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N′-(1-Phenylethylidene)isonicotinohydrazide

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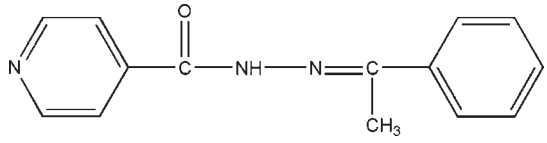
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.068; wR factor = 0.205; data-to-parameter ratio = 16.9.

The title compound, $C_{14}H_{13}N_3O$, was prepared from hypnone and isoniazid. The dihedral angle between the aromatic rings is 12.21 (2)°. In the crystal, N—H···O hydrogen bonds link the molecules into chains propagating in [001] and C—H···O interactions consolidate the packing.

Related literature

For background on Schiff bases, see: Cimerman *et al.* (1997). For a related structure, see: Chen *et al.* (2006).



Experimental

Crystal data

$C_{14}H_{13}N_3O$
M_r = 239.27
Monoclinic, $P2_1/c$
a = 25.878 (5) Å
b = 5.7100 (11) Å
c = 8.3089 (17) Å
β = 90.94 (3)°
V = 1227.6 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 K
0.35 × 0.25 × 0.25 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: none
11394 measured reflections
2821 independent reflections
2024 reflections with $I > 2\sigma(I)$
R_{int} = 0.046

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.068
$wR(F^2)$ = 0.205
S = 1.03
2821 reflections
167 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···O1^{i}	0.87 (2)	2.04 (3)	2.914 (2)	177 (2)
C4—H4A···O1^{i}	0.93	2.43	3.123 (3)	131
C7—H7A···O1^{i}	0.96	2.31	3.095 (3)	138

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); 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: HB5224).

References

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supporting information

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N′-(1-Phenylethylidene)isonicotinohydrazide

Jin-he Jiang, Jing Chen, Jie Yang and Fang-Fang Jian

S1. Comment

Schiff bases have received considerable attention in the literature. They are attractive from several points of view, such as the possibility of analytical application (Cimerman *et al.*, 1997). As part of our search for new schiff base compounds we synthesized the title compound(I) and report its crystal structure herein.

In the title compound (I) (Fig. 1), the C8=N2 bond, 1.285 (3) Å, and the C6—N3 bond, 1.351 (3) Å, are both longer than those in a related compound (Chen *et al.*, 2006). All other bond lengths are within normal ranges. The dihedral angle between the benzene and pyridine rings is 12.21 (2)°. The structure of (I) is stabilized by C—H···O,*N*—H···O and C—H···N hydrogen bonds (Table 1).

S2. Experimental

A mixture of the isoniazid (0.05 mol) and hypnone (0.05 mol) was stirred in refluxing ethanol(30 ml) for 2 h to afford the title compound (yield 78%). Colourless bars of (I) were obtained by recrystallization from ethanol at room temperature.

S3. Refinement

The N-bound H atom was located in a difference map and freely refined. The other H atoms were fixed geometrically and allowed to ride on their attached atoms, with C—H distances = 0.97 Å, and U_{iso}(H) = 1.2–1.5U_{eq}(C).

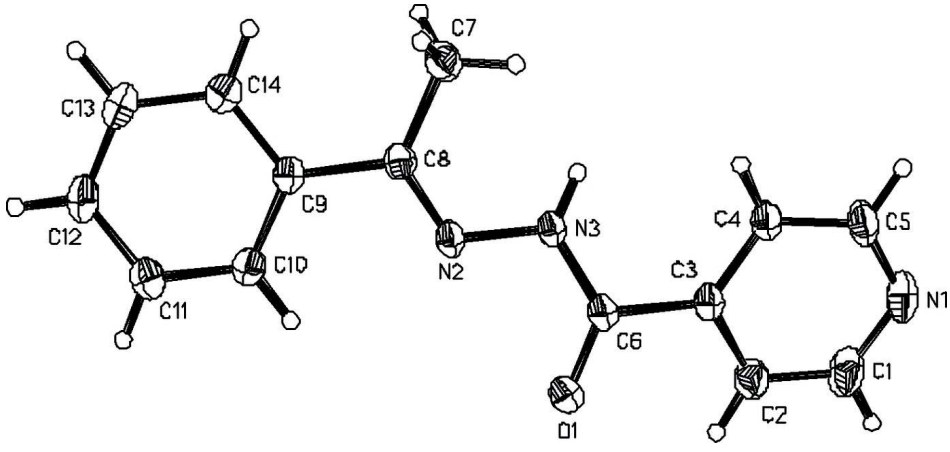

Figure 1

The molecular structure of (I) with displacement ellipsoids drawn at the 30% probability level.

