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L-Talitol

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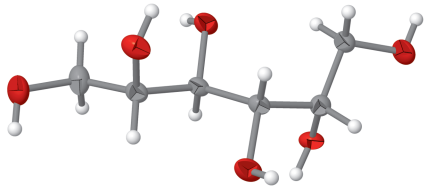
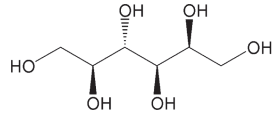
The title compound, $C_6H_{14}O_6$, the sugar alcohol corresponding to L-talose, was crystallized from aqueous solution. Colourless block-shaped single crystals suitable for single-crystal X-ray diffraction analysis were obtained. The title compound crystallizes in the monoclinic space group $P2_1$, with one molecule in the asymmetric unit. In the crystal, all six hydroxy groups act as donors in O—H···O hydrogen bonds, forming a three-dimensional hydrogen-bonded network. The crystal structure of its enantiomer, D-altritol (D-talitol), has been reported previously [Kopf *et al.* (1991). *Carbohydr. Res.* **217**, 1–6].

3D view



Chemical scheme



Structure description

L-Talitol is the sugar alcohol corresponding to the rare sugar L-talose. Systematic bioproduction strategies have expanded the availability of rare hexoses and their corresponding sugar alcohols (Izumori, 2002). Sugar alcohols possess multiple hydroxy groups and can therefore form extensive intermolecular hydrogen-bonding networks. Elucidation of their molecular conformations and crystal packing is important for understanding their solid-state properties.

The crystal structure of the enantiomer, D-altritol (D-talitol), was reported previously by Kopf *et al.* (1991; CSD refcode JOJZOX). The present study provides a modern single-crystal structure determination of the corresponding *L* enantiomer using Cu *Kα* radiation. Compared with the earlier determination, for which a conventional *R* value of 0.054 was reported, the present refinement gives a lower value of R_1 = 0.0292 and unit-cell parameters with smaller standard uncertainties. Furthermore, the anomalous-scattering data permitted assessment of the assigned absolute configuration, giving a Flack parameter of 0.07 (16) based on 570 quotients. The present determination therefore provides direct crystallographic characterization of L-talitol and a more precise modern dataset for this enantiomorphic pair.

The title compound, $C_6H_{14}O_6$ (Fig. 1), adopts an acyclic six-carbon chain structure. Single-crystal X-ray diffraction analysis revealed that it crystallizes in the monoclinic space group $P2_1$. The asymmetric unit contains one molecule of L-talitol.

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O1^{i}	0.82	2.28	2.9570 (18)	140
O2—H2···O4^{ii}	0.82	1.99	2.747 (2)	154
O3—H3···O2^{iii}	0.82	1.88	2.700 (2)	174
O4—H4···O5^{iv}	0.82	1.89	2.7027 (19)	174
O5—H5···O3^{v}	0.82	2.05	2.773 (2)	147
O6—H6···O6^{vi}	0.82	2.16	2.9502 (19)	162

Symmetry codes: (i) $-x, y+\frac{1}{2}, -z$; (ii) $x, y-1, z$; (iii) $x+1, y, z$; (iv) $x-1, y, z$; (v) $x, y+1, z$; (vi) $-x+2, y-\frac{1}{2}, -z+1$.

In the crystal, all six hydroxy groups act as hydrogen-bond donors (Table 1), all of which are intermolecular interactions. These interactions link the molecules in all three crystallographic directions, producing a three-dimensional hydrogen-bonded network, as illustrated in Fig. 2.

Synthesis and crystallization

Commercially available L-talitol [Tokyo Chemical Industry Co., Ltd. (TCI)] was used as received without further purification. The sample was dissolved in water, and the solution was allowed to evaporate slowly at room temperature. Colorless block-shaped single crystals suitable for single-crystal X-ray diffraction analysis were obtained.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The absolute configuration was assigned on the basis of the known configuration of the commercially available L-talitol sample and was further supported by the refined Flack parameter. The Flack parameter was 0.07 (16), determined using 570 quotients of the type $[(I^+) - (I^-)]/[(I^+) + (I^-)]$ (Parsons *et al.*, 2013).

