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2-Chloro-4-methylpyridin-3-amine

H. S. Yathirajan,[a] S. Bindya,[a] A. M. Vijesh,[b] B. Narayana[b] and Michael Bolte[c]*

[a]Department of Studies in Chemistry, University of Mysore, Manasagangotri, Mysore 570 006, India, [b]Department of Chemistry, Mangalore University, Mangalagangotri 574 199, India, and [c]Institut für Anorganische Chemie, J. W. Goethe-Universität Frankfurt, Max-von-Laue-Strasse 7, 60438 Frankfurt/Main, Germany

Correspondence e-mail: bolte@chemie.uni-frankfurt.de

Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.002 Å
R factor = 0.034
wR factor = 0.093
Data-to-parameter ratio = 13.3

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

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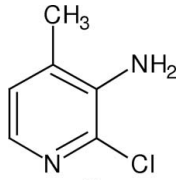
Geometric parameters of the title compound, $C_6H_7ClN_2$, are in the usual ranges. The molecular structure shows one intramolecular N—H···Cl contact and the crystal packing is stabilized by an intermolecular N—H···N hydrogen bond.

Comment

Pyridine is an important structural unit found in many known therapeutic agents (Proudfoot *et al.*, 1995). Pyridine and its derivatives are important in industrial organic chemistry as fundamental building blocks (Sherman, 2004). Many pyridinyl thiazoles have proved to possess a wide range of biological activities such as cardiotonic, anti-asthmatic, anti-inflammatory and also shown to be selective inhibitors of cytochrome P-450 2A6 (Denton *et al.*, 2005). Pyridine derivatives are known for their cardiac effects (Schoepke & Shideman, 1962). In view of the importance of pyridine derivatives, the crystal structure of the title compound, (I), is reported.



(I)

A perspective view of (I) is shown in Fig. 1. Bond lengths and angles can be regarded as normal (Cambridge Structural Database, Version 5.27, November 2005 update, August 2006;

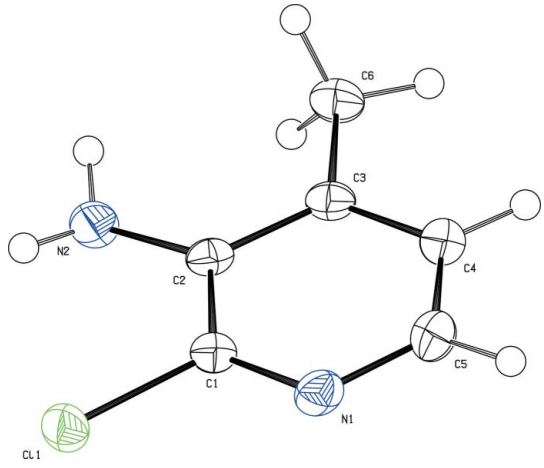


Figure 1
The molecular structure of the title compound with the atom numbering; displacement ellipsoids are drawn at the 50% probability level.

MOGUL Version 1.1; Allen, 2002; Bruno *et al.*, 2004). As expected the molecule is planar (r.m.s. deviation for all non-H atoms 0.012 Å). The molecular conformation is characterized by an N—H···Cl contact and the crystal packing is stabilized by an N—H···N hydrogen bond, forming chains along the *c* axis (Table 1).

Experimental

A pure sample of the title compound was obtained from Srides Arco Laboratory, Mangalore, India. The sample was crystallized from acetone by slow evaporation (m.p. 333–335 K).

Crystal data

$C_6H_7ClN_2$
M_r = 142.59
Monoclinic, $P2_1/c$
a = 3.9877 (8) Å
b = 12.8468 (15) Å
c = 12.8408 (19) Å
β = 90.872 (14)°
V = 657.75 (18) Å^3
Z = 4
D_x = 1.440 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.48 mm^{-1}
T = 173 (2) K
Rod, colourless
0.48 × 0.21 × 0.20 mm

Data collection

Stoe IPDS-II two-circle diffractometer
ω scans
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)
T_{min} = 0.802, T_{max} = 0.910
3879 measured reflections
1226 independent reflections
1109 reflections with $I > 2\sigma(I)$
R_{int} = 0.050
θ_{max} = 25.6°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.093
S = 1.08
1226 reflections
92 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0536P)^2 + 0.1927P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.034 (8)

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···Cl1	0.86 (3)	2.55 (3)	2.9796 (17)	111.9 (19)
N2—H2B···N1^{i}	0.84 (2)	2.28 (2)	3.089 (2)	162 (2)

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

H atoms were found in a difference map, but those bonded to C were refined using a riding model, with C—H = 0.95 Å for aromatic or C—H = 0.98 Å for methyl H atoms. U_{iso}(H) values were set at $1.2U_{eq}$(C) or $1.5U_{eq}$(methyl C). The methyl group was allowed to rotate but not to tip. H atoms bonded to nitrogen were refined freely.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; 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: *PLATON* and *SHELXL97*.

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