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Crystal and molecular structure of 8-hydroxyquinoline.

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8-Hydroxyquinoline, C_9H_7NO, crystallizes in the orthorhombic space group *Fdd*2, with $a = 29{\cdot}18$, $b = 25{\cdot}36$, $c = 3{\cdot}91$ Å, and sixteen molecules per unit cell. $R = 8{\cdot}3\%$. An important feature of the structure is the closest approach of the O atom of one molecule to the N atom of the neighbouring molecule.

Unit-cell dimensions were measured from rotation and zero-layer Weissenberg photographs. The very short *c* axis and the principal indices of refraction (1·69, slightly greater than 1·69, and 1·55, when the vibrations are parallel to the *a*, *b* and *c* axes respectively) measured with white light suggested that the nearly flat 8-hydroxyquinoline molecule has a definite tendency to arrange itself more or less in a plane very close to (001). The approximate positional parameters were obtained by a combination of a weighted reciprocal-lattice plot (Hanson, Lipson & Taylor, 1953; Taylor, 1952) for the *hk*0 reflections and the trial-and-error method. The trial structure was compatible with the optical data and cell structure. Least-squares refinement with 450 reflection intensities, obtained from *c* axis Weissenberg photographs with Cu *Kα* radiation and estimated visually, led to the solution of the structure with a final residual of 8·3%. In

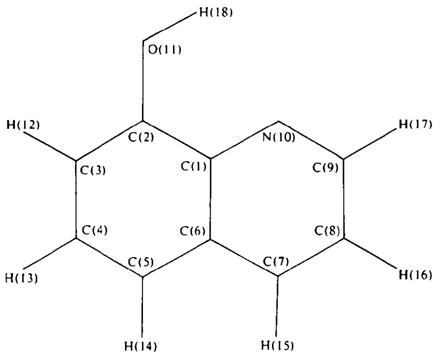

Fig. 1. Conventional structural formula of 8-hydroxyquinoline and the numbering of the atoms.

Table 1. *Positional parameters* (×10⁴) *of the non-hydrogen atoms and their estimated standard deviations*

	x	*y*	*z*
C(1)	2940 (5)	3364 (6)	2861 (60)
C(2)	2521 (6)	3528 (6)	4328 (62)
C(3)	2453 (5)	4054 (6)	5392 (62)
C(4)	2807 (6)	4428 (5)	4646 (63)
C(5)	3208 (6)	4295 (5)	3129 (62)
C(6)	3293 (5)	3753 (5)	2194 (62)
C(7)	3703 (5)	3587 (6)	555 (63)
C(8)	3751 (6)	3042 (6)	−458 (63)
C(9)	3391 (6)	2689 (6)	464 (62)
N(10)	2996 (4)	2841 (4)	1967 (52)
O(11)	2180 (3)	3161 (4)	5044 (53)

Table 2. *Bond lengths* (Å) *with their estimated standard deviations in parentheses*

C(1)–C(2)	1·411 (19)	C(1)–N(10)	1·383 (16)
C(2)–C(3)	1·412 (20)	C(6)–C(7)	1·423 (20)
C(3)–C(4)	1·431 (20)	C(7)–C(8)	1·443 (20)
C(4)–C(5)	1·357 (20)	C(8)–C(9)	1·428 (20)
C(5)–C(6)	1·443 (19)	C(9)–N(10)	1·350 (17)
C(6)–C(1)	1·449 (19)	C(2)–O(11)	1·390 (17)

Table 3. *Bond angles* (°) *with their estimated standard deviations in parentheses*

C(2)–C(1)–C(6)	119·3 (1·3)	C(4)–C(5)–C(6)	119·8 (1·4)
C(2)–C(1)–N(10)	119·1 (1·4)	C(5)–C(6)–C(1)	118·7 (1·4)
C(6)–C(1)–N(10)	121·5 (1·4)	C(5)–C(6)–C(7)	122·7 (1·4)
C(1)–C(2)–C(3)	121·2 (1·4)	C(1)–C(6)–C(7)	118·6 (1·3)
C(1)–C(2)–O(11)	120·3 (1·3)	C(6)–C(7)–C(8)	119·2 (1·4)
C(3)–C(2)–O(11)	118·2 (1·4)	C(7)–C(8)–C(9)	117·4 (1·3)
C(2)–C(3)–C(4)	117·8 (1·4)	C(8)–C(9)–N(10)	124·1 (1·4)
C(3)–C(4)–C(5)	123·0 (1·3)	C(9)–N(10)–C(1)	119·0 (1·3)

