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The crystal and molecular structure of 1,2-*O*-isopropylidene-α-D-*xylo*-pentodialdo-1,4-furanose. A dimeric form in the crystalline state

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Abstract

1,2-*O*-isopropylidene-α-D-*xylo*-pentodialdo-1,4-furanose (1), $C_{16}H_{24}O_{10}$, $M_r = 376.4$, is orthorhombic, space group $P2_12_12_1$ with $a = 10.3028(10)$, $b = 11.1875(3)$, $c = 15.7484(13)$ Å, $V = 1815.2(4)$ Å^3, $D_c = 1.377$ gcm^{-3}, $\mu(\mathrm{Cu}K\alpha) = 9.5$ cm^{-1} and $Z = 4$. The structure was refined to $R = 0.033$ and $R_w = 0.045$ for 1984 observed reflections. Crystalline **1** has a dimeric cyclic acetal–hemiacetal structure, formed by self aldol condensation of two monomers. The absolute configuration at the condensation centers, C-5 and C-5′, were assigned as 5*R* and 5*S*, respectively. In the dimer **1**, the xylofuranose rings adopt different conformations, one is a twist $^3T_4$, whereas the second is an envelope E_4 slightly distorted towards the $^3T_4$ conformation; their fused 1,2-*O*-isopropylidene rings adopt $^{\text{O-2}}E$ and $^{\text{O-2}}T_{\text{C-6}}$ conformations, respectively. The 1,3-dioxane ring has a distorted chair conformation with puckering parameters $Q = 0.516$ Å, $\phi = 90.9$, and $\theta = 11.0°$. The molecules are linked in the crystal through intermolecular hydrogen-bonding interactions that involve the two hydroxyl groups, OH-3 and OH-5′, and the isopropylidene ring oxygen atoms, O-2 and O-1′, as donor and acceptor, respectively.

1. Introduction

1,2-*O*-isopropylidene-α-D-*xylo*-pentodialdo-1,4-furanose [1,2] (**1**) is a compound of potential utility, particularly in the synthesis of ^{13}C-labeled aldoses [3,4] that have become widely accessible for use in chemical and biological studies [5]. For

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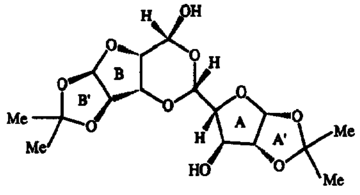
example, condensation of **1** with (^{13}C) cyanide yields C-6 epimeric (6-^{13}C) cyanohydrins that can be readily reduced with H_2 and Pd–$BaSO_4$, to give (6-^{13}C)aldehyde intermediates [6,7]. These intermediates may serve as the parent aldoses in cyanohydrin-reduction reactions [8,9], providing a route to (6-^{13}C)heptoses, or reduction with NaB^2H_4 to give biologically important mono-C-6-deuterated aldohexoses that are not readily accessible by other methods. They may also be used in the synthesis of (6-^{13}C)hexouronic acids [10,11] that are useful in the studies of glycosaminoglycan structures. Compound **1** has also been considered as a suitable starting material in the preparation of a variety of biologically active 4′-hydroxymethyl nucleosides [12,13], as well as various derivatives of griseolic acid [14] that have been the subject of numerous biochemical studies on account of their potent inhibitory activities [15–17].



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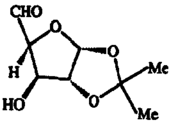

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The crystalline substance **1** was first reported as a monomer (**2**) [18]. However, Schaffer and Isbell [2] concluded, on the bases of the molecular weight determination, infrared absorption measurements, and prolonged acetylation of **1** with acetic anhydride in pyridine, that it was a dimer having a cyclic acetal–hemiacetal structure formed by self aldol condensation of two monomers. Consequently, new asymmetric centers were produced at the carbon atoms where the condensation has taken place to give rise to four diastereomers. No evidence was yet available for assigning the configurations at these centers nor the conformations of various ring systems of **1**. Thus, the importance of the 5-aldol derivative for synthetic purposes and the need for definitive proof of its structure and configuration has led us to undertake a detailed study of its conformation and 3D molecular structure by X-ray crystallography.

