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CRYSTAL AND MOLECULAR STRUCTURE OF THE DIHYDRATE OF THE ARTIFICIAL SWEETENER LACTITOL: 4-O-β-D-GALACTOPYRANOSYL-D-GLUCITOL.2H_2O

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ABSTRACT

Crystallization of lactitol from aqueous ethanol readily yields crystals of the monohydrate, the structure of which has recently been reported Slow evaporation of very concentrated aqueous syrups results in the crystalline dihydrate The space group is $P4_32_12$ with $a=8\ 762(2)$, $c=45\ 508(8)$ Å, $V=3493\ 8(13)$ Å^3, $Z=8$, $D_c=1\ 446$ g cm^{-3}, $R=0\ 037$ for 2017 unique observed reflections and 310 variables The galactopyranosyl ring has the $^4C_1$ chair conformation and the carbon chain of the glucitol fragment has a non-planar, bent *MAA* conformation The conformations about the glycosidic C(1)-O(1) and O(1)-C(14) bonds are different from those observed in the monohydrate the torsion angles O(5)-C(1)-O(1)-C(14) and C(1)-O(1)-C(14)-C(13) differ by 29 6° and 15 0°, respectively The orientations of the terminal C(11)–O(11) bonds with respect to the carbon-atom chain of the glucitol fragment also differ appreciably in the dihydrate the pertinent torsion angle is −47 3(3)° and in the monohydrate 75 5(2)° All hydroxyl groups are involved in a complex three-dimensional system of hydrogen bonds, in which the two water molecules constitute an important cohesive element

INTRODUCTION

Lactitol, 4-O-β-D-galactopyranosyl-D-glucitol, belongs to the class of glycosyl-alditols The growing interest in this class of sugar alcohols relates to their use as non-toxic, low-nutritive sweeteners which renders them very suitable as sugar-substituting food additives Their sweet property raises questions as to the relation between structure and sweet taste and, in this respect, the glycosyl-alditols represent useful model compounds As a first step in this type of investigation accurate information should be available on the conformation of these flexible molecules Although a wealth of structural knowledge exists

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for the two constituting moieties, cyclic α- and β-pyranoses and acyclic alditols respectively, only the crystal structures of five glycosyl-alditols have been reported in the literature cellobiotol (4-O-β-D-glucopyranosyl-D-glucitol) [1], maltitol (4-O-α-D-glucopyranosyl-D-glucitol) [2], isomaltitol (6-O-α-D-glucopyranosyl-D-glucitol) [3], 4-O-β-D-galactopyranosyl-L-rhamnitol [4] and 1-O-α-D-glucopyranosyl-D-mannitol [5] Recently, we have reported the crystal structure of lactitol monohydrate [6], which can easily be crystallized from 50% aqueous ethanol However, the preparation of good-quality single crystals of the dihydrate, which is mentioned in the literature [7], is troublesome After many attempts, single crystals were obtained by slow cooling over prolonged periods of aqueous concentrated syrups In this paper, we report the crystal and molecular structure of the dihydrate with emphasis on its conformational differences with respect to the monohydrate

TABLE 1

Fractional coordinates and equivalent isotropic thermal parameters ($A^{**}2$) (estimated standard deviations given in parentheses)