N′-(1-Phenylethylidene)isonicotinohydrazide

Crystal data

$C_{14}H_{13}N_3O$
$M_r = 239.27$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 25.878$ (5) Å
$b = 5.7100$ (11) Å
$c = 8.3089$ (17) Å
$\beta = 90.94$ (3)°
$V = 1227.6$ (4) Å^3
$Z = 4$
$F(000) = 504$
$D_x = 1.295$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2024 reflections
$\theta = 3.2$–27.5°
$\mu = 0.09$ mm^{-1}
$T = 293$ K
Bar, colourless
0.35 × 0.25 × 0.25 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
11394 measured reflections
2821 independent reflections
2024 reflections with $I > 2\sigma(I)$
$R_{int} = 0.046$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.2°$
$h = -33 \rightarrow 33$
$k = -7 \rightarrow 7$
$l = -9 \rightarrow 10$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.068$
$wR(F^2) = 0.205$
$S = 1.03$
2821 reflections
167 parameters
0 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.1014P)^2 + 0.6215P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.29$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
N3	0.28050 (6)	0.2893 (3)	0.9742 (2)	0.0401 (4)
N2	0.23151 (7)	0.3104 (3)	1.0394 (2)	0.0414 (5)
C6	0.31164 (7)	0.1224 (4)	1.0382 (2)	0.0366 (5)
O1	0.30052 (6)	0.0099 (3)	1.15887 (18)	0.0472 (4)

C9	0.15153 (7)	0.4982 (4)	1.0663 (2)	0.0364 (5)
C8	0.20515 (8)	0.4938 (4)	1.0019 (2)	0.0356 (5)
C3	0.36258 (7)	0.0813 (4)	0.9583 (2)	0.0375 (5)
C4	0.38721 (8)	0.2432 (4)	0.8623 (3)	0.0446 (5)
H4A	0.3719	0.3870	0.8390	0.054*
C7	0.22348 (9)	0.6943 (4)	0.9029 (3)	0.0492 (6)
H7A	0.2583	0.6658	0.8704	0.074*
H7B	0.2223	0.8356	0.9654	0.074*
H7C	0.2016	0.7107	0.8092	0.074*
C10	0.13477 (8)	0.3243 (4)	1.1704 (3)	0.0476 (6)
H10A	0.1574	0.2058	1.2021	0.057*
C13	0.06659 (9)	0.6712 (5)	1.0781 (3)	0.0591 (7)
H13A	0.0437	0.7887	1.0468	0.071*
C11	0.08489 (9)	0.3254 (5)	1.2275 (3)	0.0564 (7)
H11A	0.0744	0.2092	1.2982	0.068*
C14	0.11683 (9)	0.6724 (5)	1.0213 (3)	0.0501 (6)
H14A	0.1273	0.7911	0.9524	0.060*
C2	0.38778 (9)	−0.1288 (5)	0.9907 (3)	0.0526 (6)
H2B	0.3728	−0.2414	1.0561	0.063*
N1	0.45942 (8)	−0.0143 (5)	0.8287 (3)	0.0630 (7)
C12	0.05063 (8)	0.4978 (5)	1.1801 (3)	0.0558 (7)
H12A	0.0169	0.4965	1.2170	0.067*
C5	0.43514 (9)	0.1864 (5)	0.8015 (3)	0.0564 (7)
H5A	0.4514	0.2966	0.7373	0.068*
C1	0.43566 (10)	−0.1669 (5)	0.9235 (4)	0.0658 (8)
H1B	0.4523	−0.3078	0.9460	0.079*
H3A	0.2875 (9)	0.349 (5)	0.881 (3)	0.045 (7)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N3	0.0333 (9)	0.0442 (10)	0.0431 (9)	0.0044 (7)	0.0129 (7)	0.0055 (8)
N2	0.0334 (9)	0.0454 (11)	0.0459 (9)	0.0043 (7)	0.0134 (7)	0.0031 (8)
C6	0.0323 (9)	0.0408 (11)	0.0368 (9)	−0.0011 (8)	0.0055 (8)	−0.0025 (8)
O1	0.0431 (8)	0.0558 (11)	0.0431 (8)	0.0037 (7)	0.0106 (7)	0.0078 (7)
C9	0.0321 (9)	0.0400 (11)	0.0372 (10)	0.0010 (8)	0.0026 (8)	−0.0047 (8)
C8	0.0348 (10)	0.0366 (11)	0.0355 (9)	0.0004 (8)	0.0044 (8)	−0.0050 (8)
C3	0.0308 (9)	0.0431 (12)	0.0387 (10)	−0.0001 (8)	0.0042 (8)	−0.0065 (9)
C4	0.0328 (10)	0.0499 (13)	0.0513 (12)	−0.0003 (9)	0.0073 (9)	0.0020 (10)
C7	0.0497 (13)	0.0392 (13)	0.0590 (13)	0.0002 (9)	0.0154 (11)	0.0030 (10)
C10	0.0359 (11)	0.0496 (14)	0.0573 (13)	0.0044 (9)	0.0049 (10)	0.0088 (11)
C13	0.0416 (12)	0.0639 (18)	0.0720 (17)	0.0195 (11)	0.0061 (12)	0.0028 (13)
C11	0.0399 (12)	0.0642 (17)	0.0654 (15)	−0.0024 (11)	0.0128 (11)	0.0112 (13)
C14	0.0454 (12)	0.0478 (14)	0.0572 (13)	0.0081 (10)	0.0071 (11)	0.0061 (11)
C2	0.0435 (12)	0.0449 (14)	0.0697 (15)	0.0046 (10)	0.0102 (11)	0.0025 (12)
N1	0.0366 (10)	0.0716 (17)	0.0813 (16)	0.0040 (10)	0.0147 (10)	−0.0137 (13)
C12	0.0310 (10)	0.0702 (19)	0.0662 (15)	0.0045 (10)	0.0087 (10)	−0.0048 (13)
C5	0.0349 (11)	0.0729 (19)	0.0619 (14)	−0.0045 (11)	0.0135 (10)	0.0007 (13)

