Acta Cryst. (1974). B**30**, 873

The Crystal Structure of 1-β-D-Arabinofuranosyluracil*

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(*Received* 16 *October* 1973; *accepted* 19 *November* 1973)

An independent determination of the crystal structure of 1-*β*-D-arabinofuranosyluracil is described, and the results are compared with those previously reported [Tollin, Wilson & Young (1973) *Nature, New Biol.* **247**, 49–50; *Acta Cryst.* B**29**, 1641–1647]. Crystals of arabinofuranosyluracil are orthorhombic, space group $P2_12_12_1$, with cell dimensions $a=6\cdot826$ (3), $b=6\cdot888$ (2), $c=20\cdot973$ (5) Å; $Z=4$. Two octants of reciprocal space were surveyed using a Datex-automated G.E. XRD-5 diffractometer and Cu $K\alpha$ radiation. 2034 data were used in the least-squares refinement which converged at an R index of 0·030. The absolute configuration of the arabinose was confirmed by utilizing the anomalous scattering properties of oxygen and nitrogen. Standard deviations in the heavy-atom coordinates are 0·001–0·0015 Å, one-third as large as in the earlier study. There are no significant differences in the atomic coordinates resulting from the two refinements; however, there are systematic discrepancies between the two sets of temperature parameters.

Introduction

As part of a study on the conformations of arabinosyl nucleosides and nucleotides being carried out in this laboratory, we have carried out a crystal structure investigation of 1-*β*-D-arabinofuranosyluracil (ara-U). After our work was completed, we became aware of an independent crystal structure determination of the same compound (Tollin, Wilson & Young, 1973*a*), details of which have recently been published (Tollin, Wilson & Young, 1973*b*; hereinafter TWY). Since the formal e.s.d.'s in our resulting atomic parameters are smaller, by a factor of about 3, than those of TWY, we feel it appropriate to report our results and to compare them with those of TWY. The results of the comparison are, in general, highly gratifying.

Experimental

A sample of ara-U was furnished by the Cancer Chemotherapy National Service Center. It was recrystallized from water and a small, irregularly-shaped fragment with maximum dimensions approximately 0·10 × 0·16 × 0·18 mm was mounted along what turned out to be the [$\bar{1}$10] direction. Unit-cell dimensions were obtained from a least-squares fit to 2θ values (Cu $K\alpha$; $\lambda=1\cdot5418$ Å) for 13 reflections carefully centered on a Datex-automated General-Electric three-circle diffractometer; they are compared with the values of TWY in Table 1. The crystal density was measured by flotation in a CCl_4–CH_2Br_2 solution.

Table 1. *Crystal data*

$C_9H_{12}N_2O_6$ F.W. 244·2
Space group: $P2_12_12_1$ $Z=4$

	SM*	TWY†
a	6·826 (3) Å	6·810 (5) Å
b	6·888 (2)	6·870 (5)
c	20·973 (5)	20·98 (1)
D_x	1·645 g cm^{-3}	1·652 g cm^{-3}
D_m	1·62 (1)	
μ	12·2 cm^{-1}	1·5 cm^{-1}

* This investigation.
† Tollin, Wilson & Young (1973*b*).

Intensities for two octants (*hkl* and *hk*$\bar{l}$) were measured with θ–2θ scans at a speed of 1°/min in 2θ; backgrounds were counted for 40 s at each scan extremum. Four check reflections ($\bar{4}00$, $22\bar{2}$, $\overline{225}$, $\overline{335}$) were monitored periodically; their intensities decayed by about 2% during the course of data collection. The 43 strongest reflections were re-collected at reduced tube current to check on coincidence losses and counter overflow. Of a total of 2034 reflections having $2\theta \le 150°$ (Cu $K\alpha$ radiation), 2001 had net intensities greater than zero. Observational variances $\sigma^2(I)$ were based on

Table 2. *Enantiomorph determination*

	(L)	(D)
R*	0·0331	0·0329
Goodness of fit†	2·085	2·078

* $\sum||F_o|-|F_c||/\sum|F_o|$.
† $[\sum w(F_o^2-F_c^2)^2/(M-S)]^{1/2}$ for $M=2034$ data and $S=203$ parameters.