Acknowledgements

The authors gratefully acknowledge Professor Genta Sakane (Okayama University of Science) for valuable discussions and technical guidance, and Kei Takeshita (FUSHIMI Pharmaceutical Co., Ltd.) for helpful suggestions. This work was supported by the JST Support for Pioneering Research Initiated by the Next Generation (SPRING) program, Japan.

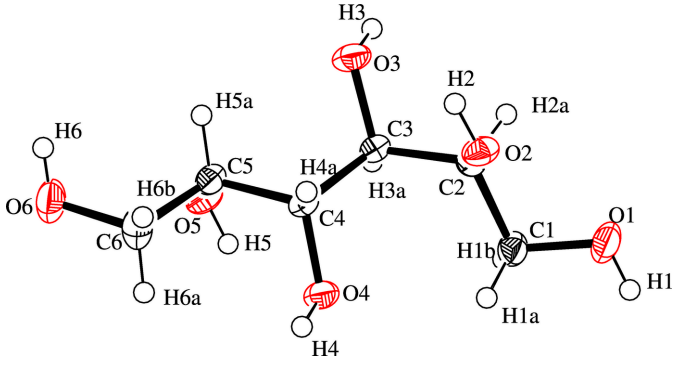


Figure 1
Molecular structure of L-talitol, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level, and hydrogen atoms are shown as spheres of arbitrary radii.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_6H_{14}O_6$
M_r	182.17
Crystal system, space group	Monoclinic, $P2_1$
Temperature (K)	296
a, b, c (Å)	4.8901 (3), 5.1671 (3), 16.3657 (10)
β (°)	100.136 (4)
V (Å^3)	407.07 (4)
Z	2
Radiation type	Cu $K\alpha$
μ (mm^{-1})	1.17
Crystal size (mm)	0.10 × 0.10 × 0.10
Data collection	
Diffractometer	Rigaku R-AXIS RAPID
Absorption correction	Multi-scan (*ABSCOR*; Rigaku, 1995)
T_{min}, T_{max}	0.711, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	4278, 1446, 1399
R_{int}	0.059
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.602
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.029, 0.075, 1.08
No. of reflections	1446
No. of parameters	116
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.20, −0.12
Absolute structure	Flack x determined using 570 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.07 (16)

Computer programs: *RAPID-AUTO* (Rigaku, 2009), *SHELXT2018/2* (Sheldrick, 2015*a*), *SHELXL2018/3* (Sheldrick, 2015*b*) and *OLEX2* 1.3 (Dolomanov *et al.*, 2009).

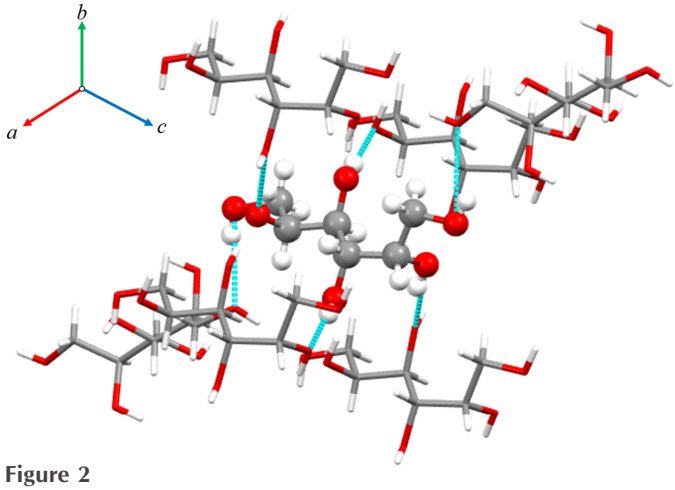


Figure 2
Crystal packing of L-talitol, showing part of the three-dimensional hydrogen-bonded network, with the unit-cell directions indicated. The cyan dashed lines indicate the O···O contacts associated with the O—H···O hydrogen bonds. The central molecule is shown using a ball-and-stick representation, whereas the surrounding molecules are shown using a capped-stick representation.