2. Experimental

The sample of 1,2-*O*-isopropylidene-α-D-*xylo*-pentodialdo-1,4-furanose (**1**) was kindly provided by Professor Hassan El Khadem from Dr. H.S. Isbell's collection of rare sugars at The American University, Washington, DC. Suitable crystals for X-ray diffraction were obtained from benzene–ethyl acetate by slow evaporation at room temperature.

Data collection and processing.—A colorless crystal with dimensions of 0.22 × 0.25 × 0.37 mm was used for the structure determination. Intensity data were collected on an Enraf–Nonius CAD4 diffractometer equipped with graphite-monochromated Cu$K\alpha$ radiation ($\lambda = 1.54184$ Å) at 22°C. Unit-cell parameters

Table 1
Crystallographic data for 1,2-*O*-isopropylidene-α-D-xylo-pentodialdo-1,4-furanose (1)

Molecular formula	$C_{16}H_{24}O_{10}$
Molecular weight	376.4
Melting point (°C)	199-200 (dec)
Crystal dimensions (mm)	0.22×0.25×0.37
Space group	$P2_12_12_1$
Cell dimensions (Å)	
a	10.3028(10)
b	11.1875(3)
c	15.7484(13)
Volume (Å^3)	1815.2(4)
Z (molecules/cell)	4
θ_{max} (°)	75
μ (cm^{-1})	9.5
Radiation (graphite monochromator)	Cu*K*α
Calculated density (g cm^{-3})	1.377
Unique reflections	2131
Observed data	1984
S (284 variables)	2.824
Final residual factors	
R	0.033
R_w	0.045

were determined by least-squares refinement using 25 accurately centered reflections ($32 < 2\theta < 56°$). A total of 2154 reflections was measured by $\omega - 2\theta$ scans (one octant having $4 < 2\theta < 150°$) with variable scan rate (0.55–3.30 deg min^{-1}). Systematic absences were deleted to yield 2131 unique data; 1984 reflections with $I > 3\sigma(I)$ were used in the refinement. Crystal stability was monitored by recording three standard reflections every 10000 s; no significant variation was noted. Absorption correlations were based on a series of Ψ scans, and the minimum relative transmission coefficient was 91.8%. Systematic absences uniquely specified that the crystal belongs to space group $P2_12_12_1$ with Z = 4 (see Table 1).

Structural analysis.—The structure was solved by direct methods using the program MULTAN-80 [19], and completed by difference Fourier methods. It was refined by full-matrix least-squares based upon F, using data for which $I > 3\sigma$(I), weights $w = 4F_o^2\ [\sigma^2(I) + (0.02\ F_o^2)^2]^{-1}$ using the MolEN programs [20]. Nonhydrogen atoms were refined anisotropically. The H-atom coordinates were located by ΔF syntheses and hydrogen atoms were refined isotropically, except for those of methyl groups, which were placed in calculated positions. Atomic coordinates and equivalent isotropic thermal parameters are given in Table 2 *. Final R = 0.033 for 1984 observed data (0.037 for all 2131 data), $R_w = 0.045$, and $S = 2.824$ for 284

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* Lists of observed and calculated structure-amplitudes, anisotropic thermal parameters, hydrogen coordinates and isotropic thermal parameters, and torsion angles for this compound have been deposited with the Cambridge Crystallographic Data Centre and may be obtained on request, from the Director, Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge, CB2 1EZ, UK.

Table 2
Atomic coordinates and equivalent isotropic thermal parameters for 1,2-*O*-isopropylidene-α-D-*xylo*-pentodialdo-1,4-furanose (**1**)

