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1-(4-Aminophenyl)ethanone isonicotinoylhydrazone

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.006 Å
R factor = 0.100
wR factor = 0.183
Data-to-parameter ratio = 9.6

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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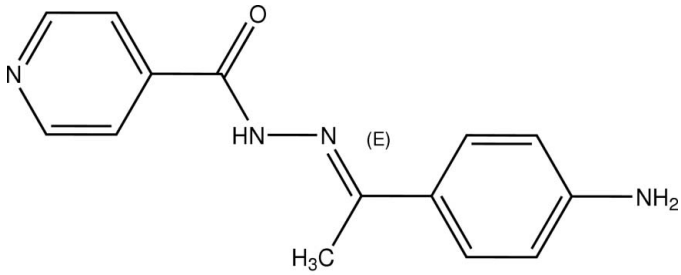
The title molecule, $C_{14}H_{14}N_4O$, adopts a *trans* configuration with respect to the C=N double bond. The dihedral angle between the two rings is 73.1 (4)°. The crystal structure is stabilized by intermolecular N—H···N and N—H···O hydrogen bonds which link the molecules into a chain along the *c* axis.

Comment

The background to this study is described in the first paper of this series (Xie *et al.*, 2006).



(I)

In the title compound, (I) (Fig. 1), the C7=N2 bond, 1.277 (5) Å, and the C9—N3 bond, 1.340 (5) Å, are both shorter than normal because of conjugation effects. All other bond lengths are within normal ranges (Allen *et al.*, 1987). The dihedral angle between the benzene and pyridine rings [73.1 (4)°] is significantly larger than normal due to the steric effect of the C8 methyl substituent. The structure of (I) is stabilized by intermolecular N—H···N and N—H···O hydrogen bonds, forming chains along the *c* axis (Table 1 and Fig. 2).

Experimental

1-(4-Aminophenyl)ethanone (0.2 mmol, 27 mg) and isonicotinohydrazide (0.2 mmol, 27.4 mg) were dissolved in methanol (10 ml). The

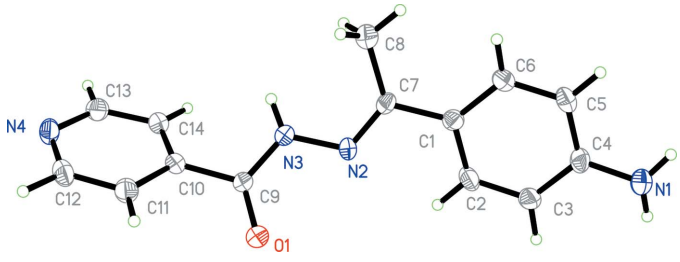


Figure 1
The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

mixture was stirred at room temperature for 10 min. to give a clear yellow solution. The solution was set aside for 8 d to allow slow evaporation of the solvent. Large colourless block-shaped crystals separated; these were collected and washed three times with water.

Crystal data

$C_{14}H_{14}N_4O$
$M_r = 254.29$
Monoclinic, $P2_1/n$
$a = 7.9137\ (15)$ Å
$b = 5.3466\ (10)$ Å
$c = 29.650\ (6)$ Å
$\beta = 95.415\ (3)^\circ$
$V = 1248.9\ (4)$ Å^3
$Z = 4$
$D_x = 1.352$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1324 reflections
$\theta = 5.2$–53.9°
$\mu = 0.09$ mm^{-1}
$T = 298\ (2)$ K
Block, colourless
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min} = 0.974$, $T_{max} = 0.982$
5756 measured reflections
2193 independent reflections
1936 reflections with $I > 2\sigma(I)$
$R_{int} = 0.043$
$\theta_{max} = 25.0^\circ$
$h = -9 \rightarrow 9$
$k = -6 \rightarrow 6$
$l = -29 \rightarrow 35$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.100$
$wR(F^2) = 0.183$
$S = 1.33$
2193 reflections
228 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.034P)^2 + 1.5639P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···N4^{i}	0.84 (5)	2.20 (5)	3.018 (6)	164 (4)
N3—H3A···O1^{ii}	0.85 (4)	2.48 (4)	3.320 (5)	169 (3)

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

All H atoms were initially located in a difference Fourier map and were refined freely with isotropic displacement parameters, giving N—H distances in the range 0.84 (5) to 0.87 (5) and C—H distances in the range 0.89 (5) to 1.01 (4) Å.

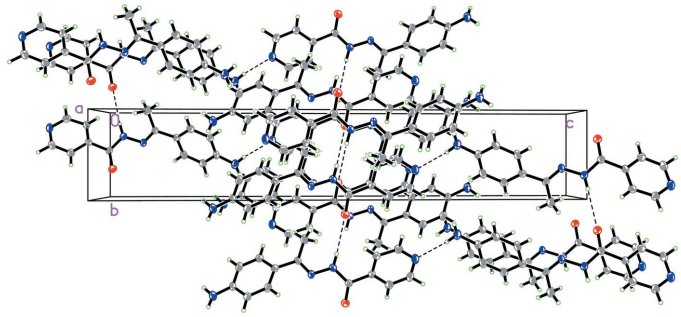


Figure 2
The crystal packing of (I), viewed along the *a* axis. Dashed lines indicate intermolecular hydrogen bonds.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); 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: *SHELXL97*.

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References

Allen, F. H., Kennard, O.,Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bruker (2000). *SHELXTL*. Version 6.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2002). *SADABS*, *SAINT* and *SMART*. Bruker AXS Inc., Madison, Winconsin.
Sheldrick G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Xie, Y.-H., Sheng, L.-Q., Zhu, W. & Shao, S.-C. (2006). *Acta Cryst.* E**62**, o26–o27.