	x	y	z	$U(\mathrm{eq})^a$
O(1)	0 8180(2)	0 2624(2)	0 03819(3)	0 0229(5)
O(2)	0 7108(2)	−0 0296(2)	0 05285(5)	0 0374(5)
O(3)	0 9485(2)	−0 2383(2)	0 06712(4)	0 0285(5)
O(4)	1 2040(2)	−0 0537(2)	0 05999(4)	0 0341(6)
O(5)	1 0333(2)	0 2252(2)	0 06593(3)	0 0240(5)
O(6)	1 2418(2)	0 3631(2)	0 10793(4)	0 0348(6)
O(11)	1 1329(2)	0 6690(2)	0 02300(5)	0 0451(6)
O(12)	1 0984(2)	0 4540(2)	−0 02549(4)	0 0327(6)
O(13)	0 7941(2)	0 4155(2)	−0 01400(4)	0 0268(5)
O(15)	0 6587(2)		0 03915(4)	0 0305(5)
O(16)	0 4647(2)	0 6488(2)	0 08114(6)	0 0507(8)
O(111)	0 4700(3)	0 5172(2)	0 08534(5)	0 0382(6)
O(112)	0 9825(3)	0 8286(2)	0 11112(5)	0 0470(7)
C(1)	0 8784(3)	0 5430(3)	0 06205(5)	0 0217(6)
C(2)	0 8662(3)	0 1835(3)	0 05394(5)	0 0239(6)
C(3)	0 9457(3)	0 0162(3)	0 07680(5)	0 0235(6)
C(4)	1 1054(3)	−0 0828(3)	0 08407(5)	0 0247(6)
C(5)	1 0988(3)	−0 0245(3)	0 09047(5)	0 0230(6)
C(6)	1 2547(3)	0 1468(3)	0 09570(6)	0 0299(7)
C(11)	1 1622(3)	0 2141(3)	0 02380(6)	0 0313(7)
C(12)	1 0530(3)	0 5090(3)	0 00403(5)	0 0243(6)
C(13)	0 8875(3)	0 4245(3)	0 00880(5)	0 0205(6)
C(14)	0 8249(3)	0 4766(3)	0 03863(5)	0 0199(6)
C(15)	0 6645(3)	0 4268(2)	0 04448(5)	0 0246(6)
C(16)	0 6114(3)	0 4885(3)	0 07546(7)	0 042(1)
		0 4563(3)		

$^a U(\mathrm{eq}) = 1/3 \,\mathrm{sum}(i)\,\mathrm{sum}(j)\; U(ij)a(i^*)a(j^*)a(i)a(j)$

TABLE 2

Hydrogen atom positions and isotropic thermal parameters

	x	*y*	*z*	*U*(Iso)
H(C1)	0 830(3)	0 207(3)	0 0789(6)	0 0234(-)
H(C2)	0 916(3)	−0 005(3)	0 0341(6)	0 0293(-)
H(C3)	0 895(3)	−0 079(3)	0 0946(6)	0 0272(-)
H(C4)	1 143(3)	−0 081(3)	0 1032(5)	0 0278(-)
H(C5)	1 044(3)	0 169(3)	0 1096(6)	0 0255(-)
H(C6)	1 308(3)	0 158(3)	0 1109(6)	0 0327(-)
H′(C6)	1 309(3)	0 221(3)	0 0777(6)	0 0327(-)
H(O2)	0 666(3)	0 021(3)	0 0396(6)	0 039(-)
H(O3)	1 020(3)	−0 256(3)	0 0521(6)	0 0341(-)
H(O4)	1 284(3)	−0 098(3)	0 0650(6)	0 0368(-)
H(O6)	1 312(3)	0 420(3)	0 0980(6)	0 0357(-)
H(C11)	1 145(3)	0 476(3)	0 0428(6)	0 0358(-)
H′(C11)	1 267(3)	0 483(3)	0 0184(6)	0 0358(-)
H(C12)	1 066(3)	0 318(3)	0 0100(5)	0 0257(-)
H(C13)	0 880(3)	0 586(3)	0 0068(5)	0 0209(-)
H(C14)	0 892(3)	0 466(3)	0 0545(5)	0 0239(-)
H(C15)	0 602(3)	0 439(3)	0 0306(6)	0 0286(-)
H(C16)	0 685(4)	0 497(3)	0 0904(6)	0 0434(-)
H′(C16)	0 609(4)	0 358(3)	0 0787(7)	0 0434(-)
H(O11)	1 196(4)	0 708(4)	0 0194(8)	0 0446(-)
H(O12)	1 064(4)	0 398(4)	−0 0357(7)	0 0348(-)
H(O13)	0 751(3)	0 487(3)	−0 0196(6)	0 0273(-)
H(O15)	0 719(4)	0 680(4)	0 0443(7)	0 0318(-)
H(O16)	0 470(4)	0 615(4)	0 0798(7)	0 0514(-)
H(O111)	0 471(4)	0 876(4)	0 1012(7)	0 0409(-)
H′(O111)	0 538(4)	0 855(4)	0 0761(7)	0 0409(-)
H(O112)	1 070(4)	0 488(4)	0 1108(7)	0 0468(-)
H′(O112)	0 988(4)	0 612(4)	0 1000(7)	0 0468(-)