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* Contribution No. 4779 from the A. A. Noyes Laboratory of Chemical Physics. This investigation was supported in part by Public Health Service Research Grant No. GM 16966 from the National Institute of General Medical Sciences, National Institutes of Health. One of us (JSS) was supported in part by Research Training Grant 5T01 GM-01262-09-BCH.

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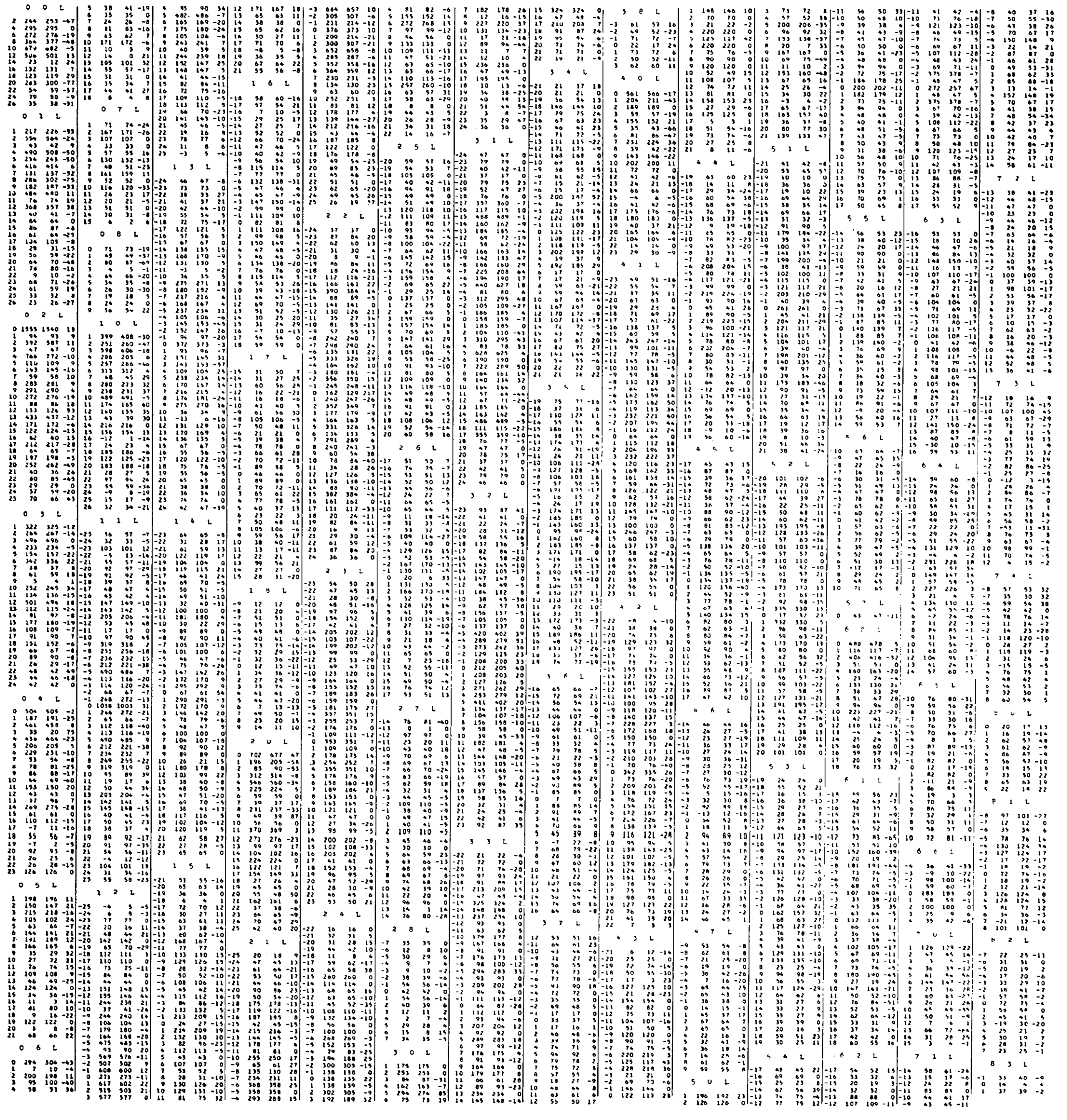
counting statistics plus an additional term $(0{\cdot}02S)^2$, where S is the scan count. Absorption effects were neglected ($\mu R_{\max} \approx 0{\cdot}16$). During the solution and preliminary refinement of the structure, data from the two octants of reciprocal space were averaged; later, they were separated.

