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# 4-(Methylamino)pyridine

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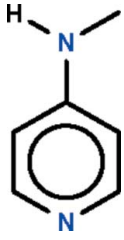
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.044; $wR$ factor = 0.102; data-to-parameter ratio = 9.1.

The non-H atoms of the title compound, $C_6H_8N_2$, lie in a common plane (r.m.s. deviation = 0.034 Å). In the crystal, adjacent molecules are linked by intermolecular N—H···N hydrogen bonds into a zigzag chain running along the $c$ axis.

## Related literature

For the non-linear optical activity of co-crystals with substituted 4-nitrophenol, see; Huang *et al.* (1997). For the crystal structure of 4-aminopyridine, see: Anderson *et al.* (2005) and for that of 4-dimethylpyridine, see: Ohms & Guth (1984).




## Experimental

### Crystal data

$C_6H_8N_2$
$M_r$ = 108.14
Orthorhombic, $Pna2_1$
$a$ = 6.5645 (18) Å
$b$ = 7.1230 (19) Å
$c$ = 12.489 (4) Å
$V$ = 584.0 (3) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.08 mm$^{-1}$
$T$ = 100 K
0.12 × 0.12 × 0.02 mm

### Data collection

Bruker SMART APEX diffractometer
5127 measured reflections
707 independent reflections
521 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.093

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.102
$S$ = 0.99
707 reflections
78 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.18 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.20 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1···N2$^{i}$ | 0.88 (1) | 2.06 (1) | 2.930 (3) | 168 (3) |

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

I thank the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5213).

## References

Anderson, F. P., Gallagher, J. F., Kenny, P. T. M. & Lough, A. J. (2005). *Acta Cryst.* E**61**, o1350–o1353.
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Ohms, U. & Guth, H. (1984). *Z. Kristallogr.* **166**, 213–219.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2010). *publCIF*. In preparation.

# supplementary materials

*Acta Cryst.* (2010). E**66**, o823 [ **doi:10.1107/S1600536810008986** ]

# 4-(Methylamino)pyridine

**S. W. Ng**

## Comment

The amino nitrogen atom in 4-aminopyridine, a drug used for treating multiple sclerosis, is pyramidal; the amino group engages in a N–H···N hydrogen bonding interaction with adjacent pyridyl rings to generate a chain. The amino group uses its other nitrogen atom to form an N–H···$\pi$ interaction with other pyridyl rings (Anderson *et al.*, 2005).

In the title monomethyl-substituted analogue (Scheme I, Fig. 1), all non-hydrogen atoms lie in a common plane. However, the amino nitrogen atom is slightly pyramidal, this being displaced out of the trigonal plane by 0.18 (2) Å (Σangles 353 °). On the other hand, the amino nitrogen atom in 4-dimethylaminopyridine has unambiguously planar configuration (Ohms & Guth, 1984). In the present structure, adjacent molecules are linked by an N–H···N hydrogen bond to generate a helical chain motif (Table 1).

The compound belongs to a non-centrosymmetric space group, a feature that may render it useful for second-harmonic generation, particularly as it co-crystal with 2-methoxy-4-nitrophenol shows NLO activity (Huang *et al.*, 1997).

## Experimental

4-Methylaminopyridine, as purchased from the Aldrich Chemical Company, is a crystalline material.

## Refinement

Due to the absence of anomalous scatterers, 644 Friedel pairs were merged. Carbon-bound H-atoms were placed in calculated positions (C—H 0.95 Å) and were included in the refinement in the riding model approximation, with $U$(H) set to 1.2$U_{eq}$(C). The amino H-atom was located in a difference Fourier map and it was refined with a distance restraint of N–H 0.88±0.01 Å.

## Figures

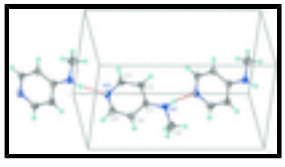

Fig. 1. Anisotropic displacement ellipsoid plot (Barbour, 2001) of a portion of the hydrogen-bonded chain structure of 4-methylaminopyridine at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

## 4-(Methylamino)pyridine

*Crystal data*

| | |
|---|---|
| $C_6H_8N_2$ | $F(000) = 232$ |
| $M_r = 108.14$ | $D_x = 1.230$ Mg m$^{-3}$ |

| | |
|---|---|
| Orthorhombic, $Pna2_1$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: P 2c -2n | Cell parameters from 379 reflections |
| $a = 6.5645$ (18) Å | $\theta = 3.3–21.5°$ |
| $b = 7.1230$ (19) Å | $\mu = 0.08$ mm$^{-1}$ |
| $c = 12.489$ (4) Å | $T = 100$ K |
| $V = 584.0$ (3) Å$^3$ | Plate, colorless |
| $Z = 4$ | 0.12 × 0.12 × 0.02 mm |

*Data collection*

| | |
|---|---|
| Bruker SMART APEX diffractometer | 521 reflections with $I > 2\sigma(I)$ |
| Radiation source: fine-focus sealed tube | $R_{int} = 0.093$ |
| graphite | $\theta_{max} = 27.5°$, $\theta_{min} = 3.3°$ |
| ω scans | $h = -7\rightarrow8$ |
| 5127 measured reflections | $k = -9\rightarrow8$ |
| 707 independent reflections | $l = -16\rightarrow16$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.044$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.102$ | H atoms treated by a mixture of independent and constrained refinement |
| $S = 0.99$ | $w = 1/[\sigma^2(F_o^2) + (0.0518P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 707 reflections | $(\Delta/\sigma)_{max} = 0.001$ |
| 78 parameters | $\Delta\rho_{max} = 0.18$ e Å$^{-3}$ |
| 2 restraints | $\Delta\rho_{min} = -0.20$ e Å$^{-3}$ |

