference map and refined isotropically, other H atoms were placed in geometrically idealized positions and allowed to ride on their parent atoms,*C*—H=0.93, with $U_{iso}$(H)=1.2$U_{eq}$(C). In the absence of any significant anomalous scatterers in the molecule, the 1215 Friedel pairs were merged before the final refinement.

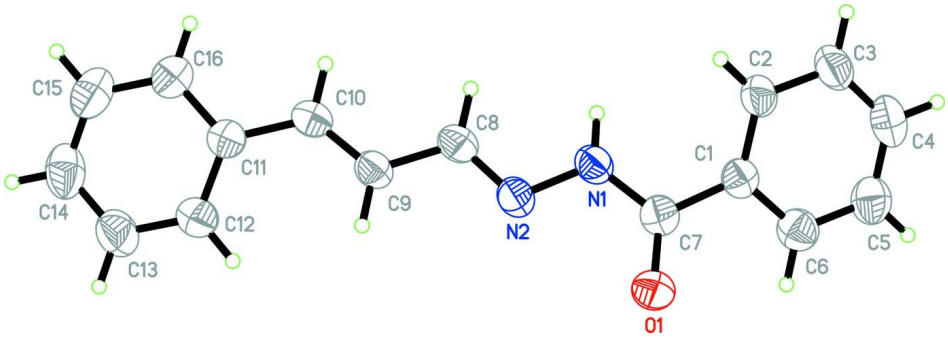


**Figure 1**

The molecular structure of (I) showing the atomic numbering and 30% probability displacement ellipsoids.

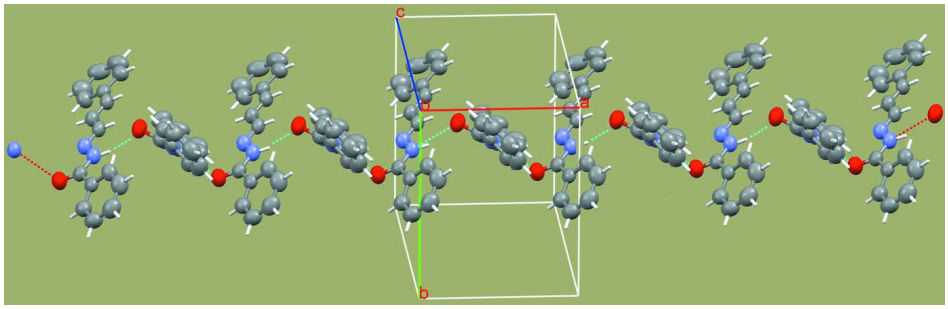


**Figure 2**

A portion of the packing, viewed down the *a* axis. The dashed lines represent the intermolecular hydrogen bonds.

### (*E*)-*N*′-[(*E*)-3-Phenylallylidene]benzohydrazide

*Crystal data*

$C_{16}H_{14}N_2O$
$M_r = 250.29$
Orthorhombic, $Pna2_1$
Hall symbol: P 2c -2n
$a = 8.427$ (3) Å
$b = 10.439$ (4) Å
$c = 15.724$ (6) Å
$V = 1383.2$ (9) Å$^3$
$Z = 4$
$F(000) = 528.0$
$D_x = 1.202$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 968 reflections
$\theta = 0.5$–$3.2°$
$\mu = 0.08$ mm$^{-1}$
$T = 296$ K
Block, yellow
0.16 × 0.13 × 0.10 mm

*Data collection*

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and $\omega$ scans
6868 measured reflections
1761 independent reflections
1361 reflections with $I > 2\sigma(I)$
$R_{int} = 0.040$
$\theta_{max} = 28.2°$, $\theta_{min} = 2.3°$
$h = -11 \rightarrow 11$
$k = -12 \rightarrow 13$
$l = -14 \rightarrow 20$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.096$
$S = 1.01$
1761 reflections
176 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0355P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.09$ e Å$^{-3}$
$\Delta\rho_{min} = -0.12$ e Å$^{-3}$

