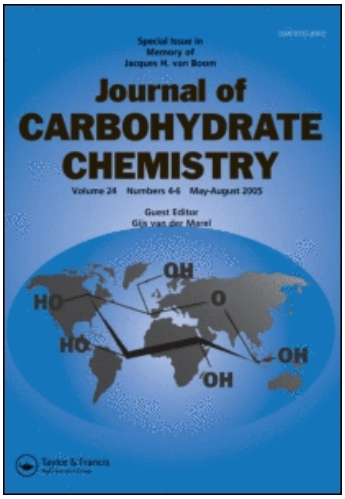

Journal of Carbohydrate Chemistry
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713617200

THE CRYSTAL STRUCTURES OF d-PINITOL AND l-QUEBRACHITOL BY LOW-TEMPERATURE X-RAY DIFFRACTION

Michael K. Dowd[a]; Edwin D. Stevens[b]
[a] Southern Regional Research Center, ARS, USDA, New Orleans, Lousiana, USA [b] Department of Chemistry, University of New Orleans, New Orleans, Lousiana, USA

Online publication date: 16 September 2002

To cite this Article Dowd, Michael K. and Stevens, Edwin D.(2002) 'THE CRYSTAL STRUCTURES OF d-PINITOL AND l-QUEBRACHITOL BY LOW-TEMPERATURE X-RAY DIFFRACTION', Journal of Carbohydrate Chemistry, 21: 5, 373 — 383
To link to this Article: DOI: 10.1081/CAR-120014901
URL: http://dx.doi.org/10.1081/CAR-120014901

MARCEL DEKKER, INC. • 270 MADISON AVENUE • NEW YORK, NY 10016

JOURNAL OF CARBOHYDRATE CHEMISTRY
Vol. 21, No. 5, pp. 373–383, 2002

THE CRYSTAL STRUCTURES OF D-PINITOL AND L-QUEBRACHITOL BY LOW-TEMPERATURE X-RAY DIFFRACTION

Michael K. Dowd[1,*] and Edwin D. Stevens[2]

[1]Southern Regional Research Center, ARS, USDA,
1100 Robert E. Lee Blvd., New Orleans, Louisiana, USA
[2]Department of Chemistry, University of New Orleans,
New Orleans, Louisiana, USA

ABSTRACT

The crystal and molecular structures of D-pinitol and L-quebrachitol were determined from low temperature x-ray diffraction data. Pinitol crystallizes in an orthorhombic system, $P2_12_12_1$ ($Z=4$), with unit cell dimensions of $a=$ 6.8345(8) Å, $b=9.3233(10)$ Å, and $c=12.8911(14)$ Å. Quebrachitol crystallizes in a monoclinic system, $P2_1$ ($Z=2$), with unit cell dimensions of $a=6.6289(4)$ Å, $b=7.1895(4)$ Å, $c=8.6843(5)$ Å, and $\beta=90.5690(10)°$. No unusual bond lengths or valence angles are present within either structure. Both rings are in chair conformations, with the majority of the pendent groups in equatorial orientations. As found for many compounds with multiple hydroxyl groups, the structures have extensive networks of hydrogen bonds. Both structures have infinite chain sequences of hydrogen bonds incorporating the O-1 and O-4 hydroxyl groups and finite chain sequences incorporating the other hydroxyl groups.

*Corresponding author. Fax: 504-286-4367; E-mail: mkdowd@srrc.ars.usda.gov

DOI: 10.1081/CAR-120014901 0732-8303 (Print); 1532-2327 (Online)

INTRODUCTION

Cyclitols and polyols are found throughout the plant kingdom. One role of these compounds is to help plants survive adverse environmental conditions. D-Pinitol (3-methyl-D-*chiro*-inositol) has been widely studied in this regard.[1–8] The compound has been found to accumulate in many plants during periods of elevated temperature and drought.[1–4] It is also found in high concentrations in halophytes, and it accumulates in salt tolerant plants when exposed to elevated salt concentrations.[6–8] Because pinitol has been shown to act as a hypoglycemic agent in mice,[9] it is of medical interest and has been patented for its ability to alleviate symptoms associated with diabetes.[10,11] L-Quebrachitol (2-methyl-L-*chiro*-inositol) is also a natural plant product. It occurs in high concentration in rubber trees (*Heava brasiliensis*) and is conveniently isolated from latex waste liquor.[12–14] Several biologically active classes of compounds, including other inositols, L- and pseudo-monosaccharides, aminoglycoside- and aminocycitol-based antibiotics, and compounds functioning as enzyme inhibitors, have been synthesized from quebrachitol.[13]