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full crystallographic data

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L-Talitol

Crystal data

$C_6H_{14}O_6$
M_r = 182.17
Monoclinic, $P2_1$
a = 4.8901 (3) Å
b = 5.1671 (3) Å
c = 16.3657 (10) Å
β = 100.136 (4)°
V = 407.07 (4) Å^3
Z = 2
$F(000)$ = 196
D_x = 1.486 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54187 Å
Cell parameters from 1932 reflections
θ = 5.5–68.2°
μ = 1.17 mm^{-1}
T = 296 K
Block, clear light colourless
0.1 × 0.1 × 0.1 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (ABSCOR; Rigaku, 1995)
T_{min} = 0.711, T_{max} = 1.000
4278 measured reflections
1446 independent reflections
1399 reflections with $I > 2\sigma(I)$
R_{int} = 0.059
θ_{max} = 68.2°, θ_{min} = 5.5°
h = −5→5
k = −6→6
l = −19→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.075
S = 1.08
1446 reflections
116 parameters
1 restraint
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0295P)^2 + 0.0407P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.12 e Å^{-3}
Extinction correction: SHELXL-2018/3 (Sheldrick, 2015b), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.027 (4)
Absolute structure: Flack x determined using 570 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.07 (16)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. All non-hydrogen atoms were refined anisotropically. Hydroxy H atoms were placed in geometrically calculated positions and treated as rotating groups, with O—H = 0.82 Å. C-bound H atoms were placed in calculated positions and refined using riding models, with C—H = 0.98 Å for CH groups and 0.97 Å for CH_2 groups. For all H atoms, U_{iso}(H) was constrained to $1.2U_{eq}$ of the parent C or O atom.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.1487 (4)	0.2244 (3)	0.00353 (9)	0.0387 (5)
H1	0.049895	0.334701	−0.022940	0.046*
O2	0.2665 (3)	−0.0647 (3)	0.14835 (9)	0.0251 (4)
H2	0.351707	−0.178860	0.176956	0.030*
O3	0.8391 (3)	−0.0087 (3)	0.23126 (9)	0.0287 (4)
H3	0.960388	−0.023251	0.202749	0.034*
O4	0.3808 (3)	0.5215 (3)	0.25422 (8)	0.0260 (4)
H4	0.256058	0.531070	0.281637	0.031*
O5	0.9447 (3)	0.5638 (3)	0.33441 (9)	0.0277 (4)
H5	0.849284	0.676689	0.308092	0.033*
O6	0.8543 (4)	0.4580 (4)	0.49996 (9)	0.0400 (5)
H6	0.939124	0.322089	0.511232	0.048*
C1	0.2905 (5)	0.3341 (5)	0.07904 (12)	0.0268 (5)
H1A	0.158245	0.404113	0.110957	0.032*
H1B	0.411851	0.472857	0.067510	0.032*
C2	0.4582 (4)	0.1203 (4)	0.12684 (12)	0.0223 (5)
H2A	0.563950	0.035165	0.088863	0.027*
C3	0.6663 (4)	0.2077 (4)	0.20298 (12)	0.0205 (4)
H3A	0.781593	0.347156	0.186723	0.025*
C4	0.5431 (4)	0.2952 (4)	0.27779 (11)	0.0202 (4)
H4A	0.422927	0.158257	0.293084	0.024*
C5	0.7699 (4)	0.3574 (4)	0.35239 (12)	0.0229 (5)
H5A	0.885797	0.202833	0.364967	0.027*
C6	0.6458 (5)	0.4218 (6)	0.42847 (12)	0.0326 (5)
H6A	0.535703	0.578391	0.418094	0.039*
H6B	0.523187	0.282646	0.438795	0.039*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0476 (11)	0.0336 (10)	0.0273 (8)	0.0020 (9)	−0.0144 (7)	0.0010 (7)
O2	0.0235 (8)	0.0178 (7)	0.0326 (8)	0.0016 (6)	0.0010 (6)	0.0039 (6)
O3	0.0253 (8)	0.0309 (9)	0.0311 (8)	0.0116 (7)	0.0082 (6)	0.0070 (7)
O4	0.0250 (8)	0.0290 (9)	0.0250 (7)	0.0096 (7)	0.0073 (6)	0.0054 (6)
O5	0.0195 (7)	0.0287 (9)	0.0336 (8)	0.0001 (7)	0.0007 (6)	0.0071 (7)
O6	0.0508 (11)	0.0401 (10)	0.0238 (7)	0.0001 (9)	−0.0080 (7)	−0.0046 (7)
C1	0.0335 (12)	0.0224 (10)	0.0222 (9)	−0.0014 (10)	−0.0011 (8)	0.0014 (9)
C2	0.0228 (10)	0.0227 (10)	0.0217 (9)	0.0010 (9)	0.0043 (8)	−0.0004 (8)
C3	0.0191 (10)	0.0203 (10)	0.0215 (9)	0.0022 (8)	0.0015 (8)	0.0033 (8)
C4	0.0198 (10)	0.0203 (10)	0.0199 (8)	0.0028 (8)	0.0022 (7)	0.0042 (8)

