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Structure of 1-(2-Hydroxyethyl)uracil

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Abstract. $C_6H_8N_2O_3$, $M_r = 156\cdot14$, orthorhombic, *Pccn*, $a = 10\cdot993\ (1)$, $b = 19\cdot032\ (1)$, $c = 6\cdot625\ (1)$ Å, $V = 1386\cdot1\ (2)$ Å^3, $Z = 8$, $D_m = 1\cdot498$, $D_x = 1\cdot496$ g cm^{-3}, Cu $K\alpha$, $\lambda = 1\cdot54184$ Å, $\mu = 10\cdot5$ cm^{-1}, $F(000) = 656$, room temperature, $R = 0\cdot068$ for 962 reflexions. The uracil moieties form a pair through N(3)—H···O(2) hydrogen bonds around a twofold axis. The hydroxyl groups are hydrogen-bonded with O(4) atoms of the stacked pairs, constructing the columns along the *c* axis. There are no unusual bond distances or angles.

Introduction. As part of a series of studies on hydrogen bonds between hydroxyl groups and nucleic acid bases (Shibata, Takenaka, Sasada & Ohki, 1985*a,b*), the present paper deals with the structure of 1-(2-hydroxyethyl)uracil.

Experimental. 1-(2-Hydroxyethyl)uracil was synthesized by the reaction of uracil, its sodium salt and ethylene carbonate in dry dimethylformamide at 403 K (Prystaš & Gut, 1962). Purification was by fractional crystallization of a methanol solution, a small amount of acetone being added. Recrystallization from an ethanol solution gave colourless columnar crystals. D_m by flotation in a mixture of chloroform and cyclohexane. Rigaku four-circle diffractometer; graphite-monochromated Cu $K\alpha$ radiation; crystal $0\cdot6 \times 0\cdot3 \times 0\cdot2$ mm; unit-cell dimensions determined with 30 high-angle reflexions; intensities measured for $3 < 2\theta < 125°$; h 0–12, k 0–21, l 0–7; ω-scan mode; scan rate 8° (ω) min^{-1}; scan width 2° (ω); five reference reflexions showed no significant intensity deterioration; corrections for Lorentz and polarization factors, but not for absorption or extinction; 1109 independent reflexions; 126 zero reflexions; standard deviations $\sigma^2(F_o) = \sigma_p^2(F_o) + qF_o^2$, where $\sigma_p(F_o)$ was evaluated by counting statistics and q was estimated to be $5\cdot0 \times 10^{-5}$. Structure solved by the direct method; full-matrix least-squares refinement; all H atoms found on difference map; $\sum w(|F_o| - |F_c|)^2$ minimized, where $w = 1/\sigma^2(F_o)$; zero reflexions with $|F_c| > F_{\rm lim}$ ($F_{\rm lim} = 1\cdot719$) included in the refinement with the assumption $F_o = F_{\rm lim}$ and $w = w(F_{\rm lim})$; final $R = 0\cdot068$ for 962 reflexions with $F_o > 3\sigma$ ($wR = 0\cdot078$, $S = 3\cdot883$); $(\Delta/\sigma)_{\max} = 0\cdot1$ for non-H atoms; $\Delta\rho$ peak $0\cdot41$ e Å^{-3}; atomic scattering factors from *International Tables for X-ray Crystallography* (1974); program *MULTAN*78 (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978), *LSAP*80 (Takenaka & Sasada, 1980), *DCMS*82 (Takenaka & Sasada, 1982) and *LISTUP* (Takenaka & Sasada, 1983).

Discussion. Final atomic parameters are given in Table 1.* Fig. 1 shows the bond distances and angles. The dimensions of the uracil moiety are in good agreement with those of 1-methyluracil (Green, Mathews & Rich,

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* Lists of structure factors, anisotropic thermal parameters and atomic parameters for H atoms have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42304 (8 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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1962), 1-(2-carboxyethyl)uracil (Fujita, Takenaka & Sasada, 1982, 1983), 1-(2-carbamoylethyl)uracil (Fujita, Takenaka & Sasada, 1984) and uridine (Green, Rosenstein, Shiono, Abraham, Trus & Marsh, 1975). The pyrimidine ring is planar within 0·015 Å. Torsion angles are 274·1 (5)° for C(2)—N(1)—C(7)—C(8) and 292·3 (5)° for N(1)—C(7)—C(8)—O(9).