*Special details*

**Geometry**. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on $F^2$, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative $F^2$. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on $F^2$ are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 1.0668 (3) | 0.6483 (2) | 0.48249 (16) | 0.0652 (6) |
| C2 | 0.9616 (3) | 0.7307 (2) | 0.44374 (17) | 0.0759 (7) |
| H2 | 0.9252 | 0.8027 | 0.4727 | 0.091* |
| C3 | 0.9099 (3) | 0.7064 (3) | 0.36146 (18) | 0.0946 (9) |
| H3 | 0.8373 | 0.7612 | 0.3357 | 0.114* |
| C4 | 0.9659 (4) | 0.6012 (4) | 0.3178 (2) | 0.0980 (9) |
| H4 | 0.9308 | 0.5851 | 0.2628 | 0.118* |
| C5 | 1.0721 (4) | 0.5212 (3) | 0.3549 (2) | 0.0919 (8) |
| H5 | 1.1107 | 0.4508 | 0.3251 | 0.110* |
| C6 | 1.1229 (3) | 0.5441 (3) | 0.4371 (2) | 0.0832 (7) |
| H6 | 1.1957 | 0.4889 | 0.4622 | 0.100* |
| C7 | 1.1258 (3) | 0.6639 (2) | 0.57099 (17) | 0.0686 (6) |
| C8 | 0.9802 (3) | 0.8064 (2) | 0.75525 (16) | 0.0697 (7) |
| H8 | 0.8937 | 0.8469 | 0.7302 | 0.084* |
| C9 | 1.0068 (3) | 0.8183 (2) | 0.84500 (16) | 0.0689 (7) |
| H9 | 1.0972 | 0.7808 | 0.8680 | 0.083* |
| C10 | 0.9088 (3) | 0.8803 (2) | 0.89690 (17) | 0.0720 (7) |
| H10 | 0.8252 | 0.9235 | 0.8710 | 0.086* |
| C11 | 0.9157 (3) | 0.8892 (2) | 0.98938 (17) | 0.0670 (6) |
| C12 | 1.0264 (3) | 0.8252 (3) | 1.03800 (18) | 0.0859 (8) |
| H12 | 1.1026 | 0.7750 | 1.0112 | 0.103* |
| C13 | 1.0268 (4) | 0.8341 (3) | 1.1250 (2) | 0.1066 (10) |
| H13 | 1.1025 | 0.7899 | 1.1565 | 0.128* |
| C14 | 0.9169 (5) | 0.9073 (3) | 1.1655 (2) | 0.1060 (11) |
| H14 | 0.9170 | 0.9130 | 1.2245 | 0.127* |
| C15 | 0.8062 (4) | 0.9724 (3) | 1.1190 (2) | 0.1051 (11) |
| H15 | 0.7315 | 1.0233 | 1.1465 | 0.126* |
| C16 | 0.8049 (3) | 0.9630 (2) | 1.03158 (18) | 0.0849 (8) |
| H16 | 0.7284 | 1.0070 | 1.0006 | 0.102* |
| H1A | 0.938 (3) | 0.761 (2) | 0.6107 (14) | 0.062 (7)* |
| N1 | 1.0322 (3) | 0.7305 (2) | 0.62472 (13) | 0.0713 (6) |
| N2 | 1.0757 (2) | 0.7398 (2) | 0.70954 (13) | 0.0714 (6) |
| O1 | 1.25170 (19) | 0.61572 (17) | 0.59406 (13) | 0.0867 (5) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0605 (13) | 0.0711 (14) | 0.0640 (16) | −0.0100 (13) | 0.0033 (13) | 0.0047 (13) |
| C2 | 0.0778 (15) | 0.0902 (17) | 0.0597 (16) | 0.0012 (13) | 0.0077 (16) | 0.0089 (15) |
| C3 | 0.094 (2) | 0.125 (2) | 0.064 (2) | 0.0053 (19) | −0.0004 (17) | 0.0212 (19) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C4 | 0.108 (2) | 0.125 (2) | 0.0611 (19) | −0.021 (2) | 0.0000 (18) | 0.0016 (19) |
| C5 | 0.107 (2) | 0.0881 (18) | 0.080 (2) | −0.0092 (18) | −0.0003 (17) | −0.0115 (18) |