A recent survey of the Cambridge Crystal Structure Database[15] indicated that the only structural information available for the monomethylated inositols was for sequoyitol (5-methyl-*myo*-inositol).[16] A room temperature diffraction study of L-quebrachitol has been reported,[17] but hydrogen coordinates were not refined and hydrogen bonding was not discussed. To increase the information available for methylated cyclitols, single crystals of D-pinitol and L-quebrachitol were prepared, and their structures were determined by x-ray diffraction at low temperature.

METHODS

Both compounds were purchased from Sigma–Aldrich Chemical Co. (St. Louis, MO, USA). Initial attempts at forming crystals by diffusing acetone into an aqueous pinitol solution resulted in microcrystals that were unsuitable for diffraction. Inspection of the process revealed that a reddish-brown impurity coprecipitated with the addition of acetone and promoted the nucleation of pinitol. The contaminant was removed by repeated fractional crystallizations from the same solvents. Diffusion of acetone into an aqueous solution of the purified compound yielded small, wedge-shaped, octahedral crystals, similar in shape to those pictured by Lee and Morris.[18] A crystal 0.08 mm × 0.08 mm × 0.2 mm was selected for diffraction.

Large rod-shaped crystals of L-quebrachitol were easily prepared from the same solvents. The crystal selected for diffraction was cut to 0.25 mm × 0.4 mm × 0.6 mm.

Diffraction data were collected for both compounds at 150(2) K with a Siemens diffractometer fitted with a graphite monochromator (MoKα, $\lambda = 0.71073$ Å) and a SMART 1K CCD detector. The SHELXTL NT system (version 5.10) was used for structure solution and refinement. After data collection, the individual data frames were integrated, and Lorenz, polarization, and adsorption corrections were applied. Direct methods were used to obtain the initial structures (SHELXS-97), and both structures were refined by full-matrix least-squares optimization of F^2 over all unique reflections (SHELXL-97). Hydrogen atoms were located from difference maps and were refined with an isotropic model. A small correction for extinction was included in the re-

Table 1. Crystal and Diffraction Data for D-Pinitol (**1**) and L-Quebrachitol (**2**)

	1	**2**
Crystal data		
Empirical formula, weight	$C_7H_{14}O_6$, 194.18	$C_7H_{14}O_6$, 194.18
Color, habit	colorless, wedge shaped	colorless, cube shaped
Size, mm	$0.08 \times 0.08 \times 0.2$	$0.25 \times 0.4 \times 0.6$
Crystal system	orthorhombic	monoclinic
Space group	$P2_12_12_1$	$P2_1$
Symmetry	$x, y, z;\ 1/2-x, -y, 1/2+z;\ 1/2+x, 1/2-y, -z;$ $-x, 1/2+y, 1/2-z$	$x, y, z;\ -x, 1/2+y, -z$
Unit cell dimensions, Å	$a=6.8345(8)$, $b=9.3233(10)$, $c=12.8911(14)$	$a=6.6289(4)$, $b=7.1895(4)$, $c=8.6843(5)$
Unit cell angles, °	$\alpha=\beta=\gamma=90$	$\alpha=\gamma=90$, $\beta=90.5690(10)$
Volume, Å^3	821.42(16)	413.86(4)
Z	4	2
Density (calc.), g/cm^3	1.5702(3)	1.5583(2)
Absorption coef., mm^{-1}	0.138	0.137
F(000)	416	208
Data collection		
Radiation	MoKα, $\lambda=0.71073$ Å	MoKα, $\lambda=0.71073$ Å
Temperature, K	150(2)	150(2)
Source	graphite monochromator	graphite monochromator
Detector	CCD area detector	CCD area detector
2θ range	5.40 to 52.78	6.14 to 69.00
Index range	$-8<h<8;\ -11<k<11;\ -16<l<16$	$-10<h<10;\ -11<k<11;\ -13<l<13$

(*continued*)

