Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2,4,6-Collidine

Andrew D. Bond* and John E. Davies

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

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

Key indicators

Single-crystal X-ray study
T = 180 K
Mean σ(C–C) = 0.004 Å
R factor = 0.071
wR factor = 0.193
Data-to-parameter ratio = 15.8

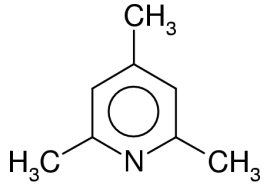
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 26 October 2001
Accepted 30 October 2001
Online 10 November 2001

The crystal structure of 2,4,6-collidine (2,4,6-trimethylpyridine, $C_8H_{11}N$) has been determined at 180 (2) K following *in situ* crystal growth from the liquid. In space group $P2_1/c$, there are two molecules in the asymmetric unit. Molecules are linked into one-dimensional chains *via* C—H···N interactions.

Comment

This work forms 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 recently the crystal structures of 3-methylpyridine (3-picoline) and 2-methylpyridine (2-picoline) (Bond & Davies, 2001*a*,*b*), and report here the structure of the trisubstituted molecule 2,4,6-trimethylpyridine (2,4,6-collidine), (I).



(I)

In space group $P2_1/c$, there are two molecules in the asymmetric unit (Fig. 1). The two independent molecules form an interplanar angle of *ca* 68° and the C3*A*—H3*A*···N1*B* angle of 154° is indicative of a directional hydrogen-bond interaction (H3*A*···N1*B* = 2.75 Å). These interactions, together with a second C—H···N contact [H5*B*···N1*A*^{i} = 2.56 Å, C5*B*—H5*B*···N1*A*^{i} = 171°; symmetry code (i): $-1+x$, y, $-1+z$] link the molecules into one-dimensional chains running along the vector [101] (Fig. 2). Between adjacent chains, pyridyl rings adopt both face-to-face offset (with interplanar separation *ca* 3.6 Å), and edge-to-face arrangements (Fig. 3).

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 using a technique described previously (Davies & Bond, 2001). In this case, however, the sample remained liquid at the low-temperature limit of the cooling device (*ca* 110 K), and the initial solid material could only be obtained by immersing the sealed capillary tube directly in liquid nitrogen. The capillary was then transferred to the diffractometer and warmed, and the crystal was grown at *ca* 212 K (a temperature only slightly less than the melting point of the solid in the capillary tube). Once formed, the crystal was

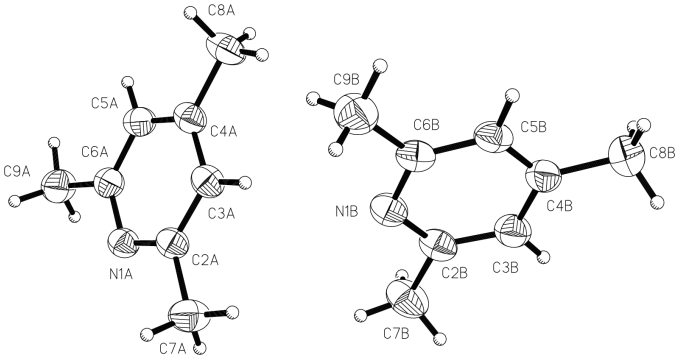


Figure 1
Molecular structure and atom-labelling scheme for (I) showing displacement ellipsoids at the 50% probability level for non-H atoms. The two molecules in the asymmetric unit are denoted by the suffixes *A* and *B*, and disorder of the H atoms in the methyl group C8*B* has been omitted for clarity.

cooled to 180 (2) K for data collection. Although the diffraction pattern contained contributions from more than one crystal, the pattern associated with the major crystal component was indexed successfully, and only reflections associated with this component were included in the integration. The length of the cylindrical crystal could not be estimated accurately, but it exceeded the diameter of the collimator (0.35 mm).

