plane of the molecule and consequently O(6) is *trans* to HC(5) whilst in methyl α-glucoside O(6) is approximately in the plane of the ring and *trans* to C(4) (Berman & Kim, 1968).

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The Crystal and Molecular Structure of 5-Iodouridine

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The crystal structure of 5-iodouridine ($C_9H_{11}IN_2O_6$) has been determined from data collected on a Hilger and Watts linear diffractometer. The crystals are monoclinic, space group $P2_1$, with cell dimensions: $a=4{\cdot}683\pm0{\cdot}005$, $b=17{\cdot}14\pm0{\cdot}01$, $c=14{\cdot}58\pm0{\cdot}01$ Å and $\beta=90{\cdot}85\pm0{\cdot}1°$. The structure was solved by the heavy-atom method and the positional and thermal parameters were refined by the method of least-squares. The final R value for 2143 observed reflexions is 0·061. There are two molecules in the asymmetric unit and the dihedral angle between the base and sugar planes in both is 69°. However, the glycosidic torsion angle, φ_{CN}, is $-13{\cdot}2°$ in molecule I and $-58{\cdot}7°$ in molecule II. In molecule I atom C(3′) of the sugar ring is displaced 0·54 Å *endo*, and in molecule II atom C(2′) is displaced 0·63 Å *endo*. The orientation of the C(5′)–O(5′) bond is *gauche* to both the C(4′)–O(1′) and C(4′)–C(3′) bonds in molecule I, but in molecule II it is *trans* to C(4′)–O(1′) and *gauche* to C(4′)–C(3′).

Introduction

The structure determination of 5-iodouridine (IUR) (Fig. 1) was undertaken as part of a series of structure determinations of nucleic acid components and their analogues. Single-crystal studies of nucleosides and nucleotides give important information about the bond lengths and angles, and about the conformations of the molecules, which can be used when molecular models of polynucleotide structures are constructed. It was mainly to obtain information about the conformation of the molecule that IUR was studied. Knowledge of the crystal and molecular structure of IUR was also desirable as a first step in the study of the effects of ionizing radiations on single crystals of IUR by electron-spin resonance. Such studies have already been made on 5-iodo-2′-deoxyuridine (Nice & Rorke, 1969). It is hoped that similar studies will eventually elucidate the effects of ionizing radiations on the nucleic acids themselves, and explain the change in sensitivity when certain analogues are incorporated into the structure in place of a normal component. A preliminary account of the conformations of the molecules has been given recently (Rahman & Wilson, 1970).

Experimental

Crystal of 5-iodouridine ($C_9H_{11}IN_2O_6$) were obtained by evaporation from aqueous solutions. The unit-cell dimensions were first obtained from Weissenberg photographs and were then refined on a Wooster four-circle diffractometer using Cu $K\alpha$ radiation. The crystals are monoclinic and elongated along the a axis. The unit-cell dimensions are:

$a = 4{\cdot}683 \pm 0{\cdot}005$, $b = 17{\cdot}14 \pm 0{\cdot}01$, $c = 14{\cdot}58 \pm 0{\cdot}01$ Å, $\beta = 90{\cdot}85 \pm 0{\cdot}1°$

(λ Cu $K\alpha_1 = 1{\cdot}54050$ Å, λ Cu $K\alpha_2 = 1{\cdot}54434$ Å).

Systematic absences of the $0k0$ reflexions when k is odd show that the space group is either $P2_1$ or $P2_1/m$, and the optical activity of the nucleoside establishes the space group as $P2_1$. If there were two molecules in the unit cell the density would be only 1·051 g.cm^{-3} which is too low, and this suggests that there are four molecules in the unit cell, and hence two molecules in the asymmetric unit. The calculated density is then 2·102 g.cm^{-3}.

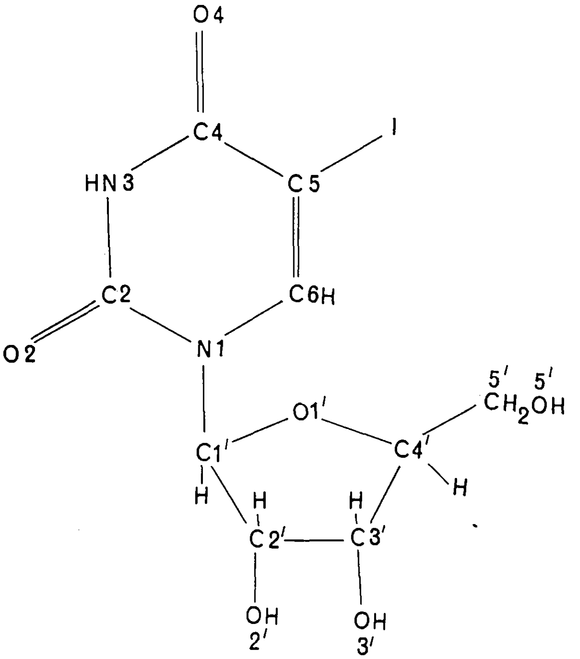
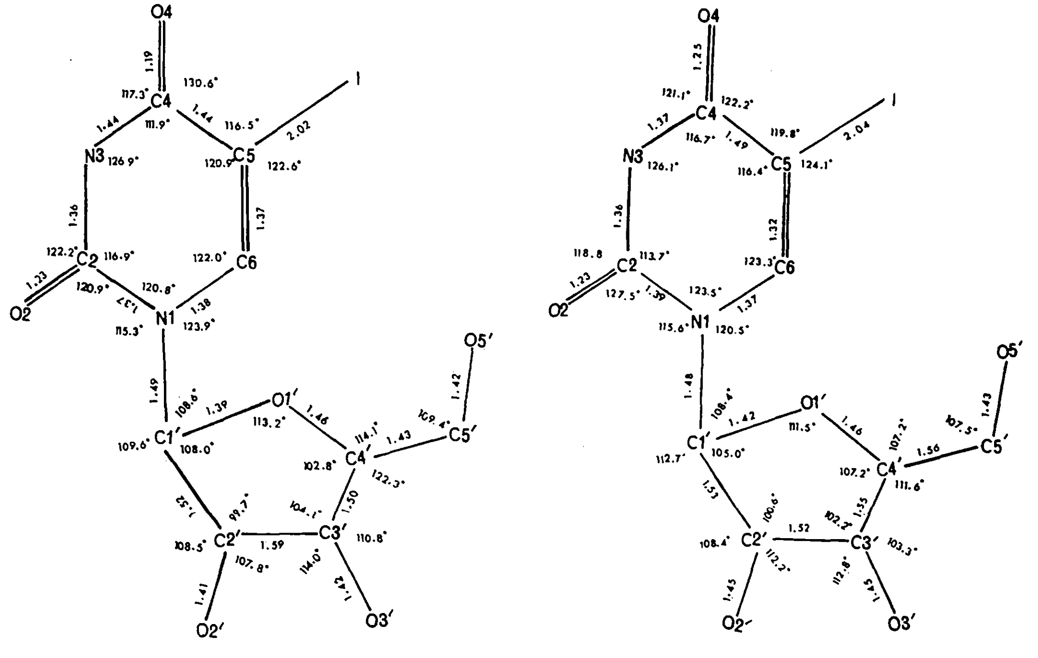


Fig. 1. The 5-iodouridine ($C_9H_{11}IN_2O_6$) molecule and the atom numbering.

The intensities of 2143 unique reflexions were measured on a Hilger and Watts linear diffractometer, using molybdenum K radiation and balanced filters, and a few were measured on a Wooster four-circle diffractometer using copper $K\alpha$ radiation, to check the setting of one of the crystals. The data were collected to a $\sin\theta$ value corresponding to the radius of the limiting sphere for copper $K\alpha$ radiation, and the measurable reflexions represented 80% of the total possible number. In the final stages of the analysis it was found that seven reflexions which should have been recorded had not been measured and visual estimates of the intensities of these reflexions were made. Two crystals were used for collecting the intensity data, one mounted along the a axis and the other along the b axis. The first crystal had length 0·26 mm parallel to **a** and cross section 0·17 × 0·09 mm perpendicular to **a**; the second crystal had length 0·22 mm parallel to **b** and cross section 0·13 × 0·09 mm perpendicular to **b**. The data on layer planes 0 to 5 were collected about the a axis, and layer planes 0 to 3 about the b axis, on the linear diffractometer. The absorption coefficient for molybdenym radiation is 2·8 cm^{-1} and no absorption corrections were applied.



(*a*) (*b*)

Fig. 2. Bond lengths and angles in (*a*) molecule I, and (*b*) molecule II.

Structure determination

The positions of the iodine atoms were first determined from two-dimensional Patterson syntheses using the $0kl$ and the $h0l$ intensities, and the coordinates were confirmed by a three-dimensional Patterson synthesis. A three-dimensional Fourier synthesis was calculated using the observed structure factors and the phases calculated from the iodine atoms alone. The presence of two iodine atoms in the asymmetric unit means that the Fourier syntheses are easier to interpret than if only one iodine atom were present and the pyrimidine rings were clearly observed in this synthesis. Structure factors were calculated for these atoms using scattering factors from *International Tables for X-ray Crystallography* (1962), with $B=4{\cdot}5$ Å^2 for all atoms; the iodine scattering factor was corrected for anomalous dispersion according to the expression:

$$f_{\text{corrected}}=\sqrt{\{(f_o+\Delta f')^2+(\Delta f'')^2\}}\,,$$

where $\Delta f'$ and $\Delta f''$ are those listed in *International Tables for X-ray Crystallography* (1962). The R value, defined by $R=\sum||F_o|-|F_c||/\sum|F_o|$, was 0·26. A second Fourier synthesis, using the phases derived from the iodine atom and the atoms of the bases, revealed all the other atoms in the molecules, other than hydrogen atoms. A structure-factor calculation, using all the atoms revealed in the electron density map, and with the same B value of 4·5 Å^2 gave an R value of 0·21.

Refinement

The structure was refined by the method of least squares, using the block-diagonal approximation and a program written by Professor J. Trotter (Toronto University), modified and adapted for use on an Elliott 4130 computer by the staff of the Computing Laboratory of the University of Dundee.