MARCEL DEKKER, INC. • 270 MADISON AVENUE • NEW YORK, NY 10016

Table 1. Continued

Reflections collected	8616	8403
Unique reflections	1698	3360
Obs. reflections ($>2\sigma(I)$)	722	3206
R_{int}	0.0674	0.0289
Completeness to 2θ, %	100	97.7
Absorption correction	empirical $T_{min} = 0.85129$; $T_{max} = 1.00000$	empirical $T_{min} = 0.77710$; $T_{max} = 1.00000$
Refinement		
System used	SHELXTL NT, version 5.1	SHELXTL NT, version 5.1
Solution method	direct methods, SHELXL-97	direct methods, SHELXL-97
Refinement method	full-matrix least-squares on F^2	full-matrix least-squares on F^2
Weighting scheme	$w = 1/[\sigma^2(F_o^2) + (0.005P)^2]$, where $P = (F_o^2 + 2F_c^2)/3$	$w = 1/[\sigma^2(F_o^2) + (0.077P)^2]$, where $P = (F_o^2 + 2F_c^2)/3$
Extinction correction	none	$k = 0.039(12)$, where $F_c = F_c\ k\ [1 + 0.001F_c^2\lambda^3/\sin(2\theta)]^{-1/4}$
Hydrogen atoms	mixed	mixed
Flack parameter	− 1.6(1.4)	− 0.1(5)
Parameters refined	174	175
Final R indices (obs.)	$R_1 = 0.0261$, $wR_2 = 0.0296$	$R_1 = 0.0353$, $wR_2 = 0.0896$
Final R indices (all data)	$R_1 = 0.0626$, $wR_2 = 0.0314$	$R_1 = 0.0373$, $wR_2 = 0.0912$
GOF	0.467	1.085
Largest residual peak, $e/\text{Å}^3$	0.163	0.368
Largest residual hole, $e/\text{Å}^3$	− 0.138	− 0.309
RMS diff., $e/\text{Å}^3$	0.035	0.078

finement of L-quebrachitol. A summary of the crystal and diffraction data and the refinement methods used for the structure determinations is given in Table 1.

RESULTS AND DISCUSSION

Fractional coordinates and equivalent temperature factors for the two compounds are given in Tables 2 and 3, and ORTEP representations of the structures are shown in Figures 1 and 2. For the D-pinitol structure, the carbon–carbon bond lengths vary from 1.516(4) to 1.540(4) Å; the carbon–oxygen bond lengths vary from 1.413(3) Å to 1.436(3) Å; and the non-hydrogen atom valance angles vary from 107.6(2) to 114.9(2)°. Similar bond lengths and valence angles exist within the L-quebrachitol structure. The variation for these distances and angles is comparable to the variation of the same parameters for the room-temperature L-quebrachitol structure[16] and the nonmethylated L-*chiro*-inositol structure.[19]

Table 2. Fractional Coordinates ($\times 10^4$) and Equivalent or Isotropic Displacement Parameters ($Å^2 \times 10^3$) for the Atom Coordinates of D-Pinitol

	x	y	z	U_{eq},[a] U_{iso}
C-1	8362(4)	− 65(3)	932(2)	11.2(7)
C-2	6663(3)	− 856(3)	438(2)	12.1(7)
C-3	4925(4)	139(3)	197(2)	11.4(6)
C-4	4314(4)	963(3)	1164(2)	10.0(7)
C-5	6035(4)	1816(3)	1600(2)	11.0(7)
C-6	7727(4)	835(3)	1875(2)	11.8(7)
C-7	2920(5)	− 642(4)	1236(2)	21.1(8)
O-1	9180(3)	880(2)	173(2)	17.6(6)
O-2	7217(3)	− 1516(2)	− 517(1)	16.7(5)
O-3	3274(2)	− 679(2)	− 141(1)	14.2(5)
O-4	2677(3)	1881(2)	950(1)	14.9(5)
O-5	5524(3)	2613(2)	2492(2)	15.9(5)
O-6	7215(3)	− 136(2)	2696(1)	15.8(5)
H-1	9370(30)	− 770(20)	1216(15)	0(6)
H-2	6090(30)	− 1570(20)	966(14)	0(6)
H-3	5240(30)	760(20)	− 382(16)	9(7)
H-4	3870(30)	340(20)	1694(15)	0(7)
H-5	6410(30)	2480(20)	1026(14)	0(6)
H-6	8800(30)	1450(20)	2108(14)	0(7)
H-11	10120(30)	1070(30)	311(19)	5(9)
H-12	7470(40)	− 2230(20)	− 433(19)	23(11)
H-14	2990(30)	2540(20)	678(15)	0(8)
H-15	4540(40)	3120(20)	2321(19)	23(10)
H-16	7130(50)	240(30)	3162(16)	25(11)
H-7a	1760(30)	− 790(30)	− 1400(20)	26(9)
H-7b	3670(30)	− 1320(20)	− 1544(16)	5(8)
H-7c	3190(30)	460(30)	− 1630(18)	59(10)

