Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-(Methylamino)pyridine

Seik Weng Ng

Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

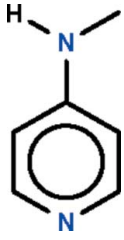
Received 9 March 2010; accepted 9 March 2010

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(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
μ = 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.
Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Bruker (2009). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Huang, K.-S., Britton, D. E., Etter, M. C. & Byrn, S. R. (1997). *J. Mater. Chem.* **7**, 713–720.
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.

supporting information

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

4-(Methylamino)pyridine

Seik Weng Ng

S1. 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···π 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).

S2. Experimental

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

S3. 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 1.2U_{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.

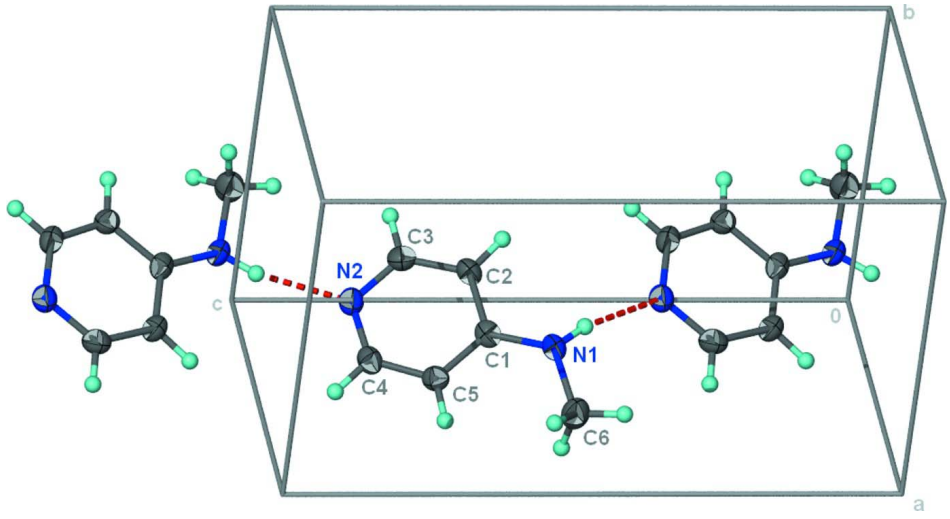


Figure 1

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

$C_6H_8N_2$
$M_r = 108.14$
Orthorhombic, $Pna2_1$
Hall symbol: P 2c -2n
$a = 6.5645\ (18)$ Å
$b = 7.1230\ (19)$ Å
$c = 12.489\ (4)$ Å
$V = 584.0\ (3)$ Å^3
$Z = 4$
$F(000) = 232$
$D_x = 1.230$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 379 reflections
$\theta = 3.3–21.5°$
$\mu = 0.08$ mm^{-1}
$T = 100$ K
Plate, colorless
0.12 × 0.12 × 0.02 mm

Data collection

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

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.102$
$S = 0.99$
707 reflections
78 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0518P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.18$ e Å^{-3}
$\Delta\rho_{min} = -0.20$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	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 (Å²)

	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, º)

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, º)

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*−1/2.