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## Structure Reports

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# *N'*-[(*E*)-3-Pyridylmethylidene]benzohydrazide

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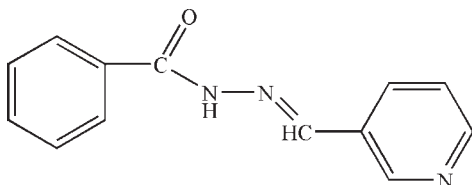
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 Key indicators: single-crystal X-ray study;  $T = 298$  K; mean  $\sigma(\text{C}-\text{C}) = 0.007$  Å;  $R$  factor = 0.042;  $wR$  factor = 0.104; data-to-parameter ratio = 7.4.

The title compound,  $\text{C}_{13}\text{H}_{11}\text{N}_3\text{O}$ , was prepared by the reaction of benzohydrazide and nicotinaldehyde. The dihedral angle between the planes of the two aromatic rings is  $47.78$  ( $9$ )°. The crystal structure is stabilized by intermolecular  $\text{N}-\text{H}\cdots\text{N}$  hydrogen-bonding interactions.

## Related literature

 For related structures, see: Yin *et al.* (2008).


## Experimental

## Crystal data

 $\text{C}_{13}\text{H}_{11}\text{N}_3\text{O}$ 
 $M_r = 225.25$ 

 Orthorhombic,  $P2_12_12_1$ 
 $a = 7.6193$  (13) Å

 $b = 10.6291$  (17) Å

 $c = 13.530$  (2) Å

 $V = 1095.7$  (3) Å<sup>3</sup>
 $Z = 4$ 

 Mo  $K\alpha$  radiation  
 $\mu = 0.09$  mm<sup>-1</sup>
 $T = 298$  K  
 $0.21 \times 0.18 \times 0.08$  mm

## Data collection

 Siemens SMART CCD  
 diffractometer  
 Absorption correction: multi-scan  
 (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.981$ ,  $T_{\max} = 0.993$ 

 5473 measured reflections  
 1136 independent reflections  
 612 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.073$ 

## Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.042$   
 $wR(F^2) = 0.104$   
 $S = 1.18$   
 1136 reflections

 154 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.20$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.20$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H1}\cdots\text{N3}^i$	0.86	2.40	3.236 (5)	164

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

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2228).

## References

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 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.  
 Siemens (1996). *SMART* and *SAINTE*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.  
 Yin, H., Cui, J. & Qiao, Y. (2008). *Polyhedron*, **27**, 2157–2166.

**supplementary materials**

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## *N'*-[(*E*)-3-Pyridylmethylidene]benzohydrazide

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### Comment

Acylhydrazones, as an example of Schiff bases, and their metal complexes have been widely studied due to their versatile applications in the fields of analytical and medicinal chemistry and biotechnology. These ligands, owing to their facile keto-enol tautomerization and the availability of several potential donor sites, can coordinate with metals (Yin *et al.*, 2008). We report here the synthesis and structure of the title compound. The molecular structure of the title compound is shown in Fig. 1. The hydrazone molecule crystallizes as an *E* isomer. In the crystal structure, there exist intermolecular N—H...N hydrogen bonds (Table 1). As seen in Fig. 2, the molecules are linked into one-dimensional extended chain structure.

### Experimental

A mixture of benzohydrazide (10 mmol) and nicotinaldehyde (10 mmol) was refluxed in ethanol (40 ml) for 2 h at 353K. After the solution had cooled down to room temperature yellow sediment appeared. The product was crystallized from a solution of methanol to yield yellow block-shaped crystals of the title compound (yield 78%). Anal. Calcd (%) for C<sub>13</sub>H<sub>11</sub>N<sub>3</sub>O (Mr = 225.25): C, 69.32; H, 4.92; N, 18.65. Found (%): C, 69.21; H, 4.97; N, 18.76.

### Refinement

In the absence of significant anomalous scattering effects, Friedel pairs were averaged. The C—H and N—H H atoms were positioned with idealized geometry (N—H = 0.86 Å and C—H = 0.93 Å) and were refined using a riding model approximation with  $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C}, \text{N})$ .

### Figures

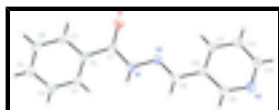


Fig. 1. The molecule of the title compound, shown with 50% probability displacement ellipsoids.

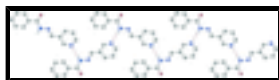


Fig. 2. A view of the one-dimensional extended chain structure in the title compound.