EXPERIMENTAL

Crystallography

$C_{12}H_{24}O_{11}\ 2H_2O$, $M=380.36$, tetragonal, space group $P4_32_12$, $a=8.762(2)$, $c=45\ 508(8)$ Å, $V=3493.8(13)$ Å^3, $Z=8$, $D_c=1\ 446$ g cm^{-3}, $F(000)=1632$, λ(Mo $K\alpha$) $=0\ 71073$ Å, $\mu=1.2$ cm^{-1}, crystal dimensions $0\ 2\times0\ 2\times0\ 15$ mm^3

Data collection

A transparent, colourless crystal was selected for the collection of data, which was performed using Zr-filtered Mo $K\alpha$ radiation on an Enraf-Nonius CAD 4 diffractometer The cell dimensions were derived from the setting angles of 25 reflections with $12\ 3° \leqslant \theta \leqslant 19\ 6°$ A total of 5077 reflections were measured

TABLE 3

Bond distances (Å), bond angles (deg) and torsion angles (deg) (estimated standard deviations given in parentheses)

O(1)-C(1)	1 392(3)	O(16)-C(16)	1 416(3)
O(1)-C(14)	1 442(2)	C(1)-C(2)	1 515(4)
O(2)-C(2)	1 420(3)	C(2)-C(3)	1 523(3)
O(3)-C(3)	1 432(3)	C(3)-C(4)	1 526(4)
O(4)-C(4)	1 419(3)	C(4)-C(5)	1 530(4)
O(5)-C(1)	1 417(3)	C(5)-C(6)	1 507(4)
O(5)-C(5)	1 431(3)	C(11)-C(12)	1 508(4)
O(6)-C(6)	1 424(3)	C(12)-C(13)	1 536(4)
O(11)-C(11)	1 426(3)	C(13)-C(14)	1 528(3)
O(12)-C(12)	1 425(3)	C(14)-C(15)	1 529(4)
O(13)-C(13)	1 426(3)	C(15)-C(16)	1 511(4)
O(15)-C(15)	1 426(3)		
C(1)-O(5)-C(5)	110 9(2)	C(4)-C(5)-C(6)	112 3(2)
C(1)-O(1)-C(14)	118 0(2)	O(6)-C(6)-C(5)	110 4(2)
O(1)-C(1)-O(5)	109 5(2)	O(11)-C(11)-C(12)	110 7(2)
O(1)-C(1)-C(2)	105 3(2)	O(12)-C(12)-C(11)	107 2(2)
O(5)-C(1)-C(2)	110 3(2)	O(12)-C(12)-C(13)	110 1(2)
O(2)-C(2)-C(1)	110 5(2)	C(11)-C(12)-C(13)	111 6(2)
O(2)-C(2)-C(3)	107 5(2)	O(13)-C(13)-C(12)	109 1(2)
C(1)-C(2)-C(3)	110 6(2)	O(13)-C(13)-C(14)	109 5(2)
O(3)-C(3)-C(2)	109 8(2)	C(12)-C(13)-C(14)	112 3(2)
O(3)-C(3)-C(4)	111 7(2)	O(1)-C(14)-C(13)	106 8(2)
C(2)-C(3)-C(4)	112 1(2)	O(1)-C(14)-C(15)	108 5(2)
O(4)-C(4)-C(3)	109 3(2)	C(13)-C(14)-C(15)	112 6(2)
O(4)-C(4)-C(5)	110 3(2)	O(15)-C(15)-C(14)	110 6(2)