Solution of the structure was by Patterson methods. Inspection of the $v=0$ section of a sharpened map indicated immediately the orientation of the pyrimidine ring, and packing considerations dictated the sites of substitution. Interpretation of the three Harker sections established the position of the uracil fragment of the

Table 3. *Observed and calculated structure factors*

The three columns of data contain values of $10|F_o|$, $10|F_c|$, and $10(F_o^2-F_c^2)/\sigma(F_o^2)$. A negative sign preceding F_o signifies that the net intensity was less than zero; these reflections were included in the least-squares refinement but were omitted in calculating the R index.



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      0   0   L          5   38   41  -19
                         6   35   35    0
  2  244  253  -47       7   24   26   -8
  4  295  295    0       8   81   83  -16
  6  272  276  -19       9   63   62    7
  8  364  377  -48      10  171  172   -6
 10  679  682   -5      11   10    3    9
 12  506  501   13      12   14    0   21
 14   23   12   24      13  105  101   32
 16  132  131    7      14   55   57  -17
 18  123  119   29      15   31   31    0
 20  263  300  -77      16   35   34    7
 22   54   59  -37      17   44   41   27
 24   79   80   -9      18    8    4    8
 26   35   38  -31
                              0   7   L
     0   1   L
                         1   71   74  -24
  1  217  226  -53       2  167  171  -26
  2  554  564  -24       3  107  107    0
  3   43   42    9       4   33   33    0
  4  490  508  -50       5   57   55   16
  5  234  243  -50       6  130  132  -13
  6  416  414    6       7   48   51  -23
  7  131  137  -52       8  161  159   13
  8  286  302  -75       9   52   52    0
  9  182  187  -33      10  116  120  -33
 10  484  480   11      11   26   23   17
 11   76   74   19      12   20   21   -5
 12  368  357   38      13   51   51    0
 13   40   41   -7      14   30   31   -8
 14   64   64    0      15    6    2    6
 15   86   87   -8
 16   61   64  -25          0   8   L
 17  134  105   -8
 18   28   31  -15       0   71   73  -19
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molecule, and subsequent structure-factor, Fourier, and tangent refinement calculations yielded the locations of the remaining heavy atoms. The *R* index was 0·20.

Refinement was by least-squares minimization of the quantity $\sum w(F_o^2 - F_c^2)^2$, with weights w equal to $\sigma^{-2}(F_o^2)$. Preliminary coordinates for the hydrogen atoms were recovered from a difference map, and were included, with isotropic temperature factors, in subsequent refinements. Form factors for hydrogen were those of Stewart, Davidson & Simpson (1965); others were from *International Tables for X-ray Crystallography* (1962). Eventually, a total of 203 parameters – coordinates for 29 atoms, anisotropic temperature coefficients for 17 heavy atoms, isotropic temperature coefficients for 12 hydrogen atoms, a scale factor and a secondary extinction parameter (Larson, 1967) – were included in a single matrix. Refinement converged at a goodness-of-fit of 2·53 for 1214 reflections and an *R* index of 0·026 for 1200 reflections with averaged intensities greater than zero.

At this stage the observed data were divided into the two Friedel-related portions (*hkl* and $hk\bar{l}$), and the form factors for nitrogen and oxygen were corrected for anomalous dispersion [$\Delta f' = 0{\cdot}049$ and $\Delta f'' = 0{\cdot}032$ for oxygen, $\Delta f' = 0{\cdot}032$ and $\Delta f'' = 0{\cdot}019$ for nitrogen; see Sherfinski & Marsh (1973)]. Structure factors were calculated for both the D and L enantiomer; results are summarized in Table 2. Hamilton's (1965) ratio test applied to both the *R* index and the goodness-of-fit indicates that confirmation of the expected D configuration is significant at the $\alpha = 0{\cdot}005$ level.