## *N'*-[(*E*)-3-Pyridylmethylidene]benzohydrazide

### Crystal data

C<sub>13</sub>H<sub>11</sub>N<sub>3</sub>O

$M_r = 225.25$

Orthorhombic,  $P2_12_12_1$

$F_{000} = 472$

$D_x = 1.365 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073 \text{ \AA}$

# supplementary materials

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Hall symbol: P 2ac 2ab  
 $a = 7.6193$  (13) Å  
 $b = 10.6291$  (17) Å  
 $c = 13.530$  (2) Å  
 $V = 1095.7$  (3) Å<sup>3</sup>  
 $Z = 4$

Cell parameters from 764 reflections  
 $\theta = 2.4$ – $25.1^\circ$   
 $\mu = 0.09$  mm<sup>-1</sup>  
 $T = 298$  K  
Block, yellow  
 $0.21 \times 0.18 \times 0.08$  mm

## Data collection

Siemens SMART CCD  
diffractometer  
Radiation source: fine-focus sealed tube  
Monochromator: graphite  
 $T = 298$  K  
 $\varphi$  and  $\omega$  scans  
Absorption correction: multi-scan  
(SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.981$ ,  $T_{\max} = 0.993$   
5473 measured reflections

1136 independent reflections  
612 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.073$   
 $\theta_{\text{max}} = 25.0^\circ$   
 $\theta_{\text{min}} = 2.4^\circ$   
 $h = -9 \rightarrow 8$   
 $k = -12 \rightarrow 11$   
 $l = -12 \rightarrow 16$

## Refinement

Refinement on  $F^2$   
Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.042$   
 $wR(F^2) = 0.104$   
 $S = 1.18$   
1136 reflections  
154 parameters  
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map  
Hydrogen site location: inferred from neighbouring sites  
H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0242P)^2 + 0.2399P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.20$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.20$  e Å<sup>-3</sup>  
Extinction correction: none

## Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å<sup>2</sup>)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.1276 (5)	0.7488 (3)	0.4106 (3)	0.0430 (12)
H1	0.1551	0.8129	0.3750	0.052*
N2	0.1085 (5)	0.7596 (4)	0.5111 (3)	0.0410 (11)
N3	0.1881 (5)	1.0185 (4)	0.7966 (3)	0.0450 (12)
O1	0.0701 (5)	0.5389 (3)	0.4181 (2)	0.0544 (10)
C1	0.1015 (7)	0.6334 (4)	0.3688 (4)	0.0386 (13)
C2	0.1109 (6)	0.6291 (4)	0.2602 (3)	0.0327 (12)
C3	0.0535 (7)	0.7257 (4)	0.2001 (4)	0.0438 (14)
H3	0.0107	0.7992	0.2285	0.053*
C4	0.0588 (7)	0.7150 (5)	0.0986 (4)	0.0523 (15)
H4	0.0175	0.7805	0.0594	0.063*

C5	0.1247 (7)	0.6078 (5)	0.0548 (4)	0.0559 (17)
H5	0.1301	0.6013	-0.0137	0.067*
C6	0.1826 (7)	0.5105 (4)	0.1136 (4)	0.0515 (15)
H6	0.2268	0.4376	0.0848	0.062*
C7	0.1748 (6)	0.5212 (4)	0.2156 (4)	0.0448 (14)
H7	0.2132	0.4547	0.2547	0.054*
C8	0.1525 (6)	0.8640 (5)	0.5499 (3)	0.0446 (14)
H8	0.1941	0.9288	0.5101	0.054*
C9	0.1968 (6)	0.9926 (4)	0.6998 (3)	0.0432 (14)
H9	0.2460	1.0533	0.6588	0.052*
C10	0.1383 (6)	0.8825 (4)	0.6558 (4)	0.0365 (13)
C11	0.0676 (6)	0.7933 (4)	0.7186 (4)	0.0416 (14)
H11	0.0272	0.7173	0.6933	0.050*
C12	0.0567 (7)	0.8168 (5)	0.8183 (4)	0.0492 (15)
H12	0.0094	0.7572	0.8610	0.059*
C13	0.1173 (6)	0.9306 (5)	0.8537 (4)	0.0497 (15)
H13	0.1080	0.9465	0.9211	0.060*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
N1	0.066 (3)	0.036 (2)	0.026 (2)	-0.006 (2)	0.001 (2)	-0.0031 (19)
N2	0.051 (3)	0.039 (2)	0.033 (3)	-0.002 (2)	0.003 (2)	0.0001 (19)
N3	0.048 (3)	0.046 (2)	0.041 (3)	-0.003 (2)	0.001 (2)	-0.008 (2)
O1	0.080 (3)	0.0399 (19)	0.044 (2)	-0.009 (2)	-0.004 (2)	0.0059 (18)
C1	0.043 (3)	0.036 (3)	0.037 (3)	-0.005 (3)	-0.006 (3)	-0.003 (3)
C2	0.030 (3)	0.033 (3)	0.035 (3)	-0.004 (3)	0.002 (3)	-0.004 (2)
C3	0.057 (4)	0.033 (3)	0.042 (4)	0.004 (3)	0.005 (3)	-0.005 (3)
C4	0.063 (4)	0.054 (3)	0.040 (4)	-0.002 (3)	-0.007 (3)	0.003 (3)
C5	0.077 (4)	0.056 (4)	0.035 (3)	-0.002 (3)	0.002 (3)	-0.006 (3)
C6	0.063 (4)	0.037 (3)	0.055 (4)	0.004 (3)	0.005 (3)	-0.011 (3)
C7	0.050 (4)	0.036 (3)	0.049 (4)	-0.004 (3)	0.000 (3)	-0.001 (3)
C8	0.057 (4)	0.039 (3)	0.038 (3)	-0.003 (3)	0.001 (3)	0.003 (3)
C9	0.056 (4)	0.038 (3)	0.036 (3)	-0.002 (3)	0.002 (3)	0.000 (3)
C10	0.044 (3)	0.035 (3)	0.030 (3)	-0.002 (3)	0.000 (3)	0.002 (2)
C11	0.045 (4)	0.038 (3)	0.042 (4)	-0.002 (3)	0.000 (3)	-0.002 (3)
C12	0.060 (4)	0.048 (3)	0.039 (3)	-0.010 (3)	0.004 (3)	0.006 (3)
C13	0.052 (4)	0.061 (3)	0.037 (3)	-0.002 (3)	0.004 (3)	-0.006 (3)