Atom	x	y	z	B_{eq} (Å^2) [a]
O-1′	0.6219(1)	0.1315(1)	0.41680(9)	4.04(3)
O-1	0.9504(2)	0.0.8290(2)	0.27349(9)	6.02(4)
O-2	0.9766(1)	0.8025(2)	0.41326(9)	4.50(3)
O-2′	0.4848(1)	0.2467(1)	0.4940(1)	3.72(2)
O-3	0.6351(1)	0.8000(1)	0.4551(1)	4.85(3)
O-3′	0.6327(1)	0.5134(1)	0.41504(8)	3.52(2)
O-4′	0.6165(2)	0.2889(1)	0.32130(8)	4.31(3)
O-4	0.7410(1)	0.7581(1)	0.28587(9)	4.63(3)
O-5	0.6251(1)	0.5352(1)	0.26779(8)	4.18(3)
O-5′	0.4000(2)	0.5234(2)	0.2596(1)	6.39(4)
C-1	0.8268(2)	0.8503(2)	0.3085(2)	4.51(4)
C-1′	0.6593(2)	0.2505(2)	0.4022(1)	3.34(3)
C-2′	0.5858(2)	0.3244(2)	0.4677(1)	3.28(3)
C-2	0.8468(2)	0.8431(2)	0.4045(1)	3.84(4)
C-3′	0.5305(2)	0.4273(2)	0.4171(1)	3.39(3)
C-3	0.7543(2)	0.7450(2)	0.4333(1)	3.33(3)
C-4′	0.5099(2)	0.3697(2)	0.3309(1)	3.75(4)
C-4	0.7433(2)	0.6715(2)	0.3524(1)	3.20(3)
C-5	0.6230(2)	0.5951(2)	0.3462(1)	3.55(4)
C-5′	0.5155(2)	0.4584(2)	0.2584(1)	4.57(4)
C-6′	0.5336(2)	0.1275(2)	0.4872(1)	3.62(4)
C-6	1.0452(2)	0.8306(3)	0.3365(1)	4.98(5))
C-7	1.1052(3)	0.9521(4)	0.3441(2)	9.82(8)
C-7′	0.4239(3)	0.0460(2)	0.4650(2)	5.27(5)
C-8′	0.6075(3)	0.0920(3)	0.5660(2)	6.40(7)
C-8	1.1413(3)	0.7336(5)	0.3195(2)	9.5(1)

[a] $B_{eq} = (8\pi^2/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$.

variables. In the final cycle of refinement, the maximum shift was 0.01σ, maximum residual density 0.16, minimum -0.12 eÅ^{-3}, and extinction coefficient $g = 2.9(2) \times 10^{-6}$ where the factor $(1 + gI_C)^{-1}$ was applied to F_C. All calculations were performed on VAX 3600 computer. Atomic scattering factors were obtained from the International Tables for X-ray Crystallography [21]. The crystal structure is represented as an ORTEP [22] drawing (Fig. 1), which also shows the atom numbering in the molecule.

3. Discussion

The molecular structure of the title compound **1** shows clearly that the molecule has a dimeric cyclic acetal–hemiacetal structure, formed by self aldol condensation of two monomers; each consists of a furanose ring in the D-*xylo* configuration, sharing C-1 and C-2 with a 1,2-dioxolane ring. The two monomeric partners are interconnected through ether bridges formed by the addition of the OH-3 function

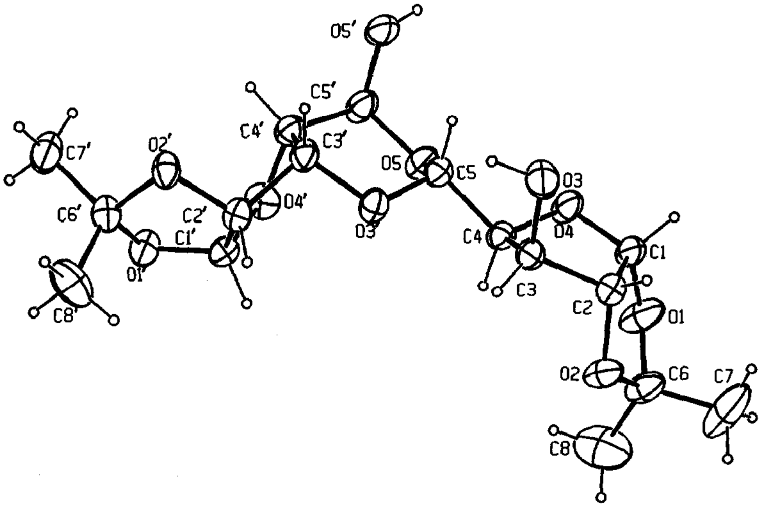

Fig. 1. Molecular structure and atomic numbering of the title compound **1**. Nonhydrogen atoms are represented by 30% ellipsoids and hydrogen atoms with circles of arbitrary radius.

of one monomer to the keto group of the second monomer, thus forming a central 1,3-dioxane ring. These results confirm that the previously assigned chemical structure [2] of **1** is correct.