[a]For non-hydrogen atoms, U_{eq} is 1/3 of the trace of the orthogonalized U_{ij} tensor.

MARCEL DEKKER, INC. • 270 MADISON AVENUE • NEW YORK, NY 10016

Table 3. Fractional Coordinates ($\times 10^4$) and Equivalent or Isotropic Displacement Parameters ($Å^2 \times 10^3$) for the Atom Coordinates of L-Quebrachitol

	x	y	z	U_{eq},[a] U_{iso}
C-1	8398(1)	5550(1)	2858(1)	11.0(1)
C-2	6454(1)	4469(1)	2513(1)	11.1(1)
C-3	6860(1)	2818(1)	1455(1)	11.8(1)
C-4	8506(1)	1549(1)	2140(1)	11.9(1)
C-5	10433(1)	2641(1)	2508(1)	12.0(1)
C-6	9976(1)	4255(1)	3586(1)	11.5(1)
C-7	4383(1)	7182(1)	2685(1)	18.8(2)
O-1	9197(1)	6324(1)	1469(1)	15.1(1)
O-2	4953(1)	5604(1)	1783(1)	16.0(1)
O-3	5037(1)	1795(1)	1242(1)	17.1(1)
O-4	8880(1)	42(1)	1114(1)	17.1(1)
O-5	11908(1)	1441(1)	3192(1)	17.0(1)
O-6	9239(1)	3503(1)	4989(1)	15.2(1)
H-1	8190(20)	6540(30)	3570(16)	16(3)
H-2	5910(20)	4070(30)	3503(16)	14(3)
H-3	7320(20)	3250(20)	397(15)	11(3)
H-4	7910(30)	990(30)	3090(20)	30(4)
H-5	10990(20)	3150(20)	1547(17)	14(3)
H-6	11250(20)	4960(30)	3760(20)	27(4)
H-11	8990(30)	7630(30)	1440(20)	34(5)
H-13	5080(20)	1330(30)	380(17)	18(3)
H-14	9540(40)	500(40)	210(30)	68(8)
H-15	12950(20)	1470(30)	2640(20)	24(4)
H-16	8950(30)	4200(40)	5630(30)	45(5)
H-7a	3020(20)	7510(30)	2280(18)	22(4)
H-7b	4250(20)	6850(30)	3803(18)	24(4)
H-7c	5340(30)	8200(40)	2517(20)	28(4)

[a]For non-hydrogen atoms, U_{eq} is 1/3 of the trace of the orthogonalized U_{ij} tensor.

Both compounds have similar ring conformations. The ring form of D-pinitol is $^4C_1$ with Cremer-Pople (C-P) puckering coordinates of $q = 0.563(3)$ Å, $\theta = 175.1(3)°$, and $\phi = 20(3)°$. Because of the difference in absolute configuration, the ring form of L-quebrachitol is $^1C_4$ with puckering coordinates of $q = 0.587(1)$ Å, $\theta = 2.8(1)°$, $\phi = 319(2)°$. Both conformations place four of the pendant groups, including the methoxy group, in equatorial positions and two of the hydroxyl units in axial positions. After accounting for absolute configuration, the ring conformations of these compounds are similar to the ring conformation of L-*chiro*-inositol ($q = 0.561$ Å, $\theta = 4.4°$, $\phi = 51.2°$).[19] The NMR coupling constants of both compounds indicate that the same ring forms are found in solution.[20–22]

All of the hydroxyl groups of each structure participate in hydrogen bonds (Tables 4 and 5). For D-pinitol, one three-center bond is found, with the O-5 hydroxyl hydrogen donating intramolecularly to the O-4 oxygen atom and intermolecularly to an O-6 oxygen atom. Because of steric constraints, the intramolecular component of this bond is very weak, as indicated by the small O–H···O angle of 110(2)° (Table 4). The

