

2,6-Lutidine

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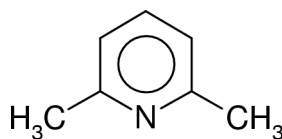
Key indicators

Single-crystal X-ray study
T = 120 K
Mean $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$
R factor = 0.057
wR factor = 0.140
Data-to-parameter ratio = 8.4For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

The crystal structure of 2,6-lutidine (2,6-dimethylpyridine, $\text{C}_7\text{H}_9\text{N}$), has been determined at 120 (2) K following *in situ* crystal growth from the liquid. In the non-centrosymmetric space group *Fdd2*, the asymmetric unit comprises half a molecule, each molecule being sited on a crystallographic diad axis. Molecules are linked *via* linear $\text{C}-\text{H}\cdots\text{N}$ interactions into one-dimensional chains that align in a parallel manner, giving rise to macroscopically polar crystals.

Comment

2,6-Lutidine (2,6-dimethylpyridine, $\text{C}_7\text{H}_9\text{N}$), (I), is present in many complexes, coordinated to a metal centre (see, for example, Engelhardt *et al.*, 1985). The free base (unprotonated and not coordinated to any metal centre) has also been observed in the crystal structures of three solvates, usually hydrogen bonded to the principal component of the structure (Bowmaker *et al.*, 1997; Linti *et al.*, 1996; Caira *et al.*, 1999). The crystal structure of (I) itself, however, has not been reported to date, probably as a result of the difficulties associated with obtaining suitable single crystals of (I), which is liquid at room temperature. We report here the crystal structure of (I), determined at 120 (2) K, following *in situ* crystal growth from the liquid. This work forms part of a continuing study devoted to improving the techniques for determining the crystal structures of substances that are liquids at room temperature (see, for example, Bond & Davies, 2001*a,b*).



(I)

In the non-centrosymmetric space group *Fdd2*, the asymmetric unit comprises half a molecule of (I), with a crystallographic diad axis passing through atoms N1 and C4 (Fig. 1). Molecules of (I) are linked into one-dimensional chains propagating along the diad axis (parallel to [001]) by linear $\text{C}-\text{H}\cdots\text{N}$ interactions (Fig. 2; $\text{H}4\cdots\text{N}1^1 = 2.63 \text{ \AA}$ and $\text{C}4-\text{H}4\cdots\text{N}1 = 180^\circ$; symmetry code: (i) $x, y, 1+z$). Adjacent chains are parallel such that the structure is macroscopically polar; this observation may be of interest to researchers seeking organic molecular materials for non-linear optic (NLO) applications, particularly frequency doubling through second harmonic generation (SHG) (Bosshard *et al.*, 1995).

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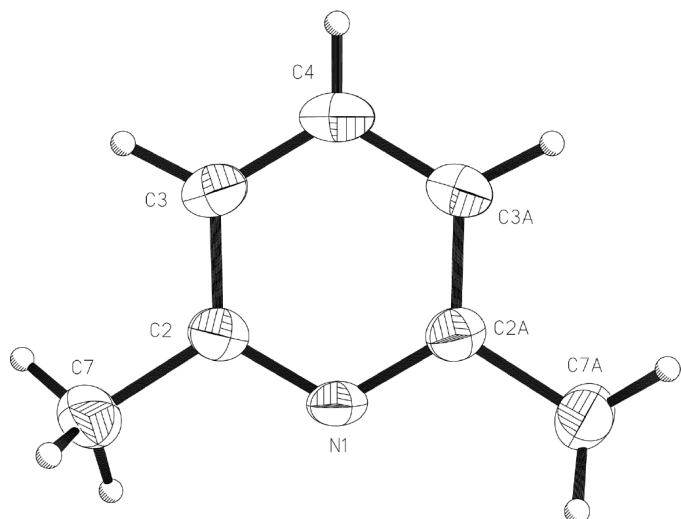


Figure 1
The molecular structure and atom-labelling scheme for (I) showing displacement ellipsoids at the 50% probability for non-H atoms. Atoms related by the diad axis are denoted by the suffix *A* (*XP*; Sheldrick, 1993).

The presence of the methyl substituents in the 2- and 6-positions prevents adoption of an edge-to-face geometry between molecules (that might otherwise be expected), and the planes through the pyridyl rings of molecules in adjacent chains remain essentially parallel (Fig. 3).