Initially, refinement of the positional and isotropic thermal parameters, and a scale factor, was carried out, with all but the very strongest reflexions given equal weight. After five cycles of refinement the R value was 0·12 and at this stage anisotropic temperature parameters were introduced for the iodine atoms. After three cycles of refinement the R value was 0·09. At this stage three-dimensional Fourier and difference-Fourier syntheses were calculated. These verified that there were no molecules of water of crystallization present, but the difference-Fourier did not reveal the positions of the hydrogen atoms. Hydrogen atom positions were calculated on the basis of normal bond lengths and angles, the positions of those attached to atoms O(2′), O(3′) and O(5′) being placed according to the suggested hydrogen-bonding scheme.

All the non-hydrogen atoms were then refined anisotropically, the hydrogen atoms being kept in fixed positions. After three cycles of refinement the R value was 0·075. At this stage a new weighting scheme was introduced in which the weight ω is given by

$$\omega=1/\{1+(|F_o|-b)^2/a^2\}\,,$$

where a and b are constants. The values of the constants a and b were chosen so that the average value of $\omega\Delta^2$ was approximately constant for all structure amplitudes, and the values were modified as required, as the refinement proceeded. The anisotropic temperature factor was of the form

$$\exp\{-(B_{11}h^2+B_{22}k^2+B_{33}l^2+B_{12}hk+B_{23}kl+B_{13}hl)\}\quad.$$

Four cycles of refinement were carried out with the new weighting scheme and the final R value for the observed reflexions was 0·061. Including the unobserved reflexions with structure factors of zero resulted in an increase in the R value to 0·062.

At the final stage of refinement the maximum positional parameter shift was 0·0011 Å, corresponding to 0·30σ, and the maximum thermal parameter shift was

Table 1. *Positional parameters of the non-hydrogen atoms with estimated standard deviations in fractional coordinates*

	Molecule I			Molecule II		
	x/a	*y/b*	*z/c*	*x/a*	*y/b*	*z/c*
N(1)	0·5398 (35)	0·6997 (8)	0·8541 (10)	0·7826 (30)	0·6063 (7)	0·4307 (9)
C(2)	0·5682 (36)	0·7626 (8)	0·7968 (11)	0·6588 (30)	0·5384 (10)	0·4637 (10)
O(2)	0·4182 (25)	0·7690 (7)	0·7268 (8)	0·4652 (27)	0·5329 (6)	0·5194 (8)
N(3)	0·7652 (30)	0·8171 (7)	0·8213 (9)	0·7662 (28)	0·4719 (7)	0·4261 (10)
C(4)	0·9441 (58)	0·8170 (9)	0·9024 (13)	0·9638 (34)	0·4680 (8)	0·3577 (10)
O(4)	1·1048 (27)	0·8700 (6)	0·9122 (10)	1·0526 (33)	0·4036 (7)	0·3289 (8)
C(5)	0·8749 (44)	0·7532 (10)	0·9629 (12)	1·0726 (31)	0·5441 (11)	0·3216 (7)
I	1·0901 (3)	0·7502 (1)	1·0844 (1)	1·3415 (2)	0·5445 (1)	0·2123 (1)
C(6)	0·6864 (29)	0·6965 (8)	0·9364 (10)	0·9831 (41)	0·6072 (9)	0·3630 (11)
C(1′)	0·3284 (32)	0·6398 (10)	0·8231 (11)	0·6600 (34)	0·6801 (8)	0·4653 (11)
O(1′)	0·2664 (25)	0·5917 (5)	0·8969 (7)	0·5411 (25)	0·7219 (6)	0·3895 (8)
C(2′)	0·4582 (34)	0·5870 (9)	0·7484 (9)	0·8861 (37)	0·7345 (8)	0·5064 (10)
O(2′)	0·2355 (29)	0·5598 (6)	0·6928 (9)	0·9244 (30)	0·7152 (7)	0·6026 (9)
C(3′)	0·5802 (40)	0·5197 (8)	0·8096 (10)	0·7413 (34)	0·8131 (8)	0·4928 (10)
O(3′)	0·6081 (28)	0·4484 (7)	0·7615 (10)	0·4933 (26)	0·8230 (6)	0·5504 (7)
C(4′)	0·3685 (32)	0·5119 (8)	0·8854 (11)	0·6089 (41)	0·8050 (9)	0·3949 (10)
C(5′)	0·4357 (40)	0·4730 (11)	0·9693 (14)	0·8339 (42)	0·8223 (10)	0·3191 (12)
O(5′)	0·6618 (30)	0·5128 (9)	1·0149 (10)	0·9125 (30)	0·9026 (7)	0·3270 (9)

0.22σ. The final values of the parameters of the heavy atoms, together with their estimated standard deviations are given in Tables 1 and 2. The observed and calculated structure factors are listed in Table 3. Table 4 lists the intramolecular bond lengths and angles in the two molecules, and these are also shown in Fig. 2.

Discussion

The pyrimidine bases

In discussing the results the molecules are referred to as molecules I and II.

The pyrimidine base in molecule II is planar, and the maximum deviation of a ring atom from the least-squares plane of the ring is 0·02 Å. However, the pyrimidine ring in molecule I is less planar and the maximum deviation in this case is 0·05 Å. The equations of the least-squares planes through the six-membered rings of molecules I and II respectively are:

$$-0{\cdot}7239x+0{\cdot}5151y+0{\cdot}4590z-10{\cdot}2313=0$$

and $$0{\cdot}7241x-0{\cdot}0461y+0{\cdot}6882z-\ 6{\cdot}4153=0,$$

where X, Y and Z are coordinates, in Å, measured in the directions **a**, **b** and **c***.

Atom C(1′) of the sugar is displaced 0·06 Å above the pyrimidine plane in molecule I, as viewed in Fig. 1, and is displaced 0·12 Å below the plane in molecule II. Similar displacements are observed in other nucleosides (Haschmeyer & Rich, 1967). The deviations of the atoms from the pyrimidine planes are given in Table 5.

The pyrimidine base is in the diketo form and the average value of the length of the four C=O bonds is 1·23 Å, although they differ amongst themselves by 0·06 Å. The C–N bonds in both molecules vary from 1·36 to 1·38 Å, with the exception of the N(1)–C(6) bond in molecule I which is 1·42 Å. The mean value of 1·35 Å for the C(5)–C(6) bond indicates its double-bond character, and the mean value of 1·47 Å for the C(4)–C(5) bond indicates its single-bond character. Both C(5)–I bond lengths are normal.

Comparison of the pyrimidine bases with that in 5-iodo-2′-deoxyuridine (Camerman & Trotter, 1965) shows that they are in good agreement, and comparison with the more accurate structure determination of thymidine (Young, Tollin & Wilson, 1969) shows that substitution of iodine for the methyl group does not alter the structure of the base significantly. The values of 126·1 and 126·9° for the angles C(2)–N(3)–C(4) in the two molecules are consistent with a hydrogen atom being attached to atom N(3) (Singh, 1965).

The sugars

Sugar rings in nucleosides and nucleotides are usually puckered with either atom C(2′) or atom C(3′) displaced out of the plane of the other four atoms. The amount of the displacement is normally about 0·6 Å and the most common type of pucker is with either C(2′) or C(3′) *endo*, *i.e.* lying on the same side

Table 2. *Thermal parameters of the non-hydrogen atoms with their estimated standard deviations in brackets,* $\times 10^4$

	Molecule I							Molecule II					
	B_{11}	B_{22}	B_{33}	B_{12}	B_{23}	B_{13}		B_{11}	B_{22}	B_{33}	B_{12}	B_{23}	B_{13}
N(1)	626 (79)	19 (4)	34 (6)	95 (31)	−12 (8)	43 (38)	N(1)	439 (62)	8 (3)	36 (6)	5 (25)	12 (7)	68 (31)
C(2)	464 (70)	11 (4)	33 (6)	−19 (29)	−2 (8)	99 (34)	C(2)	331 (56)	20 (4)	38 (6)	70 (35)	18 (11)	7 (32)
C(2)	371 (49)	26 (4)	29 (4)	−10 (24)	−9 (7)	−34 (25)	O(2)	612 (58)	12 (4)	42 (5)	11 (24)	1 (7)	155 (27)
N(3)	405 (61)	16 (4)	26 (5)	28 (27)	−5 (8)	5 (30)	N(3)	354 (56)	10 (3)	44 (6)	1 (25)	−2 (8)	57 (31)
C(4)	1050 (157)	8 (4)	39 (8)	−73 (42)	20 (9)	12 (59)	C(4)	405 (69)	11 (4)	30 (6)	−13 (29)	3 (9)	−82 (34)
O(4)	450 (56)	12 (3)	60 (7)	80 (23)	0 (8)	−38 (33)	O(4)	789 (81)	16 (3)	34 (5)	−76 (30)	11 (8)	17 (35)
C(5)	664 (101)	12 (4)	36 (7)	−25 (40)	8 (10)	−21 (45)	C(5)	418 (58)	16 (3)	25 (5)	−63 (41)	−5 (11)	63 (28)
I	652 (7)	48 (1)	33 (1)	23 (4)	5 (1)	−45 (3)	I	459 (4)	24 (1)	33 (1)	−7 (3)	0 (1)	66 (2)
C(6)	243 (52)	19 (4)	34 (6)	−89 (26)	−1 (9)	60 (30)	C(6)	622 (93)	15 (4)	24 (6)	−76 (35)	−1 (9)	51 (39)
C(1′)	282 (61)	22 (5)	33 (6)	−2 (31)	1 (9)	68 (32)	C(1′)	409 (70)	8 (4)	34 (7)	9 (29)	0 (8)	11 (36)
O(1′)	470 (53)	8 (3)	34 (5)	−72 (21)	−4 (6)	76 (26)	O(1′)	441 (52)	12 (3)	38 (5)	23 (22)	4 (7)	−94 (27)
C(2′)	367 (68)	20 (5)	17 (5)	−79 (31)	−9 (9)	20 (32)	C(2′)	514 (76)	13 (4)	23 (5)	21 (31)	−4 (8)	−57 (34)
O(2′)	556 (62)	18 (4)	43 (6)	−28 (25)	5 (7)	−23 (32)	C(2′)	540 (65)	23 (4)	46 (6)	−47 (29)	1 (9)	−37 (34)
C(3′)	582 (87)	9 (2)	20 (5)	−54 (30)	−4 (7)	16 (37)	C(3′)	342 (64)	14 (4)	30 (6)	−4 (30)	16 (8)	−30 (33)
O(3′)	404 (57)	21 (3)	75 (7)	−29 (25)	52 (8)	23 (35)	O(3′)	459 (54)	14 (3)	31 (5)	−14 (23)	4 (7)	60 (27)
C(4′)	320 (62)	9 (3)	45 (7)	18 (28)	13 (9)	104 (34)	C(4′)	563 (87)	12 (4)	26 (6)	11 (34)	−3 (9)	−5 (40)
C(5′)	386 (77)	24 (5)	53 (9)	18 (38)	−13 (12)	15 (45)	C(5′)	644 (89)	17 (5)	38 (7)	32 (37)	−1 (10)	155 (40)
O(5′)	466 (66)	41 (5)	51 (7)	−5 (32)	−24 (10)	−93 (36)	O(5′)	533 (63)	21 (4)	59 (6)	10 (28)	−35 (8)	91 (34)

Table 3. *Observed and calculated structure factors*

The values based on visual estimations are indicated with an asterisk.