MARCEL DEKKER, INC. • 270 MADISON AVENUE • NEW YORK, NY 10016

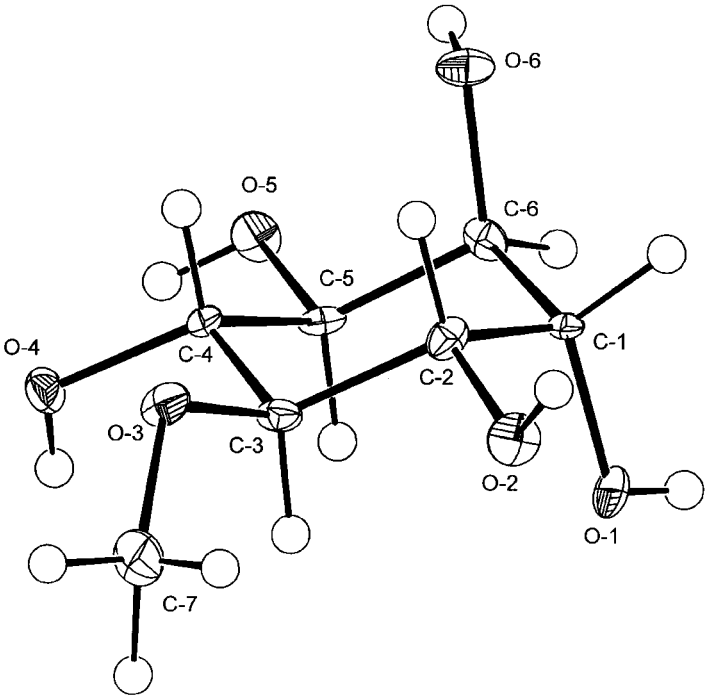

Figure 1. ORTEP diagram of D-pinitol.

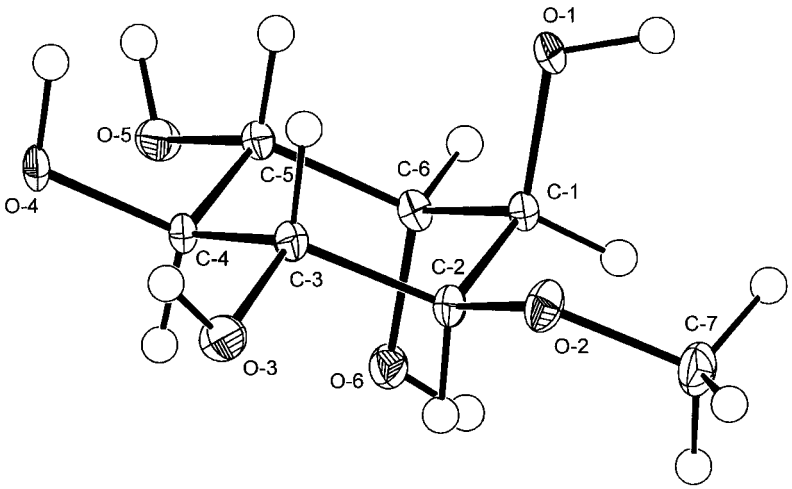

Figure 2. ORTEP diagram of L-quebrachitol.

Table 4. Hydrogen Bonding Within Crystalline D-Pinitol

Bond	Acceptor Symmetry Code[a]	d(D–H) Å	d(H···A) Å	d(D···A) Å	∠(D–H···A)°
O1–H11···O4	1655	0.69(2)	2.07(2)	2.754(3)	169(3)
O2–H12···O3	3545	0.70(2)	2.16(2)	2.843(2)	169(3)
O4–H14···O1	3455	0.74(2)	2.01(2)	2.740(3)	170(2)
O5–H15···O4	1555	0.85(2)	2.47(2)	2.865(3)	110(2)
O5–H15···O6	4655	0.85(2)	2.02(2)	2.823(3)	157(2)
O6–H16···O2	2655	0.70(2)	2.13(2)	2.799(3)	162(4)

[a]Symmetry code for related molecules. Codes are defined as nxyz, where n = identifies the asymmetric unit within the cell ($1 = x, y, z$; $2 = 1/2 - x, -y, 1/2 + z$; $3 = 1/2 + x, 1/2 - y, -z$; $4 = -x, 1/2 + y, 1/2 - z$), and z, y, z represent the unit cell position relative to a central cell of 555.

intramolecular interaction does not appear to have a significant influence on the intermolecular interaction, as this hydrogen bond has typical distances and angles (Table 4). No multi-center hydrogen bonds are present within the L-quebrachitol structure.

