solution/solid-state reactivity difference is due to the difference between the range of allowable motions in solution and the solid state.

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Neutron Diffraction Refinement of Partially Deuterated β-L-Arabinopyranose and α-L-Xylopyranose at 123 K*

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Abstract

Refinement of the hydrogen–deuterium neutron scattering parameters for partially deuterated β-L-arabinopyranose and α-L-xylopyranose at 123 K showed no evidence of preferential substitution, despite the presence of anomeric hydroxyls and a large difference in some hydrogen-bond lengths. Comparison with the results of room-temperature studies of the undeuterated crystals showed that the marked difference in the thermal contraction in the two structures was due primarily to a weak hydrogen bond in the β-L-arabinopyranose structure.

Introduction

The experiment described herein was carried out to explore the use of partial deuterium exchange in hydroxyl groups as a probe of differences in hydrogen

bonding and electronic structure in carbohydrate molecules. If equilibrium is reached in a carbohydrate crystal grown in a deuterium–water mixture, it is anticipated that the deuteron will have a preference for the hydroxyl bonds with the greatest force constants (Coppens, 1970). Hydroxyl-bond force constants in carbohydrates may differ for two reasons; because of differences in molecular electronic structure, due to the anomeric effect, for example (cf. Jeffrey, 1979), and because of differences in hydrogen bonding due to the crystal structure. It is debatable, however, to what degree we would expect hydrogen bonding in the crystal to influence the exchange since this process presumably takes place in solution prior to crystallization. If any effects are observed, the deuterons are expected to have a greater population in those hydroxyls which form the weaker hydrogen bonds.

The two carbohydrate crystals studied were β-L-arabinopyranose, (I), and α-L-xylopyranose, (II).
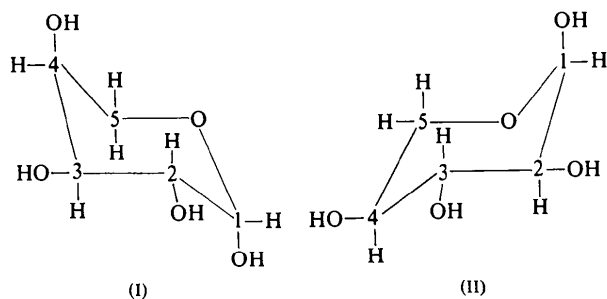
The H/D ratio was 1:4, and the neutron diffraction data were measured at 123 ± 1 K. Neutron diffraction refinements of the undeuterated crystals at room temperature, 298 K, had previously been carried out by Takagi & Jeffrey (1977, 1979).

Experimental

The crystals of (I) and (II) were grown by very slow evaporation from a 1:4 $H_2O:D_2O$ solution. The unit-cell constants and three-dimensional neutron diffraction data were obtained at 123 ± 1 K using a closed-cycle helium refrigerator, DISPLEX®, Model CS-202 (Air Products and Chemicals, Inc.) on a Brookhaven High-Flux Reactor diffractometer. The procedures used for data collection were the same as those used for the room-temperature studies (Takagi & Jeffrey, 1977, 1979). The crystal data and experimental details relevant to this particular experiment are given in Table 1.

The atomic coordinates from the room-temperature neutron diffraction structure determination of the undeuterated crystals were used as starting parameters for full-matrix least-squares refinement (Busing, Martin & Levy, 1962). In the final refinement cycles, aniso-

Table 1. *Crystal data and neutron diffraction experimental data for β-L-arabinopyranose, (I), and α-L-xylopyranose, (II), at 123 K*

