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6-Methylpyridin-3-amine

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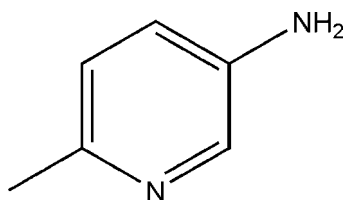
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Key indicators: single-crystal X-ray study; $T = 294$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.057; wR factor = 0.154; data-to-parameter ratio = 15.2.

In the molecule of the title compound, $\text{C}_6\text{H}_8\text{N}_2$, the methyl C and amine N atoms are 0.021 (2) and 0.058 (2) Å from the pyridine ring plane. In the crystal structure, intermolecular $\text{N}-\text{H}\cdots\text{N}$ hydrogen bonds link the molecules.

Related literature

For a related structure, see: Sawanishi *et al.* (1987). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$\text{C}_6\text{H}_8\text{N}_2$
 $M_r = 108.14$
 Monoclinic, $P2_1/n$
 $a = 8.4240$ (17) Å
 $b = 7.0560$ (14) Å
 $c = 10.658$ (2) Å
 $\beta = 105.23$ (3)°

$V = 611.3$ (2) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.07$ mm⁻¹
 $T = 294$ (2) K
 $0.30 \times 0.20 \times 0.10$ mm

Data collection

Enraf–Nonius CAD-4 diffractometer
 Absorption correction: ψ scan (North *et al.*, 1968)
 $T_{\min} = 0.978$, $T_{\max} = 0.993$
 1183 measured reflections

1106 independent reflections
 746 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.059$
 3 standard reflections
 frequency: 120 min
 intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.057$
 $wR(F^2) = 0.154$
 $S = 1.02$
 1106 reflections

73 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.19$ e Å⁻³
 $\Delta\rho_{\min} = -0.19$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N2}-\text{H2B}\cdots\text{N1}^i$	0.86	2.29	3.131 (3)	165

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

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2583).

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supplementary materials

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6-Methylpyridin-3-amine

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Comment

Some derivatives of 3-pyridinecarboxylic acid are important chemical materials. We report herein the crystal structure of the title compound.

In the molecule of the title compound (Fig. 1) the bond lengths (Allen *et al.*, 1987) and angles are within normal ranges. Atoms C1 and N2 are 0.021 (2) Å and 0.058 (2) Å away from the pyridine ring plane.

In the crystal structure, intermolecular N-H...N hydrogen bonds (Table 1) link the molecules, in which they may be effective in the stabilization of the structure.

Experimental

For the preparation of the title compound, bromine (17.3 g) was added slowly to sodium hydroxide solution (303 ml, 5%), and then 3-pyridinecarboxamide (13 g) was added in about 20 min at 273-278 K. The mixture was heated in an oil bath at 343-353 K for 4 h. The product was extracted with CH₂Cl₂, washed with water and dried (yield; 8 g, 77.6%) (Sawanishi *et al.*, 1987). Crystals suitable for X-ray analysis were obtained by slow evaporation of a methanol solution.

Refinement

H atoms were positioned geometrically, with N-H = 0.86 Å (for NH₂) and C-H = 0.93 and 0.96 Å for aromatic and methyl H, respectively, and constrained to ride on their parent atoms with $U_{\text{iso}}(\text{H}) = xU_{\text{eq}}(\text{C,N})$, where $x = 1.5$ for methyl H, and $x = 1.2$ for all other H atoms.

Figures

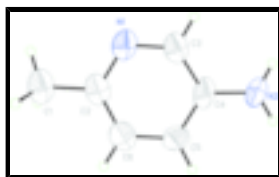


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

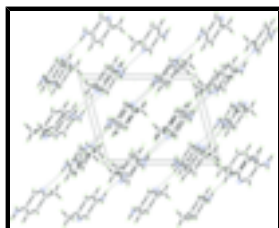


Fig. 2. A partial packing diagram of the title compound. Hydrogen bonds are shown as dashed lines.