C1	0.0445 (13)	0.0534 (16)	0.100 (2)	0.0129 (11)	0.0110 (14)	−0.0080 (15)

Geometric parameters (Å, º)

N3—C6	1.351 (3)	C7—H7C	0.9600
N3—N2	1.392 (2)	C10—C11	1.382 (3)
N3—H3A	0.87 (2)	C10—H10A	0.9300
N2—C8	1.285 (3)	C13—C12	1.371 (4)
C6—O1	1.229 (2)	C13—C14	1.391 (3)
C6—C3	1.504 (3)	C13—H13A	0.9300
C9—C14	1.387 (3)	C11—C12	1.378 (4)
C9—C10	1.391 (3)	C11—H11A	0.9300
C9—C8	1.496 (3)	C14—H14A	0.9300
C8—C7	1.492 (3)	C2—C1	1.385 (3)
C3—C4	1.384 (3)	C2—H2B	0.9300
C3—C2	1.390 (3)	N1—C5	1.324 (4)
C4—C5	1.385 (3)	N1—C1	1.332 (4)
C4—H4A	0.9300	C12—H12A	0.9300
C7—H7A	0.9600	C5—H5A	0.9300
C7—H7B	0.9600	C1—H1B	0.9300
C6—N3—N2	116.69 (17)	C11—C10—C9	120.8 (2)
C6—N3—H3A	119.8 (16)	C11—C10—H10A	119.6
N2—N3—H3A	121.1 (16)	C9—C10—H10A	119.6
C8—N2—N3	117.33 (18)	C12—C13—C14	120.4 (2)
O1—C6—N3	122.91 (18)	C12—C13—H13A	119.8
O1—C6—C3	119.80 (19)	C14—C13—H13A	119.8
N3—C6—C3	117.27 (18)	C12—C11—C10	120.4 (2)
C14—C9—C10	118.20 (19)	C12—C11—H11A	119.8
C14—C9—C8	121.05 (19)	C10—C11—H11A	119.8
C10—C9—C8	120.74 (18)	C9—C14—C13	120.6 (2)
N2—C8—C7	125.95 (18)	C9—C14—H14A	119.7
N2—C8—C9	114.75 (18)	C13—C14—H14A	119.7
C7—C8—C9	119.30 (18)	C1—C2—C3	118.5 (2)
C4—C3—C2	117.99 (19)	C1—C2—H2B	120.7
C4—C3—C6	124.4 (2)	C3—C2—H2B	120.7
C2—C3—C6	117.5 (2)	C5—N1—C1	116.4 (2)
C3—C4—C5	118.5 (2)	C13—C12—C11	119.6 (2)
C3—C4—H4A	120.8	C13—C12—H12A	120.2
C5—C4—H4A	120.8	C11—C12—H12A	120.2
C8—C7—H7A	109.5	N1—C5—C4	124.5 (2)
C8—C7—H7B	109.5	N1—C5—H5A	117.8
H7A—C7—H7B	109.5	C4—C5—H5A	117.8
C8—C7—H7C	109.5	N1—C1—C2	124.1 (3)
H7A—C7—H7C	109.5	N1—C1—H1B	117.9
H7B—C7—H7C	109.5	C2—C1—H1B	117.9

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*A*···O1^{i}	0.87 (2)	2.04 (3)	2.914 (2)	177 (2)
C4—H4*A*···O1^{i}	0.93	2.43	3.123 (3)	131
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