

## 3,5-Lutidine

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## Key indicators

Single-crystal X-ray study

$T = 150$  K

Mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å

$R$  factor = 0.069

$wR$  factor = 0.214

Data-to-parameter ratio = 19.8

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

The crystal structure of 3,5-lutidine (3,5-dimethylpyridine,  $\text{C}_7\text{H}_9\text{N}$ ) has been determined at 150 (2) K following *in situ* crystal growth from the liquid. In space group  $I2/a$ , the asymmetric unit comprises half a molecule, each molecule possessing a crystallographic diad axis. Molecules are linked by linear  $\text{C}-\text{H}\cdots\text{N}$  interactions into extended polar chains aligned in a parallel manner to form polar sheets. Adjacent sheets are arranged in an anti-parallel manner.

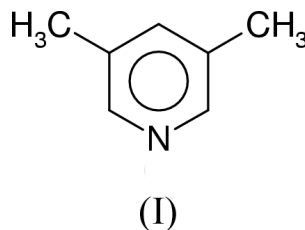
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## Comment

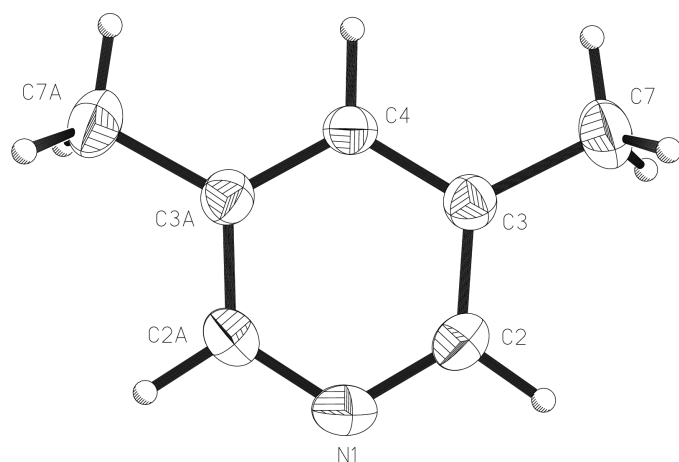
As part of a study devoted to improving the techniques for determining the crystal structures of substances that are liquids at room temperature, we have reported previously the crystal structure of 2,6-lutidine (2,6-dimethylpyridine) (Bond *et al.*, 2001). We report here the crystal structure of the isomeric molecule, 3,5-lutidine, (I), determined at 150 (2) K following *in situ* crystal growth from the liquid.



In space group  $I2/a$ , the asymmetric unit comprises half a molecule, each molecule possessing a crystallographic diad axis passing through N1 and C4 (Fig. 1). Molecules are linked *via* linear  $\text{C}-\text{H}\cdots\text{N}$  interactions [ $\text{C4}-\text{H4}\cdots\text{N1}^i = 2.51$  (3) Å and  $\text{C4}-\text{H4}\cdots\text{N1}^i = 180^\circ$ ; symmetry code: (i)  $x, 1+y, z$ ] into extended polar chains, similar to those observed in the crystal structure of 2,6-lutidine. All chains propagate parallel to [010], forming polar sheets (Fig. 2) parallel to (101). Chains in adjacent sheets are arranged in an anti-parallel manner (Fig. 3) so that the crystal is not macroscopically polar. This is in contrast to the structure of 2,6-lutidine in which a change in the position of the methyl substituents produces a macroscopically polar structure in space group  $Fdd2$ , where all sheets are arranged in a parallel fashion. This observation may be of interest to researchers seeking organic molecular materials for non-linear optic (NLO) applications.

## Experimental

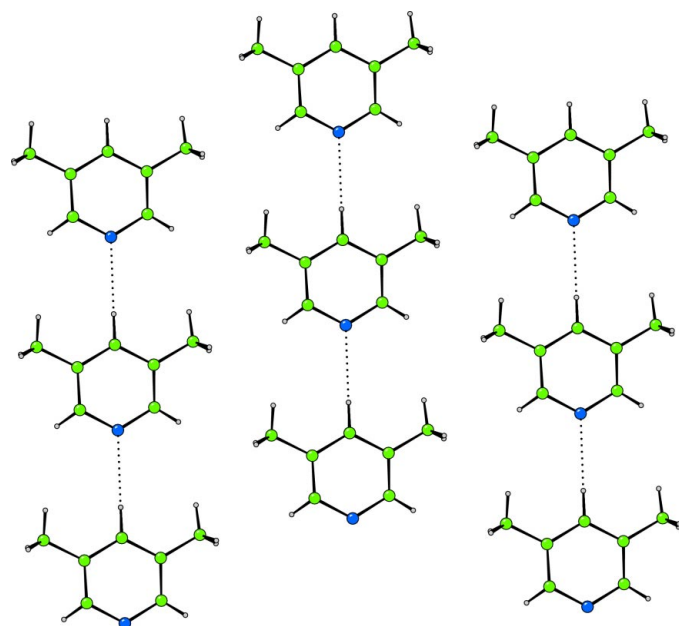
The sample (99%) was obtained from the Aldrich Company and used without further purification. The crystal was grown in a 0.3 mm glass capillary tube at *ca* 256 K (a temperature only slightly less than the melting point of the solid in the capillary) using a technique described