Crystal data

$C_8H_{11}N$	D_x = 1.049 Mg m^{-3}
M_r = 121.18	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 16 950 reflections
a = 8.7773 (5) Å	θ = 1.0–25.0°
b = 20.3849 (11) Å	μ = 0.06 mm^{-1}
c = 8.9935 (4) Å	T = 180 (2) K
β = 107.427 (3)°	Cylinder, colourless
V = 1535.29 (14) Å^3	0.15 mm (radius)
Z = 8	

Data collection

Nonius KappaCCD diffractometer	2056 reflections with $I > 2\sigma(I)$
Thin-slice ω and φ scans	R_{int} = 0.069
Absorption correction: multi-scan (*SORTAV*; Blessing, 1997)	θ_{max} = 25.1°
T_{min} = 0.796, T_{max} = 0.955	$h = -10 \rightarrow 10$
11 768 measured reflections	$k = -24 \rightarrow 24$
2701 independent reflections	$l = -10 \rightarrow 10$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0746P)^2 + 0.8878P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.071	$(\Delta/\sigma)_{max}$ = 0.024
$wR(F^2)$ = 0.193	$\Delta\rho_{max}$ = 0.21 e Å^{-3}
S = 1.13	$\Delta\rho_{min}$ = −0.19 e Å^{-3}
2701 reflections	
171 parameters	
H-atom parameters constrained	

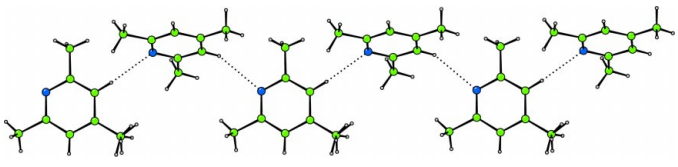


Figure 2
Molecules of (I) linked into one-dimensional chains *via* C—H···N interactions.

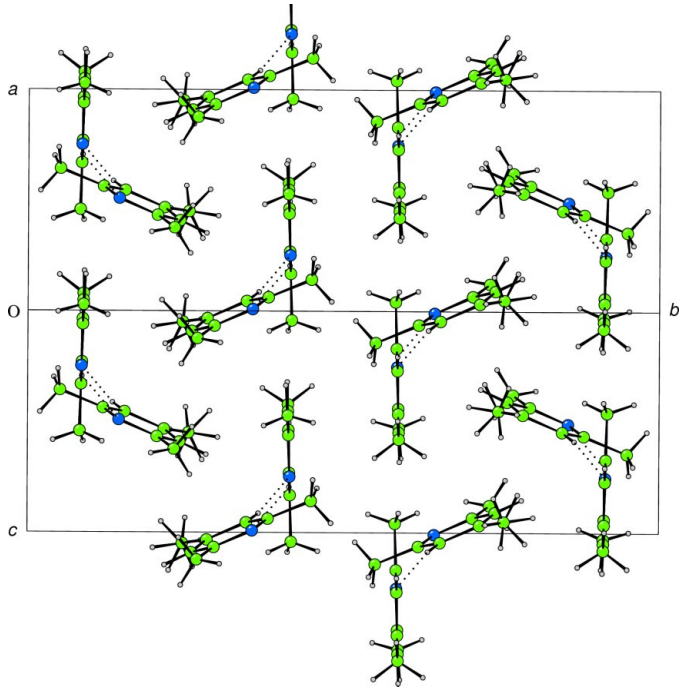


Figure 3
Projection on to (101) showing chains of (I) running perpendicular to the plane of the page.

The methyl-H atoms associated with atom C8*B* are disordered and were modelled as two sets of idealized positions. All H atoms were placed geometrically and allowed to refine with isotropic displacement parameters (one common parameter for all methyl-H atoms and one common displacement parameter for the other H atoms). Each methyl group was allowed to rotate about its local threefold axis.

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); molecular graphics: *XP* (Sheldrick, 1993) and *CAMERON* (Watkin *et al.*, 1996); software used to prepare material for publication: *SHELXL*97.

We thank the EPSRC for financial assistance towards the purchase of the Nonius CCD diffractometer.

References

Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M. C., Polidori, G. & Camalli, M. (1994). *J. Appl. Cryst.* **27**, 435–436.
Blessing, R. H. (1997). *J. Appl. Cryst.* **30**, 421–429.
Bond, A. D. & Davies, J. E. (2001*a*). *Acta Cryst.* E**57**, o1087–o1088.
Bond, A. D. & Davies, J. E. (2001*b*). *Acta Cryst.* E**57**, o1089–o1090.
Davies, J. E. & Bond, A. D. (2001). *Acta Cryst.* E**57**, o947–o949.
Nonius (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter & R. M. Sweet, pp. 307–326. London: Academic Press.
Sheldrick, G. M. (1993). *XP*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXL*97. University of Göttingen, Germany.
Watkin, D. J., Prout, C. K. & Pearce, L. J. (1996). *CAMERON*. Chemical Crystallography Laboratory, University of Oxford, UK.