Final full-matrix refinement of the D enantiomer proceeded until no heavy-atom parameter shifted by as much as $0{\cdot}3\sigma$ nor any hydrogen-atom parameter by as much as $0{\cdot}5\sigma$. The final *R* index was 0·030 for 2001 reflections with $F_o^2 > 0$ and the goodness-of-fit was 1·96 for all 2034 reflections surveyed. As is usual, the largest magnitudes of the residuals $\sqrt{w}(F_o^2 - F_c^2)$ tended to be associated with low-angle reflections, and the most prominent features on a final difference map were peaks ranging up to 0·3 e Å^{-3} located midway between pairs of bonded atoms. A listing of observed and calculated structure factors is given in Table 3.

Discussion

Our final atomic coordinates and their standard deviations are given in Table 4. We also include in Table 4 the values of Δ/σ, where Δ is the difference between our value of a coordinate and the value reported by TWY and σ is the standard deviation of that difference. The agreement is excellent. The goodness of fit, $[\sum(\Delta/\sigma)^2/n]^{1/2}$, is 1·04 for the 51 heavy-atom parameters and 1·01

Table 4. *Atomic coordinates*

Values in parentheses are e.s.d.'s of this investigation, σ_{SM}. Values of Δ/σ are ratios between the difference in the coordinates found in the two investigations ($\Delta x = x_{SM} - x_{TWY}$) and their pooled standard deviation $\sigma_x = (\sigma_{SM2} + \sigma_{TWY2})^{1/2}$. We presume that the correct values of σ_{TWY} for the hydrogen atoms are larger by a factor of 10 than the values reported in Table 2 of TWY.

	$x(\times 10^5)$	Δ/σ	$y(\times 10^5)$	Δ/σ	$z(\times 10^5)$	Δ/σ
N(1)	33774 (17)	0·3	−1098 (17)	0·0	29509 (5)	−1·0
C(2)	51353 (20)	−1·2	−252 (22)	−1·3	26427 (6)	−1·1
O(2)	67166 (14)	−1·4	−1004 (18)	−1·2	29158 (4)	1·7
N(3)	50217 (16)	−1·4	1263 (19)	−0·7	19916 (5)	−0·7
C(4)	33450 (22)	1·0	3615 (20)	−0·5	16282 (6)	0·6
O(4)	34825 (16)	0·1	5360 (16)	−0·2	10503 (4)	−0·6
C(5)	15658 (21)	0·2	3478 (23)	0·0	19939 (6)	1·9
C(6)	16320 (20)	0·6	1036 (23)	2·3	26239 (6)	0·0
C(1′)	33955 (20)	−1·0	−3236 (20)	0·5	36494 (5)	−0·3
O(1′)	17152 (16)	−0·3	−13959 (15)	−2·1	38188 (4)	1·7
C(2′)	32684 (20)	−0·1	15928 (21)	−1·3	40139 (6)	−2·0
O(2′)	20575 (14)	0·7	29619 (15)	−1·4	37099 (9)	1·9
C(3′)	24343 (20)	0·0	8789 (21)	−1·1	46457 (6)	−0·6
O(3′)	40441 (14)	0·0	1917 (17)	0·7	50099 (4)	−1·0
C(4′)	10702 (21)	1·8	−7794 (20)	−0·2	44499 (4)	0·0
C(5)′	−10764 (21)	0·6	−2932 (23)	0·9	44198 (7)	−0·6
O(5′)	−14551 (15)	0·7	13172 (17)	−0·2	40058 (5)	−0·4
	$x(\times 10^4)$	Δ/σ	$y(\times 10^4)$	Δ/σ	$z(\times 10^4)$	Δ/σ
H(1)	6034 (24)	−1·8	−2 (24)	1·7	1800 (8)	1·7
H(2)	363 (23)	0·6	518 (24)	0·4	1786 (7)	0·1
H(3)	489 (25)	1·3	38 (23)	−1·2	2881 (7)	0·5
H(4)	4570 (22)	−0·8	−1039 (23)	0·5	3767 (7)	−0·7
H(5)	1057 (35)	1·1	2772 (32)	−0·4	3790 (10)	1·3
H(6)	4536 (26)	−0·7	2136 (26)	−0·2	4089 (8)	0·5
H(7)	3695 (28)	0·2	6 (28)	1·5	5371 (9)	−0·6
H(8)	1687 (25)	0·6	1926 (26)	0·5	4879 (7)	−0·8
H(9)	1239 (24)	−0·5	−1876 (25)	−0·5	4736 (7)	2·0
H(10)	−2022 (31)	−0·4	968 (35)	0·8	3682 (9)	−0·9
H(11)	−1397 (22)	1·8	35 (24)	−0·9	4862 (8)	1·5
H(12)	−1839 (26)	1·0	−1452 (28)	0·9	4277 (8)	−0·6

