Quinoline

John E. Davies and Andrew D. Bond*

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

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

Key indicators

Single-crystal X-ray study
$T = 150$ K
Mean σ(C–C) = 0.002 Å
R factor = 0.045
wR factor = 0.124
Data-to-parameter ratio = 13.3

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

The crystal structure of quinoline, C_9H_7N, has been determined at 150 (2) K. In space group $P2_1/c$, the asymmetric unit comprises two independent molecules. Molecules are linked *via* C—H···N interactions into two orthogonal sets of chains which are linked *via* an extensive network of edge-to-face C—H···π interactions.

Comment

Although the structure of naphthalene was one of the first determined by X-ray crystallography (Bragg, 1922), this is the first report of the structure of quinoline. This long delay may be attributed to the difficulty of obtaining a suitable single crystal of quinoline. This work forms part of a study devoted to improving the techniques for determining the crystal structures of substances which are liquids at room temperature [see, for example, Bond *et al.* (2001)].

(I)
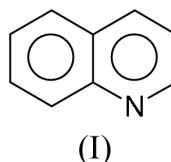
Quinoline, (I), crystallizes in the space group $P2_1/c$ with the asymmetric unit comprising two independent molecules (denoted *A* and *B*, Fig. 1). Molecules of type *A* are linked *via* C—H···N interactions into chains running parallel to the *c* direction [H6A···N1A^i = 2.89 (2) Å, C6A—H6A···N1A^i = 141.1 (1)°; symmetry code: (i) $x, \frac{1}{2} - y, \frac{1}{2} + z$]. Molecules of type *B* are also linked *via* C—H···N interactions into chains running parallel to the *b* direction [H3B···N1B^{ii} = 2.68 (2) Å, C3B—H3B···N1B^{ii} = 171.1 (1)°; symmetry code: (ii) $2 - x, \frac{1}{2} + y, \frac{3}{2} - z$]. Thus, there exist in (I) two orthogonal sets of C—H···N hydrogen-bonded chains. Between these chains, an extensive network of edge-to-face C—H···π interactions exists (Desiraju & Steiner, 1999). This network may be visualized most conveniently by considering that each edge of a molecule of (I) exposed in a type *B* chain is 'capped' by a molecule of type *A*, and that these capped chains interlock to form two-dimensional layers parallel to ($\bar{1}01$) (Fig. 2). The layers may then be considered to stack in an *ABCABC* arrangement perpendicular to ($\bar{1}01$) with the C—H···N interactions between type *A* molecules linking the layers (Fig. 3).
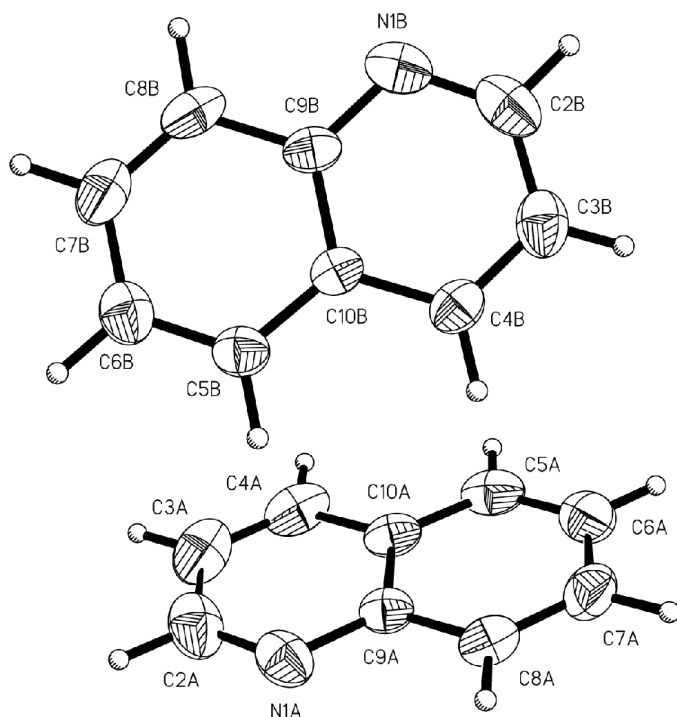
Experimental