C(3)-C(4)-C(5)	109 6(2)	O(15)-C(15)-C(16)	109 4(2)
O(5)-C(5)-C(4)	109 7(2)	C(14)-C(15)-C(16)	112 3(2)
O(5)-C(5)-C(6)	107 4(2)	O(16)-C(16)-C(15)	112 3(2)
C(14)-O(1)-C(1)-O(5)	−56 7(3)	O(4)-C(4)-C(5)-C(6)	−55 5(3)
C(14)-O(1)-C(1)-C(2)	−175 4(2)	C(3)-C(4)-C(5)-O(5)	−56 5(2)
C(1)-O(1)-C(14)-C(13)	131 8(2)	C(3)-C(4)-C(5)-C(6)	−175 9(2)
C(1)-O(1)-C(14)-C(15)	−106 7(2)	O(5)-C(5)-C(6)-O(6)	72 3(2)
C(5)-O(5)-C(1)-O(1)	179 6(2)	C(4)-C(5)-C(6)-O(6)	−166 9(2)
C(5)-O(5)-C(1)-C(2)	−65 0(2)	O(11)-C(11)-C(12)-O(12)	73 3(3)
C(1)-O(5)-C(5)-C(4)	65 7(2)	O(11)-C(11)-C(12)-C(13)	−47 3(3)
C(1)-O(5)-C(5)-C(6)	−171 9(2)	O(12)-C(12)-C(13)-O(13)	50 0(3)
O(1)-C(1)-C(2)-O(2)	−67 6(2)	O(12)-C(12)-C(13)-C(14)	171 6(2)
O(1)-C(1)-C(2)-C(3)	173 4(2)	C(11)-C(12)-C(13)-O(13)	169 0(2)
O(5)-C(1)-C(2)-O(2)	174 3(2)	C(11)-C(12)-C(13)-C(14)	−69 4(3)
O(5)-C(1)-C(2)-C(3)	55 4(2)	O(13)-C(13)-C(14)-O(1)	55 9(2)
O(2)-C(2)-C(3)-O(3)	66 0(2)	O(13)-C(13)-C(14)-C(15)	−63 0(2)
O(2)-C(2)-C(3)-C(4)	−169 2(2)	C(12)-C(13)-C(14)-O(1)	−65 4(3)
C(1)-C(2)-C(3)-O(3)	−173 3(2)	C(12)-C(13)-C(14)-C(15)	175 7(2)
C(1)-C(2)-C(3)-C(4)	−48 5(3)	O(1)-C(14)-C(15)-O(15)	−168 0(2)
O(3)-C(3)-C(4)-O(4)	51 8(3)	O(1)-C(14)-C(15)-C(16)	69 5(2)
O(3)-C(3)-C(4)-C(5)	172 8(2)	C(13)-C(14)-C(15)-O(15)	−50 1(2)
C(2)-C(3)-C(4)-O(4)	−71 9(3)	C(13)-C(14)-C(15)-C(16)	−172 6(2)
C(2)-C(3)-C(4)-C(5)	49 0(3)	O(15)-C(15)-C(16)-O(16)	55 2(3)
O(4)-C(4)-C(5)-O(5)	63 9(3)	C(14)-C(15)-C(16)-O(16)	178 3(2)

using the ω–2θ scan technique (h. $0 \leqslant 11$, k. $0 \leqslant 11$, l: $0 \leqslant 59$; $2\theta_{max} = 55°$) of which, after merging equivalent reflections, 2017 unique reflections remained with I above the $2.5\sigma(I)$ level. Two standard reflections (211 and $2\bar{1}1$) measured every hour showed insignificant variations. Intensities were corrected for Lorentz and polarization effects, but not for absorption

