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N′-(But-2-enylidene)isonicotinohydrazide

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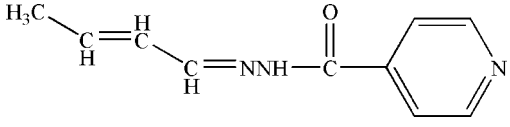
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.034; wR factor = 0.101; data-to-parameter ratio = 9.9.

In the title Schiff base compound, $C_{10}H_{11}N_3O$, the pyridine ring is twisted with respect to the mean plane containing the hydrazine chain, making a dihedral angle of 31.40 (9)°. The NH group interacts with the N atom of the pyridine ring through N—H···N hydrogen bonds to build up a zigzag chain developing parallel to the $(\bar{1}01)$ plane.

Related literature

For general background, see: Kahwa *et al.* (1986); Santos *et al.* (2001).



Experimental

Crystal data

$C_{10}H_{11}N_3O$
M_r = 189.22
Monoclinic, *Cc*
a = 9.5779 (8) Å
b = 12.6191 (11) Å
c = 9.2095 (8) Å
β = 113.511 (1)°
V = 1020.70 (15) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 (2) K
0.25 × 0.23 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.969, T_{max} = 0.974
4639 measured reflections
1264 independent reflections
1225 reflections with $I > 2\sigma(I)$
R_{int} = 0.012

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.101
S = 1.08
1264 reflections
128 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 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
N2—H2···N3^{i}	0.86	2.17	2.991 (2)	160

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996), *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2003).; software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2392).

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supporting information

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S1. Comment

The chemistry of Schiff bases has attracted a great deal of interest in recent years. These compounds play an important role in the development of various proteins and enzymes(Kahwa *et al.*, 1986; Santos *et al.*, 2001). As part of our interest in the study of the coordination chemistry of Schiff bases, we have synthesized the title compound (I) and reported its cyrstal structure.

In the title compound. the pyridine ring is twisted with respect to the mean plane containing the hydrazine chain making a dihedral angle of 31.40 (9)° (Fig. 1). The NH interacts with the nitrogen atom of the pyridine ring through N-H···N hydrogen bond to build up a zig-zag chain developing parallel to the (-1 0 1) plane (Table 1, Fig. 2).

S2. Experimental

Pyridine-4-carboxylic acid hydrazide (1 mmol, 0.137 g) was dissolved in anhydrous methanol, H_2SO_4 (98% 0.5 ml) was added to this, the mixture was stirred for several minitutes at 351 K, 3,4-dichlorobenzyaldehyde (1 mmol 0.070 g) in methanol (8 ml) was added dropwise and the mixture was stirred at refluxing temperature for 2 h. The product was isolated and recrystallized in dichloromethane, brown single crystals of (I) was obtained after 5 d.

S3. Refinement

H atoms were placed in calculated position and treated as riding with C—H= 0.93Å (aromatic), 0.96Å(methyl) and N-H= 0.86\%A with U_{iso}(H)=1.2U_{eq}(C,N) or U_{iso}(H)=1.5U_{eq}(methyl).

In the absence of significant anomalous scattering, the absolute structure could not be reliably determined and then the Friedel pairs were merged and any references to the Flack parameter were removed.

Figure 1

Molecular view of (I) with the atom-labeling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are presented as small spheres of arbitrary radii.