6-Methylpyridin-3-amine

Crystal data

$C_6H_8N_2$	$F_{000} = 232$
$M_r = 108.14$	$D_x = 1.175 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
Hall symbol: -P 2yn	$\lambda = 0.71073 \text{ \AA}$
$a = 8.4240 (17) \text{ \AA}$	Cell parameters from 25 reflections
$b = 7.0560 (14) \text{ \AA}$	$\theta = 10\text{--}12^\circ$
$c = 10.658 (2) \text{ \AA}$	$\mu = 0.07 \text{ mm}^{-1}$
$\beta = 105.23 (3)^\circ$	$T = 294 (2) \text{ K}$
$V = 611.3 (2) \text{ \AA}^3$	Block, colorless
$Z = 4$	$0.30 \times 0.20 \times 0.10 \text{ mm}$

Data collection

Enraf-Nonius CAD-4 diffractometer	$R_{\text{int}} = 0.059$
Radiation source: fine-focus sealed tube	$\theta_{\text{max}} = 25.3^\circ$
Monochromator: graphite	$\theta_{\text{min}} = 2.8^\circ$
$T = 294(2) \text{ K}$	$h = 0 \rightarrow 9$
$\omega/2\theta$ scans	$k = 0 \rightarrow 8$
Absorption correction: ψ scan (North <i>et al.</i> , 1968)	$l = -12 \rightarrow 12$
$T_{\text{min}} = 0.978$, $T_{\text{max}} = 0.993$	3 standard reflections
1183 measured reflections	every 120 min
1106 independent reflections	intensity decay: 1%
746 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.057$	H-atom parameters constrained
$wR(F^2) = 0.154$	$w = 1/[\sigma^2(F_o^2) + (0.05P)^2 + 0.5P]$
$S = 1.02$	where $P = (F_o^2 + 2F_c^2)/3$
1106 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
73 parameters	$\Delta\rho_{\text{max}} = 0.19 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\text{min}} = -0.19 \text{ e \AA}^{-3}$
	Extinction correction: none

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.8161 (3)	0.0759 (3)	0.11504 (18)	0.0480 (6)
N2	1.0351 (3)	0.4188 (3)	0.3558 (2)	0.0595 (7)
H2A	0.9692	0.5137	0.3361	0.071*
H2B	1.1237	0.4285	0.4177	0.071*
C1	0.8752 (4)	-0.2454 (4)	0.0569 (3)	0.0616 (8)
H1B	0.7734	-0.2235	-0.0076	0.092*
H1C	0.8626	-0.3507	0.1105	0.092*
H1D	0.9602	-0.2730	0.0148	0.092*
C2	0.9206 (4)	-0.0734 (4)	0.1390 (2)	0.0483 (7)
C3	0.8578 (3)	0.2310 (4)	0.1886 (2)	0.0474 (7)
H3A	0.7857	0.3333	0.1709	0.057*
C4	0.9987 (3)	0.2519 (4)	0.2884 (2)	0.0478 (7)
C5	1.1033 (3)	0.0962 (4)	0.3130 (2)	0.0503 (7)
H5A	1.2009	0.1007	0.3788	0.060*
C6	1.0608 (4)	-0.0656 (4)	0.2385 (2)	0.0544 (7)
H6A	1.1290	-0.1713	0.2566	0.065*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0679 (13)	0.0494 (13)	0.0253 (10)	-0.0054 (11)	0.0098 (9)	0.0006 (10)
N2	0.0703 (15)	0.0579 (15)	0.0413 (13)	0.0013 (12)	-0.0013 (11)	-0.0182 (11)
C1	0.096 (2)	0.0527 (17)	0.0366 (14)	-0.0081 (15)	0.0191 (14)	-0.0067 (13)
C2	0.0835 (18)	0.0426 (14)	0.0242 (12)	-0.0001 (13)	0.0234 (12)	0.0044 (11)
C3	0.0707 (16)	0.0446 (14)	0.0302 (13)	0.0036 (12)	0.0190 (12)	0.0017 (11)
C4	0.0772 (17)	0.0489 (15)	0.0206 (11)	-0.0019 (13)	0.0187 (11)	-0.0033 (11)
C5	0.0622 (15)	0.0554 (16)	0.0301 (12)	0.0096 (13)	0.0062 (11)	0.0047 (12)
C6	0.0844 (19)	0.0481 (15)	0.0326 (13)	0.0087 (14)	0.0190 (13)	0.0038 (12)