TABLE 4

Geometry of the hydrogen bonds of lactitol dihydrate

Donor	Acceptor	D---A (Å)	D–H (Å)	H---A (Å)	D–H---A (deg)	Sym op[a]
O(2)–H	O(12)	2 806(3)	0 85(3)	2 08(3)	144(2)	2 545
O(3)–H	O(11)	2 702(3)	0 94(3)	1 78(3)	167(2)	1 545
O(4)–H	O(111)	2 798(3)	0 83(3)	1 98(3)	166(3)	1 645
O(6)–H	O(16)	2 669(3)	0 91(3)	1 76(3)	173(2)	1 655
O(11)–H	O(13)	2 739(2)	0 67(3)	2 08(3)	167(4)	2 655
O(12)–H	O(4)	3 007(2)	0 74(3)	2 27(3)	170(3)	2 645
O(13)–H	O(15)	2 734(2)	0 77(3)	1 97(3)	172(3)	2 555
O(15)–H	O(2)	2 922(2)	0 64(3)	2 58(3)	117(4)	1 565
O(15)–H	O(3)	3 008(2)	0 64(3)	2 37(3)	172(4)	1 565
O(16)–H	O(111)	2 736(2)	0 86(4)	1 98(3)	168(3)	1 555
O(111)–H	O(112)	2 686(3)	0 83(3)	1 86(3)	172(3)	3 465
O(111)–H	O(2)	2 860(3)	0 77(3)	2 11(3)	169(4)	1 565
O(112)–H	O(6)	2 769(3)	0 91(3)	1 87(3)	175(3)	1 555
O(112)–H	O(3)	2 788(3)	0 79(3)	2 02(3)	164(3)	1 565

[a]The symmetry operation is performed on the acceptor oxygen atom The first digit indicates one of the following symmetry operations (1) x,y,z, (2) $y,x,-z$, (3) $0\,5+x, 0\,5-y, 0\,25-z$ The last set of numbers specifies the lattice translations, e g 1 645 is a-b translated from 1 555

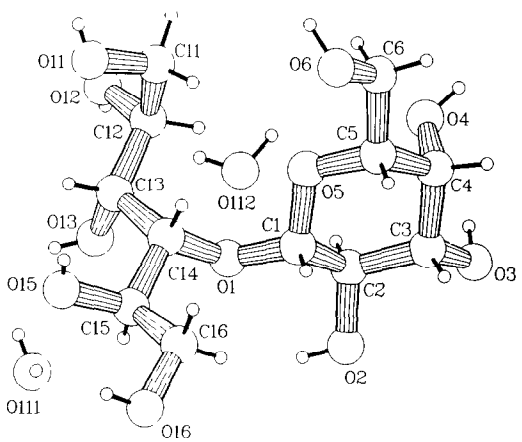

Fig 1 Perspective view of lactitol dihydrate with adopted numbering scheme

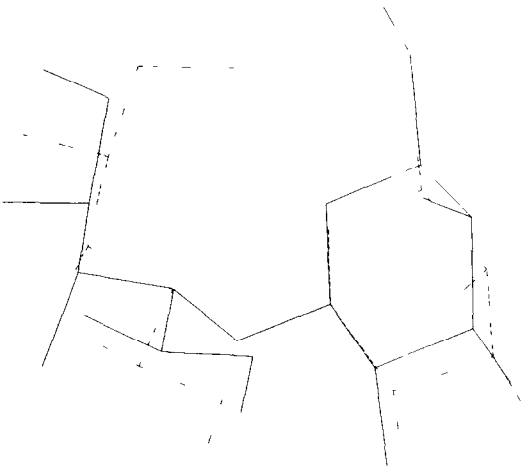

Fig 2 Molecular superposition of the lactitol fragments of the monohydrate (- - -) and dihydrate (—) by a least-squares fit of atoms C(1), O(1) and C(14) of the glycosidic linkage

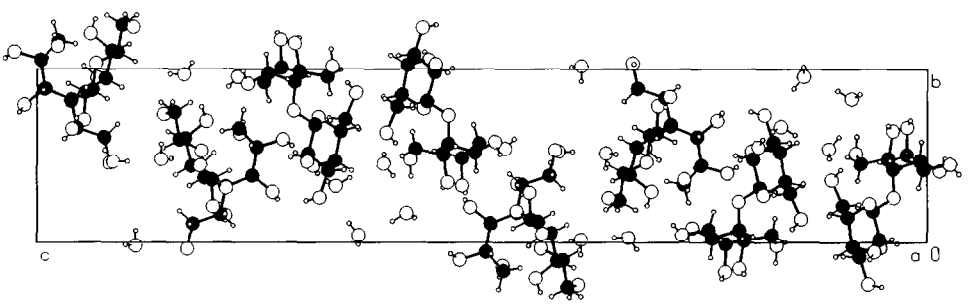

Fig 3 View of the contents of the unit cell of lactitol dihydrate along the *a* axis