Although the absolute configuration at the asymmetric centers produced as a result of dimerization at C-5 and C-5′ was not directly determined, it can be assigned as 5*R* and 5′*S*, respectively, based on the known configurations of the other chiral centers (for atom numbering see Fig. 1). The orientation of O-5′ about the C-5′–C-4′ bond is *trans–gauche* to O-4′ and C-3′, with the torsion angles O-5′–C-5′–C-4′–O-4′ and O-5–C-5′–C-4′–C-3′ being 170.0(2)° and 46.4(2)°, respectively. Similarly, the orientation of O-5 about O-5–C-5 bond is *trans–gauche* to C-3 and O-4 with the torsion angles O-5–C-5–C-4–C-3 and O-5–C-5–C-4–O-4 being 179.0(2)° and 62.0(2)°, respectively. The bond lengths, bond angles and selected torsion angles in the molecule with their estimated standard deviations are given in Tables 3, 4, and 5, respectively.

In contrast to the crystalline state, compound **1** was found to exist in solution, mainly, in the monomeric form **2**. This was evident from the presence of a signal attributable to an aldehydic proton in its ^{1}H NMR spectrum [23] measured at 400 MHz ($\delta = 9.57$ ppm in acetonitrile-d_3). This was further supported by the fact that the monomeric form **2** could be readily isolated as its crystalline 1,3-diphenylimidazolidine derivative in an overall yield of 74% from 1,2-*O*-isopropylidene-α-D-glucofuranose by treatment of the oxidation product **2** with *N*,*N*′-diphenylethylidenediamine in methanol containing acetic acid [13].

The results of the conformational calculations on the various ring systems in **1** are presented in Table 6. The analysis of the torsion angles and puckering parameters [24] indicates that the furanose rings have different conformations. For simplicity, one will be called ring A, and the other ring, ring B, in the subsequent

Table 3
Bond lengths for 1,2-*O*-isopropylidene-α-D-*xylo*-pentodialdo-1,4-furanose (1)

Atoms	Length (Å)	Atoms	Length (Å)	Atoms	Length (Å)
O-1′–C-1′	1.405(2)	O-3′–C-5	1.421(2)	C-2′–C-3′	1.511(3)
O-1′–C-6′	1.435(2)	O-4′–C-1′	1.415(2)	C-2–C-3	1.522(3)
O-1–C-1	1.408(3)	O-4′–C-4′	1.430(3)	C-3′–C-4′	1.518(3)
O-1–C-6	1.392(3)	O-4–C-1	1.404(3)	C-3–C-4	1.522(3)
O-2–C-2	1.419(3)	O-4–C-4	1.428(2)	C-4′–C-5′	1.515(3)
O-2–C-6	1.436(3)	O-5–C-5	1.406(2)	C-4–C-5	1.508(3)
O-2′–C-2′	1.418(2)	O-5–C-5′	1.427(3)	C-6′–C-7′	1.495(3)
O-2′–C-6′	1.429(2)	O-5′–C-5′	1.395(3)	C-6′–C-8′	1.509(3)
O-3–C-3	1.416(2)	C-1–C-2	1.529(3)	C-6–C-7	1.498(5)
O-3′–C-3′	1.428(2)	C-1′–C-2′	1.523(3)	C-6–C-8	1.493(5)

