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N′-[1-(2-Pyridyl)ethylidene]nicotinohydrazide

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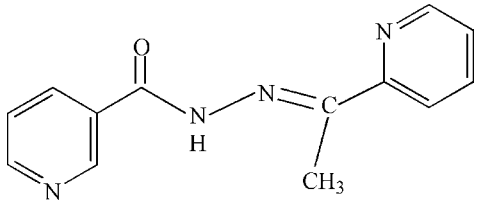
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.038; wR factor = 0.106; data-to-parameter ratio = 12.8.

In the the title compound, $C_{13}H_{12}N_4O$, the dihedral angle between the aromatic ring planes is 21.7 (3)°. In the crystal structure, intermolecular N—H···O hydrogen bonds lead to $C(4)$ chains.

Related literature

For related literature, see: Tai *et al.* (2003).



Experimental

Crystal data

$C_{13}H_{12}N_4O$
M_r = 240.27
Orthorhombic, *Pbcn*
a = 18.264 (3) Å
b = 7.9300 (9) Å
c = 16.471 (2) Å
V = 2385.5 (5) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 (2) K
0.46 × 0.43 × 0.40 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.960, T_{max} = 0.965
9146 measured reflections
2107 independent reflections
1568 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.106
S = 1.06
2107 reflections
164 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.86	2.27	3.125 (2)	171

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); 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: HB2634).

References

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Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
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supplementary materials

Acta Cryst. (2008). E**64**, o65 [**doi:10.1107/S1600536807056024**]

N'-[1-(2-Pyridyl)ethylidene]nicotinohydrazide

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Comment

As part of our ongoing studies of the coordination chemistry of aroylhydrazones ligands (Tai *et al.*, 2003), we now report the synthesis and structure of the title compound, (I), (Fig. 1).

In the molecule of (I), both C8—N2 [1.284 (2) Å] and C1—O1 [1.220 (2) Å] are close to double-bond separations, indicating that the Lewis structure shown in the scheme is only an approximation to the electron distribution in the molecule. Otherwise, the geometrical parameters for (I) are normal. The dihedral angle between the pyridine ring mean planes is 21.7 (3)°, indicating that the molecule is significantly twisted, perhaps for steric reasons.

In the crystal, an N—H···O hydrogen bond (Table 1) leads to C(4) chains.

Experimental

10 mmol of 2-acetylpyridine (10 mmol) was added to a solution of nicotinic acid hydrazine (10 mmol) in 10 ml of ethanol. The mixture was continuously stirred for 3 h at refluxing temperature, evaporating some ethanol, then, upon cooling, the solid product was collected by filtration and dried *in vacuo* (yield 68%). Colourless blocks of (I) were obtained by evaporation from a methanol solution after two weeks.

Refinement

The H atoms were placed geometrically (C—H = 0.93–0.96 Å, N—H = 0.86 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(carrier) or 1.5U_{eq}(methyl C).

Figures

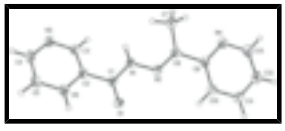

Fig. 1. The molecular structure of (I) showing 30% displacement ellipsoids (arbitrary spheres for the H atoms).

N'-[1-(2-Pyridyl)ethylidene]nicotinohydrazide

Crystal data

$C_{13}H_{12}N_4O$	D_x = 1.338 Mg m^{-3}
M_r = 240.27	Mo $K\alpha$ radiation λ = 0.71073 Å
Orthorhombic, *Pbcn*	Cell parameters from 2977 reflections
a = 18.264 (3) Å	θ = 2.2–27.1°

b = 7.9300 (9) Å	μ = 0.09 mm^{-1}
c = 16.471 (2) Å	T = 298 (2) K
V = 2385.5 (5) Å^3	Block, colourless
Z = 8	0.46 × 0.43 × 0.40 mm
F_{000} = 1008	

Data collection

Bruker SMART CCD diffractometer	2107 independent reflections
Radiation source: fine-focus sealed tube	1568 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.041
T = 298(2) K	θ_{max} = 25.0º
ω scans	θ_{min} = 2.5º
Absorption correction: multi-scan (SADABS; Bruker, 2000)	h = −17→21
T_{min} = 0.960, T_{max} = 0.965	k = −9→8
9146 measured reflections	l = −19→16

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.038	$w = 1/[\sigma^2(F_o^2) + (0.0375P)^2 + 1.131P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.106	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.06	$\Delta\rho_{max}$ = 0.21 e Å^{-3}
2107 reflections	$\Delta\rho_{min}$ = −0.17 e Å^{-3}
164 parameters	Extinction correction: SHELXL, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0194 (13)
Secondary atom site location: difference Fourier map	