for the 36 hydrogen-atom parameters; the points on a half-normal probability plot (Abrahams & Keve, 1971) fall close to a line with slope and intercept of 1·0 and 0·0. We point out that the terms in the denominator, σ, are determined primarily by the standard deviations reported by TWY, which are about three times larger than our values. Thus, the excellent match between the observed and expected parameter differences is a strong vindication of the standard deviations reported by TWY but says little about the reliability of our e.s.d'.s beyond confirming that they are much smaller than those of TWY.

Anisotropic temperature factors are given in Table 5. At first glance, the agreement with the values of TWY is less satisfactory. However, the differences reflect, almost entirely, a larger isotropic component – by 0·0044 Å^2 in units of U(= mean square displacement) – in our values compared to those of TWY. When this component is subtracted from the diagonal elements of our values, the goodness-of-fit among the 102 pairs of values becomes 1·07.

One is tempted to suggest that the systematic differences between the two sets of temperature factors, as well as the differences in unit-cell dimensions, reflect the difference in climate between Dundee and Pasadena. However, we find it difficult to imagine that the Dundee experiments were carried out at a temperature far enough below ours (about 22°C) to cause so large a difference. Crystals of approximately the same size were used in both investigations, and in both cases absorption effects should have been very small; in any event, since TWY used molybdenum radiation while we used copper, any errors due to absorption would be expected to have produced errors in the temperature factors in the opposite sense from that observed. Neglect of secondary extinction by TWY could have caused temperature parameter errors in the right direction, but once again we estimate the effect to be far too small. Finally, we note that our value of the extinction parameter, 65 (5) × 10^{-7} e^{-2}, brings into close agreement the observed and calculated F values reported by TWY for the strongest reflection, 020; thus, there was apparently no great difference in the degree of perfection of the crystals used in the two laboratories. In sum, while we presume that the difference in the isotropic component of the temperature parameters represents a systematic error in one or both data sets, we have no clue as to the source of the error.

Table 5. *Anisotropic temperature parameters of the heavy atoms* ($\times 10^5$)

Standard deviations are in parentheses. The temperature factor expression is of the form $\exp[-(\beta_{11}h^2\cdots\beta_{23}kl)]$. Values of Δ/σ are as in Table 3, except that Δ includes the quantity 0·0044 $[2\pi^2(a_i^*)^2]$ added to the diagonal terms β_{ii} of TWY (see text).

