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2-Picoline

Andrew D. Bond* and John E. Davies

Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge CB2 1EW, England

Correspondence e-mail: adb29@cam.ac.uk

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Key indicators

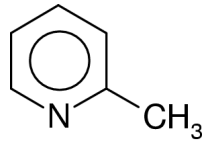
Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.003 Å
Disorder in main residue
R factor = 0.062
wR factor = 0.181
Data-to-parameter ratio = 10.5

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

The crystal structure of 2-picoline (2-methylpyridine, C_6H_7N) has been determined at 120 (2) K following *in situ* crystal growth from the liquid. Molecules pack in a herring-bone-type arrangement in the non-centrosymmetric space group $P2_12_12_1$, with C—H···N contacts indicative of directional hydrogen bonds.

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 2-picoline (m.p. 206 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 (Fig. 2) in the non-centrosymmetric space group $P2_12_12_1$. Between molecules, C—H···N contacts exist that are close to linear [H4···N1^{i} = 2.60 Å and C4—H4···N1^{i} = 146.6°; H6···N1^{ii} = 2.79 Å and C6—H6···N1^{ii} = 170.1°; symmetry codes: (i) $\frac{1}{2}-x$, $-y$, $\frac{1}{2}+z$; (ii) $-\frac{1}{2}+x$, $-y$, $-z$], indicative of directional hydrogen bonds.

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 206 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 subsequently cooled to 120 (2) K for data collection. The length of the cylindrical crystal was not estimated, but it exceeded the diameter of the collimator (0.35 mm).

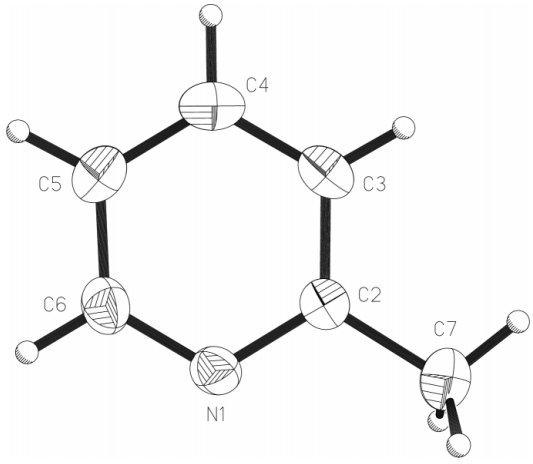


Figure 1
The molecular structure and atom-labelling scheme for (I) showing displacement ellipsoids at the 50% probability level for non-H atoms (*XP*; Sheldrick, 1993). Disorder of the H atoms in the methyl group has been omitted for clarity.

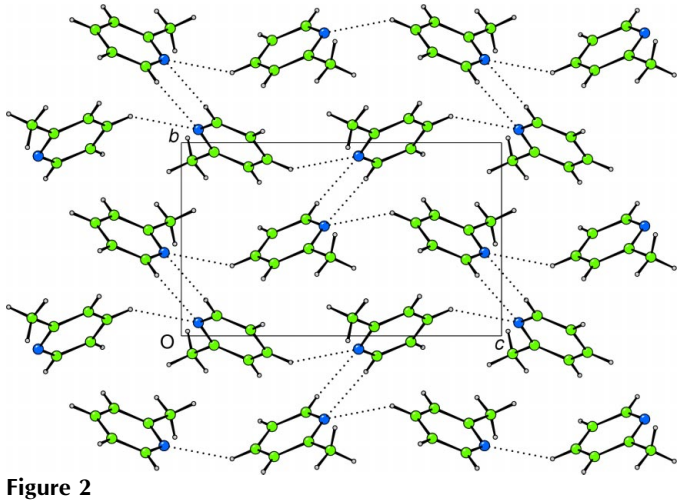


Figure 2
Projection onto (100) showing the herring-bone packing in (I) (*CAMERON*; Watkin *et al.*, 1996). C—H···N interactions are shown as dotted lines.

Crystal data

C_6H_7N
M_r = 93.13
Orthorhombic, $P2_12_12_1$
a = 6.6593 (5) Å
b = 7.0878 (6) Å
c = 11.7358 (7) Å
V = 553.93 (7) Å^3
Z = 4
D_x = 1.117 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4571 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
3477 measured reflections
749 independent reflections
672 reflections with $I > 2\sigma(I)$
R_{int} = 0.110
θ_{max} = 27.5°
$h = -4 \rightarrow 8$
$k = -9 \rightarrow 7$
$l = -15 \rightarrow 10$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.181
S = 1.10
749 reflections
71 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.1425P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

The methyl H atoms are disordered and were modelled as two sets of idealized positions. All H atoms were placed geometrically and allowed to refine with independent isotropic displacement parameters (one common parameter for all methyl H atoms). The methyl group was allowed to rotate about its local threefold axis. Friedel pairs (486) were averaged before merging of data in $P2_12_12_1$; the reported value of R_{int} corresponds to subsequent merging of equivalent reflections in this space group.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *HKL DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; 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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