H	K	L	FOBS	FCALC
0	0	1	*46.48	46.31
0	0	3	*54.75	56.18
0	0	5	19.04	19.39
0	0	6	63.32	62.93
0	0	7	133.34	131.98
0	0	8	53.92	55.61
0	0	9	53.42	55.97
0	0	10	75.19	77.25
0	0	11	20.78	19.10
0	0	12	12.41	11.08
0	0	13	24.49	25.73
0	0	14	22.75	24.83
0	0	16	25.25	26.12
0	0	17	35.37	38.94
0	0	18	9.89	9.65
0	1	1	*55.[illegible]	60.79
0	1	3	*55.[illegible]	65.59
0	1	4	95.71	101.14
0	1	5	40.81	43.23
0	1	6	77.41	81.42
0	1	7	43.53	44.37
0	1	8	95.96	96.51
0	1	9	58.86	63.56
0	1	10	40.56	40.81
0	1	11	22.26	23.26
0	1	12	14.59	13.58
0	1	13	39.57	42.73
0	1	14	26.96	28.72
0	1	15	39.57	43.24
0	1	16	25.00	27.86
0	1	17	13.36	15.08
0	1	18	12.37	15.28
0	2	0	*53.88	53.23
0	2	1	*48.15	44.63
0	2	2	132.81	134.81
0	2	3	60.35	59.24
0	2	4	110.76	109.13
0	2	5	126.63	127.42
0	2	6	85.08	82.51
0	2	7	24.73	23.85
0	2	8	3.71	7.75
0	2	9	80.38	78.03
0	2	10	19.54	17.78
0	2	11	54.41	55.33
0	2	12	65.29	69.46
0	2	13	26.71	28.67
0	2	14	16.82	18.71
0	2	16	12.86	13.69
0	3	1	*61.49	56.56
0	3	2	51.94	48.26
0	3	3	151.12	153.18
0	3	4	140.34	131.63
0	3	5	10.39	9.71
0	3	6	97.69	95.75
0	3	7	56.86	53.17
0	3	8	31.41	29.52
0	3	9	48.48	46.48
0	3	10	74.44	75.90
0	3	11	42.05	43.36
0	3	12	22.26	23.68
0	3	13	57.13	58.62
0	3	14	29.18	32.59
0	3	15	14.59	23.58
0	3	16	12.37	12.23
0	3	17	13.60	18.17
0	3	18	14.59	14.89
0	4	0	212.95	217.88
0	4	1	87.06	84.48
0	4	2	85.08	81.37
0	4	3	82.36	76.62
0	4	4	63.81	62.31
0	4	5	24.49	25.37
0	4	6	63.07	61.09
0	4	7	85.08	87.05
0	4	8	27.45	30.46
0	4	9	47.24	46.27
0	4	10	68.51	68.57
0	4	11	17.56	19.79
0	4	12	32.40	32.03
0	4	13	19.54	20.12
0	4	14	27.21	30.07
0	4	15	11.13	9.12
0	4	16	20.53	23.18
0	4	17	24.73	29.30
0	5	1	113.77	113.62
0	5	2	144.19	140.15
0	5	3	44.02	42.55
0	5	4	13.11	16.61
0	5	5	66.53	64.02
0	5	6	73.46	70.72
0	5	7	28.94	29.95
0	5	8	102.89	102.93
0	5	9	71.97	72.18
0	5	11	14.84	12.12
0	5	12	15.83	15.94
0	5	14	29.43	31.93
0	5	15	36.36	38.36
0	5	16	30.92	32.98
0	5	18	8.90	9.54
0	6	0	127.13	124.16
0	6	1	52.43	51.11
0	6	2	50.45	51.17
0	6	3	66.28	59.46
0	6	4	41.55	42.88
0	6	5	69.50	68.68
0	6	6	76.92	73.74
0	6	7	87.55	84.82
0	6	8	26.22	24.93
0	6	9	37.13	37.97
0	6	10	50.95	49.03
0	6	11	36.36	37.08
0	6	12	43.78	45.04
0	6	13	24.24	23.89
0	6	14	22.26	23.27
0	6	15	18.55	21.03
0	6	16	18.80	21.44
0	6	17	23.50	27.09
0	6	18	12.37	13.80
0	7	1	40.31	37.76
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1	10	13	22.76	20.05
1	10	14	10.88	10.74
1	10	15	27.21	25.09
1	10	16	13.36	10.19
1	11	-15	21.52	20.30
1	11	-14	20.78	18.74
1	11	-12	30.67	31.92
1	11	-11	19.79	16.66
1	11	-10	26.71	27.95
1	11	-9	20.03	21.07
1	11	-8	31.66	28.83
1	11	-7	43.53	44.35
1	11	-6	35.61	37.78
1	11	-5	59.11	59.14
1	11	-4	33.88	34.08
1	11	-3	47.73	47.77
1	11	-2	20.53	20.97
1	11	-1	46.90	47.03
1	11	0	36.36	37.36
1	11	1	36.60	38.26
1	11	2	48.48	49.50
1	11	3	40.81	41.08
1	11	4	51.69	52.22
1	11	5	40.07	39.68
1	11	6	28.94	27.51
1	11	7	25.72	28.43
1	11	8	27.70	28.59
1	11	9	43.78	44.81
1	11	11	26.22	25.49
1	11	12	24.24	24.59
1	11	13	27.45	26.08
1	11	14	26.46	27.40
1	11	15	13.85	12.86
1	11	16	20.28	19.66
1	12	-15	12.37	7.85
1	12	-14	22.26	21.00
1	12	-13	29.48	30.01
1	12	-12	17.31	18.34
1	12	-11	25.47	25.41
1	12	-10	11.13	10.24
1	12	-8	15.35	14.58
1	12	-7	39.57	39.66
1	12	-6	41.06	42.67
1	12	-5	13.36	14.92
1	12	-4	36.60	37.53
1	12	-3	26.71	28.27
1	12	-2	11.38	11.49
1	12	0	52.93	53.55
1	12	1	56.39	57.83
1	12	2	22.26	22.08
1	12	3	63.81	62.72
1	12	4	32.15	31.91
1	12	5	24.24	25.80
1	12	6	17.81	15.98
1	12	7	32.65	32.23
1	12	8	29.68	30.80
1	12	9	10.86	8.74
1	12	10	41.59	43.13
1	12	11	18.05	19.69
1	13	-14	14.54	15.94
1	13	-12	18.30	19.53
1	13	-10	34.87	38.65
1	13	-9	16.57	13.54
1	13	-8	37.84	41.71
1	13	-7	31.90	32.52
1	13	-6	39.34	39.27
1	13	-5	51.44	54.41
1	13	-4	25.23	25.88
1	13	-3	38.98	41.07
1	13	-2	15.43	16.92
1	13	-1	24.98	25.94
1	13	0	33.67	32.49
1	13	1	41.30	44.15
1	13	2	58.56	60.15
1	13	3	23.50	23.38
1	13	4	48.23	48.63
1	13	5	14.59	13.84
1	13	6	18.55	18.33
1	13	7	34.63	34.43
1	13	8	17.56	22.32
1	13	9	36.34	36.56
1	13	10	14.54	14.73
1	13	11	22.01	22.14
1	13	12	15.29	13.73
1	13	13	11.38	9.93
1	13	14	16.57	14.00
1	14	-14	16.98	16.66
1	14	-12	21.92	21.91
1	14	-11	25.23	24.36
1	14	-10	3.71	3.23
1	14	-9	27.21	25.18
1	14	-8	22.51	24.21
1	14	-6	28.94	30.46
1	14	-5	19.29	23.03
1	14	-4	38.83	38.93
1	14	-3	18.30	20.89
1	14	-2	49.71	50.52
1	14	-1	47.96	50.11
1	14	0	11.13	13.04
1	14	1	31.41	32.93
1	14	2	31.90	31.31
1	14	3	44.92	45.37
1	14	4	30.42	31.87
1	14	5	29.93	31.90
1	14	6	34.63	36.76
1	14	7	15.33	12.86
1	14	8	25.97	27.05
1	14	9	14.34	14.26
1	14	10	16.57	16.11
1	14	11	17.07	13.26
1	14	12	22.01	22.58
1	14	14	16.57	12.29
1	15	-13	4.20	3.47
1	15	-10	24.98	27.50
1	15	-9	23.50	22.44
1	15	-8	18.05	15.15
1	15	-7	30.17	32.15
1	15	-6	3.46	3.50
1	15	-5	25.97	26.38
1	15	-4	15.09	15.49
1	15	-3	34.38	35.71
1	15	-2	13.60	14.82
1	15	-1	43.53	43.05
1	15	0	24.73	23.32
1	15	2	43.03	42.27
1	15	3	28.94	30.99
1	15	4	34.38	37.03
1	15	5	12.37	12.33
1	15	6	17.31	20.61
1	15	7	35.67	33.07
1	15	8	3.71	3.00
1	15	9	19.79	22.66
1	15	11	19.04	17.13
1	16	-12	13.36	12.92
1	16	-11	26.46	24.60
1	16	-9	18.05	16.80
1	16	-8	11.47	14.15
1	16	-7	23.25	22.37
1	16	-6	26.46	28.07
1	16	-5	12.86	13.73
1	16	-4	19.54	17.63
1	16	-3	23.50	24.91
1	16	-2	25.23	28.34
1	16	-1	26.22	29.99
1	16	1	31.41	29.72
1	16	3	35.41	37.29
1	16	5	20.53	21.25
1	16	6	20.53	19.63
1	16	9	21.27	20.74
1	16	10	24.73	25.56
1	16	11	19.54	17.58
1	16	12	12.37	10.99
1	17	-8	19.54	17.75
1	17	-7	27.70	27.02
1	17	-6	20.28	21.34
1	17	-5	31.90	30.90
1	17	-3	17.81	17.41
1	17	-1	28.94	28.16
1	17	0	18.05	18.92
1	17	1	20.28	20.30
1	17	2	36.95	37.14
1	17	4	32.40	32.69
1	17	5	19.79	17.73
1	17	7	13.36	13.11
1	17	8	18.05	16.30
1	17	9	18.55	19.90
1	17	11	12.56	14.65
1	18	-9	14.59	16.42
1	18	-6	25.72	24.68
1	18	-4	27.95	30.58
1	18	-2	18.55	21.76
1	18	-1	25.23	26.87
1	18	0	16.08	16.32
1	18	1	18.50	17.81
1	18	3	22.51	25.39
1	18	4	19.54	17.25
1	18	6	24.24	25.39
1	18	7	13.85	13.52
1	18	9	15.33	11.08
1	18	10	15.58	14.17
1	19	-8	11.38	9.08
1	19	-6	10.63	7.28
1	19	-5	13.11	13.76
1	19	-3	25.47	26.55
1	19	-2	14.34	15.02
1	19	-1	12.86	13.86
1	19	0	18.30	19.94
1	19	2	13.36	15.83
1	19	4	17.31	18.09
1	19	5	11.13	8.73
1	19	6	13.60	16.53
1	19	7	21.27	20.24
1	20	-6	17.56	15.49
1	20	-2	17.07	17.95
1	20	-1	11.62	15.33
1	20	1	21.76	20.54
1	20	3	12.37	13.59
1	20	5	21.02	20.68
1	20	7	12.61	10.77
1	21	-5	20.33	17.47
1	21	-4	12.61	9.02
1	21	-3	17.31	21.13
1	21	-2	11.13	8.02
1	21	-1	17.56	13.73
1	21	0	20.53	21.24
1	21	2	18.05	20.95
1	21	5	18.80	17.24
1	21	6	14.34	11.74
2	0	-17	3.96	3.38
2	0	-14	11.38	8.15
2	0	-13	62.57	64.01
2	0	-12	31.41	31.52
2	0	-11	2.97	5.56
2	0	-10	75.43	75.21
2	0	-9	9.89	9.11
2	0	-8	41.30	43.05
2	0	-7	35.37	32.71
2	0	-6	72.96	77.17
2	0	-5	24.73	26.13
2	0	-4	49.96	50.38
2	0	-3	148.40	156.32
2	0	-2	26.71	27.39
2	0	-1	37.59	35.23
2	0	0	27.95	23.40
2	0	1	23.00	21.21
2	0	2	9.40	10.61
2	0	3	74.20	84.83
2	0	4	117.23	120.85
2	0	5	49.98	53.64
2	0	6	25.97	32.98
2	0	8	2.72	0.03
2	0	9	11.13	10.43
2	0	10	45.26	44.81
2	0	11	42.79	41.28
2	0	12	11.13	9.24
2	0	13	37.54	36.41
2	0	14	26.71	26.74
2	0	17	13.36	15.25
2	1	-17	14.84	13.54
2	1	-16	19.54	21.36
2	1	-15	13.85	10.19
2	1	-14	34.87	35.52
2	1	-13	10.39	13.43
2	1	-12	35.61	33.79
2	1	-11	47.73	45.10
2	1	-10	33.39	32.91
2	1	-9	29.18	30.17
2	1	-7	53.67	54.86
2	1	-6	81.86	79.38
2	1	-5	37.84	39.92