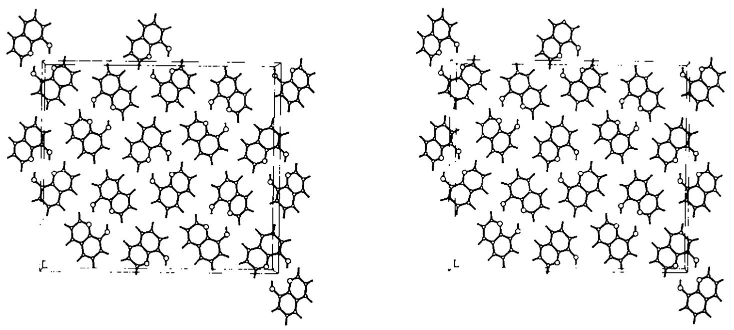

Fig. 2. A stereoscopic view of the structure of 8-hydroxyquinoline.

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the final cycles of refinement the positional and anisotropic thermal parameters were included for all atoms except H. The contributions of these atoms were included in the structure-factor calculations, keeping the atoms fixed in their calculated positions and with their isotropic temperature factors equal to those of the atoms to which they are covalently bonded. These factors were obtained from the earlier cycles of refinement. The final values of the coordinates of the non-hydrogen atoms are given in Table 1.*

Bond lengths and angles are given in Tables 2 and 3. An important feature of the structure is the closest approach of the O atom of one molecule to the N atom of the neighbouring molecule. This distance was found to be 2·858 Å, which reveals hydrogen bonding between these atoms. All other contacts are consistent with the sum of the van der Waals radii. The numbering scheme is shown in Fig. 1 and a stereoview of the structure is given in Fig. 2.

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* Lists of anisotropic thermal parameters, hydrogen atom parameters and structure factors have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 33230 (10 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

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A neutron diffraction study of the crystal structure of β-D-fructopyranose: errata.

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The atomic coordinates in the paper by Takagi & Jeffrey [*Acta Cryst.* (1977), B**33**, 3510–3515] refer to the L enantiomer. To obtain the data for the D enantiomer, a – sign should be added to the *z* coordinates. Fig. 1 in the paper is the stereoview of the L enantiomer. That of the D enantiomer is now given. The signs of the torsion angles in Fig. 2 should be changed. The ring conformation is $^{2}C_{5}$–*D* and the Cremer & Pople [*J. Am. Chem. Soc.* (1975), **97**, 1354–1358] parameters are $q_3 = -0{\cdot}555$ Å, $\varphi_2 = 47{\cdot}9°$, $\theta = 177{\cdot}3°$. In Table 3, the signs of T_{13} and T_{23} should be interchanged; the signs of ω_{13} and ω_{23} should be –. Corrected values for the directions relative to the axes are given.

A stereoview of the molecule of β-D-fructopyranose is given in Fig. 1.

In Table 3 of Takagi & Jeffrey (1977) the directions relative to the axes should be as follows:

	a	*b*	*c*
T	135·7°	77·8°	131·8°
	45·9	82·6	134·9
	93·6	165·7	103·9
ω	83·2	113·7	24·8
	26·8	110·9	106·0
	64·2	32·5	71·6

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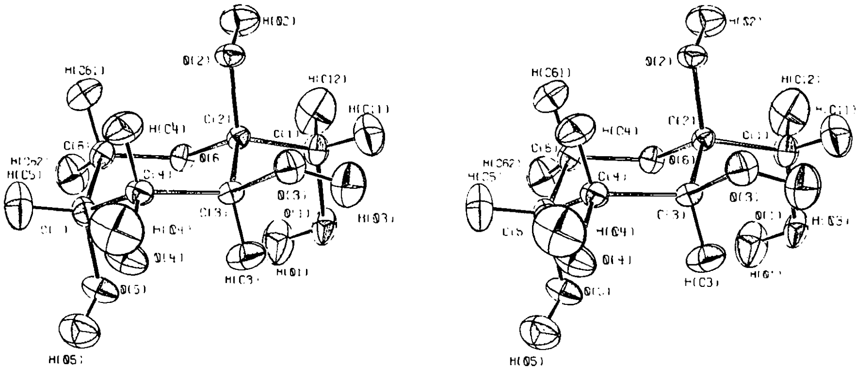

Fig. 1. Stereoview of the molecule of β-D-fructopyranose. Thermal ellipsoids are at 50% probability (Johnson, 1976).