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.74333 (8)	0.92565 (18)	0.94870 (8)	0.0347 (4)
H1	0.7208	0.8309	0.9442	0.042*
N2	0.71633 (8)	1.05276 (17)	0.99711 (9)	0.0342 (4)
N3	0.81694 (9)	0.5927 (2)	0.76098 (10)	0.0499 (5)
N4	0.55759 (8)	1.1916 (2)	1.09086 (10)	0.0472 (5)
O1	0.83904 (7)	1.08958 (17)	0.91028 (9)	0.0518 (4)
C1	0.80666 (10)	0.9551 (2)	0.90842 (11)	0.0346 (4)
C2	0.83536 (9)	0.8086 (2)	0.86108 (10)	0.0329 (4)
C3	0.79344 (10)	0.7247 (2)	0.80384 (11)	0.0399 (5)
H3	0.7460	0.7627	0.7947	0.048*
C4	0.88433 (12)	0.5398 (3)	0.77688 (13)	0.0540 (6)
H4	0.9013	0.4453	0.7493	0.065*
C5	0.93084 (11)	0.6157 (3)	0.83154 (13)	0.0553 (6)
H5	0.9778	0.5740	0.8400	0.066*
C6	0.90614 (10)	0.7548 (3)	0.87343 (12)	0.0451 (5)
H6	0.9367	0.8113	0.9094	0.054*
C7	0.60952 (12)	0.8730 (3)	1.03313 (15)	0.0600 (6)
H7A	0.5709	0.8875	0.9942	0.090*
H7B	0.5888	0.8539	1.0859	0.090*
H7C	0.6391	0.7779	1.0180	0.090*
C8	0.65592 (10)	1.0280 (2)	1.03520 (10)	0.0352 (4)
C9	0.63030 (9)	1.1754 (2)	1.08347 (10)	0.0339 (4)
C10	0.67883 (10)	1.2881 (2)	1.11839 (11)	0.0390 (5)
H10	0.7291	1.2719	1.1133	0.047*
C11	0.65202 (12)	1.4242 (3)	1.16058 (13)	0.0503 (5)
H11	0.6837	1.5011	1.1847	0.060*
C12	0.57744 (12)	1.4446 (3)	1.16657 (14)	0.0561 (6)
H12	0.5576	1.5366	1.1938	0.067*
C13	0.53299 (12)	1.3260 (3)	1.13141 (14)	0.0560 (6)
H13	0.4826	1.3399	1.1361	0.067*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0408 (9)	0.0252 (8)	0.0381 (8)	−0.0008 (7)	0.0054 (7)	−0.0048 (7)
N2	0.0403 (9)	0.0279 (8)	0.0344 (8)	0.0058 (7)	0.0007 (6)	−0.0029 (7)
N3	0.0511 (11)	0.0497 (10)	0.0490 (10)	0.0043 (9)	−0.0005 (8)	−0.0147 (9)
N4	0.0367 (9)	0.0506 (11)	0.0542 (10)	0.0046 (8)	0.0029 (7)	−0.0111 (9)
O1	0.0480 (8)	0.0377 (8)	0.0698 (10)	−0.0094 (7)	0.0109 (7)	−0.0114 (7)
C1	0.0365 (10)	0.0304 (10)	0.0370 (10)	0.0005 (8)	−0.0021 (8)	−0.0010 (8)
C2	0.0357 (10)	0.0316 (10)	0.0313 (9)	−0.0005 (8)	0.0058 (7)	0.0018 (8)
C3	0.0381 (10)	0.0393 (11)	0.0422 (11)	0.0032 (9)	0.0008 (8)	−0.0026 (9)
C4	0.0550 (13)	0.0546 (14)	0.0523 (13)	0.0154 (11)	0.0061 (10)	−0.0168 (11)
C5	0.0416 (12)	0.0690 (15)	0.0552 (13)	0.0182 (11)	−0.0003 (10)	−0.0128 (12)

C6	0.0389 (11)	0.0552 (13)	0.0413 (11)	0.0016 (9)	−0.0003 (8)	−0.0074 (10)
C7	0.0580 (14)	0.0460 (13)	0.0760 (16)	−0.0101 (11)	0.0213 (12)	−0.0188 (12)
C8	0.0368 (10)	0.0335 (10)	0.0352 (10)	0.0011 (8)	0.0012 (8)	−0.0009 (8)
C9	0.0376 (10)	0.0338 (10)	0.0304 (9)	0.0013 (8)	0.0019 (7)	0.0003 (8)
C10	0.0389 (10)	0.0403 (11)	0.0378 (10)	−0.0005 (9)	0.0025 (8)	−0.0033 (9)
C11	0.0559 (13)	0.0454 (12)	0.0495 (12)	−0.0060 (10)	0.0033 (10)	−0.0136 (10)
C12	0.0605 (14)	0.0483 (13)	0.0594 (13)	0.0099 (11)	0.0116 (11)	−0.0154 (11)
C13	0.0425 (12)	0.0581 (14)	0.0672 (15)	0.0111 (11)	0.0059 (11)	−0.0127 (12)