Table 3 (*cont.*)

H	K	L	FOBS	FCALC
2	1	-4	106.10	108.39
2	1	-3	46.50	45.91
2	1	-2	59.36	59.93
2	1	-1	44.02	49.86
2	1	0	50.70	51.26
2	1	1	68.51	67.18
2	1	2	91.26	84.24
2	1	3	66.78	75.48
2	1	4	41.30	40.80
2	1	5	94.73	95.36
2	1	6	38.58	38.27
2	1	7	58.37	58.61
2	1	8	26.71	26.06
2	1	9	31.16	30.24
2	1	10	33.39	33.08
2	1	11	28.44	28.01
2	1	12	38.34	37.61
2	1	13	44.27	41.07
2	1	14	21.52	23.57
2	1	16	10.14	8.38
2	2	-17	25.72	23.38
2	2	-15	38.34	38.75
2	2	-14	23.00	27.09
2	2	-13	22.26	22.81
2	2	-12	17.07	16.53
2	2	-11	27.21	25.06
2	2	-10	23.50	25.12
2	2	-9	34.13	35.44
2	2	-8	77.66	78.22
2	2	-7	39.08	40.86
2	2	-6	21.02	20.01
2	2	-5	58.62	55.90
2	2	-4	37.35	36.46
2	2	-3	25.72	26.16
2	2	-2	41.55	46.77
2	2	-1	106.35	117.85
2	2	0	87.06	74.54
2	2	1	73.46	70.17
2	2	2	57.38	54.14
2	2	3	37.59	36.58
2	2	4	28.19	26.52
2	2	5	42.05	38.17
2	2	6	98.68	96.19
2	2	7	28.94	26.36
2	2	8	43.78	46.18
2	2	9	76.92	75.26
2	2	10	50.21	46.20
2	2	11	10.14	9.71
2	2	12	11.62	6.29
2	2	13	27.95	25.59
2	2	14	11.62	7.11
2	2	15	32.89	28.16
2	2	16	33.64	31.59
2	2	17	15.58	10.87
2	3	-17	18.55	19.90
2	3	-16	29.68	29.93
2	3	-14	27.95	29.53
2	3	-13	21.27	22.28
2	3	-12	26.71	26.71
2	3	-11	28.69	29.20
2	3	-10	38.83	38.62
2	3	-9	60.59	61.53
2	3	-8	13.11	13.09
2	3	-7	73.46	77.34
2	3	-6	69.75	71.41
2	3	-5	27.21	24.80
2	3	-4	33.39	33.85
2	3	-3	55.15	54.30
2	3	-2	64.80	66.88
2	3	-1	35.86	36.62
2	3	0	119.21	107.39
2	3	1	77.66	70.72
2	3	2	19.79	28.08
2	3	3	27.21	26.74
2	3	4	20.03	16.88
2	3	5	45.26	45.13
2	3	6	25.23	27.41
2	3	7	85.82	83.53
2	3	8	61.09	59.41
2	3	9	24.24	22.41
2	3	10	24.98	22.00
2	3	12	23.50	20.82
2	3	13	27.21	27.99
2	3	14	29.43	28.37
2	3	15	20.78	17.47
2	3	17	18.55	17.18
2	4	-17	17.56	15.12
2	4	-15	15.83	17.38
2	4	-14	14.59	14.60
2	4	-13	39.82	39.22
2	4	-12	22.75	21.63
2	4	-11	17.81	16.19
2	4	-10	46.00	47.64
2	4	-9	30.42	32.17
2	4	-8	38.58	36.44
2	4	-7	30.17	30.07
2	4	-6	80.13	78.96
2	4	-5	23.25	26.28
2	4	-4	78.90	76.22
2	4	-3	94.97	92.02
2	4	-2	49.47	47.60
2	4	-1	56.39	52.77
2	4	0	54.66	50.20
2	4	1	24.73	28.57
2	4	2	42.54	46.07
2	4	3	107.34	102.20
2	4	4	108.08	105.63
2	4	5	48.97	48.48
2	4	6	27.70	24.64
2	4	7	26.46	28.86
2	4	8	27.95	28.56
2	4	9	29.93	29.83
2	4	10	43.03	44.20
2	4	11	49.22	47.09
2	4	13	27.21	26.85
2	4	14	23.50	23.19
2	4	15	24.49	21.72
2	4	16	20.28	18.29
2	4	17	14.59	11.80
2	5	-14	35.37	34.65
2	5	-12	43.53	43.85
2	5	-11	63.56	63.43
2	5	-10	9.89	10.37
2	5	-8	20.03	22.31
2	5	-7	35.61	35.36
2	5	-6	22.51	21.44
2	5	-5	77.91	78.92
2	5	-4	109.81	109.43
2	5	-3	17.31	14.98
2	5	-2	76.42	75.70
2	5	-1	44.52	45.20
2	5	0	16.32	15.37
2	5	1	17.31	18.19
2	5	2	82.33	83.26
2	5	3	93.24	87.32
2	5	4	20.53	19.34
2	5	5	55.90	56.29
2	5	6	50.45	49.29
2	5	7	10.39	5.02
2	5	8	20.03	18.53
2	5	9	34.87	32.40
2	5	10	15.09	13.01
2	5	11	29.68	27.28
2	5	12	41.06	39.32
2	5	13	39.08	33.89
2	6	-15	21.27	25.54
2	6	-14	17.07	15.96
2	6	-13	32.65	28.63
2	6	-12	33.14	30.54
2	6	-11	26.96	27.68
2	6	-10	26.46	27.87
2	6	-9	37.59	37.07
2	6	-8	37.59	37.03
2	6	-7	42.05	42.31
2	6	-6	39.57	40.08
2	6	-5	32.65	31.49
2	6	-4	47.49	45.73
2	6	-3	60.10	59.44
2	6	-2	36.60	33.11
2	6	-1	78.90	77.88
2	6	0	34.87	33.21
2	6	1	27.95	28.61
2	6	2	87.80	82.90
2	6	3	53.17	51.91
2	6	4	72.71	71.15
2	6	5	29.18	27.48
2	6	6	47.49	46.92
2	6	7	25.23	24.30
2	6	8	28.19	26.67
2	6	9	46.90	45.47
2	6	10	40.07	37.47
2	6	11	30.92	28.79
2	6	12	22.51	22.38
2	6	13	25.47	23.48
2	6	14	21.52	17.59
2	6	15	15.09	15.04
2	6	16	17.07	18.49
2	7	-16	25.97	24.66
2	7	-15	12.61	11.81
2	7	-14	22.01	23.16
2	7	-13	20.03	22.60
2	7	-11	12.37	13.38
2	7	-10	49.96	50.77
2	7	-9	32.59	35.93
2	7	-8	26.71	28.08
2	7	-7	62.08	61.78
2	7	-6	57.63	56.91
2	7	-5	35.86	33.34
2	7	-4	35.86	35.65
2	7	-3	60.35	60.86
2	7	-2	61.56	61.26
2	7	-1	31.41	32.19
2	7	0	56.64	56.94
2	7	1	84.34	79.93
2	7	3	28.19	28.34
2	7	5	32.89	30.16
2	7	6	46.29	45.43
2	7	7	70.98	70.42
2	7	8	60.84	58.91
2	7	9	26.96	23.30
2	7	10	29.43	27.12
2	7	11	27.45	26.91
2	7	13	16.57	15.63
2	7	14	36.60	32.39
2	7	15	18.55	17.40
2	7	16	11.62	8.62
2	8	-15	26.46	27.56
2	8	-14	19.29	16.92
2	8	-12	22.01	21.75
2	8	-11	23.74	24.09
2	8	-10	27.95	28.48
2	8	-9	30.92	30.84
2	8	-8	49.22	47.98
2	8	-7	46.99	45.67
2	8	-6	48.48	47.54
2	8	-5	42.79	41.11
2	8	-4	29.93	30.03
2	8	-3	35.61	34.16
2	8	-2	39.82	41.24
2	8	-1	72.47	72.52
2	8	0	42.05	40.28
2	8	1	43.93	40.09
2	8	2	76.18	70.65
2	8	3	24.73	23.21
2	8	4	39.57	39.57
2	8	5	46.00	44.64
2	8	6	50.21	48.75
2	8	7	23.25	21.49
2	8	8	39.08	38.13
2	8	9	30.92	29.23
2	8	10	26.46	26.13
2	8	11	20.03	20.87
2	8	13	19.54	17.62
2	8	15	24.98	23.49
2	8	16	18.05	15.71
2	9	-16	15.09	12.91
2	9	-14	30.92	29.41
2	9	-13	3.71	6.29
2	9	-12	36.11	35.52
2	9	-11	46.50	48.74
2	9	-10	14.34	17.38
2	9	-9	13.85	15.50
2	9	-8	22.51	21.97
2	9	-7	19.04	17.86
2	9	-6	21.52	23.11
2	9	-5	59.36	60.95
2	9	-4	60.35	59.59
2	9	-2	60.35	58.65
2	9	-1	30.42	28.98
2	9	0	24.49	26.14
2	9	1	35.12	33.23
2	9	2	38.58	38.69
2	9	3	55.90	54.03
2	9	4	21.76	21.10
2	9	5	46.00	46.52
2	9	6	49.96	45.24
2	9	7	32.15	29.89
2	9	8	16.32	18.48
2	9	9	13.85	12.76
2	9	10	10.14	9.36
2	9	11	14.84	13.92
2	9	12	33.14	32.18
2	9	13	22.75	23.87
2	9	14	12.12	10.26
2	10	-13	27.21	25.86
2	10	-12	21.52	20.76
2	10	-11	18.55	19.04
2	10	-10	37.59	32.84
2	10	-9	12.61	11.49
2	10	-8	13.85	16.88
2	10	-6	56.88	55.02
2	10	-5	33.88	34.13
2	10	-4	48.97	47.96
2	10	-3	61.58	62.24
2	10	-2	44.02	41.66
2	10	-1	31.41	30.06
2	10	1	39.92	38.46
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3	14	-10	11.87	12.38
3	14	-7	32.65	33.49
3	14	-5	27.45	24.44
3	14	-4	17.31	14.21
3	14	0	23.25	22.82
3	14	3	20.03	23.26
3	14	4	10.63	11.51
3	14	7	16.82	17.35
3	14	8	13.11	13.13
3	14	9	20.53	20.65
3	15	-9	13.85	10.92
3	15	-8	14.34	10.91
3	15	-7	18.05	15.55
3	15	-6	24.24	23.36
3	15	-5	11.13	7.31
3	15	-4	17.31	17.44
3	15	-1	23.00	21.82
3	15	0	23.00	23.16
3	15	3	14.59	15.39
3	15	4	23.74	25.22
3	15	6	14.84	12.82
3	15	7	13.11	10.32
3	15	8	24.24	24.63
3	16	-5	23.74	19.64
3	16	-4	17.31	16.91
3	16	-1	3.71	1.59
3	16	0	14.10	16.11
3	16	4	14.34	13.00
3	16	5	12.12	13.50
3	16	6	10.63	6.36
3	17	-6	12.12	9.87
3	17	-4	23.00	21.23
3	17	-1	21.02	21.75
3	17	0	10.88	7.92
3	17	3	16.32	14.39
3	17	5	14.10	17.14
3	17	6	11.87	16.15
3	17	7	13.60	8.24
3	18	-1	10.88	8.54
3	18	3	12.86	11.18
3	18	5	14.84	10.26
3	19	-1	14.84	14.90
4	0	-13	18.30	14.60
4	0	-12	5.69	1.15
4	0	-11	14.34	11.86
4	0	-10	13.60	9.12
4	0	-9	37.10	35.42
4	0	-8	13.11	13.94
4	0	-7	23.25	20.49
4	0	-6	33.14	31.49
4	0	-5	14.59	16.22
4	0	-4	1.98	6.26
4	0	-3	15.33	11.33
4	0	-2	29.18	25.51
4	0	-1	2.47	6.12
4	0	0	41.55	32.54
4	0	2	2.23	0.61
4	0	3	2.47	3.42
4	0	4	15.58	15.72
4	0	5	19.04	22.21
4	0	7	34.87	38.19
4	0	8	26.96	22.77
4	0	9	14.10	12.88
4	0	10	11.87	13.37
4	1	-13	14.59	11.78
4	1	-12	19.29	18.90
4	1	-11	8.41	7.95
4	1	-10	23.00	23.65
4	1	-9	15.83	13.38
4	1	-8	42.29	39.93
4	1	-7	19.79	20.16
4	1	-6	12.86	14.12
4	1	-5	26.96	30.69
4	1	-4	9.15	9.74
4	1	-3	37.59	32.54
4	1	-2	23.00	19.07
4	1	2	39.32	40.75
4	1	3	17.56	16.81
4	1	4	16.57	19.95
4	1	5	9.65	11.20
4	1	6	14.34	15.75
4	1	7	20.28	20.02
4	1	8	14.10	6.91
4	1	9	21.76	22.89
4	1	10	11.87	16.65
4	1	11	16.32	21.70
4	1	13	5.44	6.37
4	2	-13	17.07	13.95
4	2	-12	15.09	12.96
4	2	-11	31.41	26.22
4	2	-10	22.01	18.36
4	2	-9	19.79	17.78
4	2	-8	8.41	9.27
4	2	-7	22.51	22.50
4	2	-6	9.89	10.57
4	2	-5	25.47	27.02
4	2	-4	44.77	49.56
4	2	-3	15.83	18.32

