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6-Methylpyridin-3-amine

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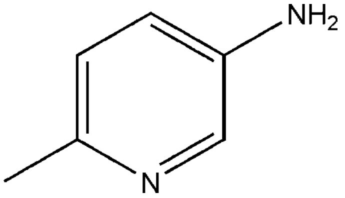
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.004 Å; R factor = 0.057; wR factor = 0.154; data-to-parameter ratio = 15.2.

In the molecule of the title compound, $C_6H_8N_2$, 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 N—H···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

$C_6H_8N_2$
M_r = 108.14
Monoclinic, $P2_1/n$
a = 8.4240 (17) Å
b = 7.0560 (14) Å
c = 10.658 (2) Å
β = 105.23 (3)°
V = 611.3 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 294 (2) K
0.30 × 0.20 × 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_{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—H···A	D—H	H···A	D···A	D—H···A
N2—H2B···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

Acta Cryst. (2009). E**65**, o124 [**doi:10.1107/S1600536808040531**]

6-Methylpyridin-3-amine

K. Zhu, **N. Xun**, **P. Wei** and **P.-F. Han**

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 CH_2Cl_2, 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 NH_2) and C-H = 0.93 and 0.96 Å for aromatic and methyl H, respectively, and constrained to ride on their parent atoms with $U_{iso}(H) = xU_{eq}(C,N)$, where x = 1.5 for methyl H, and x = 1.2 for all other H atoms.

Figures

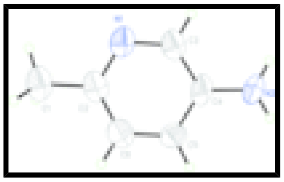

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

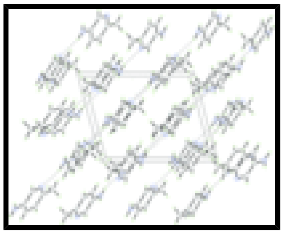

Fig. 2. A partial packing diagram of the title compound. Hydrogen bonds are shown as dashed lines.

6-Methylpyridin-3-amine

Crystal data

$C_6H_8N_2$

$M_r = 108.14$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 8.4240$ (17) Å

$b = 7.0560$ (14) Å

$c = 10.658$ (2) Å

$\beta = 105.23$ (3)°

$V = 611.3$ (2) Å^3

$Z = 4$

$F_{000} = 232$

$D_x = 1.175$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å

Cell parameters from 25 reflections

$\theta = 10–12$°

$\mu = 0.07$ mm^{-1}

$T = 294$ (2) K

Block, colorless

0.30 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 294(2)$ K

$\omega/2\theta$ scans

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 $I > 2\sigma(I)$

$R_{\rm int} = 0.059$

$\theta_{\max} = 25.3$°

$\theta_{\min} = 2.8$°

$h = 0\rightarrow9$

$k = 0\rightarrow8$

$l = -12\rightarrow12$

3 standard reflections

every 120 min

intensity decay: 1%

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.057$

$wR(F^2) = 0.154$

$S = 1.02$

1106 reflections

73 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.05P)^2 + 0.5P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.19$ e Å^{-3}

$\Delta\rho_{\min} = -0.19$ e Å^{-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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{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 (Å²)

	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 (Å, °)

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

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 (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2B···N1^{i}	0.86	2.29	3.131 (3)	165

Symmetry codes: (i) *x*+1/2, −*y*+1/2, *z*+1/2.

Fig. 1

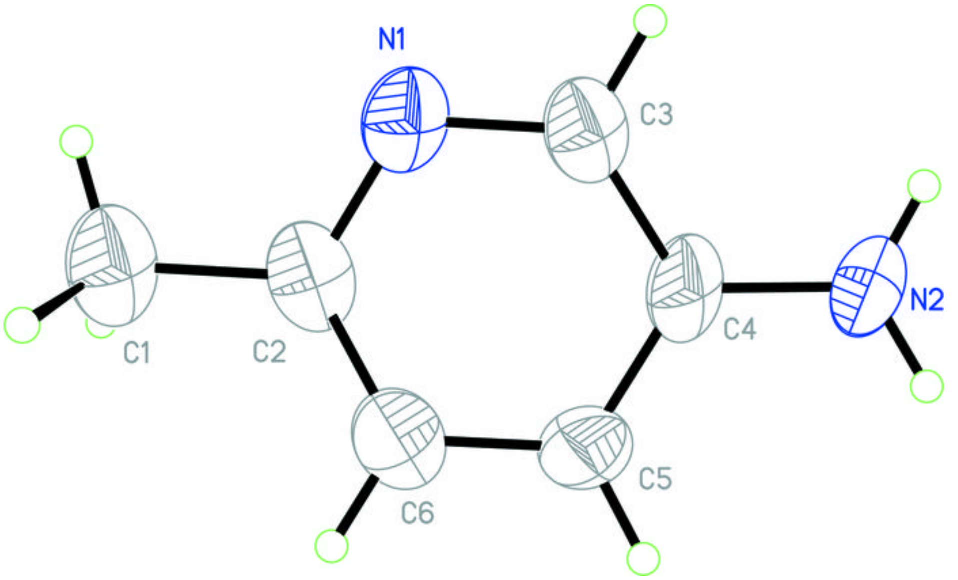

Fig. 2