Geometric parameters (\AA , $^\circ$)

N1—C3	1.338 (3)	C1—H1D	0.9600
N1—C2	1.353 (3)	C2—C6	1.365 (4)

supplementary materials

N2—C4	1.371 (3)	C3—C4	1.378 (4)
N2—H2A	0.8600	C3—H3A	0.9300
N2—H2B	0.8600	C4—C5	1.390 (4)
C1—C2	1.487 (3)	C5—C6	1.383 (4)
C1—H1B	0.9600	C5—H5A	0.9300
C1—H1C	0.9600	C6—H6A	0.9300
C3—N1—C2	117.9 (2)	N1—C3—C4	125.4 (2)
C4—N2—H2A	120.0	N1—C3—H3A	117.3
C4—N2—H2B	120.0	C4—C3—H3A	117.3
H2A—N2—H2B	120.0	N2—C4—C3	121.6 (2)
C2—C1—H1B	109.5	N2—C4—C5	122.5 (2)
C2—C1—H1C	109.5	C3—C4—C5	115.9 (2)
H1B—C1—H1C	109.5	C6—C5—C4	119.2 (2)
C2—C1—H1D	109.5	C6—C5—H5A	120.4
H1B—C1—H1D	109.5	C4—C5—H5A	120.4
H1C—C1—H1D	109.5	C2—C6—C5	121.3 (3)
N1—C2—C6	120.2 (2)	C2—C6—H6A	119.3
N1—C2—C1	118.1 (2)	C5—C6—H6A	119.3
C6—C2—C1	121.7 (3)		
C3—N1—C2—C6	2.2 (3)	N2—C4—C5—C6	-178.1 (2)
C3—N1—C2—C1	-179.6 (2)	C3—C4—C5—C6	-0.3 (4)
C2—N1—C3—C4	-0.5 (4)	N1—C2—C6—C5	-2.9 (4)
N1—C3—C4—N2	177.4 (2)	C1—C2—C6—C5	178.9 (2)
N1—C3—C4—C5	-0.4 (4)	C4—C5—C6—C2	1.9 (4)

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2—H2B \cdots N1 ⁱ	0.86	2.29	3.131 (3)	165

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

Fig. 1

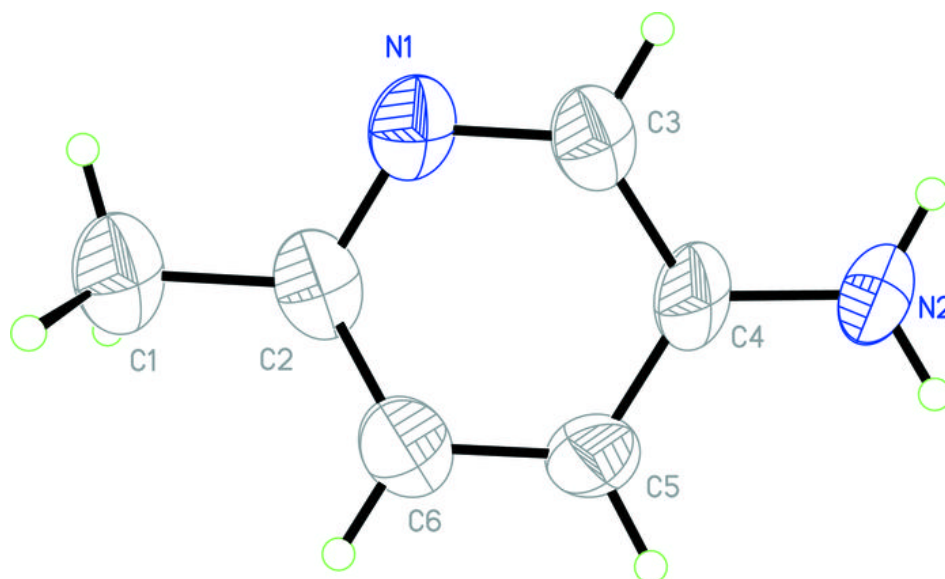


Fig. 2

