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N′-[(*E*)-3-Pyridylmethylidene]benzohydrazide

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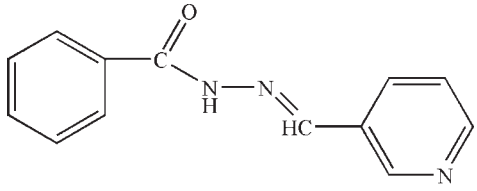
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.007 Å; R factor = 0.042; wR factor = 0.104; data-to-parameter ratio = 7.4.

The title compound, $C_{13}H_{11}N_3O$, 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 N—H···N hydrogen-bonding interactions.

Related literature

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



Experimental

Crystal data

$C_{13}H_{11}N_3O$
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^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 K
0.21 × 0.18 × 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_{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
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···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).

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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 $C_{13}H_{11}N_3O$ (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_{iso}(H) = 1.2 U_{eq}(C, N).

Figures

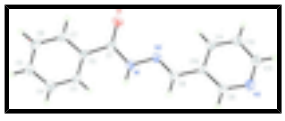

Fig. 1. The molecule of the title compound, shown with 50% probability displacement ellipsoids.

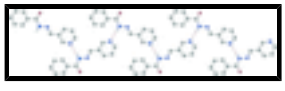

Fig. 2. A view of the one-dimensional extended chain structure in the title compound.

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

Crystal data

$C_{13}H_{11}N_3O$	F_{000} = 472
M_r = 225.25	D_x = 1.365 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation, λ = 0.71073 Å

Hall symbol: P 2ac 2ab	Cell parameters from 764 reflections
a = 7.6193 (13) Å	θ = 2.4–25.1º
b = 10.6291 (17) Å	μ = 0.09 mm^{-1}
c = 13.530 (2) Å	T = 298 K
V = 1095.7 (3) Å^3	Block, yellow
Z = 4	0.21 × 0.18 × 0.08 mm

Data collection

Siemens SMART CCD diffractometer	1136 independent reflections
Radiation source: fine-focus sealed tube	612 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.073
T = 298 K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 2.4º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -9 \rightarrow 8$
T_{min} = 0.981, T_{max} = 0.993	$k = -12 \rightarrow 11$
5473 measured reflections	$l = -12 \rightarrow 16$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.042	H-atom parameters constrained
$wR(F^2)$ = 0.104	$w = 1/[\sigma^2(F_o^2) + (0.0242P)^2 + 0.2399P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.18	$(\Delta/\sigma)_{max} < 0.001$
1136 reflections	$\Delta\rho_{max}$ = 0.20 e Å^{-3}
154 parameters	$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{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 (Å^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 (Å, °)

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

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 (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···N3^{i}	0.86	2.40	3.236 (5)	164

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

Fig. 1

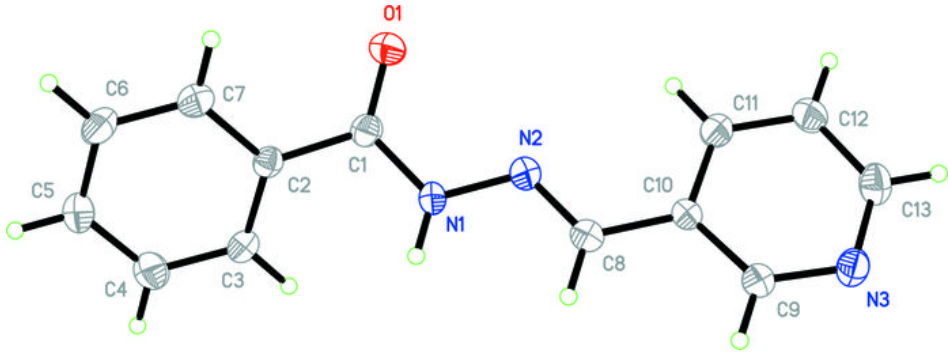

Fig. 2