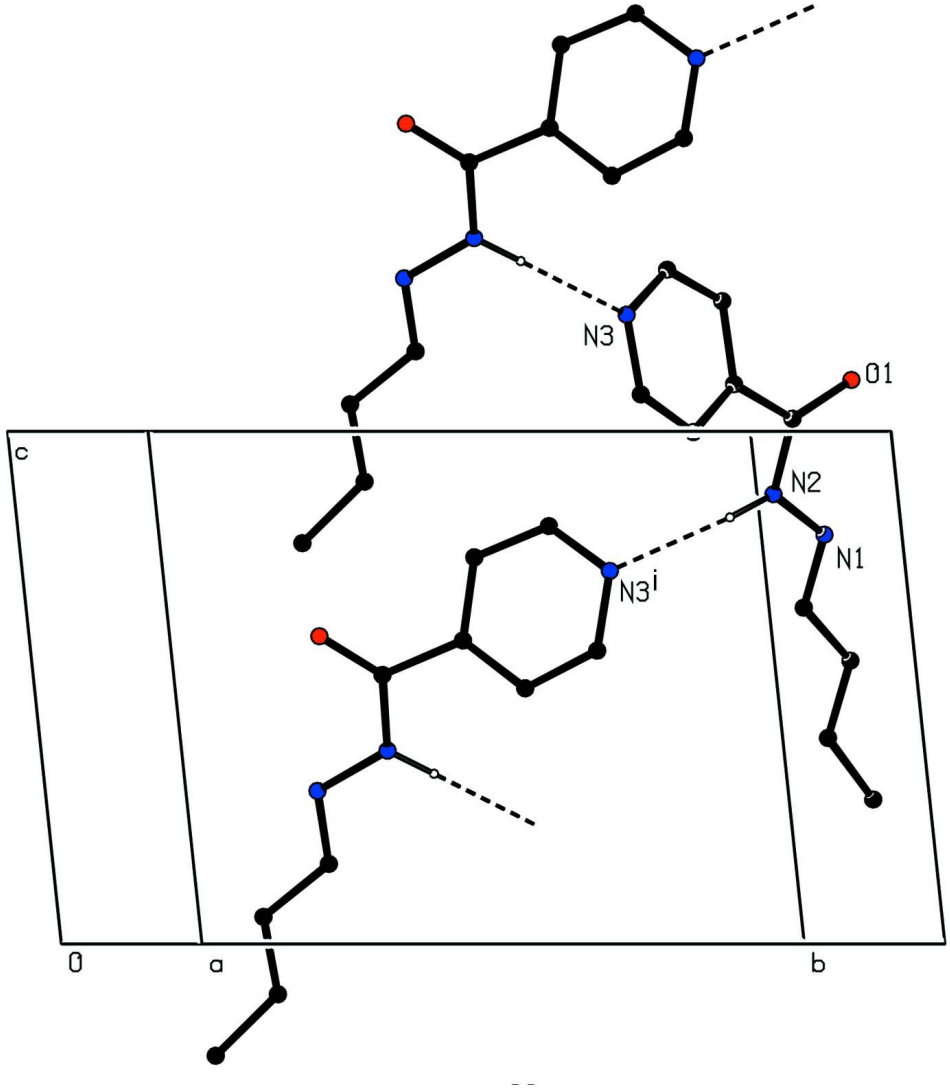

Figure 2

Partial packing view showing the formation of the zig-zag chain through N-H···N hydrogen bonds which are shown as dashed lines. H atoms not involved in hydrogen bondings have been omitted for clarity.[Symmetry code: (i) x-1/2, -y+3/2, z-1/2]

N′-(But-2-enylidene)isonicotinohydrazide

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$C_{10}H_{11}N_3O$
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Hall symbol: C -2yc
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$c = 9.2095\ (8)$ Å
$\beta = 113.511\ (1)°$
$V = 1020.70\ (15)$ Å^3
$Z = 4$
$F(000) = 400$
$D_x = 1.231$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2994 reflections
$\theta = 2.4–23.8°$
$\mu = 0.08$ mm^{-1}
$T = 293$ K
Block, brown
0.25 × 0.23 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.969, T_{max} = 0.974
4639 measured reflections
1264 independent reflections
1225 reflections with $I > 2\sigma(I)$
R_{int} = 0.012
θ_{max} = 28.3°, θ_{min} = 2.8°
h = −12→12
k = −16→16
l = −12→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.101
S = 1.08
1264 reflections
128 parameters
2 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0744P)^2 + 0.0728P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.12 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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}
N1	0.12133 (17)	1.06196 (12)	0.79852 (17)	0.0441 (3)
N2	0.21940 (16)	0.98057 (11)	0.87720 (16)	0.0398 (3)
H2	0.2126	0.9200	0.8322	0.048*
N3	0.6220 (2)	0.73212 (13)	1.2278 (2)	0.0512 (4)
O1	0.33989 (17)	1.07888 (10)	1.10035 (17)	0.0542 (4)
C1	−0.2651 (3)	1.1633 (3)	0.2819 (3)	0.0800 (8)
H1A	−0.2643	1.2313	0.3292	0.120*
H1B	−0.3661	1.1344	0.2431	0.120*
H1C	−0.2337	1.1712	0.1957	0.120*
C2	−0.1590 (3)	1.0910 (2)	0.4019 (3)	0.0625 (5)
H2A	−0.1514	1.0222	0.3696	0.075*
C3	−0.0728 (2)	1.11582 (19)	0.5528 (2)	0.0546 (5)
H3	−0.0819	1.1824	0.5913	0.066*
C4	0.0338 (2)	1.04042 (16)	0.6560 (2)	0.0475 (4)
H4	0.0388	0.9732	0.6170	0.057*
C5	0.32562 (18)	0.99674 (12)	1.02479 (18)	0.0366 (3)