discussion (see the line drawing of **1**). Their fused, 1,2-*O*-isopropylidene rings will be called ring A′ and B′, respectively. The furanose ring A adopts an envelope E_4 conformation slightly distorted towards $^3T_4$. Four atoms, C-1, C-2, C-3, and O-4 are nearly coplanar within deviations of 0.02–0.03 Å. The flap atom, C-4, is displaced from this plane in the *exo* direction by 0.564(2) Å. The mean plane of the furanose ring A makes a dihedral angle of 67.6(1)° with the mean plane of the fused 1,2-*O*-isopropylidene ring A′. The hydroxyl group on C-3 is quasiequatorially oriented and adopts *gauche–gauche* dispositions with respect to the 1,3-dioxane ring atom C-5 and the isopropylidene ring atom, O-2, respectively; the O-3–C-3–C-4–C-5 and O-2–C-2–C-3–O-3 torsion angles being −43.8(2) and 157.9(2)°, respectively. Unlike ring A, ring B has a twist conformation, presumably due to its

Table 4
Bond angles for 1,2-*O*-isopropylidene-α-D-*xylo*-pentodialdo-1,4-furanose (1)

Atoms	Angle (°)	Atoms	Angle (°)	Atoms	Angle (°)
C-1′–O-1′–C-6′	109.2(1)	C-1′–C-2′–C-3′	104.1(1)	O-3′–C-5–O-5	111.3(2)
C-1–O-1–C-6	110.7(2)	O-2–C-2–C-1	103.9(2)	O-3′–C-5–C-4	104.9(1)
C-2–O-2–C-6	108.2(2)	O-2–C-2–C-3	109.3(2)	O-5–C-5–C-4	108.3(2)
C-2′–O-2′–C-6′	107.0(1)	C-1–C-2–C-3	104.4(2)	O-5–C-5′–O-5′	111.1(2)
C-3′–C-3′–C-5	113.5(1)	O-3′–C-3′–C-2′	104.4(1)	O-5–C-5′–C-4′	110.3(2)
C-1′–O-4′–C-4′	109.6(1)	O-3′–C-3′–C-4′	111.7(2)	O-5′–C-5′–C-4′	107.4(2)
C-1–O-4–C-4	107.6(2)	C-2′–C-3′–C-4′	101.6(2)	O-1′–C-6′–O-2′	104.6(1)
C-5–O-5–C-5′	111.5(1)	O-3–C-3–C-2	107.5(2)	O-1′–C-6′–C-7′	108.5(2)
O-1–C-1–O-4	110.2(2)	O-3–C-3–C-4	111.9(2)	O-1′–C-6′–C-8′	108.9(2)
O-1–C-1–C-2	104.8(2)	C-2–C-3–C-4	100.7(2)	O-2′–C-6′–C-7′	108.7(2)
O-4–C-1–C-2	107.3(2)	O-4′–C-4′–C-3′	104.8(2)	O-2′–C-6′–C-8′	111.2(2)
O-1′–C-1′–O-4′	110.4(2)	O-4′–C-4′–C-5′	107.7(2)	C-7′–C-6′–C-8′	114.4(2)
O-1′–C-1′–C-2′	105.5(2)	C-3′–C-4′–C-5′	113.0(2)	O-1–C-6–O-2	104.6(2)
O-4′–C-1′–C-2′	106.8(2)	O-4–C-4–C-3	104.4(2)	O-1–C-6–C-7	111.0(2)
O-2′–C-2′–C-1′	103.3(2)	O-4–C-4–C-5	108.9(1)	O-1–C-6–C-8	109.2(2)
O-2′–C-2′–C-3′	110.2(2)	C-3–C-4–C-5	114.9(2)	O-2–C-6–C-7	108.5(2)
O-2–C-6–C-8	108.5(2)	C-7–C-6–C-8	113.6(3)		

Table 5
Endocyclic torsion angles of various ring systems in 1,2-*O*-isopropylidene-α-D-*xylo*-pentodialdo-1,4-furanose (**1**)

