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N-(3-Pyridyl)urea

Sumod George and Ashwini Nangia*

School of Chemistry, University of Hyderabad, Hyderabad 500 046, India

Correspondence e-mail: ansc@uohyd.ernet.in

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.045
wR factor = 0.134
Data-to-parameter ratio = 15.4

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

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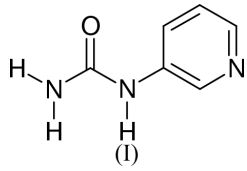
The crystal structure of the title compound, $C_6H_7N_3O$, exhibits packing typical of amides, with N—H···O hydrogen-bond dimers forming a corrugated tape and N—H···N bonds connecting the tapes.

Comment

In a recent monograph on the role of amides in non-covalent syntheses (Palmore & MacDonald, 2000), the urea functional group is considered as part of the amide family. In connection with an ongoing crystallographic study of aromatic ureas (George *et al.*, 2001), we have determined the crystal structure of *N*-(3-pyridyl) urea, (I).



(I)

The pyridyl ring in (I) is tilted to the urea plane by 163.94 (14)° (C8/N7/C6/C5, Fig. 1). The crystal structure of (I) contains a corrugated tape of (*syn*) N10—H8···O9 and (*anti*) N10—H9···O9 hydrogen-bond dimers along the *a* axis, with an (*anti*) N7—H7···N4 bond connecting screw-axis-related molecules in the *b* direction (*syn* and *anti* refer to ureido H atoms) (Fig. 2). The *a* axis of 4.8558 (10) Å in (I) is smaller than the characteristic 5.1 Å packing in carboxylic amides because of the zigzag corrugated pattern. A crystal structure assembled by N—H···N hydrogen bonding interaction was published recently in this journal (Lynch & McClenaghan, 2001). In contrast to the structure of (I), the molecular conformation and crystal packing in *N*-(2-pyridyl)urea (Velikova *et al.*, 1997) are quite different. This latter structure contains parallel zigzag ribbons of molecules hydrogen bonded through (*syn*) N—H···O dimers along the *ab* diagonal. The molecule adopts a planar conformation because of an intramolecular (*anti*) N—H···N interaction. Thus, isomeric 2- and 3-pyridylurea have very different crystal structures.

Experimental

Compound (I) was synthesized by slowly adding NaOCN (130 mg, 2 mmol) dissolved in hot water (1 ml) to a solution of 3-aminopyridine (188 mg, 2 mmol) in glacial AcOH (0.2 ml) with stirring. The aqueous solution was neutralized and extracted with chloroform to remove the unreacted 3-aminopyridine. Column chromatography and recrystallization from EtOAc afforded crystals of (I) (m.p. 472–474 K).

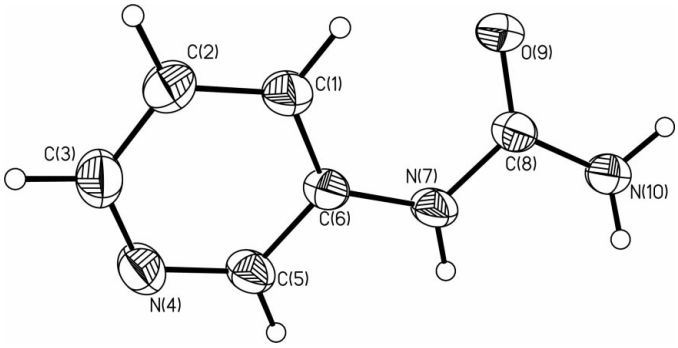


Figure 1
*ORTEP*II (Johnson, 1976) plot of (I) with 50% probability ellipsoids.

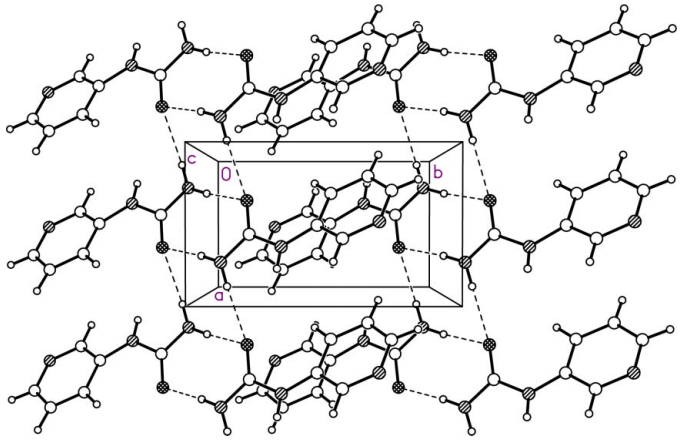


Figure 2
The corrugated tape of N—H···O hydrogen bonds along [100]. For clarity, the N—H···N bond is not shown. Notice the van der Waals packing of pyridyl rings between the hydrogen-bond tapes.

Crystal data

$C_6H_7N_3O$	D_x = 1.445 Mg m^{-3}
M_r = 137.15	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 25 reflections
a = 4.8558 (10) Å	θ = 9.0–10.6°
b = 8.1621 (16) Å	μ = 0.10 mm^{-1}
c = 15.919 (3) Å	T = 293 (2) K
β = 92.16 (3)°	Cube, colourless
V = 630.5 (2) Å^3	0.12 × 0.11 × 0.10 mm
Z = 4	

Data collection

Enraf–Nonius CAD-4 diffractometer	$h = 0 \rightarrow 6$
ω scans	$k = 0 \rightarrow 11$
2021 measured reflections	$l = -22 \rightarrow 22$
1835 independent reflections	3 standard reflections
1362 reflections with $I > 2\sigma(I)$	every 150 reflections
R_{int} = 0.010	frequency: 90 min
θ_{max} = 30.0°	intensity decay: none

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0665P)^2 + 0.1436P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.045	$(\Delta/\sigma)_{max}$ = 0.019
$wR(F^2)$ = 0.134	$\Delta\rho_{max}$ = 0.25 e Å^{-3}
S = 1.08	$\Delta\rho_{min}$ = −0.25 e Å^{-3}
1835 reflections	
119 parameters	
All H-atom parameters refined	

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

D—H···A	D—H	H···A	D···A	D—H···A
N7—H7···N4^{i}	0.888 (19)	2.156 (18)	2.984 (2)	155.0 (16)
N10—H8···O9^{ii}	0.92 (2)	2.05 (2)	2.9657 (19)	173.0 (18)
N10—H9···O9^{iii}	0.842 (19)	2.193 (19)	2.9734 (19)	154.2 (18)
C2—H2···O9^{iv}	0.97 (2)	2.67 (2)	3.629 (2)	168.4 (16)

Symmetry codes: (i) $-\frac{1}{2}-x, y-\frac{1}{2}, \frac{3}{2}-z$; (ii) $-x, 1-y, 2-z$; (iii) $x-1, y, z$; (iv) $1-x, 2-y, 2-z$.

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989); cell refinement: *CAD*-4 *Software*; data reduction: *Xtal*3.5 (Hall *et al.*, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLUTON*-(*C*) (Spek, 1979–1997); software used to prepare material for publication: *SHELXL*97.

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