	β_{11}	Δ/σ	β_{22}	Δ/σ	β_{33}	Δ/σ
N(1)	953 (22)	−0·5	1649 (28)	−1·1	99 (2)	0·3
C(2)	1014 (27)	−1·0	1422 (29)	0·9	102 (3)	−1·2
O(2)	1047 (20)	−0·3	2745 (32)	−0·1	130 (2)	0·6
N(3)	1018 (24)	−0·8	1698 (30)	−0·3	101 (2)	1·1
C(4)	1329 (29)	−0·1	1172 (28)	−1·4	112 (2)	−1·5
O(4)	1822 (25)	−1·2	2039 (26)	−1·5	102 (2)	3·0
C(5)	1043 (28)	−0·1	1743 (34)	0·7	141 (3)	−1·1
C(6)	922 (27)	0·7	1754 (34)	−0·7	146 (3)	−0·9
C(1′)	1082 (27)	−0·5	1358 (29)	−1·3	104 (2)	−0·7
O(1′)	1635 (24)	1·3	1302 (21)	−2·0	130 (2)	3·5
C(2′)	988 (29)	0·4	1315 (30)	0·1	107 (3)	0·9
O(2′)	1254 (24)	1·4	1292 (21)	−0·9	162 (2)	0·0
C(3′)	970 (27)	1·0	1375 (29)	0·9	101 (3)	−2·7
O(3′)	1268 (22)	0·7	2297 (30)	2·2	105 (2)	1·7
C(4′)	1285 (32)	−0·8	1354 (30)	3·5	100 (2)	−1·0
C(5′)	1160 (31)	−0·4	1760 (37)	1·0	161 (3)	0·9
O(5′)	1352 (25)	−0·4	1798 (26)	−0·3	197 (3)	−0·5

	β_{12}	Δ/σ	β_{13}	Δ/σ	β_{23}	Δ/σ
N(1)	398 (61)	−0·2	−30 (13)	−0·4	−1 (12)	0·2
C(2)	309 (66)	−0·8	−90 (16)	0·4	−3 (15)	0·5
O(2)	373 (58)	1·1	−54 (14)	0·3	−106 (11)	−0·4
N(3)	206 (58)	−0·6	−94 (14)	−0·2	90 (13)	0·9
C(4)	14 (65)	−1·9	−94 (14)	−0·5	−139 (16)	0·4
O(4)	−30 (55)	−0·7	−23 (12)	0·3	−104 (13)	0·3
C(5)	272 (70)	−0·9	−86 (18)	0·7	−182 (16)	−1·4
C(6)	215 (73)	0·6	−79 (18)	0·0	−26 (16)	0·8
C(1′)	202 (62)	−0·9	58 (15)	1·4	24 (16)	−0·1
O(1′)	−700 (47)	0·2	−112 (11)	0·8	176 (12)	−0·2
C(2′)	−184 (62)	−0·5	65 (15)	1·0	22 (16)	0·7
O(2′)	76 (43)	−0·4	201 (12)	0·8	71 (13)	0·9
C(3′)	56 (58)	0·0	7 (14)	0·1	15 (14)	−1·3
O(3′)	48 (52)	0·2	118 (14)	−0·2	−104 (12)	−0·3
C(4′)	−151 (61)	0·4	95 (16)	0·4	56 (16)	1·0
C(5′)	−471 (68)	0·3	67 (19)	−1·0	38 (18)	0·8
O(5′)	−99 (53)	0·0	27 (15)	−1·9	−198 (14)	−1·8

Table 6. *Temperature factors of the hydrogen atoms*

	B(Å^2)		B(Å^2)
H(1)	2·8 (0·4)	H(7)	4·4 (0·5)
H(2)	2·2 (0·3)	H(8)	2·8 (0·4)
H(3)	2·8 (0·4)	H(9)	2·4 (0·3)
H(4)	1·9 (0·3)	H(10)	5·3 (0·5)
H(5)	6·0 (0·6)	H(11)	2·7 (0·3)
H(6)	3·2 (0·4)	H(12)	3·6 (0·4)

Table 7. *Bond lengths and angles involving the hydrogen atoms*

Standard deviations are approximately 0·02 Å and 1·5°.