| C6 | 0.0847 (16) | 0.0818 (16) | 0.083 (2) | −0.0035 (14) | −0.0061 (17) | −0.0025 (16) |
| C7 | 0.0635 (14) | 0.0725 (15) | 0.0697 (18) | −0.0098 (13) | −0.0013 (14) | 0.0004 (14) |
| C8 | 0.0603 (14) | 0.0779 (17) | 0.0708 (18) | −0.0045 (13) | −0.0098 (14) | 0.0068 (14) |
| C9 | 0.0631 (14) | 0.0798 (17) | 0.0639 (17) | −0.0003 (13) | −0.0082 (13) | 0.0039 (13) |
| C10 | 0.0632 (15) | 0.0773 (16) | 0.0756 (18) | 0.0023 (14) | −0.0107 (14) | 0.0051 (14) |
| C11 | 0.0671 (14) | 0.0620 (13) | 0.0718 (18) | −0.0046 (13) | −0.0022 (15) | 0.0013 (12) |
| C12 | 0.0867 (18) | 0.0919 (18) | 0.079 (2) | 0.0115 (17) | −0.0065 (16) | 0.0057 (18) |
| C13 | 0.139 (3) | 0.106 (2) | 0.075 (2) | 0.012 (2) | −0.015 (2) | 0.011 (2) |
| C14 | 0.166 (3) | 0.0823 (19) | 0.069 (2) | −0.018 (2) | 0.009 (2) | 0.0045 (17) |
| C15 | 0.138 (3) | 0.081 (2) | 0.097 (3) | 0.000 (2) | 0.030 (2) | −0.0086 (18) |
| C16 | 0.0878 (19) | 0.0784 (16) | 0.088 (2) | 0.0029 (16) | 0.0050 (16) | −0.0050 (15) |
| N1 | 0.0655 (13) | 0.0850 (15) | 0.0634 (15) | −0.0003 (12) | −0.0073 (13) | 0.0041 (12) |
| N2 | 0.0702 (12) | 0.0839 (13) | 0.0601 (14) | −0.0021 (11) | −0.0045 (11) | 0.0042 (10) |
| O1 | 0.0694 (10) | 0.1060 (12) | 0.0847 (13) | 0.0098 (10) | −0.0118 (10) | −0.0070 (10) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C2 | 1.378 (3) | C9—C10 | 1.330 (3) |
| C1—C6 | 1.384 (3) | C9—H9 | 0.9300 |
| C1—C7 | 1.486 (3) | C10—C11 | 1.458 (3) |
| C2—C3 | 1.389 (4) | C10—H10 | 0.9300 |
| C2—H2 | 0.9300 | C11—C12 | 1.379 (4) |
| C3—C4 | 1.378 (4) | C11—C16 | 1.380 (4) |
| C3—H3 | 0.9300 | C12—C13 | 1.371 (4) |
| C4—C5 | 1.356 (4) | C12—H12 | 0.9300 |
| C4—H4 | 0.9300 | C13—C14 | 1.359 (5) |
| C5—C6 | 1.382 (4) | C13—H13 | 0.9300 |
| C5—H5 | 0.9300 | C14—C15 | 1.366 (4) |
| C6—H6 | 0.9300 | C14—H14 | 0.9300 |
| C7—O1 | 1.229 (3) | C15—C16 | 1.378 (4) |
| C7—N1 | 1.349 (3) | C15—H15 | 0.9300 |
| C8—N2 | 1.284 (3) | C16—H16 | 0.9300 |
| C8—C9 | 1.434 (3) | N1—N2 | 1.386 (3) |
| C8—H8 | 0.9300 | N1—H1A | 0.88 (2) |
| | | | |
| C2—C1—C6 | 118.9 (3) | C8—C9—H9 | 118.4 |
| C2—C1—C7 | 124.1 (2) | C9—C10—C11 | 128.2 (2) |
| C6—C1—C7 | 117.0 (2) | C9—C10—H10 | 115.9 |
| C1—C2—C3 | 120.0 (3) | C11—C10—H10 | 115.9 |
| C1—C2—H2 | 120.0 | C12—C11—C16 | 117.5 (3) |
| C3—C2—H2 | 120.0 | C12—C11—C10 | 123.3 (3) |
| C4—C3—C2 | 120.2 (3) | C16—C11—C10 | 119.2 (3) |
| C4—C3—H3 | 119.9 | C13—C12—C11 | 121.5 (3) |
| C2—C3—H3 | 119.9 | C13—C12—H12 | 119.3 |
| C5—C4—C3 | 120.2 (3) | C11—C12—H12 | 119.3 |
| C5—C4—H4 | 119.9 | C14—C13—C12 | 120.2 (3) |