Structure analysis and refinement

The structure was solved by direct routine methods of MULTAN-78 [8] and refined by full-matrix least-squares using XRAY-76 [9] All hydrogen atoms were located from difference Fourier maps and were included in the refinement with fixed isotropic thermal parameters equal to those of the carrier atoms Refinement of 310 parameters, including scale factor, coordinates and anisotropic thermal parameters of carbon and oxygen atoms and coordinates of the hydrogen atoms, converged at R and R_w values of 0 037 and 0 049, respectively The quantity minimized was $\Sigma w(|F_o|-|F_c|)^2$ with $w=[\sigma^2(F_o)+0\ 0004F_o^2]^{-1}$ Minimum and maximum residual densities in the final Fourier map amount to $-0\ 30$ and $+0\ 25$ e Å^{-3} respectively Scattering

factors for carbon and oxygen were taken from Stewart et al. [10] and for hydrogen from Cromer and Mann [11]

Results

Final positional parameters and equivalent isotropic thermal parameters of carbon and oxygen atoms are given in Table 1 and the coordinates of the hydrogen atoms are given in Table 2 The bond lengths, angles and torsion angles are listed in Table 3 and the hydrogen-bond geometries are summarized in Table 4. A perspective view of the molecule with adopted numbering is shown in Fig 1, a molecular fit of the lactitol molecules of the monohydrate and dihydrate at the atoms of the glycosidic link is shown in Fig 2 and Fig 3 shows the contents of the unit cell as seen along the *a* axis. Non-hydrogen atom anisotropic thermal parameters and listings of observed and calculated structure factors are available as supplementary data (B L L D Supplementary Publication number S U.P 26395 (12 pages))

DISCUSSION

Bond lengths and angles

The C–C bond lengths are in the range 1 507(4)–1 536(4) Å and the three terminal C–C bonds display a significant shortening, which has also been observed in analogous cellobiotol [1], maltitol [2], isomaltitol [3], in many pyranosides [12] and in some alditols [13] The C–O bonds range from 1 392(3) to 1 442(2) Å The anomeric C(1)–O(1) bond is shortened as is commonly observed in β-pyranosides [12] The C–O distances of the acetal sequence of bonds C(1)–O(5)–C(5) differ by 0 014 Å, whereas in the monohydrate the difference is negligible, this is in accordance with the observation that in β-pyranosides the differences are much smaller than in α-pyranosides [14, 15]

The C–C–C and C–C–O angles are in the range 109 6(2)–112 6(2)° and 105 3(2)–112 3(2)°, respectively The C(1)–O(1)–C(14) angle of the glycosidic link (118 0(2)°) is very close to the corresponding angle of the monohydrate (118 2(2)°), but significantly different from those of cellobiotol (115 4(3)°) [1] and galactosyl-rhamnitol (115 8(1)°) [4] and also well outside the range 115 8–117 1° reported for six β-(1→4)-linked disaccharides [16] The average differences between the corresponding distances and angles of the monohydrate and dihydrate are 0 007 Å and 1 4°, respectively In particular, the angles O(11)–C(11)–C(12), C(13)–C(12)–O(12) and C(12)–C(13)–C(14) of the glucitol chain differ appreciably· 4 5°, 5 3° and 4 1°, respectively The C–H distances average to 0 97 Å, the O–H distances average to 0 81 Å and the angles involving hydrogen atoms average to 109 1°

Molecular conformation

The endocyclic ring torsion angles are in the range 48.5(3)–65 7(2)° and the six-membered ring has a slightly distorted $^4C_1$ chair conformation as follows from the Cremer and Pople [17] puckering parameters θ and ϕ which are 8.2(2)° and 350(2)°, respectively. The exocyclic torsion angles all have values which are close to the ideal *gauche* or *trans* conformations; the average deviation is 7.3° The conformation of the exocyclic C(6)–O(6) bond is *gauche–trans* as in β-D-galactose and in the majority of galactosyl-pyranosides [18]. The pyranosyl fragment conformations of the monohydrate and dihydrate are very similar, the average deviations of the corresponding endocyclic and exocyclic torsion angles are 1 9° and 2.5°, respectively.