	(I)	(II)
Crystal data	$C_5H_{10}O_5$	
Space group	$P2_12_12_1$	
a (Å)	6·432 (2)	9·180 (4)
b (Å)	19·480 (7)	12·572 (5)
c (Å)	4·778 (2)	5·606 (2)
V (Å³)	598·66	646·99
D_{neut} (Mg m⁻³)	1·663	1·540
λ_{neut} (Å)	1·1590 (Ge, 220)	1·1597 (Ge, 220)
Experimental data		
Crystal volume (mm³)	4·3551	2·9625
Number of reflections measured	2236	2016
unique	1863	1051
Data-collection mode		
θ–2θ step scan;		
$\Delta 2\theta$ (°) for $2\theta \le 60°$	3·0	3·0
$\Delta 2\theta$ (°) for $2\theta > 60° \le 105°$	1·5 + 3·75 tan θ	1·2 + 2·97 tan θ
Absorption corrections (Templeton & Templeton, 1973)		
μ_{neut} (mm⁻¹)	0·1806	0·1872
Corrections to F_o^2: maximum	1·379	1·301
minimum	1·216	1·173
average	1·270	1·216
Anisotropic extinction parameters (× 10⁴)		
Type 1, Lorentzian distribution (Thornley & Nelmes, 1974)		
g_{11}	9·2 (9)	21 (5)
g_{22}	4·8 (4)	113 (14)
g_{33}	5·3 (2)	8 (1)
g_{12}	−0·9 (6)	−11 (5)
g_{13}	−2·0 (6)	9 (2)
g_{23}	1·3 (4)	1 (3)
Final refinement cycle		
$\sum w|F_o^2 - k^2F_c^2|^2$, $w^{-1} = \sigma_c^2(F_o^2) + (0·01\ F_o^2)^2$,		
(where σ_c is from counting statistics)		
R_{F^2}	0·024	0·032
wR_{F^2}	0·031	0·042
S	1·376	1·877

tropic extinction parameters (Becker & Coppens, 1975) and the scattering lengths of the partially deuterated atoms were varied.

The final parameters are given in Tables 2 and 3.* The atomic notation is standard for pentapyranose molecules and is the same as that used in the room-temperature studies. The results of rigid-body thermal analyses by the method of Schomaker & Trueblood (1968) have been deposited.* The r.m.s. $|\Delta U_{ij}|$'s were 0·0005 Å for (I), and 0·0010 Å for (II) for a rigid body which included all non-hydrogen atoms. This is a better fit by a factor of 3 for (I) and of 2 for (II) over the room-temperature results.

The analysis of (II) was inferior to that of (I), as shown by the larger values of R_{F^2}, wR_{F^2} and S in Table

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Table 2. *Fractional coordinates* ($\times 10^5$) *for* β-L-*arabinopyranose*, (I) *and* α-L-*xylopyranose*, (II)

	(I)				(II)		
	x	y	z		x	y	z
C(1)	74227 (9)	41846 (3)	18256 (13)		57066 (8)	48647 (6)	44377 (15)
C(2)	67767 (9)	34815 (3)	29288 (12)		64325 (8)	39837 (5)	29896 (14)
C(3)	49515 (9)	32099 (3)	12272 (12)		55031 (8)	29791 (5)	29313 (15)
C(4)	31678 (10)	37284 (3)	12907 (13)		39948 (8)	32726 (5)	20132 (15)
C(5)	39593 (10)	44203 (3)	3111 (13)		33581 (8)	41779 (6)	35015 (15)
O(1)	81593 (11)	40981 (3)	−9005 (15)		56203 (11)	45713 (7)	68261 (18)
O(2)	85362 (11)	30394 (3)	27740 (14)		78687 (10)	37998 (7)	38100 (18)
O(3)	43238 (12)	25621 (3)	23054 (15)		62066 (10)	22450 (7)	13936 (19)
O(4)	23560 (12)	37922 (4)	40489 (16)		30783 (10)	23655 (7)	21653 (17)
O(5)	57055 (10)	46420 (3)	19536 (15)		43061 (10)	50862 (6)	34557 (18)
H(C1)	86096 (20)	44136 (6)	31899 (29)		63258 (19)	56083 (12)	42146 (34)
H(C2)	62964 (21)	35483 (6)	51228 (26)		65260 (20)	42736 (13)	11494 (30)
H(C3)	54538 (22)	31440 (6)	−9531 (25)		54082 (18)	26403 (12)	47400 (30)
H(C4)	19459 (22)	35610 (8)	−1590 (30)		40990 (21)	35247 (13)	1394 (30)
H(C51)	27750 (21)	48177 (7)	5649 (33)		31904 (21)	39094 (14)	53491 (35)
H(C52)	43985 (23)	43888 (7)	−19050 (28)		23164 (19)	44392 (14)	27654 (40)
H(O1)	87290 (16)	45309 (5)	−15733 (21)		59516 (14)	51735 (10)	77663 (24)
H(O2)	85875 (17)	27453 (5)	44279 (21)		78513 (14)	33976 (9)	52955 (23)
H(O3)	40061 (17)	22723 (5)	7052 (21)		59229 (14)	15192 (9)	16734 (27)
H(O4)	11762 (18)	34956 (6)	41476 (26)		23300 (13)	24292 (9)	9407 (23)