**Figure 1**

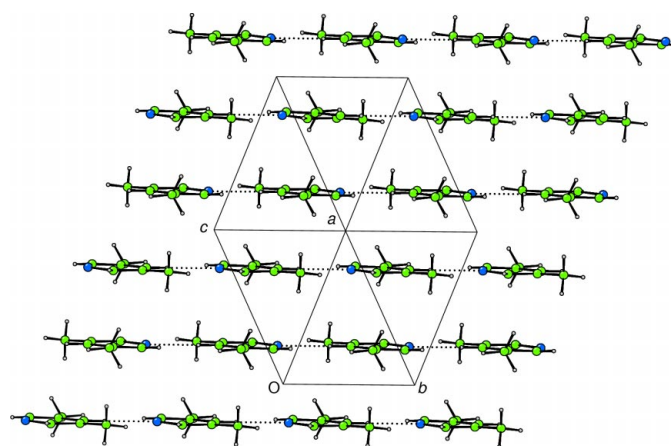
The molecular structure and atom-labelling scheme for (I), showing displacement ellipsoids at the 50% probability level. Atoms related by the crystallographic diad axis are indicated by the suffix *A* (XP; Sheldrick, 1993).

earlier (Davies & Bond, 2001). Once grown, the crystal was cooled to 150 (2) K for data collection. Although the diffraction pattern clearly contained contributions from more than one crystal (reflected to some extent in the relatively high  $R_{\text{int}}$  of 0.165), the pattern associated with the major crystal component was indexed successfully; only reflections associated with this component were included in the integration. The length of the cylindrical crystal was not estimated, but it exceeded the diameter of the collimator (0.35 mm).



**Figure 2**

Extended polar chains in (I), projected on to (101) (CAMERON; Watkin *et al.*, 1996).



**Figure 3**

Projection of (I) parallel to the layers, showing the anti-parallel alignment of adjacent layers (CAMERON; Watkin *et al.*, 1996).

#### Crystal data

$C_7H_9N$   
 $M_r = 107.15$   
 Monoclinic,  $I2/a$   
 $a = 9.7236$  (9) Å  
 $b = 6.2851$  (8) Å  
 $c = 10.517$  (2) Å  
 $\beta = 95.691$  (5)°  
 $V = 639.57$  (16) Å<sup>3</sup>  
 $Z = 4$

$D_x = 1.113$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 Cell parameters from 1914 reflections  
 $\theta = 1.0$ – $30.0^\circ$   
 $\mu = 0.07$  mm<sup>-1</sup>  
 $T = 150$  (2) K  
 Cylinder, colourless  
 0.15 mm (radius)

#### Data collection

Nonius KappaCCD diffractometer  
 Thin-slice  $\omega$  and  $\varphi$  scans  
 Absorption correction: none  
 2651 measured reflections  
 912 independent reflections  
 620 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.165$   
 $\theta_{\text{max}} = 30.0^\circ$   
 $h = -10 \rightarrow 13$   
 $k = -8 \rightarrow 8$   
 $l = -10 \rightarrow 14$

#### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.069$   
 $wR(F^2) = 0.214$   
 $S = 1.05$   
 912 reflections  
 46 parameters  
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.1018P)^2 + 0.203P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.21$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.22$  e Å<sup>-3</sup>

The H atoms of the methyl group were placed geometrically, assigned one common isotropic displacement parameter and allowed to rotate about their local threefold axis. Other H atoms were refined independently with individual isotropic displacement parameters.

Data collection: COLLECT (Nonius, 1998); cell refinement: HKL SCALEPACK (Otwinowski & Minor, 1997); data reduction: HKL SCALEPACK and DENZO (Otwinowski & Minor, 1997); program(s) used to solve structure: SIR92 (Altomare *et al.*, 1994); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: XP (Sheldrick, 1993) and CAMERON (Watkin *et al.*, 1996); software used to prepare material for publication: SHELXL97.

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