Table 3 (*cont.*)

H	K	L	FOBS	FCALC
4	2	-2	24.98	22.85
4	2	-1	17.81	16.23
4	2	0	10.43	6.97
4	2	1	7.67	11.13
4	2	2	22.76	23.74
4	2	3	58.86	51.16
4	2	4	14.10	13.24
4	2	5	20.18	27.26
4	2	6	29.58	27.63
4	2	7	17.31	17.80
4	2	8	11.13	11.33
4	2	9	18.05	15.92
4	2	10	16.78	21.64
4	2	12	16.32	19.49
4	2	13	9.89	15.02
4	3	-13	19.29	14.37
4	3	-12	33.42	25.52
4	3	-11	6.18	4.40
4	3	-10	26.40	25.43
4	3	-9	13.40	11.18
4	3	-8	21.52	21.23
4	3	-7	11.38	8.17
4	3	-6	19.29	18.32
4	3	-5	31.10	32.78
4	3	-4	7.91	8.51
4	3	-3	34.63	41.19
4	3	-2	27.21	33.13
4	3	-1	21.52	19.17
4	3	1	19.79	22.14
4	3	2	18.55	15.79
4	3	3	17.07	16.52
4	3	4	30.36	34.83
4	3	5	21.52	20.18
4	3	6	16.92	17.69
4	3	7	18.30	20.31
4	3	8	6.18	5.61
4	3	9	9.43	11.95
4	3	10	13.88	14.67
4	3	11	19.54	24.61
4	3	12	8.41	11.31
4	4	-13	13.85	8.67
4	4	-12	13.14	7.14
4	4	-11	21.76	18.95
4	4	-10	16.32	14.07
4	4	-9	28.34	27.96
4	4	-8	20.33	18.81
4	4	-7	18.35	17.16
4	4	-6	24.98	23.56
4	4	-5	14.13	19.01
4	4	-4	15.09	18.33
4	4	-3	19.34	23.31
4	4	-2	22.51	26.14
4	4	-1	15.09	17.31
4	4	0	25.07	27.43
4	4	1	48.07	44.73
4	4	2	20.73	18.47
4	4	3	24.73	23.10
4	4	4	13.60	15.49
4	4	5	22.75	22.24
4	4	6	8.66	7.07
4	4	7	22.75	23.66
4	4	8	20.78	21.64
4	4	9	11.62	12.38
4	4	10	12.96	11.11
4	4	12	8.16	9.95
4	5	-12	19.33	18.16
4	5	-10	24.98	22.11
4	5	-9	6.18	4.64
4	5	-8	35.61	36.55
4	5	-7	34.87	35.35
4	5	-5	21.27	24.50
4	5	-4	2.23	3.14
4	5	-3	17.37	18.96
4	5	-2	9.49	14.13
4	5	-1	48.23	46.80
4	5	0	29.68	29.74
4	5	1	10.88	8.93
4	5	2	31.41	26.27
4	5	3	7.91	9.42
4	5	6	24.49	24.46
4	5	7	23.90	22.98
4	5	8	13.36	14.46
4	5	9	25.23	26.98
4	5	10	11.38	13.02
4	6	-12	6.68	3.71
4	6	-11	18.80	16.81
4	6	-10	11.62	10.33
4	6	-9	28.19	27.93
4	6	-8	12.37	12.15
4	6	-7	19.79	19.49
4	6	-6	25.23	28.47
4	6	-5	17.97	16.48
4	6	-4	25.47	22.41
4	6	-3	13.36	13.58
4	6	-1	21.52	22.56
4	6	0	27.70	27.84
4	6	1	29.68	27.43
4	6	2	13.60	15.13
4	6	3	32.89	27.61
4	6	4	10.63	10.39
4	6	5	7.42	8.55
4	6	6	20.53	19.75
4	6	7	21.76	23.11
4	6	9	8.16	10.53
4	6	10	8.16	13.16
4	6	12	6.43	13.00
4	7	-12	16.57	16.95
4	7	-11	7.17	4.75
4	7	-10	20.53	17.48
4	7	-9	11.87	13.90
4	7	-8	6.68	8.15
4	7	-6	26.22	29.24
4	7	-5	29.68	33.84
4	7	-4	14.34	16.06
4	7	-3	16.32	16.26
4	7	-2	43.93	42.72
4	7	-1	15.09	16.71
4	7	0	10.63	7.15
4	7	1	26.71	23.96
4	7	2	26.48	23.42
4	7	3	16.82	15.68
4	7	4	40.31	36.97
4	7	5	18.55	18.14
4	7	7	11.13	12.44
4	7	10	8.66	13.91
4	7	11	15.83	21.64
4	8	-12	8.66	9.07
4	8	-11	25.72	22.68
4	8	-10	12.61	11.43
4	8	-9	22.75	21.57
4	8	-8	14.59	11.17
4	8	-7	9.59	13.48
4	8	-6	20.03	18.47
4	8	-5	27.95	27.06
4	8	-4	20.78	21.20
4	8	-3	15.58	17.27
4	8	-2	24.73	23.36
4	8	-1	24.98	22.68
4	8	0	28.94	25.63
4	8	1	13.85	12.10
4	8	2	21.52	18.99
4	8	3	28.19	27.40
4	8	5	22.75	21.86
4	8	6	15.09	14.14
4	8	8	10.88	15.23
4	8	10	7.91	8.47
4	9	-11	8.16	6.87
4	9	-10	20.03	19.16
4	9	-8	21.52	25.57
4	9	-7	26.96	28.29
4	9	-5	19.79	23.41
4	9	-3	15.83	15.85
4	9	-2	18.30	13.59
4	9	-1	33.14	28.61
4	9	0	30.67	29.59
4	9	1	10.14	9.58
4	9	2	14.10	12.33
4	9	3	8.66	5.09
4	9	4	17.31	15.28
4	9	5	14.34	14.18
4	9	6	15.43	18.47
4	9	7	18.30	22.94
4	9	9	12.37	15.94
4	9	10	8.16	7.48
4	9	11	7.67	13.46
4	10	-9	23.99	23.02
4	10	-8	14.59	16.04
4	10	-7	20.78	19.33
4	10	-6	18.95	18.38
4	10	-4	15.33	10.40
4	10	-3	9.40	9.60
4	10	-2	22.51	23.32
4	10	0	30.42	27.98
4	10	1	32.89	28.44
4	10	2	12.61	12.93
4	10	3	20.28	19.48
4	10	4	5.41	9.29
4	10	7	15.83	19.30
4	10	8	11.38	20.43
4	11	-10	9.89	13.38
4	11	-9	8.41	8.21
4	11	-8	19.54	19.89
4	11	-7	13.85	12.43
4	11	-6	8.16	9.42
4	11	-5	20.78	21.99
4	11	-3	16.82	14.47
4	11	-2	20.28	18.05