Including the intramolecular bond, pinitol has a hydrogen bond network consisting of an infinite chain, which extends along the **a** coordinate direction, and a finite branch chain (Figure 3). The infinite chain is composed of a sequence of hydrogen bonds between the O-4 and O-1 hydroxyl groups, and the branch is attached to the infinite chain at the O-4 oxygen atom. The branch terminates at the methylated oxygen atom (O-3). For quebrachitol, the network also consists of one infinite chain, which extends along the **b** coordinate direction, and one finite chain (Figure 4). As for pinitol, the infinite chain is composed of alternating O-4 and O-1 hydroxyl groups, and the finite chain is composed of the other hydroxyl groups. The finite chain also ends at the methylated oxygen atom (O-2). Because there is no multi-center hydrogen bond within the network, no branching exists and the two chains are separate.

Extended networks of hydrogen bonds are found within the crystal structures of carbohydrates and polyols.[23] These networks are proposed to be energetically favored because of the stabilizing influence of hydrogen bond cooperativity. Multi-center hy-

Table 5. Hydrogen Bonding Within Crystalline L-Quebrachitol

Bond	Acceptor Symmetry Code[a]	d(D–H) Å	d(H···A) Å	d(D···A) Å	∠(D–H···A)°
O1–H11···O4	1565	0.95(3)	1.76(3)	2.699(1)	170(2)
O3–H13···O2	2645	0.82(2)	1.95(2)	2.763(1)	171(2)
O4–H14···O1	2745	0.96(3)	1.79(3)	2.750(1)	179(3)
O5–H15···O3	1655	0.84(2)	1.86(2)	2.702(1)	171(2)
O6–H16···O5	2756	0.77(3)	2.00(3)	2.749(1)	165(3)

[a]Symmetry code for related molecules. Codes are defined as nxyz, where n = identifies the asymmetric unit with the cell ($1 = x, y, z$; $2 = -x, 1/2 + y, -z$), and x, y, z represent the unit cell position relative to a central cell of 555.

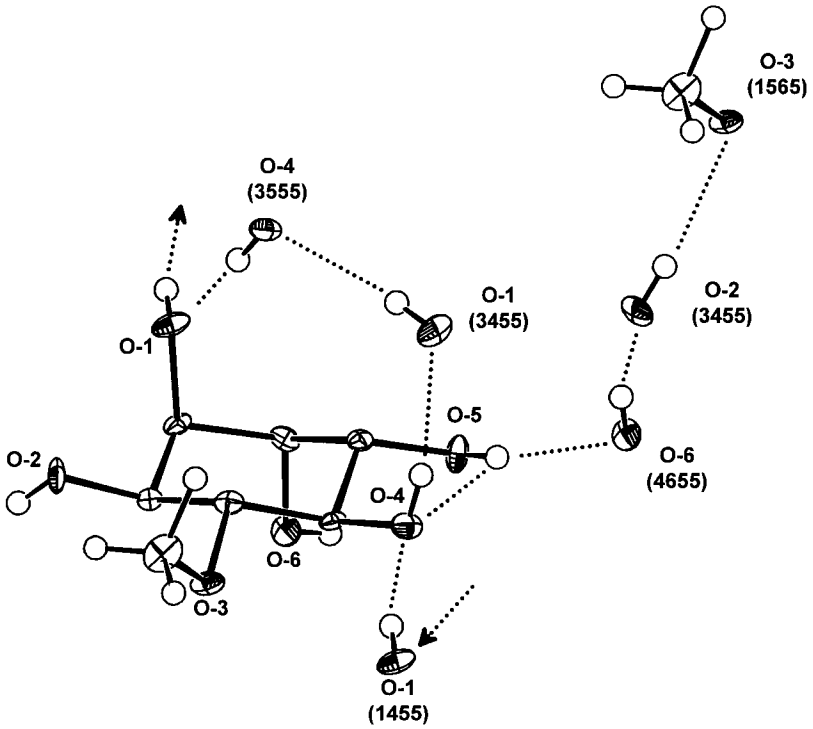

Figure 3. Network of hydrogen bonding within the D-pinitol crystal structure. Symmetry code definitions are defined in the footnote of Table 4. Arrows denote the infinite chain network.