Table 3. *Hydroxyl* H/D *atom parameters in* (I) *and* (II)

(a) Neutron scattering cross sections with standard deviations for hydroxyl H/D atoms

	(I)	(II)
H(O1)	0·4700 (22)	0·4598 (36)
H(O2)	0·4659 (22)	0·4652 (38)
H(O3)	0·4732 (23)	0·4596 (35)
H(O4)	0·4730 (24)	0·4773 (37)

(b) Values of $|\Delta_{ij}|/\sigma$, where Δ_{ij} is the difference in scattering cross sections and $\sigma = (\sigma_i^2 + \sigma_j^2)^{1/2}$

		(I)		
	H(O1)	H(O2)	H(O3)	H(O4)
H(O1)	x	1·32	1·01	0·92
(II) H(O2)	1·03	x	2·29	2·18
H(O3)	0·04	1·08	x	0·06
H(O4)	3·39	2·28	3·48	x

(c) Percentage D substitution *versus* hydrogen-bond length (Å)

	(I)			(II)	
	H/D···O	% D		H/D···O	% D
H(O2)	1·738	80·7 (1)	H(O4)	1·734	81·8 (2)
H(O1)	1·795	81·1 (1)	H(O2)	1·753	80·6 (2)
H(O3)	1·795	81·4 (1)	H(O1)	1·806	80·2 (2)
H(O4)	2·026	81·4 (1)	H(O3)	1·845	80·1 (2)

1. This results in the greater variation in the bond-length thermal-motion corrections for (II), which are shown in Table 4. It demonstrates the extreme sensitivity of thermal-motion corrections to the quality and quantity of the experimental data set.

Discussion

A previous experiment involving deuterium substitution (Coppens, 1970) had suggested that this might provide a useful numerical probe of differences in electronic structure. However, it is clear from the results given in Table 3 that the H/D exchange ratio in carbohydrates is less sensitive to differences in the hydroxyl groups than we had anticipated. Our results provide no evidence that the anomeric hydroxyls, HO(1) in carbohydrates, exchange differently from the non-anomeric hydroxyls, although they are known to form stronger hydrogen bonds (Jeffrey & Lewis, 1978; Newton, Jeffrey & Takagi, 1979). The results also showed no evidence of any sensitivity to the length of the hydrogen bonds. The correlations of bond length with H/D exchange for the two structures are in the opposite sense, as shown in Table 3(c). Therefore, in the absence of evidence to the contrary, we conclude that the deuterium exchange observed in these two structures is uniform within the experimental errors, which are underestimated by about 50% due to correlation between the H/D occupancy factors and the H/D thermal parameters. Previous experiments where significant differences were observed involved α-oxalic acid dihydrate (Coppens, 1970) where the difference in water and carboxylic acid stretching frequencies was 1560 cm^{-1}, and quinolinic acid (Takusagawa & Koetzle, 1979) where the comparison was between different types of bonds, N—H(D)···O and O—H(D)···O. With the oxalic acid dihydrate results, the difference in H/D exchange was much smaller than

Table 4. *Bond lengths* (Å) *and valence angles* (°) *in partially deuterated β-L-arabinopyranose*, (I), *and α-L-xylopyranose*, (II), *at* 123 K

The values have been corrected for thermal motion. The corrections are given in [ ] and the standard deviations in ( ), with reference to the least significant digits. The thermal-motion corrections assumed rigid-body motion of model B. E.s.d.'s for valence angles are 0·06° for (I), 0·08° for (II).