The sample (98%) was obtained from the Aldrich Company and used without further purification. The crystal was grown with difficulty in a 0.3 mm glass capillary tube, obtained from the PANTAK company
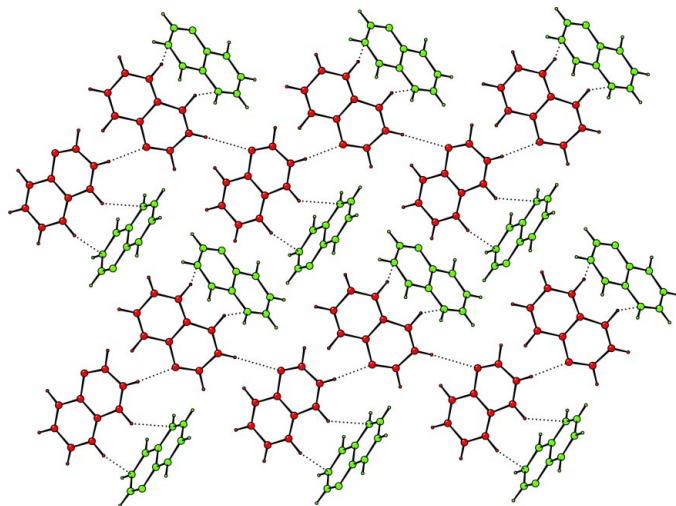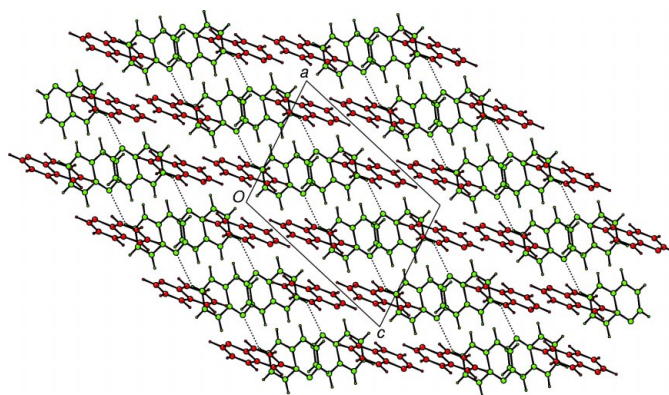
Figure 1
The asymmetric unit in (I) showing displacement ellipsoids at the 50% probability level (*XP*; Sheldrick, 1993). The two independent molecules adopt a geometry indicative of an edge-to-face C—H···π interaction.

Figure 2
Projection of (I) on to ($\bar{1}$01) showing type *B* molecules (coloured red) linked by C—H···N interactions into chains capped at each exposed edge by type *A* molecules (coloured green). Adjacent chains interlock to form two-dimensional sheets. Edge-to-face C—H···π interactions are shown as dotted lines only between the molecules at the edge of each chain (interactions between chains are not drawn for the purposes of clarity) (*CAMERON*; Watkin *et al.*, 1996).

(PANTAK Company, Unit 30, The Robert Corl Industrial Estate, Britten Road, Reading, England), at 245 K (a temperature only slightly less than the melting point of the solid in the capillary tube). With the axis of the capillary parallel to the φ axis and horizontal on the instrument, the crystal was eventually grown by moving a plug of solid material up and down the tube (the movement being controlled

Figure 3
Projection of (I) on to (010) showing layers stacked in an *ABCABC* arrangement. C—H···N interactions between type *A* molecules link the layers and are shown as dotted lines (*CAMERON*; Watkin *et al.*, 1996).

with the standard Z (height) adjustment of the goniometer head). The goniometer head was a Nonius model 1516.916 X–Y–Z (Nonius BV, Delft, The Netherlands); this head is particularly well suited to the experiment described in this paper since it has an especially wide Z translation (8 mm). This method is effectively zone refinement, similar to the industrial methods used to grow large single crystals of silicon for the electronics industry. The fine temperature control necessary for the successful growth of the crystal was provided by an Oxford Cryosystems Cryostream (Oxford Cryosystems, Lower Road, Long Hanborough, Oxford, England).

Crystal data

C_9H_7N	$D_x = 1.244$ Mg m^{-3}
$M_r = 129.16$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 6740
$a = 9.9226\,(5)$ Å	reflections
$b = 10.8473\,(7)$ Å	$\theta = 1.0$–27.5°
$c = 13.3665\,(7)$ Å	$\mu = 0.07$ mm^{-1}
$\beta = 106.578\,(3)$°	$T = 150\,(2)$ K
$V = 1378.88\,(13)$ Å^3	Cylinder, colourless
$Z = 8$	0.26 mm (radius)

Data collection

Nonius KappaCCD diffractometer	$R_{int} = 0.018$
Thin-slice ω and φ scans	$\theta_{max} = 27.4$°
4851 measured reflections	$h = -12 \rightarrow 12$
3055 independent reflections	$k = -12 \rightarrow 14$
2337 reflections with $I > 2\sigma(I)$	$l = -17 \rightarrow 17$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0556P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.045$	$+ 0.2728P]$
$wR(F^2) = 0.124$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} = 0.002$
3055 reflections	$\Delta\rho_{max} = 0.18$ e Å^{-3}
230 parameters	$\Delta\rho_{min} = -0.18$ e Å^{-3}
All H-atom parameters refined	

The positions of all H atoms were allowed to refine independently. Pairs of chemically equivalent H atoms in the two independent molecules were assigned common, isotropic displacement parameters (7 variables in total).

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: *SHELXS*97 (Sheldrick, 1997);

program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); software used to prepare material for publication: *SHELXL*97.

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