C6	0.42972 (17)	0.90326 (12)	1.09198 (17)	0.0362 (3)
C7	0.4905 (3)	0.88762 (17)	1.2543 (2)	0.0529 (5)
H7	0.4696	0.9347	1.3208	0.064*
C8	0.5828 (3)	0.80039 (19)	1.3153 (2)	0.0584 (5)
H8	0.6198	0.7887	1.4239	0.070*
C9	0.5679 (2)	0.75022 (15)	1.0721 (2)	0.0477 (4)
H9	0.5965	0.7046	1.0096	0.057*
C10	0.47069 (19)	0.83399 (13)	0.99866 (19)	0.0411 (3)
H10	0.4341	0.8433	0.8896	0.049*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0439 (8)	0.0368 (7)	0.0431 (8)	0.0086 (6)	0.0081 (6)	0.0041 (6)
N2	0.0428 (7)	0.0303 (6)	0.0381 (7)	0.0045 (5)	0.0075 (5)	−0.0011 (5)
N3	0.0596 (9)	0.0426 (8)	0.0425 (8)	0.0149 (7)	0.0108 (7)	0.0071 (6)
O1	0.0604 (8)	0.0401 (7)	0.0468 (7)	0.0119 (6)	0.0055 (6)	−0.0113 (5)
C1	0.0650 (15)	0.099 (2)	0.0570 (13)	0.0146 (14)	0.0046 (11)	0.0212 (14)
C2	0.0564 (11)	0.0683 (14)	0.0532 (12)	0.0083 (10)	0.0116 (9)	0.0077 (10)
C3	0.0481 (9)	0.0564 (11)	0.0491 (10)	0.0114 (8)	0.0086 (8)	0.0117 (8)
C4	0.0453 (9)	0.0441 (9)	0.0445 (9)	0.0048 (7)	0.0088 (7)	0.0027 (7)
C5	0.0387 (7)	0.0320 (7)	0.0351 (7)	0.0046 (5)	0.0104 (6)	−0.0001 (5)
C6	0.0381 (7)	0.0322 (7)	0.0338 (7)	0.0025 (5)	0.0096 (6)	−0.0003 (6)
C7	0.0662 (12)	0.0525 (11)	0.0334 (8)	0.0194 (9)	0.0128 (8)	−0.0008 (7)
C8	0.0720 (12)	0.0601 (12)	0.0334 (8)	0.0204 (10)	0.0108 (8)	0.0074 (8)
C9	0.0585 (10)	0.0395 (8)	0.0423 (8)	0.0146 (7)	0.0173 (8)	0.0013 (6)
C10	0.0494 (8)	0.0366 (8)	0.0332 (7)	0.0088 (6)	0.0122 (6)	0.0014 (6)

Geometric parameters (Å, º)

N1—C4	1.273 (2)	C3—C4	1.441 (3)
N1—N2	1.3853 (18)	C3—H3	0.9300
N2—C5	1.349 (2)	C4—H4	0.9300
N2—H2	0.8600	C5—C6	1.509 (2)
N3—C8	1.332 (3)	C6—C7	1.385 (2)
N3—C9	1.335 (2)	C6—C10	1.388 (2)
O1—C5	1.225 (2)	C7—C8	1.383 (3)
C1—C2	1.480 (3)	C7—H7	0.9300
C1—H1A	0.9600	C8—H8	0.9300
C1—H1B	0.9600	C9—C10	1.392 (2)
C1—H1C	0.9600	C9—H9	0.9300
C2—C3	1.340 (3)	C10—H10	0.9300
C2—H2A	0.9300		
C4—N1—N2	114.28 (15)	C3—C4—H4	118.6
C5—N2—N1	119.75 (13)	O1—C5—N2	124.64 (15)
C5—N2—H2	120.1	O1—C5—C6	121.51 (15)
N1—N2—H2	120.1	N2—C5—C6	113.84 (13)

C8—N3—C9	117.17 (16)	C7—C6—C10	118.54 (14)
C2—C1—H1A	109.5	C7—C6—C5	118.58 (14)
C2—C1—H1B	109.5	C10—C6—C5	122.85 (14)
H1A—C1—H1B	109.5	C8—C7—C6	118.48 (16)
C2—C1—H1C	109.5	C8—C7—H7	120.8
H1A—C1—H1C	109.5	C6—C7—H7	120.8
H1B—C1—H1C	109.5	N3—C8—C7	123.92 (17)
C3—C2—C1	125.9 (2)	N3—C8—H8	118.0
C3—C2—H2A	117.1	C7—C8—H8	118.0
C1—C2—H2A	117.1	N3—C9—C10	123.32 (16)
C2—C3—C4	120.8 (2)	N3—C9—H9	118.3
C2—C3—H3	119.6	C10—C9—H9	118.3
C4—C3—H3	119.6	C6—C10—C9	118.48 (15)
N1—C4—C3	122.76 (18)	C6—C10—H10	120.8
N1—C4—H4	118.6	C9—C10—H10	120.8

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···N3^{i}	0.86	2.17	2.991 (2)	160

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