N(3)–H(1)	0·81 Å	N(1)—C(1′)–H(4)	108°
C(5) –H(2)	0·94	C(2′) –C(1′)–H(4)	111
C(6) –H(3)	0·95	O(1′)–C(1′)–H(4)	110
C(1′)–H(4)	0·97	C(2′) –O(2′)–H(5)	109
O(2′)–H(5)	0·72	C(1′) –C(2′)–H(6)	112
C(2′)–H(6)	0·96	C(3′) –C(2′)–H(6)	109
O(3′)–H(7)	0·81	O(2′)–C(2′)–H(6)	110
C(3′)–H(8)	1·01	C(3′) –O(3′)–H(7)	109
C(4′)–H(9)	0·97	C(2′) –C(3′)–H(8)	112
O(5′)–H(10)	0·82	C(4′) –C(3′)–H(8)	111
C(5′)–H(11)	0·98	O(3′)–C(3′)–H(8)	112
C(5′)–H(12)	1·00	C(3′) –C(4′)–H(9)	110
		O(1′)–C(4′)–H(9)	107
		C(5′) –C(4′)–H(9)	108
C(2) –N(3)–H(1)	116°	C(5′) –O(5′)–H(10)	111
C(4) –N(3)–H(1)	117	C(4′) –C(5′)–H(11)	103
C(4) –C(5)–H(2)	119	O(5′)–C(5′)–H(11)	111
C(6) –C(5)–H(2)	120	C(4′) –C(5′)–H(12)	110
C(5) –C(6)–H(3)	123	O(5′)–C(5′)–H(12)	110
N(1)–C(6)–H(3)	115	H(11)–C(5′)–H(12)	111

Isotropic temperature parameters of the hydrogen atoms are given in Table 6, bond distances and angles are given in Fig. 1 and Table 7, and a stereoscopic view of the molecule is shown in Fig. 2. Details of the structure have already been discussed by TWY, and we wish to add only a couple of comments:

(1) The intramolecular hydrogen bond O(2′)–H(5)···O(5′) has also been noted in the crystal structure of the similar nucleoside arabinosylcytosine (Chwang & Sundaralingam, 1973; Soubeyran & Tougard, 1973; Sundaralingam & Chwang, 1973). The presence of this hydrogen bond supports the feasibility of a 2′–5′ cyclic monophosphate configuration for the arabinosylnucleotides (Cohen, 1966).

(2) The N(3)–H(1)···O(2′) hydrogen bond is quite non-linear (N–H–O = 146°), the acceptor oxygen atom lying 1·56 Å out of the plane of the donor pyrimidine ring. The hydrogen atom H(1) is also displaced from the plane of the pyrimidine ring, by 0·12 ± 0·02 Å, in the same direction as the oxygen atom. There are now many examples of out-of-plane displacements of hydrogen atoms presumably dictated by hydrogen bonding [see, for example, Lai & Marsh (1972)].

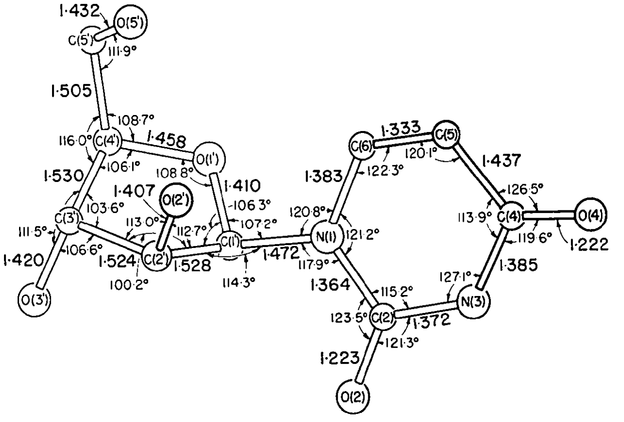

Fig. 1. Heavy-atom bond distances and angles. Estimated standard deviations are about 0·002 Å and 0·1–0·2°.