4	11	-1	19.79	21.24
4	11	0	14.84	15.41
4	11	1	12.86	11.48
4	11	2	21.02	22.62
4	11	3	6.43	5.38
4	11	5	13.11	14.15
4	11	6	7.67	9.56
4	11	7	6.93	13.34
4	11	9	9.65	13.85
4	12	-9	10.88	14.29
4	12	-7	11.38	14.09
4	12	-6	16.82	18.15
4	12	-5	11.87	12.26
4	12	-4	24.24	26.97
4	12	-2	14.84	13.62
4	12	-1	13.85	12.20
4	12	0	7.67	6.96
4	12	1	11.62	8.11
4	12	2	16.82	18.08
4	12	3	15.09	22.51
4	12	5	10.39	13.62
4	12	6	9.89	12.62
4	13	-8	11.38	14.29
4	13	-6	10.39	14.84
4	13	-5	12.61	16.01
4	13	-3	20.53	22.87
4	13	-1	8.41	9.31
4	13	0	12.12	8.65
4	13	1	9.15	8.56
4	13	2	14.59	18.39
4	13	3	9.40	9.89
4	13	4	13.11	18.13
4	14	-6	9.66	12.02
4	14	-4	7.67	9.48
4	14	-2	13.85	21.07
4	14	1	15.33	19.94
4	14	5	8.41	11.42
4	15	-5	7.17	13.16
4	15	-1	12.86	15.94
4	15	2	10.39	16.45
4	16	-1	9.16	11.85
4	16	0	6.68	11.81
5	0	-10	15.33	16.03
5	0	-8	20.53	18.15
5	0	-7	15.53	16.66
5	0	-6	13.85	12.34
5	0	-4	12.86	13.62
5	0	-3	17.31	18.73
5	0	-2	9.65	7.89
5	0	0	20.53	16.95
5	0	2	15.09	10.45
5	0	5	12.86	17.27
5	0	6	16.57	20.83
5	0	7	7.91	10.50
5	1	-10	10.39	9.39
5	1	-9	19.79	15.54
5	1	-8	9.15	5.73
5	1	-7	17.31	13.72
5	1	-6	10.14	10.37
5	1	-5	21.52	20.15
5	1	-4	8.16	7.56
5	1	-3	9.15	10.92
5	1	-2	23.00	25.64
5	1	0	12.12	11.45
5	1	2	11.87	11.12
5	1	4	8.90	7.89
5	1	5	14.34	22.08
5	1	6	7.17	4.11
5	2	-10	8.90	12.41
5	2	-9	13.60	10.21
5	2	-8	16.32	15.16
5	2	-7	9.89	7.47
5	2	-6	27.45	26.63
5	2	-5	18.55	17.78
5	2	-4	9.89	5.31
5	2	-3	10.14	13.29
5	2	-2	8.90	3.39
5	2	-1	14.34	16.48
5	2	0	13.60	11.57
5	2	1	27.95	25.47
5	2	2	20.28	21.57
5	2	4	11.13	16.93
5	3	-9	13.85	12.81
5	3	-8	13.11	9.60
5	3	-7	29.43	24.84
5	3	-6	11.13	11.69
5	3	-5	19.54	16.90
5	3	-4	16.57	14.44
5	3	-2	13.11	14.90
5	3	-1	17.31	12.30
5	3	1	8.16	9.22
5	3	2	20.28	17.92
5	3	3	19.54	20.91
5	3	4	7.42	3.53
5	4	-8	13.60	12.67
5	4	-6	8.90	9.24
5	4	-5	14.84	9.39
5	4	-4	14.34	12.85
5	4	-3	20.03	19.72
5	4	-2	10.88	6.84
5	4	-1	17.31	16.22
5	4	2	14.34	12.53
5	4	3	14.84	11.60
5	4	4	13.60	15.04
5	4	6	7.91	14.47
5	4	7	7.17	11.40
5	4	8	7.17	9.06
5	5	-9	20.53	24.17
5	5	-8	8.66	7.05
5	5	-7	14.10	13.52
5	5	-5	15.83	10.12
5	5	-3	9.65	14.84
5	5	-2	24.73	23.63
5	5	-1	7.17	8.35
5	5	1	17.07	15.92
5	5	2	9.65	10.96
5	5	4	12.37	14.25
5	5	5	12.86	20.01
5	5	8	6.68	10.10
5	6	-8	12.61	15.29
5	6	-7	7.42	7.02
5	6	-6	17.07	15.35
5	6	-5	9.65	11.14
5	6	-4	14.10	13.81
5	6	-3	14.10	14.51
5	6	-2	9.15	8.63
5	6	-1	19.04	18.76
5	6	0	16.08	15.37
5	6	1	14.34	12.90
5	6	2	9.40	10.74
5	6	3	8.41	13.01
5	6	6	9.89	16.47
5	7	-7	14.59	17.04
5	7	-6	8.16	9.28
5	7	-5	18.55	16.47
5	7	-4	18.55	18.94
5	7	-2	11.97	9.67
5	7	-1	15.09	12.67
5	7	0	12.61	12.05
5	7	1	11.87	12.45
5	7	2	15.09	15.98
5	7	3	16.32	18.78
5	7	4	6.93	3.41
5	8	-6	16.82	19.11
5	8	-3	16.57	13.84
5	8	1	14.59	18.16
5	8	2	13.85	13.97
5	8	3	8.41	11.98
5	8	4	7.67	9.88
5	9	-5	7.91	9.15
5	9	-3	9.65	12.14
5	9	-2	14.84	17.24
5	9	1	15.58	18.06
5	9	2	10.88	13.32
5	9	5	9.89	16.49
5	10	-4	8.16	13.55
5	10	-3	9.89	15.22
5	10	-1	9.65	14.43
5	11	-3	5.94	9.01
5	11	-2	9.40	12.69
5	11	0	9.40	16.45
5	11	2	8.90	7.65
5	11	3	6.43	11.38

Table 4. *The bond lengths and bond angles in the two molecules*

Bond lengths	Molecule I	Molecule II
N(1)-C(2)	1·37 Å	1·39 Å
C(2) -O(2)	1·23	1·23
C(2) -N(3)	1·36	1·36
N(3)-C(4)	1·44	1·37
C(4) -O(4)	1·19	1·25
C(4) -C(5)	1·44	1·49
C(5) -I	2·02	2·04
C(5) -C(6)	1·37	1·32
C(6) -N(1)	1·38	1·37
N(1)-C(1′)	1·49	1·48
C(1′)-O(1′)	1·39	1·42
O(1′)-C(4′)	1·46	1·46
C(1′)-C(2′)	1·52	1·53
C(2′)-O(2′)	1·41	1·45
C(2′)-C(3′)	1·59	1·52
C(3′)-O(3′)	1·42	1·45
C(3′)-C(4′)	1·50	1·55
C(4′)-C(5′)	1·43	1·56
C(5′)-O(5′)	1·42	1·43