	(I)	(II)
C(1)—C(2)	1·5276 [23] (9)	1·5305 [40] (11)
C(2)—C(3)	1·5251 [22] (9)	1·5260 [15] (10)
C(3)—C(4)	1·5314 [26] (9)	1·5255 [29] (11)
C(4)—C(5)	1·5172 [23] (10)	1·5315 [40] (11)
C(1)—O(1)	1·3981 [29] (11)	1·3934 [23] (13)
C(1)—O(5)	1·4228 [24] (9)	1·4286 [26] (12)
C(2)—O(2)	1·4265 [24] (10)	1·4179 [26] (13)
C(3)—O(3)	1·4237 [21] (10)	1·4221 [37] (12)
C(4)—O(4)	1·4249 [19] (11)	1·4210 [13] (11)
C(5)—O(5)	1·4388 [20] (10)	1·4374 [14] (12)
C(1)—H,D(C1)	1·1001 [16] (15)	1·1023 [10] (17)
C(2)—H,D(C2)	1·1021 [15] (14)	1·0992 [18] (18)
C(3)—H,D(C3)	1·0997 [15] (14)	1·1048 [17] (18)
C(4)—H,D(C4)	1·0988 [16] (16)	1·1032 [17] (18)
C(5)—H,D(C51)	1·0946 [18] (15)	1·1019 [18] (22)
C(5)—H,D(C52)	1·0991 [25] (16)	1·0943 [21] (19)
O(1)—H,D(O1)	0·9753 [15] (12)	0·9731 [18] (15)
O(2)—H,D(O2)	0·9780 [14] (12)	0·9759 [14] (15)
O(3)—H,D(O3)	0·9734 [13] (12)	0·9632 [14] (15)
O(4)—H,D(O4)	0·9564 [15] (14)	0·9762 [18] (15)
C(1)—C(2)—C(3)	109·7	111·6
C(2)—C(3)—C(4)	109·8	108·4
C(3)—C(4)—C(5)	109·2	110·1
C(4)—C(5)—O(5)	111·2	110·5
C(1)—O(5)—C(5)	113·3	112·6
O(5)—C(1)—C(2)	109·7	109·3
O(5)—C(1)—O(1)	112·3	111·8
O(1)—C(1)—C(2)	107·8	110·1
O(2)—C(2)—C(1)	108·0	110·6
O(2)—C(2)—C(3)	112·0	113·1
O(3)—C(3)—C(2)	109·5	107·3
O(3)—C(3)—C(4)	111·5	111·5
O(4)—C(4)—C(3)	110·6	109·0
O(4)—C(4)—C(5)	109·4	109·6

Puckering parameters (Cremer & Pople, 1975)

θ	1·4° ($^4C_1$)	180° ($^1C_4$)
φ	110·5°	0°
Q	0·577 Å	0·575 Å

Table 5. *Hydrogen-bond geometry in partially deuterated β-L-arabinopyranose*, (I), *and α-L-xylopyranose*, (II), *at* 123 K

The distances and angles are uncorrected for thermal motion. Values in [ ] are differences from values at 298K in undeuterated crystals. Standard deviations are 0·0012 Å and 0·06° for (I), 0·0015 Å and 0·08° for (II).

(I)	O–H/D	H/D···O	O–H/D···O
O(1)—H/D···O(5)	0·974 [+22] Å	1·795 [−25] Å	169·3 [−0·7]°
O(2)—H/D···O(3)	0·977 [−2]	1·738 [+3]	159·8 [−1·4]
O(3)—H/D···O(2)	0·972 [−3]	1·795 [−6]	163·7 [+1·1]
O(4)—H/D···O(2)	0·955 [+35]	2·026 [−175]	156·3 [+6·6]
(II)			
O(1)—H/D···O(2)	0·971 [0]	1·784 [−21]	158·8 [+0·5]
O(2)—H/D···O(4)	0·974 [+1]	1·729 [−22]	171·7 [+0·2]
O(3)—H/D···O(5)	0·962 [−8]	1·815 [−28]	165·1 [−0·1]
O(4)—H/D···O(3)	0·974 [+5]	1·716 [−15]	168·7 [−0·1]

would be predicted from the differences in stretching frequencies. In these carbohydrate molecules the hydroxyl groups are chemically similar, except for the anomeric effect. The difference in the observed O—H stretching frequencies between the short hydrogen bonds and the long bond in β-arabinose in the crystalline state is about 500 cm⁻¹ (Kanters, Kroon, Peerdeman & Vliegenthart, 1969). Under these circumstances, our results indicate that a difference in H/D ratio will not be observed.