Geometric parameters (Å, °)

N1—C1	1.354 (2)	C5—H5	0.9300
N1—N2	1.3765 (19)	C6—H6	0.9300
N1—H1	0.8600	C7—C8	1.494 (3)
N2—C8	1.284 (2)	C7—H7A	0.9600
N3—C4	1.326 (3)	C7—H7B	0.9600
N3—C3	1.333 (2)	C7—H7C	0.9600
N4—C13	1.336 (3)	C8—C9	1.489 (2)
N4—C9	1.340 (2)	C9—C10	1.384 (3)
O1—C1	1.220 (2)	C10—C11	1.374 (3)
C1—C2	1.494 (2)	C10—H10	0.9300
C2—C6	1.377 (3)	C11—C12	1.375 (3)
C2—C3	1.385 (2)	C11—H11	0.9300
C3—H3	0.9300	C12—C13	1.371 (3)
C4—C5	1.376 (3)	C12—H12	0.9300
C4—H4	0.9300	C13—H13	0.9300
C5—C6	1.377 (3)		
C1—N1—N2	117.63 (14)	C8—C7—H7A	109.5
C1—N1—H1	121.2	C8—C7—H7B	109.5
N2—N1—H1	121.2	H7A—C7—H7B	109.5
C8—N2—N1	118.61 (15)	C8—C7—H7C	109.5
C4—N3—C3	116.25 (17)	H7A—C7—H7C	109.5
C13—N4—C9	117.09 (17)	H7B—C7—H7C	109.5
O1—C1—N1	123.55 (17)	N2—C8—C9	114.28 (16)
O1—C1—C2	121.51 (16)	N2—C8—C7	127.01 (17)
N1—C1—C2	114.94 (15)	C9—C8—C7	118.68 (16)
C6—C2—C3	118.06 (17)	N4—C9—C10	122.35 (17)
C6—C2—C1	119.59 (16)	N4—C9—C8	115.81 (16)
C3—C2—C1	122.34 (16)	C10—C9—C8	121.85 (16)
N3—C3—C2	124.04 (17)	C11—C10—C9	119.30 (18)
N3—C3—H3	118.0	C11—C10—H10	120.3
C2—C3—H3	118.0	C9—C10—H10	120.3
N3—C4—C5	124.33 (19)	C10—C11—C12	118.80 (19)
N3—C4—H4	117.8	C10—C11—H11	120.6
C5—C4—H4	117.8	C12—C11—H11	120.6
C4—C5—C6	118.39 (19)	C13—C12—C11	118.39 (19)
C4—C5—H5	120.8	C13—C12—H12	120.8
C6—C5—H5	120.8	C11—C12—H12	120.8
C2—C6—C5	118.84 (19)	N4—C13—C12	124.0 (2)

C2—C6—H6	120.6	N4—C13—H13	118.0
C5—C6—H6	120.6	C12—C13—H13	118.0
C1—N1—N2—C8	179.30 (16)	N1—N2—C8—C9	−177.98 (14)
N2—N1—C1—O1	−3.1 (3)	N1—N2—C8—C7	−0.3 (3)
N2—N1—C1—C2	176.40 (14)	C13—N4—C9—C10	2.3 (3)
O1—C1—C2—C6	53.1 (3)	C13—N4—C9—C8	−177.68 (17)
N1—C1—C2—C6	−126.43 (18)	N2—C8—C9—N4	148.85 (17)
O1—C1—C2—C3	−126.2 (2)	C7—C8—C9—N4	−29.1 (3)
N1—C1—C2—C3	54.3 (2)	N2—C8—C9—C10	−31.1 (2)
C4—N3—C3—C2	1.4 (3)	C7—C8—C9—C10	150.92 (19)
C6—C2—C3—N3	1.3 (3)	N4—C9—C10—C11	−1.6 (3)
C1—C2—C3—N3	−179.39 (17)	C8—C9—C10—C11	178.37 (18)
C3—N3—C4—C5	−2.5 (3)	C9—C10—C11—C12	−0.2 (3)
N3—C4—C5—C6	0.7 (4)	C10—C11—C12—C13	1.3 (3)
C3—C2—C6—C5	−3.1 (3)	C9—N4—C13—C12	−1.2 (3)
C1—C2—C6—C5	177.58 (18)	C11—C12—C13—N4	−0.6 (4)
C4—C5—C6—C2	2.2 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.86	2.27	3.125 (2)	171

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

Fig. 1