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3-Picoline

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Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.003 Å
R factor = 0.040
wR factor = 0.106
Data-to-parameter ratio = 8.1

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

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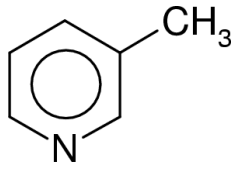
The crystal structure of 3-picoline (3-methylpyridine, C_6H_7N) has been determined at 120 (2) K following *in situ* crystal growth from the liquid. The molecules pack in a herring-bone-type arrangement in the non-centrosymmetric space group $Pna2_1$.

Comment

The picolines (methylpyridines) comprise a series of empirical formula C_6H_7N, with weak intermolecular interactions and low melting points. The crystal structure of 4-picoline (4-methylpyridine; m.p. 276 K) has been determined previously from a crystal grown using an elaborate modified Bridgman technique (Ohms *et al.*, 1985). We report here the crystal structure of 3-picoline (m.p. 255 K), determined at 120 (2) K from a crystal grown *in situ* in a 0.3 mm glass capillary. This work forms part of a study devoted to improving techniques for determining the crystal structures of substances that are liquids at room temperature (see, for example, Bond & Davies, 2001).



(I)

Molecules of (I) (Fig. 1) pack in a herring-bone-type arrangement in the non-centrosymmetric space group $Pna2_1$ (Fig. 2). There are no apparent directional C—H···N interactions: the closest contacts to N1 are made by H4 and H5, with geometric parameters H4···N1^{i} = 2.77 (3) Å and C4—H4···N1^{i} = 124 (2)°, and H5···N1^{i} = 2.90 (2) Å and C5—H5···N1^{i} = 120 (2)° [symmetry code: (i) 1.5−*x*, 0.5+*y*, 0.5+*z*].

Experimental

The sample (99%) was obtained from the Aldrich Company and was used without further purification. The crystal was grown in a 0.3 mm glass capillary tube at 240 K (a temperature only slightly less than the melting point of the solid in the capillary tube) using a technique described previously (Davies & Bond, 2001). The crystal was cooled subsequently to 120 (2) K for data collection. The length of the cylindrical crystal was not estimated, but it exceeded the 0.35 mm collimator diameter.

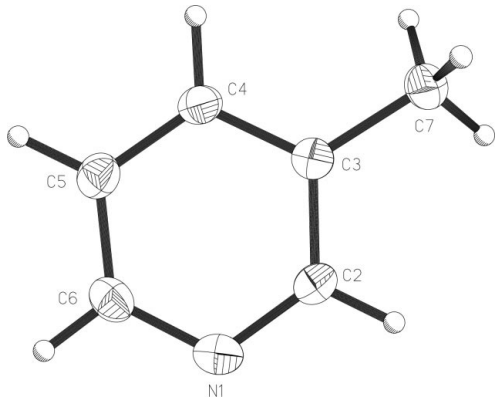


Figure 1
The molecular structure and atom-labelling scheme for (I) showing displacement ellipsoids at 50% probability for non-H atoms (*XP*; Sheldrick, 1993).

Crystal data

C_6H_7N
M_r = 93.13
Orthorhombic, $Pna2_1$
a = 9.3516 (9) Å
b = 9.7925 (10) Å
c = 5.7651 (3) Å
V = 527.94 (8) Å^3
Z = 4
D_x = 1.172 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3581 reflections
θ = 1.0–27.5°
μ = 0.07 mm^{-1}
T = 120 (2) K
Cylinder, colourless
0.15 mm (radius)

Data collection

Nonius KappaCCD diffractometer
Thin-slice ω and φ scans
Absorption correction: none
2718 measured reflections
665 independent reflections
643 reflections with $I > 2\sigma(I)$
R_{int} = 0.040
θ_{max} = 27.5°
$h = -12 \rightarrow 8$
$k = -9 \rightarrow 12$
$l = -6 \rightarrow 7$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.106
S = 1.08
665 reflections
82 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0633P)^2 + 0.0757P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

H atoms on the pyridyl ring were located in difference Fourier maps and were allowed to refine with independent isotropic displacement parameters. Methyl H atoms were placed geometrically and refined with one common isotropic displacement parameter, with the methyl group allowed to rotate about its local threefold axis. Friedel pairs (478) were averaged prior to merging of data in $Pna2_1$; the reported value of R_{int} corresponds to subsequent merging of equivalent reflections in this space group.

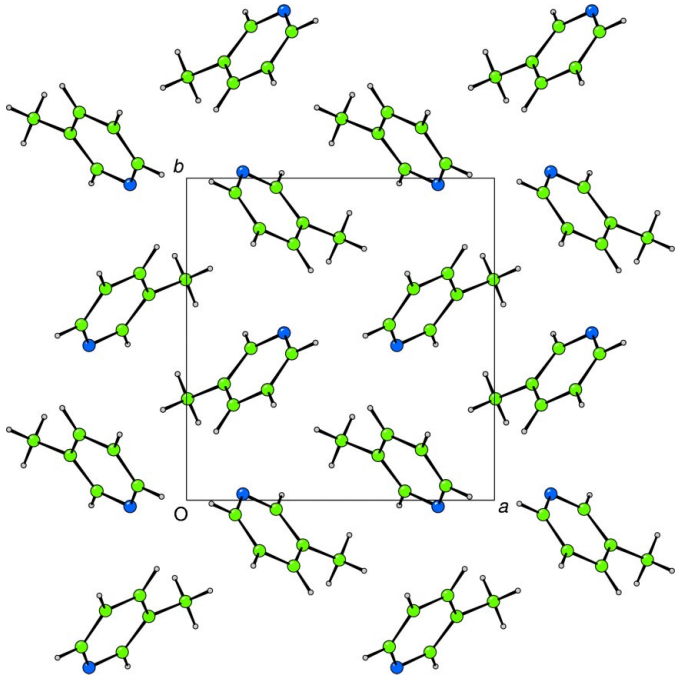


Figure 2
Projection of (I) onto (001) showing the herring-bone packing arrangement (*CAMERON*; Watkin *et al.*, 1996).

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *HKL* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *HKL*, *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); software used to prepare material for publication: *SHELXL*97.

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