Geometric parameters ( $\text{\AA}$ ,  $^\circ$ )

N1—C1	1.365 (5)	C5—H5	0.9300
N1—N2	1.372 (5)	C6—C7	1.386 (6)
N1—H1	0.8600	C6—H6	0.9300
N2—C8	1.273 (6)	C7—H7	0.9300
N3—C13	1.327 (6)	C8—C10	1.451 (6)
N3—C9	1.340 (5)	C8—H8	0.9300
O1—C1	1.229 (5)	C9—C10	1.386 (6)
C1—C2	1.473 (6)	C9—H9	0.9300

## supplementary materials

C2—C3	1.380 (6)	C10—C11	1.381 (6)
C2—C7	1.385 (6)	C11—C12	1.375 (6)
C3—C4	1.378 (6)	C11—H11	0.9300
C3—H3	0.9300	C12—C13	1.381 (6)
C4—C5	1.379 (6)	C12—H12	0.9300
C4—H4	0.9300	C13—H13	0.9300
C5—C6	1.377 (6)		
C1—N1—N2	118.1 (4)	C7—C6—H6	120.0
C1—N1—H1	121.0	C2—C7—C6	121.1 (5)
N2—N1—H1	121.0	C2—C7—H7	119.5
C8—N2—N1	117.0 (4)	C6—C7—H7	119.5
C13—N3—C9	116.4 (4)	N2—C8—C10	120.4 (5)
O1—C1—N1	122.5 (5)	N2—C8—H8	119.8
O1—C1—C2	121.7 (5)	C10—C8—H8	119.8
N1—C1—C2	115.7 (4)	N3—C9—C10	125.2 (4)
C3—C2—C7	118.1 (4)	N3—C9—H9	117.4
C3—C2—C1	123.4 (5)	C10—C9—H9	117.4
C7—C2—C1	118.5 (5)	C11—C10—C9	116.2 (4)
C4—C3—C2	121.1 (5)	C11—C10—C8	122.9 (5)
C4—C3—H3	119.5	C9—C10—C8	120.9 (5)
C2—C3—H3	119.5	C12—C11—C10	120.1 (5)
C3—C4—C5	120.5 (5)	C12—C11—H11	119.9
C3—C4—H4	119.8	C10—C11—H11	119.9
C5—C4—H4	119.8	C11—C12—C13	118.6 (5)
C6—C5—C4	119.2 (5)	C11—C12—H12	120.7
C6—C5—H5	120.4	C13—C12—H12	120.7
C4—C5—H5	120.4	N3—C13—C12	123.4 (5)
C5—C6—C7	120.0 (5)	N3—C13—H13	118.3
C5—C6—H6	120.0	C12—C13—H13	118.3

### Hydrogen-bond geometry ( $\text{\AA}$ , $^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N1-H1\cdots N3^i$	0.86	2.40	3.236 (5)	164

Symmetry codes: (i)  $-x+1/2, -y+2, z-1/2$ .

Fig. 1

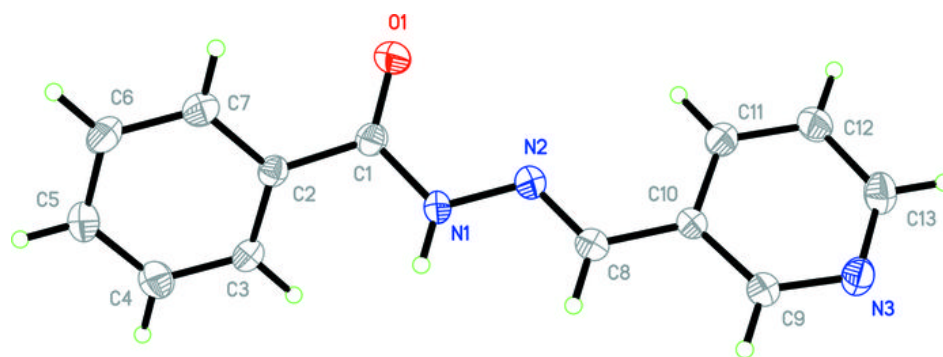


Fig. 2