| | | | |
|---|---|---|---|
| C3—C4—H4 | 119.9 | C14—C13—H13 | 119.9 |
| C4—C5—C6 | 120.0 (3) | C12—C13—H13 | 119.9 |
| C4—C5—H5 | 120.0 | C13—C14—C15 | 119.7 (3) |
| C6—C5—H5 | 120.0 | C13—C14—H14 | 120.2 |
| C5—C6—C1 | 120.8 (3) | C15—C14—H14 | 120.2 |
| C5—C6—H6 | 119.6 | C14—C15—C16 | 120.2 (3) |
| C1—C6—H6 | 119.6 | C14—C15—H15 | 119.9 |
| O1—C7—N1 | 122.1 (2) | C16—C15—H15 | 119.9 |
| O1—C7—C1 | 121.3 (2) | C15—C16—C11 | 120.9 (3) |
| N1—C7—C1 | 116.6 (2) | C15—C16—H16 | 119.5 |
| N2—C8—C9 | 120.0 (2) | C11—C16—H16 | 119.5 |
| N2—C8—H8 | 120.0 | C7—N1—N2 | 119.0 (2) |
| C9—C8—H8 | 120.0 | C7—N1—H1A | 123.6 (15) |
| C10—C9—C8 | 123.3 (2) | N2—N1—H1A | 116.9 (15) |
| C10—C9—H9 | 118.4 | C8—N2—N1 | 114.3 (2) |

| | | | |
|---|---|---|---|
| C6—C1—C2—C3 | 2.0 (3) | C9—C10—C11—C12 | −3.7 (4) |
| C7—C1—C2—C3 | −178.3 (2) | C9—C10—C11—C16 | 177.5 (2) |
| C1—C2—C3—C4 | −1.2 (4) | C16—C11—C12—C13 | 0.2 (4) |
| C2—C3—C4—C5 | −0.2 (4) | C10—C11—C12—C13 | −178.7 (3) |
| C3—C4—C5—C6 | 0.8 (4) | C11—C12—C13—C14 | −0.2 (5) |
| C4—C5—C6—C1 | 0.0 (4) | C12—C13—C14—C15 | −0.2 (5) |
| C2—C1—C6—C5 | −1.4 (3) | C13—C14—C15—C16 | 0.7 (5) |
| C7—C1—C6—C5 | 178.8 (2) | C14—C15—C16—C11 | −0.7 (5) |
| C2—C1—C7—O1 | −156.8 (2) | C12—C11—C16—C15 | 0.3 (4) |
| C6—C1—C7—O1 | 23.0 (3) | C10—C11—C16—C15 | 179.1 (2) |
| C2—C1—C7—N1 | 24.8 (3) | O1—C7—N1—N2 | −3.2 (3) |
| C6—C1—C7—N1 | −155.5 (2) | C1—C7—N1—N2 | 175.23 (19) |
| N2—C8—C9—C10 | −176.6 (2) | C9—C8—N2—N1 | 176.9 (2) |
| C8—C9—C10—C11 | 174.1 (2) | C7—N1—N2—C8 | 179.2 (2) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1*A*···O1$^{i}$ | 0.88 (2) | 2.05 (2) | 2.898 (3) | 161 (2) |

Symmetry code: (i) *x*−1/2, −*y*+3/2, *z*.