Atoms	Angle (°)	Atoms	Angle (°)
D-*xylo*-Furanose rings			
C-4–O-4–C-1–C-2	−20.2(2)	C-4′–O-4′–C-1′–C-2′	−7.6(2)
C-1–O-4–C-4–C-3	37.5(2)	C-1′–O-4′–C-4′–C-3′	27.8(2)
O-4–C-1–C-2–C-3	−4.9(2)	O-4′–C-1′–C-2′–C-3′	−15.6(2)
C-1–C-2–C-3–C-4	25.8(2)	C-1′–C-2′–C-3′–C-4′	30.9(2)
C-2–C-3–C-4–O-4	−38.5(2)	C-2′–C-3′–C-4′–O-4′	−36.0(2)
1,2-*O*-Isopropylidene rings			
C-6–O-1–C-1–C-2	−10.3(3)	C-6′–O-1′–C-1′–C-2′	−1.2(2)
C-1–O-1–C-6–O-2	24.0(3)	C-1′–O-1′–C-6′–C-2′	20.0(2)
C-6–O-2–C-2–C-1	22.2(2)	C-6′–O-2′–C-2′–C-1′	30.8(2)
C-2–O-2–C-6–O-1	28.7(3)	C-2′–O-2′–C-6′–O-1′	−32.1(2)
O-1–C-1–C-2–O-2	−7.5(2)	O-1′–C-1′–C-2′–O-2′	−18.0(2)
1,3-Dioxane ring			
C-5–O-3′–C-3′–C-4′	48.3(2)		
C-3–O-3′–C-5–O-5	−59.4(2)		
C-5′–O-5–C-5–O-3?′	63.7(2)		
C-5–O-5–C-5′–C-4′	−56.8(2)		
O-3′–C-3′–C-4′–C-5′	−42.3(2)		
C-3′–C-4′–C-5′–O-5	46.4(2)		

fusion to the 1,3-dioxane ring, which generates strain. This is corroborated by the calculation of the puckering parameters which place the ring in the $^{3}T_{4}$ conformation on the puckering diagram [25]. This conclusion is also supported by analysis of the deviations of the ring atoms from the least-squares plane passing through C-1′–O′-4–C-2′, which places C′-3 and C-4′ at positions 0.394(2) Å above and 0.178(2) Å below the plane, respectively. The mean plane of the furanose ring B makes dihedral angles of 113.5(1)° and 71.2(1)° with the mean planes of the ring B′ and 1,3-dioxane ring, respectively. The dihedral angle between the mean planes of the latter is 121.2(1)°.

The bond lengths and bond angles of the two furanose rings are almost equal and within the limits of experimental errors, except for the bond sequence C-4–O-4–C-1 in ring A. The O-4–C-1 bond [1.404(3) Å] is significantly shorter by 7σ than O-3–C-4 [1.428(2) Å]. This difference is attributable to the anomeric effect [26] distribution that is commonly observed in related structures [27–32].

The isopropylidene ring conformations differ significantly as shown by the torsion angles in Table 5 and puckering parameters in Table 6. The isopropylidene ring A′ adopts a twist $^{\mathrm{O\text{-}2}}T_{\mathrm{C\text{-}6}}$ conformation, with O-2 is displaced by 0.180(1) Å above and C-6 is 0.234(3) Å below the plane defined by O-1–C-1–C-2, whereas ring B′ has almost a perfect envelope $^{\mathrm{O\text{-}2'}}E$ conformation, with O-2′ lying in the *endo* direction by 0.449(1) Å with respect to the plane defined by the atoms C-6′, O-1′, C-1′, and C-2′, which are coplanar within deviations of 0.004(2)–0.007(2) Å. The deformation of the latter towards the envelope conformation is apparently

Table 6
Conformation and puckering parameters of the various ring systems in 1,2-*O*-isopropylidene-D-*xylo*-pentodialdo-1,4-furanose (1)

Parameters	D-*xylo*-Furanose rings		1,2-*O*-Isopropylidene rings		1,3-Dioxane ring
	Ring A	Ring B	Ring A′	Ring B′	
Puckering Parameters [a]					
ϕ (°)	315.4	297.8	232.6	173.6	90.9
q_2 (Å)	0.37	0.34	0.25	0.56	0.51
Q (Å)					0.52
θ (°)					11.0
Conformation	$E_4 \rightarrow {}^3T_4$	${}^3T_4$	${}^{O\text{-}2}T_{C\text{-}6}$	${}^{O\text{-}2'}E$	${}^1C_4$
Atom deviations (Å) from the plane defined by	C-1–C-2–C-3–C-4	C-1′–O-4′–C-2′	O-1–C-1–C-2	C-6′–O-1′–C-1–′C-2′	O-5–O-3′–C-3′–C-5′
	C-4 0.564(1)	C-3′ 0.394(2)	O-2 0.180(1)	O-2′ 0.449(1)	C-5 0.649(2)
		C-4′ −0.178(2)	C-6 −0.234(3)		C-4′ −0.547(2)

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[a] Ref 24.