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| N1 | 0.2579 (4) | 0.0086 (3) | 0.49959 (18) | 0.0219 (6) |
| H1 | 0.177 (4) | 0.027 (5) | 0.4440 (19) | 0.036 (11)* |
| N2 | −0.0105 (4) | −0.0122 (3) | 0.8044 (2) | 0.0232 (6) |
| C1 | 0.1745 (4) | −0.0004 (4) | 0.5993 (2) | 0.0193 (6) |
| C2 | −0.0127 (4) | 0.0889 (4) | 0.6198 (2) | 0.0217 (7) |
| H2 | −0.0813 | 0.1550 | 0.5645 | 0.026* |
| C3 | −0.0957 (5) | 0.0794 (4) | 0.7215 (2) | 0.0256 (7) |
| H3 | −0.2215 | 0.1417 | 0.7336 | 0.031* |
| C4 | 0.1690 (4) | −0.0944 (4) | 0.7840 (2) | 0.0220 (7) |
| H4 | 0.2337 | −0.1593 | 0.8411 | 0.026* |
| C5 | 0.2673 (4) | −0.0917 (4) | 0.6858 (2) | 0.0207 (7) |
| H5 | 0.3959 | −0.1511 | 0.6773 | 0.025* |

| | | | | |
|---|---|---|---|---|
| C6 | 0.4412 (4) | −0.0966 (5) | 0.4736 (2) | 0.0302 (8) |
| H6A | 0.5534 | −0.0546 | 0.5195 | 0.045* |
| H6B | 0.4772 | −0.0753 | 0.3984 | 0.045* |
| H6C | 0.4168 | −0.2307 | 0.4853 | 0.045* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N1 | 0.0237 (13) | 0.0242 (14) | 0.0178 (12) | 0.0021 (12) | −0.0023 (10) | 0.0025 (12) |
| N2 | 0.0277 (14) | 0.0232 (12) | 0.0189 (11) | 0.0006 (12) | 0.0005 (11) | −0.0001 (13) |
| C1 | 0.0189 (15) | 0.0192 (15) | 0.0198 (14) | −0.0048 (13) | −0.0055 (12) | −0.0010 (12) |
| C2 | 0.0231 (17) | 0.0218 (16) | 0.0201 (13) | 0.0003 (13) | −0.0031 (12) | 0.0033 (13) |
| C3 | 0.0293 (18) | 0.0210 (16) | 0.0264 (16) | 0.0046 (14) | 0.0013 (14) | −0.0005 (14) |
| C4 | 0.0248 (16) | 0.0223 (16) | 0.0188 (14) | −0.0016 (13) | −0.0039 (12) | 0.0009 (13) |
| C5 | 0.0196 (16) | 0.0205 (16) | 0.0219 (14) | 0.0009 (13) | −0.0024 (12) | −0.0011 (14) |
| C6 | 0.0242 (16) | 0.0408 (19) | 0.0256 (16) | 0.0051 (14) | 0.0028 (14) | 0.0005 (14) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| N1—C1 | 1.362 (4) | C2—H2 | 0.9500 |
| N1—C6 | 1.454 (4) | C3—H3 | 0.9500 |
| N1—H1 | 0.88 (1) | C4—C5 | 1.386 (4) |
| N2—C4 | 1.340 (4) | C4—H4 | 0.9500 |
| N2—C3 | 1.345 (4) | C5—H5 | 0.9500 |
| C1—C5 | 1.401 (4) | C6—H6A | 0.9800 |
| C1—C2 | 1.407 (4) | C6—H6B | 0.9800 |
| C2—C3 | 1.384 (4) | C6—H6C | 0.9800 |
| C1—N1—C6 | 120.8 (2) | N2—C4—C5 | 124.8 (3) |
| C1—N1—H1 | 119 (2) | N2—C4—H4 | 117.6 |
| C6—N1—H1 | 113 (2) | C5—C4—H4 | 117.6 |
| C4—N2—C3 | 115.6 (3) | C4—C5—C1 | 119.1 (3) |
| N1—C1—C5 | 123.5 (3) | C4—C5—H5 | 120.4 |
| N1—C1—C2 | 119.8 (3) | C1—C5—H5 | 120.4 |
| C5—C1—C2 | 116.7 (3) | N1—C6—H6A | 109.5 |
| C3—C2—C1 | 119.3 (3) | N1—C6—H6B | 109.5 |
| C3—C2—H2 | 120.4 | H6A—C6—H6B | 109.5 |
| C1—C2—H2 | 120.4 | N1—C6—H6C | 109.5 |
| N2—C3—C2 | 124.5 (3) | H6A—C6—H6C | 109.5 |
| N2—C3—H3 | 117.7 | H6B—C6—H6C | 109.5 |
| C2—C3—H3 | 117.7 | | |
| C6—N1—C1—C5 | 7.2 (4) | C1—C2—C3—N2 | −0.6 (5) |
| C6—N1—C1—C2 | −174.3 (3) | C3—N2—C4—C5 | −0.5 (5) |
| N1—C1—C2—C3 | −179.8 (3) | N2—C4—C5—C1 | −1.2 (5) |
| C5—C1—C2—C3 | −1.1 (4) | N1—C1—C5—C4 | −179.4 (3) |
| C4—N2—C3—C2 | 1.5 (5) | C2—C1—C5—C4 | 2.0 (4) |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|

| | | | | |
|---|---|---|---|---|
| N1—H1···N2$^{i}$ | 0.88 (1) | 2.06 (1) | 2.930 (3) | 168 (3) |

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

**Fig. 1**