C5	0.0225 (10)	0.0219 (11)	0.0227 (9)	0.0007 (8)	−0.0004 (8)	0.0028 (8)
C6	0.0327 (13)	0.0417 (13)	0.0222 (10)	−0.0032 (11)	0.0018 (9)	−0.0033 (10)

Geometric parameters (Å, º)

O1—H1	0.8200	C1—H1B	0.9700
O1—C1	1.424 (2)	C1—C2	1.510 (3)
O2—H2	0.8200	C2—H2A	0.9800
O2—C2	1.425 (3)	C2—C3	1.532 (3)
O3—H3	0.8200	C3—H3A	0.9800
O3—C3	1.429 (2)	C3—C4	1.525 (3)
O4—H4	0.8200	C4—H4A	0.9800
O4—C4	1.428 (3)	C4—C5	1.532 (2)
O5—H5	0.8200	C5—H5A	0.9800
O5—C5	1.429 (2)	C5—C6	1.515 (3)
O6—H6	0.8200	C6—H6A	0.9700
O6—C6	1.423 (2)	C6—H6B	0.9700
C1—H1A	0.9700		
C1—O1—H1	109.5	C2—C3—H3A	109.1
C2—O2—H2	109.5	C4—C3—C2	116.15 (16)
C3—O3—H3	109.5	C4—C3—H3A	109.1
C4—O4—H4	109.5	O4—C4—C3	107.77 (14)
C5—O5—H5	109.5	O4—C4—H4A	109.3
C6—O6—H6	109.5	O4—C4—C5	109.48 (17)
O1—C1—H1A	110.3	C3—C4—H4A	109.3
O1—C1—H1B	110.3	C3—C4—C5	111.66 (15)
O1—C1—C2	107.18 (18)	C5—C4—H4A	109.3
H1A—C1—H1B	108.5	O5—C5—C4	111.58 (16)
C2—C1—H1A	110.3	O5—C5—H5A	107.9
C2—C1—H1B	110.3	O5—C5—C6	110.23 (18)
O2—C2—C1	107.33 (17)	C4—C5—H5A	107.9
O2—C2—H2A	107.4	C6—C5—C4	111.25 (17)
O2—C2—C3	111.62 (16)	C6—C5—H5A	107.9
C1—C2—H2A	107.4	O6—C6—C5	111.83 (19)
C1—C2—C3	115.35 (17)	O6—C6—H6A	109.3
C3—C2—H2A	107.4	O6—C6—H6B	109.3
O3—C3—C2	107.65 (16)	C5—C6—H6A	109.3
O3—C3—H3A	109.1	C5—C6—H6B	109.3
O3—C3—C4	105.46 (14)	H6A—C6—H6B	107.9
O1—C1—C2—O2	−65.3 (2)	O5—C5—C6—O6	−60.8 (3)
O1—C1—C2—C3	169.64 (19)	C1—C2—C3—O3	−169.67 (16)
O2—C2—C3—O3	67.5 (2)	C1—C2—C3—C4	72.4 (2)
O2—C2—C3—C4	−50.4 (2)	C2—C3—C4—O4	−64.3 (2)
O3—C3—C4—O4	176.62 (16)	C2—C3—C4—C5	175.45 (19)
O3—C3—C4—C5	56.4 (2)	C3—C4—C5—O5	61.3 (2)
O4—C4—C5—O5	−57.9 (2)	C3—C4—C5—C6	−175.13 (18)

O4—C4—C5—C6	65.6 (2)	C4—C5—C6—O6	174.9 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
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