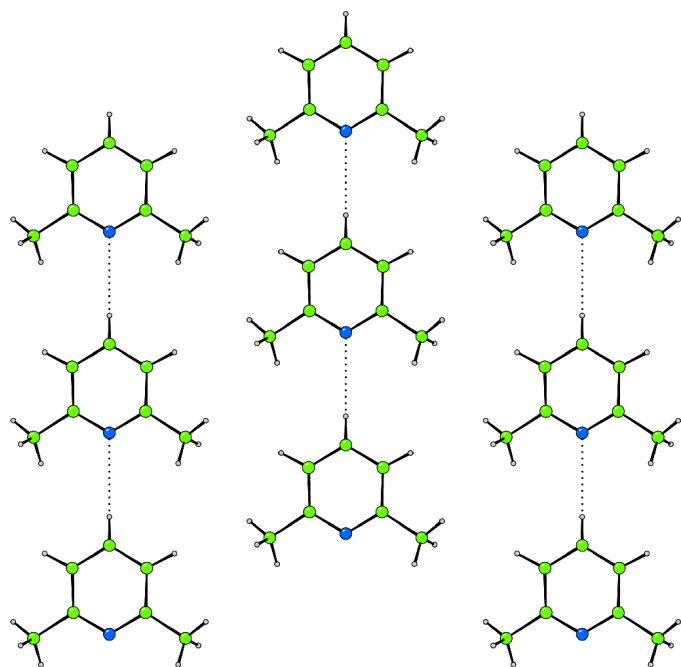


Figure 2
Chains of (I) running parallel to the *c* direction, projected onto (100). C—H...N interactions are indicated by dotted lines (*CAMERON*; Watkin *et al.*, 1996).

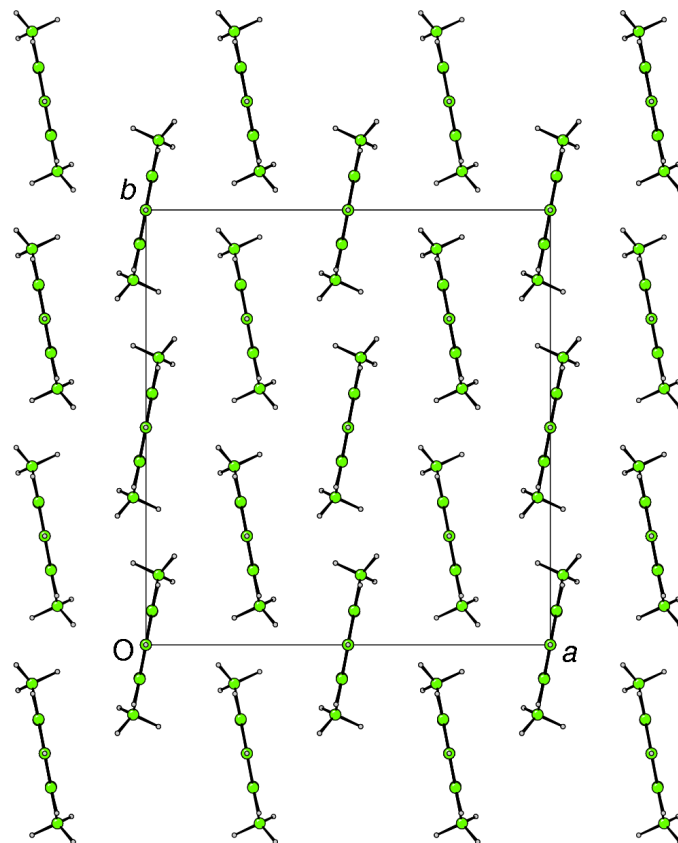


Figure 3
Projection of (I) onto (001) looking along the direction of chain propagation (*CAMERON*; Watkin *et al.*, 1996).

Experimental

A sample (99%) of the title compound 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 *ca* 260 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). Once grown, the crystal was 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).

Crystal data

C_7H_9N
 $M_r = 107.15$
Orthorhombic, *Fdd2*
 $a = 13.782$ (3) Å
 $b = 14.805$ (3) Å
 $c = 6.317$ (1) Å
 $V = 1288.9$ (4) Å³
 $Z = 8$
 $D_x = 1.104$ Mg m⁻³

Mo $K\alpha$ radiation
Cell parameters from 1553 reflections
 $\theta = 1.0$ – 27.5°
 $\mu = 0.07$ mm⁻¹
 $T = 120$ (2) K
Cylinder, colourless
0.15 mm (radius)

Data collection

Nonius KappaCCD diffractometer	$R_{int} = 0.034$
Thin-slice ω and φ scans	$\theta_{max} = 27.4^\circ$
1429 measured reflections	$h = -17 \rightarrow 13$
387 independent reflections	$k = -19 \rightarrow 15$
351 reflections with $I > 2\sigma(I)$	$l = -7 \rightarrow 8$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.057$
 $wR(F^2) = 0.140$
 $S = 1.11$
 387 reflections
 46 parameters
 H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0788P)^2 + 0.8716P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.007$
 $\Delta\rho_{\max} = 0.22 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.18 \text{ e } \text{\AA}^{-3}$

All H atoms were placed geometrically and allowed to refine with independent isotropic displacement parameters (one common displacement parameter for the methyl H atoms). The absolute structure could not be determined and Friedel pairs (288) were averaged prior to merging of data in *Fdd2*; 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: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); software used to prepare material for publication: *SHELXL97*.

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