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2,5-Lutidine

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Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.002 Å
R factor = 0.054
wR factor = 0.145
Data-to-parameter ratio = 18.2

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

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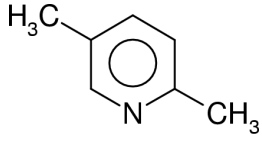
The crystal structure of 2,5-lutidine (2,5-dimethylpyridine, C_7H_9N) has been determined at 150 (2) K following *in situ* crystal growth from the liquid. In space group $P\overline{1}$, the asymmetric unit contains two independent molecules. Molecules are linked *via* C—H···N interactions into polar chains aligned in a parallel manner to form polar sheets. Adjacent sheets are packed in an anti-parallel arrangement.

Comment

This work forms part of a study devoted to improving the techniques for determining the crystal structures of substances that are liquid at room temperature. We have reported previously the crystal structures of 2,6-lutidine (Bond *et al.*, 2001) and 3,5-lutidine (Bond & Davies, 2002), and report here the structure of the isomer 2,5-lutidine, (I), determined at 150 (2) K following *in situ* crystal growth from the liquid.



(I)

In space group $P\overline{1}$, there are two independent molecules of (I) in the asymmetric unit (Fig. 1). Molecules are linked *via* C—H···N interactions into extended chains [Fig. 2; H4*B*···N1*A* = 2.66 Å, C4*B*—H4*B*···N1*A* = 159°; H4*A*···N1*B*^{i} = 2.63 Å and C4*A*—H4*A*···N1*B*^{i} = 157°; symmetry code: (i) *x*, *y*, −1+*z*]. Similar chains are observed in the crystal structures of 2,6-lutidine and 3,5-lutidine. Within the chains in (I), adjacent molecules are twisted about the direction of chain propagation with an angle between the least-squares planes through adjacent molecules of 54.0 (1)°. This twist presumably accommodates the steric requirements of the methyl substituents. Adjacent chains are arranged in a parallel manner to give polar sheets parallel to (010) (Fig. 2). Chains in adjacent sheets are arranged in an anti-parallel manner so that the crystal is not macroscopically polar (Fig. 3).

Experimental

The sample (99%) was obtained from the Lancaster company and used without further purification. The crystal was grown in a 0.3 mm glass capillary tube at *ca* 236 K (a temperature only slightly less than the melting point of the solid in the capillary tube) using a technique described earlier (Davies & Bond, 2001). Once grown, the crystal was cooled to 150 (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).

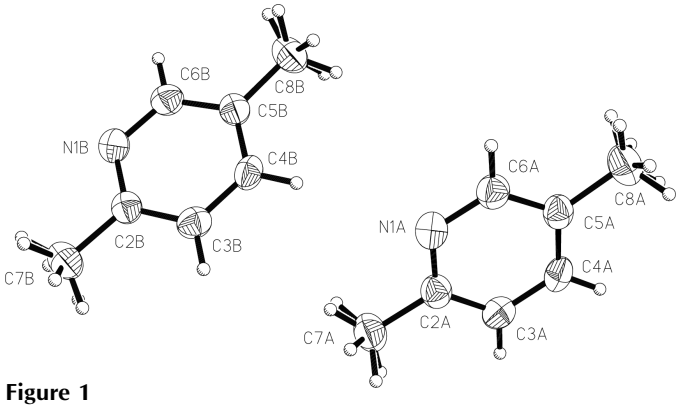


Figure 1
The asymmetric unit and atom-labelling scheme, showing displacement ellipsoids (C/N atoms) at the 50% probability level (*XP*; Sheldrick, 1993). Independent molecules are denoted by the suffixes *A* and *B*.