The glucitol carbon-atom chain has a non-planar, bent *MAA** conformation which results from a 120° rotation about C(12)–C(13), thus avoiding the unfavourable conformation with parallel C(12)–O(12)/C(14)–O(1) bonds [20]. The *MAA* conformation is also present in the monohydrate [6], the *A* form of D-glucitol [21], the D-glucitol–pyridine complex [22] and isomaltitol [3]. Cellobiotol [1] adopts the unfavourable, bent *MAP** conformation with almost parallel C(13)–O(13)/C(15)–C(16) bonds and maltitol [2] has the alternative *APP* conformation [20] which also avoids parallel C(12)–O(12)/C(14)–O(1) alignment by rotations of 120° about C(13)–C(14) and C(14)–C(15) The orientations of the terminal C–O bonds, C(11)–O(11) and C(16)–O(16), in the three glycosyl-glucitols and the two D-glucitol-containing structures show a variety of possible conformations with respect to the carbon-atom chain, which may be denoted as extended–extended, extended–bent, bent–extended and bent–bent. In cellobiotol [1], isomaltitol [3] and D-glucitol [21], the orientations are both extended, in maltitol [2] they are extended and bent respectively, in the D-glucitol–pyridine complex [22] they are both bent and in lactitol monohydrate [6] and the title compound they are bent and extended respectively The bent conformations of the C(11)–O(11) bonds in the monohydrate and dihydrate are different in that the former is *Psc** (torsion angle O(11)–C(11)–C(12)–C(13) 75 5(2)°) and the latter is *Msc** (−47 3(3)°) The *Psc* conformation of the monohydrate enables the formation of an intramolecular C(11)–H---O(6) hydrogen bond, which is not possible in the dihydrate because of the *Msc* orientation of the C(11)–O(11) bond

With the exception of the torsion angles about C(1)–O(1), O(1)–C(14) and C(11)–C(12), the corresponding torsion angles of the monohydrate and dihydrate show good agreement, the average difference being 3 3°

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*M, A and P refer to the conformation about the C–C bonds $M = Msc$, $A = ap$ and $P = Psc$ according to the convention of Klyne and Prelog [19]

Glycosidic linkage

The torsion angles characterizing the glycosidic linkage, φ_1 (O(5)–C(1)–O(1)–C(14)) and φ_2(C(1)–O(1)–C(14)–C(13)), are −56 7(3)° and 131 8(2)°, respectively. The angle φ_1 is the smallest so far observed in the class of β-(1→4)-linked glycosyl-alditols, cellobiotol (−68.2(4)°) [1] and galactopyranosyl-rhamnitol (−70 8(2)°) [4], and its value also deviates substantially from those observed in the monohydrate (−86.3(3)°) [6] and from the average of −84.9° observed in 14 β-(1→4)-linked disaccharides [23] The angle φ_2 implies a nearly eclipsed C(1)–O(1)–C(14)–H conformation (torsion angle 11(1)°), which is commonly observed in glycosyl-alditols [3] and in β-(1→4)-linked disaccharides [3].

A molecular fit of the monohydrate and dihydrate (Fig 2) at the atoms C(1), O(1) and C(14) of the link gives a view of the differences between the molecular conformations of the two lactitol modifications

Hydrogen bonding

All 13 potential hydrogen-bond donors are involved in a complex three-dimensional system of hydrogen bonds (Table 4). With the exception of ring O(5) and glycosidic link O(1), which do not accept a hydrogen bond, and O(2), O(3) and water O(111), which are double acceptors, the oxygen atoms act as single acceptors. One donor, O(15)–H forms an asymmetric, bifurcated intermolecular hydrogen bond with a four-atom planar configuration; the sum of angles about the central hydrogen atom is 359(3)°. The donor–acceptor distances span a wide range of 2 669(3) to 3.008(2) Å. The water molecules play a dominant role in the hydrogen-bond pattern by each donating two hydrogen bonds and accepting two (O(111)) and one (O(112)) hydrogen bond, respectively.

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