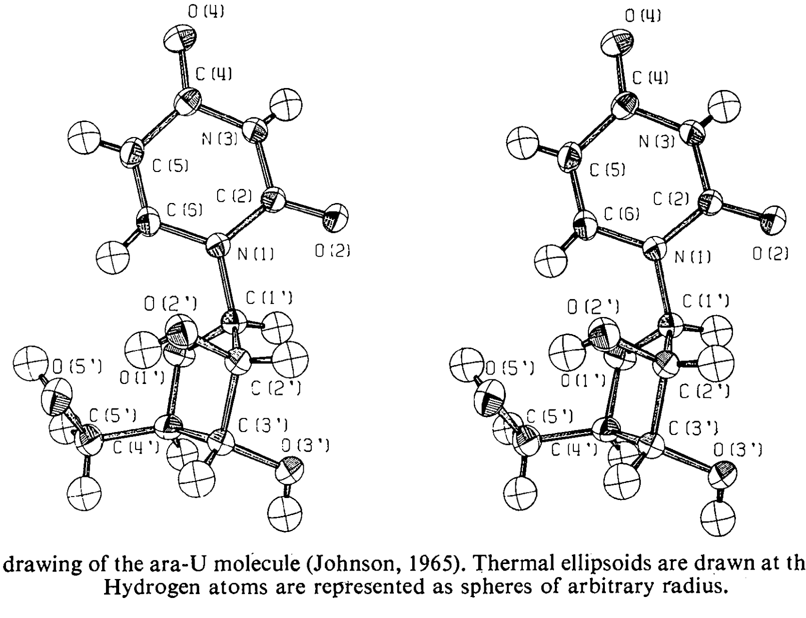

Fig. 2. A stereoscopic drawing of the ara-U molecule (Johnson, 1965). Thermal ellipsoids are drawn at the 50% probability level. Hydrogen atoms are represented as spheres of arbitrary radius.

We are grateful to Dr P. Tollin for sending us his results prior to publication.

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The Crystal Structure of *o*-Methyl β-Methylphenylcholine Ether Bromide

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(*Received* 26 *June* 1973; *accepted* 25 *November* 1973)

The crystal structure has been determined from three-dimensional counter X-ray data. The material crystallizes in the monoclinic space group $P2_1/c$ with four molecules in the unit cell. The cell parameters are $a=9·915$ (2), $b=9·204$ (2), $c=18·170$ (4) and $\beta=121·45$ (2)°. The structure was solved by Patterson and Fourier syntheses using 2859 independent reflexions and refined by block-diagonal least-squares calculations to a final R value of 0·061. The N–C–C–O system adopts the positive synclinal (*gauche*) conformation. The remaining torsional angles are close to 180°.

Introduction

The pharmacological properties of *o*-methyl β-methylphenylcholine ether bromide (OMBEM TM1) are in sharp contrast to those of phenylcholine ether bromide itself and its α-methyl substituted derivatives. Whereas the latter are all potent ganglion stimulants, OMBEM TM1 is devoid of such activity (Hey, 1952; Clark & Jana, 1966; Clark, Dawes & Williams, 1968). It has been suggested on the basis of ultraviolet spectroscopic studies that a possible reason for this lack of activity is that β-methyl substituted derivatives cannot adopt a conformation in which the Ph–O–C group of atoms are coplanar (Clark & Williams, 1967). The present study shows this deduction to be most unlikely and moreover that the conformation adopted by the molecule in the crystal is close to that which has been suggested as necessary for pharmacological activity in acetylcholine and its analogues (Chothia, 1970).

Experimental

Systematic absences were found from Weissenberg photographs for $0k0$ when $k=2n+1$, and for $h0l$ when $l=2n+1$, indicating the space group $P2_1/c$. Three-dimensional intensity data were collected on a computer-controlled Enraf–Nonius CAD4 four-circle diffractometer and measured by the moving-crystal moving-counter technique in the range $3° \le \theta \le 70°$. A control reflexion measured every 40 min showed a maximum deviation of 6%. After correction for Lorentz and polarization effects, a statistical analysis (Wilson, 1942) was carried out to determine a mean temperature factor and an absolute scale factor. No absorption corrections were made.

Crystal data

$C_{13}H_{22}ON^+Br^-$; M.W. 288. Source: Dr E. R. Clark, Dept. of Pharmacology, University of Leeds. Crystal system: monoclinic. Space group: $P2_1/c$; $a=9·915$ (2), $b=9·204$ (2), $c=18·170$ (4) Å, $\beta=121·45$ (2)°; $V=1415$ Å^3, $Z=4$, $D_c=1·351$, $D_m=1·345$ g cm^{-3}. Radiation: Graphite monochromatized Cu $K\alpha$, $\lambda=1·54051$ Å.

Structure determination and refinement

The position of the bromine atom in the asymmetric unit was found from a study of the Patterson–Harker section $(U,\frac{1}{2},W)$ and line $(0,V,\frac{1}{2})$ and confirmed by the general peak at (U,V,W). A three-dimensional