Bond angles	Molecule I	Molecule II
N(1)-C(2) -O(2)	120·9°	127·5°
C(2) -N(1)-C(6)	120·8	123·5
C(2) -N(1)-C(1′)	115·3	115·6
N(1)-C(2) -N(3)	116·9	113·7
O(2)-C(2) -N(3)	122·2	118·8
C(2) -N(3)-C(4)	126·9	126·1
N(3)-C(4) -O(4)	117·3	121·1
N(3)-C(4) -C(5)	111·9	116·7
O(4) -C(4) -C(5)	130·6	122·2
C(4) -C(5) -I	116·5	119·8
C(4) -C(5) -C(6)	120·9	116·4
I——C(5) -C(6)	122·6	124·1
C(5) -C(6) -N(1)	122·2	123·3
C(6) -N(1) -C(1′)	123·9	120·5
N(1)-C(1′)-O(1′)	108·6	108·4
N(1)-C(1′)-C(2′)	109·6	112·7
O(1′)-C(1′)-C(2′)	108·0	105·0
C(1′)-C(2′)-O(2′)	108·5	108·4
C(1′)-C(2′)-C(3′)	99·7	100·6
O(2′)-C(2′)-C(3′)	107·8	112·2
C(2′)-C(3′)-O(3′)	114·0	112·8
C(2′)-C(3′)-C(4′)	104·1	102·2
O(3′)-C(3′)-C(4′)	110·8	103·3
C(1′)-O(1′)-C(4′)	113·2	111·5
C(3′)-C(4′)-C(5′)	122·3	111·6
C(3′)-C(4′)-O(1′)	102·8	107·2
O(1′)-C(4′)-C(5′)	114·1	107·2
C(4′)-C(5′)-O(5′)	109·4	107·5

of the sugar plane as atom C(5′) and the ring of the base. In the refined molecular models of deoxyribose nucleic acid, the B-form has a C(2′) *endo* pucker of the sugar ring, while the A-form has a C(3′) *endo* pucker. In the double-stranded ribose nucleic acid molecules the pucker is also C(3′) *endo* (Arnott, Dover & Wonacott, 1969). In nucleosides and nucleotides, however, C(2′) *endo* and C(3′) *endo* puckers are observed with both ribose and deoxyribose sugars, and even the same nucleoside when in different environments can have a different type of pucker (Iball, Morgan & Wilson, 1968; Munns, Tollin, Wilson & Young, 1970).

In molecule I the sugar ring is puckered with C(3′) *endo*. The equation of the least-squares plane through the other four atoms of the sugar ring is:

$$0\cdot8997X+0\cdot2307Y+0\cdot3706Z-8\cdot1759=0$$

and the deviations of the atoms from this plane are given in Table 6. The deviation of atom C(3′) is 0·54 Å.

Table 5. *Deviation (in Å) of atoms from the least-squares plane of the pyrimidine ring*

	Molecule I	Molecule II
N(1)	−0·037	0·011
C(2)	0·029	−0·029
O(2)	0·115	−0·131
N(3)	0·011	0·016
C(4)	−0·051	0·082
C(5)	0·037	−0·034
I	0·120	−0·201
C(6)	0·002	0·022
C(1′)	−0·062	−0·121

In molecule II, however, the pucker is C(2′) *endo*, with a displacement of 0·63 Å from the least-squares plane of the other four atoms of the sugar ring. The equation of this plane is:

$$-0\cdot8996X+0\cdot1021Y+0\cdot4246Z-14139=0$$

and the deviations are also given in Table 6.

Table 6. *Deviations (in Å) of atoms from the least-squares planes of atoms* C(1′) O(1′) C(4′) C(2′) *for molecule* I *and of atoms* C(1′) O(1′) C(4′) C(3′) *for molecule* II

	Molecule I	Molecule II
C(1′)	0·031	0·035
O(1′)	−0·032	−0·055
C(2′)	−0·017	0·630
O(2′)	−1·365	0·211
C(3′)	0·540	−0·031
C(3′)	0·119	−1·460
C(4′)	0·019	0·051
C(5′)	0·586	1·451
N(1)	1·321	0·901

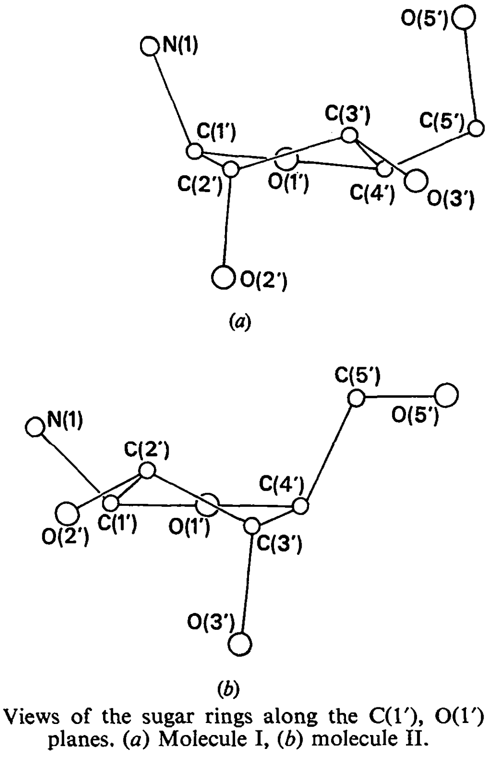
Atom O(3′) of molecule I, which is attached to the out-of-plane atom C(3′) is tipped into an equatorial-like position so that it lies 0·12 Å above the C(1′) C(2′) C(4′) O(1′) plane. Similarly, atom O(2′) of molecule II is 0·21 Å above the C(1′) C(3′) C(4′) O(1′) plane. Atom O(2′) of molecule I and atom O(3′) of molecule II lie 1·365 and 1·460 Å respectively below the corresponding planes. This arrangement must be partly due to the non-bonded O(2′)···O(3′) interactions, although similar displacements of O(3′) atoms occur in deoxyribose nucleosides and nucleotides. The displacements of atoms C(2′) and O(2′) of molecule II are larger than those of atoms C(3′) and O(3′) of molecule I. It is difficult to say whether this is related to the difference in conformation of the C(5′)–O(5′) bond about the C(4′)–C(5′) bond in the two molecules, because no other ribonucleoside has been reported with a similar conformation to molecule II. Apart from the cyclonucleotides (Coulter, 1968; Watenpaugh, Dow, Jensen & Furberg, 1968), the only nucleoside with a similar conformation about the C(4′)–C(5′) bond is 5-fluorodeoxyuridine (Harris & MacIntyre, 1964). The pucker in 5-fluorodeoxyuridine is also C(2′) *endo*, like molecule II, but the displacement of atom C(3′) is 0·022 Å and of atom O(3′) is 1.369 Å (Sundaralingam & Jensen, 1965).

With reference to the plane through atoms C(1′) O(1′) C(4′), the pucker of the sugar in molecule I is C(3′) *endo*–C(2′) *exo*, and that in molecule II is C(2′) *endo*–C(3′) *exo* (Sundaralingam, 1965). Views of the two sugar rings along the C(1′) O(1′) C(4′) plane are shown in Fig. 3. The torsion angles around the sugar rings in the two molecules are listed in Table 7, and are similar to those found in other nucleosides with similar puckering of the sugar ring (Sundaralingam, 1965).

Table 7. *Summary of the conformational parameters of the molecules, including the torsion angles around the sugar rings*

	Molecule I	Molecule II
φ_{CN}	−13·2°	−58·7°
φ_{OO}	64	172
φ_{OC}	−62	66
$\varphi_{\mathrm{O(1')-C(1')}}$	6·3	−16·9
$\varphi_{\mathrm{C(1')-C(2')}}$	−25·4	36·5
$\varphi_{\mathrm{C(2')-C(3')}}$	35·3	−41·5
$\varphi_{\mathrm{C(3')-C(4')}}$	−32·3	32·1
$\varphi_{\mathrm{C(4')-O(1')}}$	16·7	−9·6

As far as we know, this is the first time two different types of pucker have been found for the same nucleo-



(*a*)

(*b*)

Fig. 3. Views of the sugar rings along the C(1′), O(1′) C(4′) planes. (*a*) Molecule I, (*b*) molecule II.

side in the one crystal. In other cases where there is more than one molecule in the asymmetric unit, the pucker in the two molecules is the same. This is so in inosine dihydrate (Thewalt, Bugg & Marsh, 1969; Munns, Tollin, Wilson & Young, 1970), in the 3′, 5′-cyclic nucleotides of adenosine and uridine (Coulter, 1968; Watenpaugh, Dow, Jensen & Furberg, 1968), and in barium inosine-5′-phosphate (Nagashima & Iitaka, 1968). The fact that there are two different types of pucker in the one crystal is further proof that the packing forces in the crystal, and hence the environment of the molecule, determine the type of pucker in the sugar.

The bond lengths and angles in the two sugar rings are similar and agree with those found in other nucleosides and nucleotides. They are listed in Table 4. It should be noted that there is a significant difference between the lengths of the C(4′)–C(5′) bonds in the two molecules. However, the mean value is similar to that found in other nucleosides.

The conformation of the C(5′)–O(5′) bond relative to the furanose ring can be described by its rotation about the C(4′)–C(5′) bond. Shefter & Trueblood (1965) have defined the orientation in terms of the angles between the projections of the C(5′)–O(5′) bond and the C(4′)–O(1′) and C(4′)–C(3′) bonds, along the C(4′)–C(5′) bond. These angles are referred to as φ_{OO} and φ_{OC} respectively, and the values for molecules I and II are given in Table 7 and illustrated in Fig. 4. In molecule I the C(5′)–O(5′) bond is *gauche* to both C(4′)–O(1′) and to C(4′)–C(3′), so that the conformation is *gauche–gauche*. This is the conformation mostly commonly found in nucleosides and nucleotides. In molecule II, however, the C(5′)–O(5′) bond is *trans* to C(4′)–O(1′) and *gauche* to C(4′)–C(3′) so that the conformation is *trans–gauche*. The only other nucleoside which has so far been reported with a *trans–gauche* conformation is 5-fluorodeoxyuridine (Harris & MacIntyre, 1964).

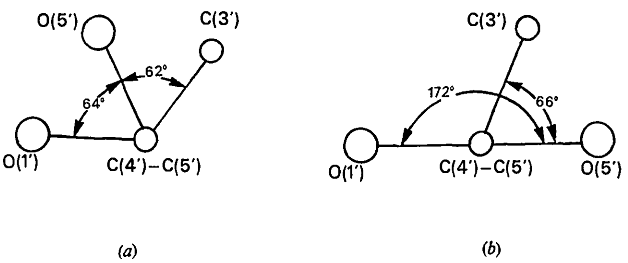


Fig. 4. The conformation of the C(4′)–C(5′) bond. (*a*) Molecule I, (*b*) molecule II.