Crystal data

C_7H_9N	$Z = 4$
$M_r = 107.15$	$D_x = 1.113$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 7.0991$ (4) Å	Cell parameters from 2259 reflections
$b = 7.7279$ (5) Å	$\theta = 1.0$–$22.5°$
$c = 12.3900$ (9) Å	$\mu = 0.07$ mm^{-1}
$\alpha = 108.139$ (4)°	$T = 150$ (2) K
$\beta = 92.399$ (4)°	Cylinder, colourless
$\gamma = 96.743$ (5)°	0.15 mm (radius)
$V = 639.26$ (7) Å^3	

Data collection

Nonius KappaCCD diffractometer	$R_{int} = 0.030$
Thin-slice ω and φ scans	$\theta_{max} = 27.5°$
Absorption correction: none	$h = 0 \rightarrow 9$
4192 measured reflections	$k = -9 \rightarrow 9$
2827 independent reflections	$l = -15 \rightarrow 15$
1643 reflections with $I > 2\sigma(I)$	

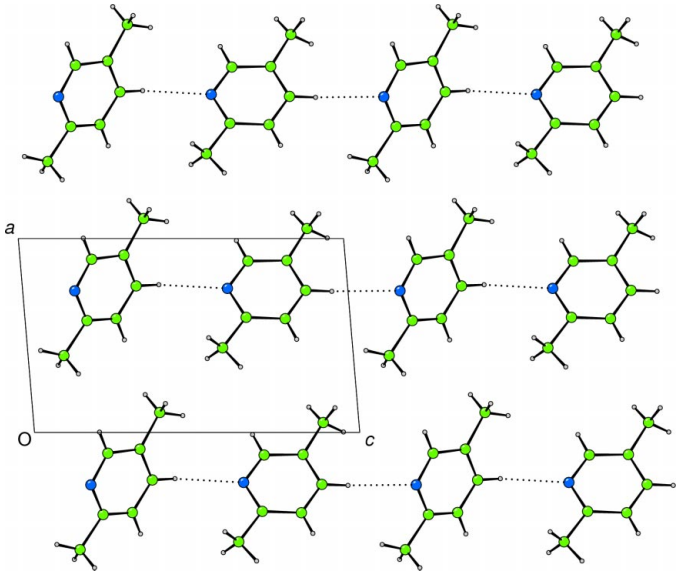


Figure 2
Projection on to (010) of a single layer of (I), showing polar chains linked by C—H···N interactions into polar sheets (*CAMERON*; Watkin *et al.*, 1996).

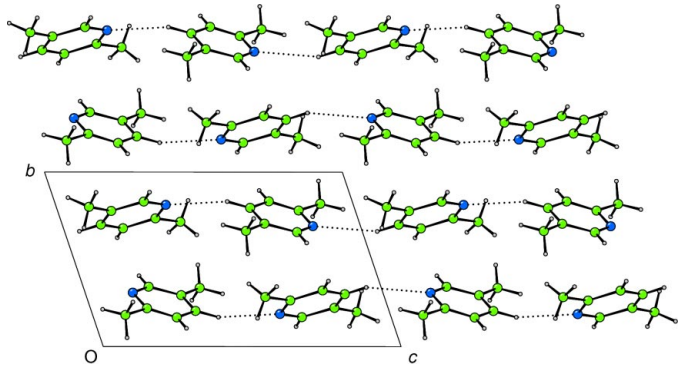


Figure 3
Projection on to (100), showing layers of (I) arranged in an antiparallel manner (*CAMERON*; Watkin *et al.*, 1996).

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0487P)^2 + 0.1043P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.054$	
$wR(F^2) = 0.145$	
$S = 1.03$	$(\Delta/\sigma)_{max} < 0.001$
2827 reflections	$\Delta\rho_{max} = 0.14$ e Å^{-3}
155 parameters	$\Delta\rho_{min} = -0.13$ e Å^{-3}
H-atom parameters constrained	

H atoms were placed geometrically and refined with isotropic displacement parameters, with common parameters assigned to chemically equivalent H atoms (one parameter for all methyl H atoms, four parameters in total). Both methyl groups are disordered and were modelled as two sets of positions, each position rotated at 60° from the other about the local threefold axis.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *HKL 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); molecular graphics: *XP* (Sheldrick, 1993) and *CAMERON* (Watkin *et al.*, 1996); software used to prepare material for publication: *SHELXL*97.

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