The molecular dimensions of (I) and (II) at 123 K are given in Table 4. The C—C and C—O bond lengths,

when corrected for rigid-body thermal motion, lie between the uncorrected and corrected values for the structures at 298 K. The corrected 123 K values are, on average, 0·0035 Å longer than the uncorrected 298 K values, for which the mean thermal-motion corrections are 0·007 Å. Interestingly, this suggests that the differences between uncorrected room-temperature data and corrected low-temperature data, extrapolated to the molecule at 0 K, will be small for carbohydrate crystals, since the thermal motion and expansion corrections are almost equal and opposite in sign, and tend to compensate.

The different configurations of (I) and (II) result in different conformations. (I) is a slightly distorted $^4C_1$ chair with two axial hydroxyls. (II) is a perfect $^1C_4$ chair with one axial hydroxyl. The geometrical constraints of the pyranose rings are such that even chemically similar bond lengths or valence angles must, in general, be different (*cf.* Dunitz & Waser, 1972). In (I), bond-length differences such that C(4)—C(3) > C(1)—C(2) ≥ C(2)—C(3) > C(4)—C(5) are observed (at both temperatures), but the C—C—C valence angles agree within 0·6°. In (II), the four C—C ring bond lengths agree within 0·0060 Å, but the C—C—C valence angles differ by 3·2°. Mathematical analysis of the relationship between ring conformation and differences in ring bond lengths and valence angles is a formidable unsolved problem for non-planar heterocyclic rings (*cf.* Britton, 1977). These results do, however, provide excellent data for testing the predictive powers of the *ab initio* quantum-mechanical calculations (*cf.* Pople, 1977) or the semi-empirical methods of molecular mechanics (*cf.* Allinger, 1976), since the agreement between experimental and theoretical molecular dimensions requires good theoretical values for the bending, stretching and torsional force constants.

The comparison with the room-temperature structures shows a quite different temperature contraction for the two structures. For (II), the 1·1% contraction in unit-cell volume for 123 K corresponds to a con-

traction in all three unit-cell directions and a very even contraction of the four hydrogen bonds by nearly the same magnitude, as shown by the data in Table 5. However, in (I), the larger 2·3%, volume contraction corresponds to a 7% contraction in the weak hydrogen bonds and a less than 1% contraction in the other three bonds. [The apparently large contraction in O(1)—H(D) is due to the riding-motion foreshortening of the O(1)—H covalent bond in the room-temperature study.] Two of the unit-cell dimensions contract by 1·2 and 1·3%, but the third shows a slight expansion.

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1,2,4,6-Tetra-O-acetyl-3-O-(2,3,4,6-tetra-O-acetyl-β-D-galactopyranosyl)-α-D-galactopyranose*

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Abstract

$C_{28}H_{38}O_{19}$ crystallizes in the space group $P2_12_12_1$, with $a = 19·194$ (1), $b = 14·719$ (1), $c = 12·415$ (1) Å, $Z = 4$, $D_x = 1·285$ Mg m^{-3}. Two sets of data (Mo and Cu radiations) and the derived results are analysed by normal probability plots. The structure was refined to $R = 0·061$ ($R_w = 0·074$). The anomeric parts have bond lengths of C(5′)—O(5′) = 1·439, O(5′)—C(1′) = 1·390, C(1′)—O(1′) = 1·435 and O(1′)—C(11′) = 1·331 Å for the α moiety and, in the same order, 1·437, 1·409, 1·407 and 1·424 Å for the β moiety. The glycosidic link has an angle of 114·5°. The distortions of the usual

$^4C_1$ chair conformation of both rings are analysed. The rings can be considered to be twisted by 75° from each other. The two galactoside substituents are attached to the rings with a difference in twist of 105°. The signs of angles which describe the relative configuration at every asymmetric C atom are defined.

Introduction

The title compound is an intermediate in the synthesis of D-galactopyranosyl-D-galactose compounds (Chacón-Fuertes & Martín-Lomas, 1975). These compounds are being studied as part of a project on con-

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* Crystal Structures of Analogues of D-Galactose. III.