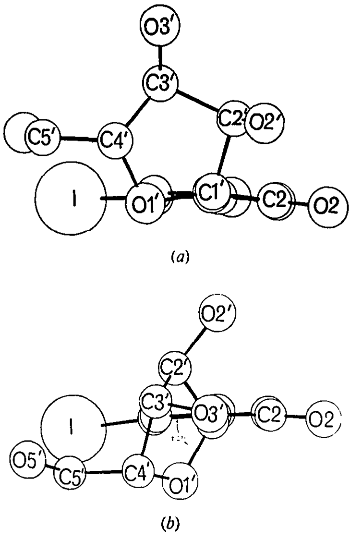


Fig. 5. Views of the molecules approximately along the glycosidic bond. (*a*) Molecule I, (*b*) molecule II.

Conformation of the molecule

The plane of the sugar ring is at a dihedral angle of 69° to the base in both molecule I and molecule II. This is similar to the values found in a number of other nucleosides (Iball, Morgan & Wilson, 1968) although it is 11° less than the corresponding angle in 5-iodo-2′-deoxyuridine (Camerman & Trotter, 1965).

The conformation of the sugar relative to the base can be specified in terms of a torsion angle, φ_{CN}, defined by Donohue & Trueblood (1960), or as defined by Haschemeyer & Rich (1967) when atom C(1′) is displaced from the plane of the base. The values of φ_{CN} for molecule I is $-13{\cdot}2°$ and for molecule II is $-58.7°$. A view of the molecules along the glycosidic bonds is shown in Fig. 5. Both molecules are in the *anti* conformation as are all other pyrimidine nucleosides and nucleotides that have so far been studied.* The values of φ_{CN} fall into the 'allowed' ranges for this angle determined by Haschemeyer & Rich (1967), and calculated on the basis of intramolecular van der Waals contacts. It should be noted that the φ_{CN} value for molecule I, which also has a C(3′) *endo* pucker of the sugar, is less than the φ_{CN} value for molecule II which has a C(2′) *endo* pucker. This is so also in the case of bromouridine and inosine molecules (Iball, Morgan & Wilson, 1968; Munns, Tollin, Wilson & Young, 1969). Arnott & Hukins (1969) have drawn attention to the fact that the mean value of the φ_{CN} angle for nucleosides and nucleotides with a C(3′) *endo* pucker is about 26° less than the mean value for φ_{CN} in nucleosides with a C(2′) *endo* pucker, and the present results are in agreement with this trend.

A summary of the conformational parameters for the two molecules is given in Table 7.

Molecular packing and hydrogen bonds

As the hydrogen atoms could not be observed in the difference Fourier synthesis, the hydrogen bonding scheme illustrated in Fig. 6 is based on interatomic distances and angles. These suggest that atom N(3) of molecule I is hydrogen bonded to atom O(4) of molecule II $(2-x, y+\frac{1}{2}, 1-z)$, since the distance between

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* An exception is thiouridine (Saenger & Scheit, 1968).

the two atoms is 2·79 Å and the angle C(2)–N(3)–O(4) is 118·4°, although atom O(4) is 1·03 Å from the plane of the pyrimidine base containing atom N(3). The distance between atom O(2′) of molecule I and O(2) of molecule II is 2·80 Å, the angle C(2′)–O(2′)–O(2) is 107°, and the displacement of atom O(2′) from the pyrimidine plane of molecule II is 0·78 Å, which suggests that a hydrogen bond between atoms O(2′) and O(2) is possible. Atom O(3′) of molecule I is 2·72 Å from atom O(5′) of molecule II $(2-x, y-\frac{1}{2}, 1-z)$ and is 2·85 Å from atom O(5′) of molecule II $(1-x, y-\frac{1}{2}, 1-z)$. The angle C(5′)–O(5′)–O(3′) involving molecule II $(2-x, y-\frac{1}{2}, 1-z)$ is 116° and the angle C(3′)–O(3′)–O(5′) is 124°. The corresponding angles involving molecule II $(1-x, y-\frac{1}{2}, 1-z)$ are 91° and 112°. Hence, if O(3′) is involved in two hydrogen bonds, the scheme with O(3′) donating to the bond to atom O(5′) of molecule II $(2-x, y-\frac{1}{2}, 1-z)$ and accepting from atom O(5′) of molecule II $(1-x, y-\frac{1}{2}, 1-z)$ is more attractive because the two C–O–O angles involved are then 116 and 112°, compared with the alternative scheme which would have angles of 124 and 91°. However, atom O(2′) is only 2·80 Å away from atom O(5′) of molecule II $(1-x, y-\frac{1}{2}, 1-z)$ and if this were a hydrogen bond atom O(5′) would be the donor because atom O(2′) is already a donor in the proposed O(2′)–O(2) hydrogen bond. The angle C(5′)–O(5′)–O(2′) is 149° which is rather large, but in the absence of direct information about the location of hydrogen atoms an unambiguous decision about the hydrogen bonds involving the O(5′) atom is not possible. Atom O(4) of molecule I is 2·88 Å from atom O(5′) of a molecule I at $(2-x, y+\frac{1}{2}, 2-z)$. The angle C(5′)–O(5′)–O(4) is 92° and the angle C(4)–O(4)–O(5′) is 159°, with atom O(5′) displaced 0·61 Å from the plane at the pyrimidine base containing the O(4) atom. An O(5′)H···O(4) hydrogen bond would thus not be in the direction of the sp^2 hybrid orbitals of the carbonyl group, although this does not eliminate the possibility of a hydrogen bond because carbonyl group hydrogen bonds are relatively insensitive to the angle between the carbonyl group and the O···O bonds (Pimentel & McClellan, 1960; Donohue, 1967).

Atom N(3) of molecule II is 2·85 Å from atom O(3′) of another molecule II at $(1-x, y-\frac{1}{2}, 1-z)$. The angle between the N(3)–H direction and the N(3)–O(3′) direction is 15°, and atom O(3′) is 0·36 Å from the pyrimidine base containing the N(3) atom, which suggests an N(3)H···O(3′) hydrogen bond. Atom O(3′) of molecule II is 2·76 Å from atom O(2) of molecule I; the angle C(3′)–O(3′)–O(2) is 128°, the angle C(2)–O(2)–O(3′) is 136°, and atom O(3′) lies 0·87 Å from the pyrimidine base containing atom O(2). This suggests an O(3′)H···O(2) hydrogen bond. The closest atom to atom O(2′) of molecule II is atom O(2) of molecule I $(1+x, y, z)$, the distance being 3·05 Å, which is rather large for an O···O hydrogen bond. The angle C(2)–O(2)–O(2′) is 91° and atom O(2′) is 0·46 Å from the plane of the pyrimidine base. Apart from this, the interatomic distances and angles are consistent with all the other hydrogen-bonding atoms taking part in the intermolecular bonding scheme.

None of the other interatomic distances in the structure is smaller than the sum of normal van der Waals

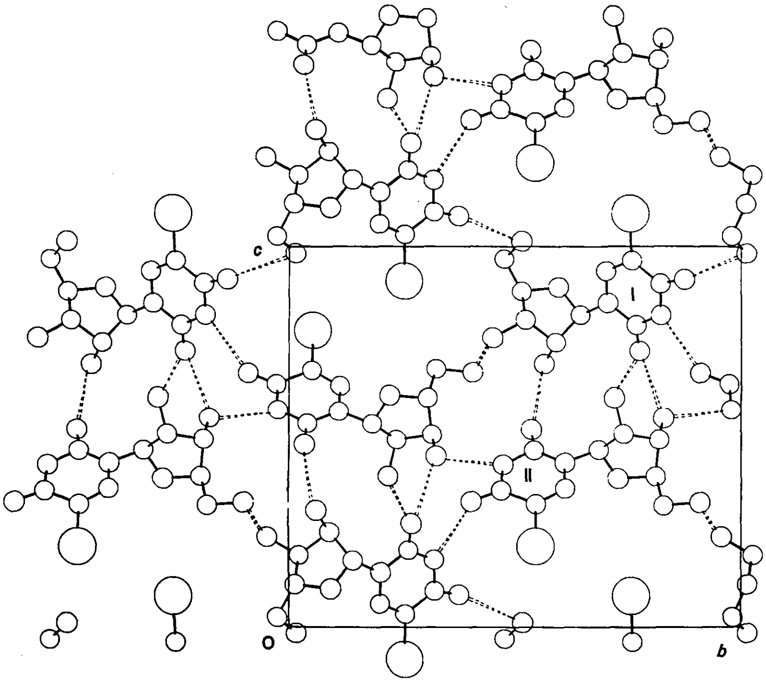

Fig. 6. A projection of the structure viewed down the *a* axis. The probable intermolecular hydrogen bonds are shown as broken lines.

radii. The separation of the iodine atoms of molecule II and molecule I (x, y, $z-1$) is 4·22 Å which means that they are in van der Waals contact, but there is no close approach to the iodine atoms comparable with that reported for 5-iodo-2′-iododeoxyuridine (Camerman & Trotter, 1965).

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The Crystal Structure and Anisotropic Thermal Expansion of β-Uranyl Dihydroxide, $UO_2(OH)_2$

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Single-crystal and powder X-ray diffraction techniques were used to determine improved positional, thermal vibration and lattice parameters for the orthorhombic β-$UO_2(OH)_2$. Values obtained for lattice parameters at 21 °C are: $a=5{\cdot}6438\pm0{\cdot}0001$, $b=6{\cdot}2867\pm0{\cdot}0001$, $c=9{\cdot}9372\pm0{\cdot}0002$ Å. Thermal expansion of this material was studied by elevated temperature X-ray diffraction and hot-stage optical microscopy. Thermal expansion up to 260 °C was strongly anisotropic, with large contractions in a, large expansions in b, and a smaller cyclic change in c. Expansion at higher temperatures was almost isotropic. Using the structural and vibrational data, the anisotropic thermal expansion is interpreted in terms of a thermally induced rotation of the oxygen octahedra surrounding all uranium atoms.

Introduction

Single crystals of β-$UO_2(OH)_2$ change in shape during heating to dehydration temperatures. This distortion can be explained if each lattice parameter is measured as a function of temperature. However, interpretation of the thermal expansion results using the crystal structure data of Roof, Cromer & Larson (1964) (hereafter referred to as RCL) is not possible owing to the large standard deviations in the RCL positional and thermal vibration parameters. The structure was therefore redetermined, giving positional and thermal vibration par-