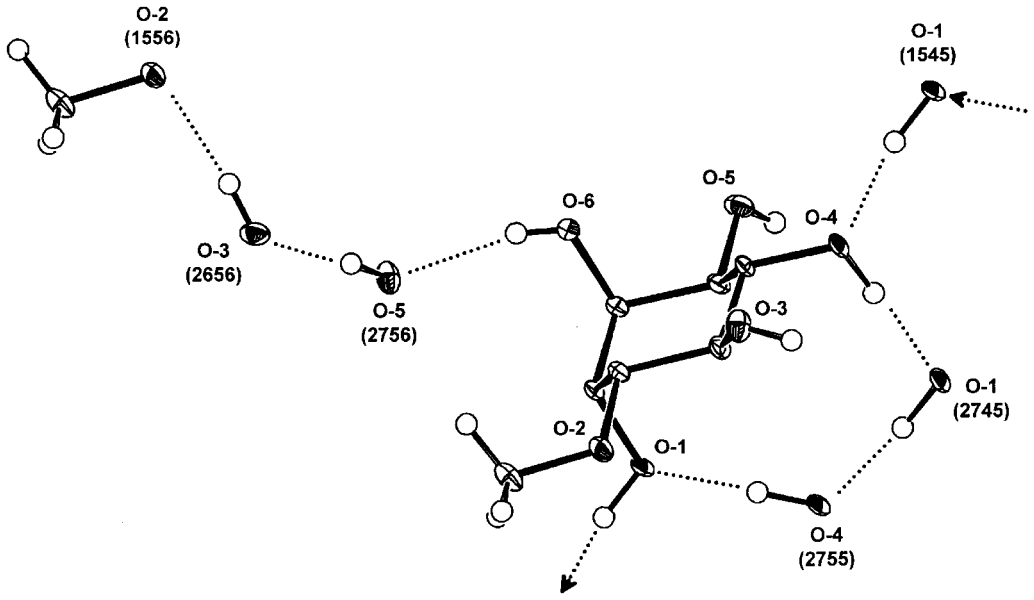

Figure 4. Network of hydrogen bonding within the L-quebrachitol crystal structure. Symmetry code definitions are defined in the footnote of Table 5. Arrows denote the infinite chain network.

drogen bonds are also observed for these compounds. These are favored because the cross-linking of the hydrogen bond networks further contributes to the cooperativity effect. In general, pyranosyl and furanosyl rings and the corresponding methyl glycosides exhibit both infinite and finite chains. Because the ring ethereal and methyl glycoside oxygen atoms can only act as hydrogen bond acceptors, finite chains occur frequently for these compounds. The networks of the methylated derivatives of *chiro*-inositol are characteristically similar to the networks of monosaccharides and their methyl glycosides.

In contrast, the hydrogen bond networks of linear polyols consist principally of infinite chains often with multi-center bonds.[23] The hydrogen bond network of L-*chiro*-inositol consists of a single infinite chain incorporating all six hydroxyl groups and one three-center bond[18] and is characteristically similar to the hydrogen bond networks of the non-cyclic polyols.

The crystallographic data for both structures have been deposited with the Cambridge Crystallographic Data Centre. The supplementary publication numbers are CCDC #172582 for D-pinitol and CCDC #172583 for L-quebrachitol. Copies of the data can be obtained, free of charge, on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (Fax: +44-1223-336033 or e-mail: deposit@ccdc.cam.ac.uk), or the data can be obtained from the authors.