The crystal structure is shown in Fig. 2. The base pairs are formed through N(3)—H···O(2) hydrogen bonds around the twofold axis. Such base pairing is different from those found in crystals of the above-mentioned compounds where N(3)—H···O(4) hydrogen bonds participate. These base pairs are stacked along the c axis. The stacking is further stabilized by the hydrogen bonds between O(4) and the hydroxyl group, as seen in Fig. 2(*b*).

Table 1. *Fractional coordinates and equivalent isotropic temperature factors*

$B_{eq} = 8\pi^2(U_1 + U_2 + U_3)/3$, where U_1, U_2, and U_3 are the principal components of the mean-square displacement matrix **U**. Values in parentheses are e.s.d.'s and those in angle brackets give the anisotropicity defined by $[\sum(B_{eq}-8\pi^2U_i)^2/3]^{1/2}$; they refer to the last decimal places.

	x	y	z	B_{eq}(Å^2)
N(1)	0·4518 (3)	0·1185 (2)	0·3455 (6)	2·1 ⟨3⟩
C(2)	0·3696 (4)	0·1712 (2)	0·3883 (7)	2·0 ⟨5⟩
O(2)	0·4031 (3)	0·2301 (1)	0·4361 (5)	2·8 ⟨10⟩
N(3)	0·2500 (4)	0·1529 (2)	0·3724 (6)	2·0 ⟨4⟩
C(4)	0·2026 (4)	0·0879 (2)	0·3201 (7)	2·2 ⟨6⟩
O(4)	0·0919 (3)	0·0806 (2)	0·3063 (5)	2·9 ⟨7⟩
C(5)	0·2927 (4)	0·0349 (2)	0·2856 (7)	2·6 ⟨5⟩
C(6)	0·4114 (4)	0·0522 (2)	0·2980 (7)	2·6 ⟨8⟩
C(7)	0·5815 (4)	0·1344 (3)	0·3600 (8)	2·9 ⟨9⟩
C(8)	0·6301 (5)	0·1660 (3)	0·165 (1)	3·7 ⟨15⟩
O(9)	0·6306 (3)	0·1174 (2)	0·0024 (6)	4·7 ⟨21⟩

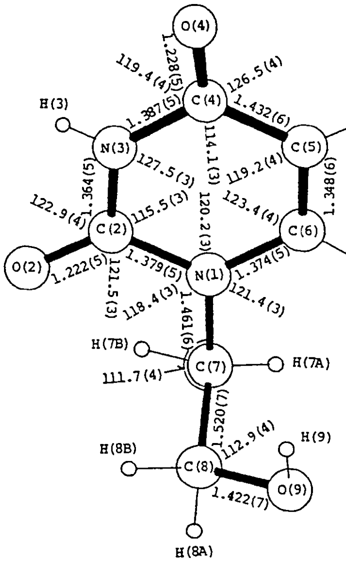

Fig. 1. Bond distances (Å) and angles (°). E.s.d.'s are shown in parentheses.

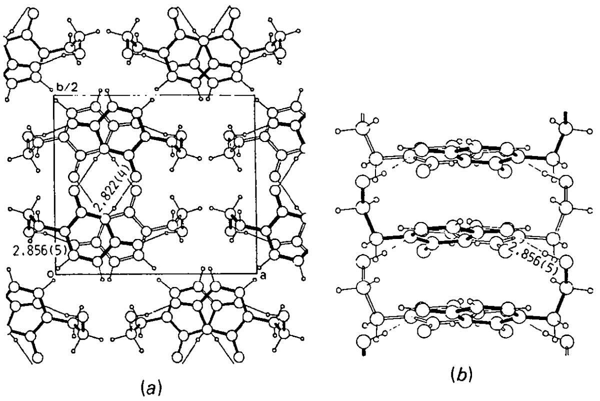

Fig. 2. (*a*) The crystal structure projected along **c**. Broken lines indicate the hydrogen bonds. (*b*) Stacking of the uracil pairs. (Distances in Å.)

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