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3,4-Diaminopyridine

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The amino group in the 3 position of the title compound, $C_5H_7N_3$, is significantly displaced out of the plane of the heteroaromatic ring. Hydrogen bonds between the amino groups and the pyridine N atom link neighbouring molecules into chains along the crystallographic *c* axis in a similar manner to that in 4-aminopyridine. Additional hydrogen bonds lead to the formation of a three-dimensional network.

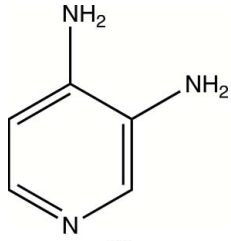
Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.003 Å
R factor = 0.036
wR factor = 0.081
Data-to-parameter ratio = 8.4

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

Comment

3,4-Diaminopyridine, (I), has been used as an amine component in Schiff base reactions (Opozda *et al.*, 2006). In this contribution, we report the crystal and molecular structure of the compound itself.



(I)

Fig. 1 shows the molecular structure and the atomic numbering scheme.. N3 is coplanar with the ring, but N2 is displaced from it by 0.131 (2) Å. C4—N3 = 1.359 (3) Å but C3—N2, is significantly longer, at 1.405 (3) Å.

N—H···N hydrogen bonds represent the strongest intermolecular interactions. Fig. 2 shows how neighbouring molecules aggregate as infinite chains along the crystallographic *c*

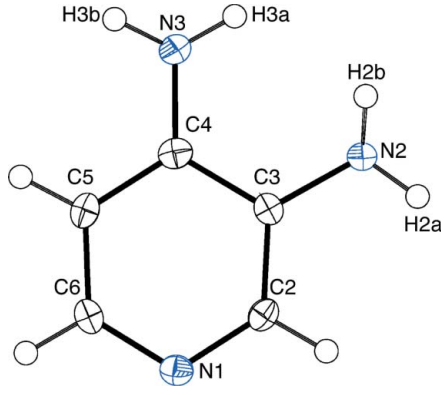


Figure 1
The molecular structure of 3,4-diaminopyridine; Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown with arbitrary radius.

axis. The chain is propagated *via* two contacts in which the amino groups donate one H atom each to the pyridine nitrogen of the next molecule, corresponding to an $R_1^2(7)$ graph-set motif (Etter *et al.*, 1990). This feature underlines the close relationship between the title compound and 4-aminopyridine (Chao & Schempp, 1977). Both compounds crystallize in the same space group with similar lattice parameters and packing. We note that space filling is superior in 3,4-diaminopyridine; its cell volume exceeds that of the monoamine only slightly, despite the presence of four additional non-H atoms per unit cell. In the crystal structure of the title compound, the presence of a second amino group allows the above-mentioned chains to interconnect into a three-dimensional hydrogen-bonding network (Fig. 3).

Experimental

Commercially available 3,4-diaminopyridine (Aldrich) was dissolved in methanol. Elongated yellow platelets were obtained by slow isothermal evaporation at room temperature.

Crystal data

$C_5H_7N_3$	$Z = 4$
$M_r = 109.13$	$D_x = 1.404$ Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation
$a = 5.5815$ (18) Å	$\mu = 0.09$ mm^{-1}
$b = 7.352$ (2) Å	$T = 120$ (2) K
$c = 12.579$ (4) Å	Platelet, yellow
$V = 516.2$ (3) Å^3	0.20 × 0.15 × 0.02 mm

Data collection

Bruker SMART CCD area-detector diffractometer	614 independent reflections
	562 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.057$
Absorption correction: none	$\theta_{max} = 25.9°$
5342 measured reflections	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.03P)^2 + 0.2P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.036$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.081$	$\Delta\rho_{max} = 0.18$ e Å^{-3}
$S = 1.09$	$\Delta\rho_{min} = -0.13$ e Å^{-3}
614 reflections	
73 parameters	
H-atom parameters constrained	

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···N1^{i}	0.90	2.50	3.184 (3)	134
N2—H2B···N1^{ii}	0.90	2.33	3.160 (3)	154
N3—H3A···N2	0.90	2.48	2.812 (3)	102
N3—H3A···N1^{ii}	0.90	2.23	3.124 (3)	174
N3—H3B···N2^{iii}	0.90	2.26	3.145 (3)	169

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

No significant anomalous dispersion effects can be expected for the elemental composition of the title compound and the wavelength used; Friedel pairs were therefore merged. All H atoms could be located in a difference Fourier map; they were, however, treated as riding in standard geometry [C—H = 0.95 or N—H = 0.90 Å and U_{iso}(H) =1.2U_{eq}(C,N)] in order to maintain an acceptable ratio between observations and variables.

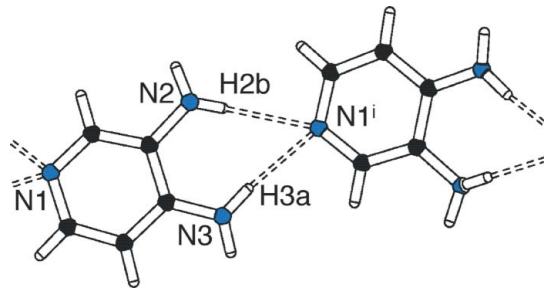


Figure 2
A chain of hydrogen-bonded molecules (dashed lines) along the *c* axis. [Symmetry code: (i) $\frac{1}{2}-x, -y, z-\frac{1}{2}$.]

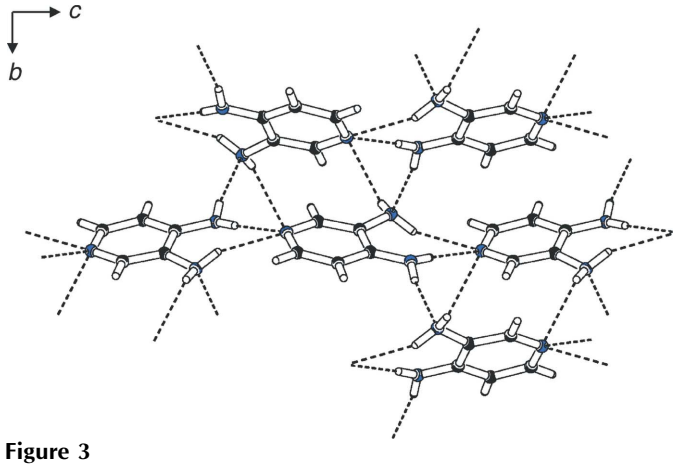


Figure 3
The hydrogen-bond (dashed lines) network in the crystal structure of 3,4-diaminopyridine.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SMART*; data reduction: *SAINT-Plus* (Bruker, 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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