REFERENCES

1. Ford, C.W. Accumulation of low molecular weight solutes in water-stressed tropical legumes. Phytochemistry **1984**, *23* (5), 1007–1015.
2. Nquyen, A.; Lamant, A. Pinitol and *myo*-inositol accumulation in water-stressed seedlings of maritime pine. Phytochemistry **1988**, *27* (11), 3423–3427.
3. Keller, F.; Ludlow, M.M. Carbohydrate metabolism in drought-stressed leaves of Pigeonpea (*Cajanus cajan*). J. Exp. Biol. **1993**, *44* (265), 1351–1359.
4. Guo, C.; Oosterhuis, D.M. Pinitol occurrence in soybean plants as affected by temperature and plant growth regulators. J. Exp. Biol. **1995**, *46* (283), 249–253.
5. Popp, M. Chemical composition of Australian mangroves. II. Low molecular weight carbohydrates. Z. Pflanzenphysiol. **1984**, *113* (5), 411–421.
6. Gorham, J.; McDonnell, E.; Wyn Jones, R.G. Pinitol and other solutes in salt-stressed *Sesbania aculeata*. Z. Pflanzenphysiol. **1984**, *114* (2), 173–178.
7. Gorham, J.; Tomar, O.S.; Wyn Jones, R.G. Salinity-induced changes in the chemical composition of *Leucaena leucocephala* and *Sesbania bispinosa*. J. Plant Physiol. **1988**, *132* (6), 678–682.
8. Orthen, B.; Popp, M.; Barz, W. Cyclitol accumulation in suspended cells and intact plants of *Cicer arietinum* L. J. Plant Physiol. **2000**, *156*, 40–45.
9. Narayanan, C.R.; Joshi, D.D.; Mujumdar, A.M.; Dhekne, V.V. Pinitol—A new anti-diabetic compound from the leaves of *Bougainvillea spectabilis*. Curr. Sci. **1987**, *56* (3), 139–141.
10. Oslund, R.E.; Sherman, W.R. Pinitol and Derivatives Thereof for the Treatment of Metabolic Disorders. US Patent #5,550,166, August 27, 1996.
11. Oslund, R.E.; Sherman, W.R. Pinitol and Derivatives Thereof for the Treatment of Metabolic Disorders. US Patent #5,827,896, October 27, 1998.

12. Udagawa, Y.; Machida, M.; Ogawa, S. Method of Recovering L-Quebrachitol from Rubber Latex Serums. US Patent #5,041,689, Aug. 20, 1991.
13. Kiddle, J.J. Quebrachitol: A versatile building block in the construction of naturally occurring bioactive materials. Chem. Rev. **1995**, *95*, 2189–2202.
14. Mun, L.C. Quebrachitol—An additional role for *Hevea* latex. Rubber Dev. **1996**, *49* (1/2), 11–13.
15. Allen, F.H.; Kennard, O. 3D Search and research using the Cambridge structural database. Chem. Des. Autom. News **1993**, *8,* 1, 31–37.
16. Cannon, J.R.; Raston, C.L.; Toia, R.F.; White, A.H. Crystal structures of (*Z*)-*O*-β-D-xylopyranosyl(1 → 6)-β-D-glucopyranosyloxy-*NNO*-azoxymethane (Macrozamin) and 5-*O*-methyl-*myo*-inositol (Sequoyitol). Aust. J. Chem. **1980**, *33*, 2229–2236.
17. Huang, K.-F.; Luo, W.-L. Crystal structure of L-quebrachitol. J. Chin. Chem. Soc. **1994**, *41*, 115–117.
18. Lee, L.S.; Morris, N.J. Isolation and identification of pinitol from peanut flour. J. Agric. Food Chem. **1963**, *11* (4), 321–322.
19. Jeffrey, G.A.; Yeon, Y. The crystal structure of L-*chiro*-inositol. Carbohydr. Res. **1987**, *159*, 211–216.
20. Angyal, S.J.; Odier, L. The effect of *O*-methylation on chemical shifts in the ^{1}H- and ^{13}C-N.M.R. Spectra of cyclic polyols. Carbohydr. Res. **1983**, *123*, 23–29.
21. Mondal, D.N.; Barik, B.R.; Dey, A.K.; Kundu, A.B.; Banerji, A.; Maiti, S. The structure and stereochemistry of D(+)-pinitol: Application of 2D-NMR spectroscopy. J. Indian Chem. Soc. **1993**, *70*, 651–652.
22. Agrawal, P.K.; Singh, A.K. Structure determination of an inositol from *Artemisia nilagirica* by high-field NMR spectroscopic methods. Indian J. Chem. **1994**, *33B*, 803–805.
23. Jeffrey, G.A.; Mitra, J. The hydrogen-bonding patterns in the pyranose and pyranoside crystal structures. Acta Crystallogr. Sect. B **1983**, *39*, 469–480.

Received December 12, 2001
Accepted May 29, 2002