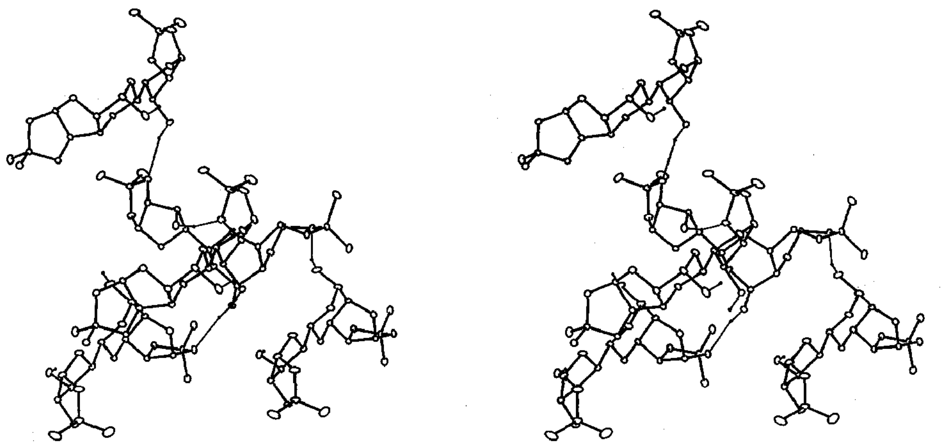

Fig. 2. Stereoview of the hydrogen bonding scheme in the crystal of **1**. For clarity, hydrogen atoms not involved in hydrogen bonding are omitted.

associated with the strain imposed on the furanose ring B by the 1,3-dioxane ring at positions C-3′ and C-4′. The conformational liability of dioxolane rings fused with a furanose ring has been previously discussed [33]. The bond lengths and angles of the two isopropylidene rings are in good agreement with each other and show no significant differences from the mean values tabulated for *O*-isopropylidene groups fused to sugar molecules [34,35]. The mean values of C–O, and $C–CH_3$ distances are: 1.414 and 1.496 Å for ring A′ and 1.422 and 1.502 Å for ring B′, respectively.

The 1,3-dioxane ring has a normal chair conformation and is more puckered at the acetal center (torsion angle magnitudes 62.0–62.4°), but flattened on the other end at the fusion with the furanose ring (torsion angle magnitudes 47.1–47.7°). A least-squares plane through O-5, O-3′, C-3′, and C-5′ shows average and maximum deviations of these atoms (from the plane) of 0.03 Å; C-5 is displaced by 0.649(2) Å above the plane and C-4′ is 0.547(2) Å below it. The molecules are linked in the crystal by a network of hydrogen bonds. It involves the two hydroxyl groups, OH-3 and OH-5′, and the isopropylidene ring oxygen atoms, O-2 and O-1′, as donor and acceptor, respectively. A stereoview of the hydrogen-bonding interactions in the crystal are shown in Fig. 2, and the relevant hydrogen–oxygen and oxygen–oxygen distances are listed in Table 7, together with angles about the H atoms.

Table 7
Geometry of the hydrogen bonds [a] in 1,2-*O*-isopropyledine-α-D-*xylo*-pentodialdo-1,4-furanose (**1**)

D [b] A	Acceptor symmetry	O···O (Å)	O–H (Å)	H···O (Å)	O–H···O (°)
O-3-H···O2	$x-0.5, 0.5+y, 1-z$	2.878(2)	0.96(3)	2.00(3)	152(3)
O-5′-H···O1′	$1-x, 0.5+y, 0.5-z$	3.038(2)	0.83(4)	2.24(4)	161(4)

[a] Estimated standard deviation in parentheses.
[b] D, donor; A, acceptor.

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