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L-Iditol

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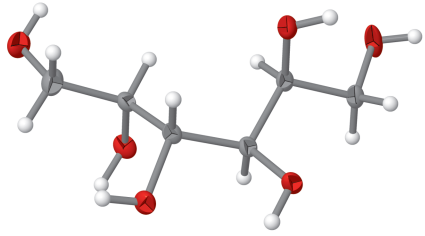
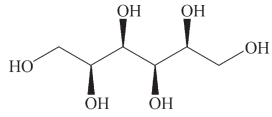
L-Iditol, $C_6H_{14}O_6$, the sugar alcohol corresponding to L-idose, was crystallized from aqueous solution. Colourless block-shaped single crystals suitable for single-crystal X-ray diffraction analysis were obtained. The title compound crystallizes in the monoclinic space group $P2_1$, with one molecule 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-iditol, has been reported previously [Azarnia *et al.* (1972). *Acta Cryst.* B**28**, 1007–1013].

3D view



Chemical scheme



Structure description

L-Iditol is the sugar alcohol corresponding to the rare sugar L-idose. 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-iditol was reported previously by Azarnia *et al.* (1972; CSD refcode IDITOL), and that of racemic D,L-iditol was reported by Kopf *et al.* (1992; CSD refcode VOMXEA). The present study provides a modern high-precision single-crystal X-ray determination of the corresponding L enantiomer. The refinement converged at R_1 = 0.0337, and the standard uncertainties of the C—C and C—O bond lengths are in the range 0.003–0.004 Å. Together with the deposited structure-factor data and detailed hydrogen-bond geometry, the present results provide an updated crystallographic description of iditol and specifically document the crystal structure of the L enantiomer.

L-iditol adopts a twisted, acyclic six-carbon chain conformation (Fig. 1). The C1—C2—C3—C4, C2—C3—C4—C5 and C3—C4—C5—C6 torsion angles are −179.9 (2), 62.2 (3) and −175.3 (2)°, respectively. Single-crystal X-ray diffraction analysis revealed that it crystallizes in the monoclinic space group $P2_1$. The asymmetric

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O3^{i}	0.82	2.04	2.834 (3)	163
O2—H2···O6^{ii}	0.82	1.95	2.764 (3)	171
O3—H3···O5^{iii}	0.82	2.01	2.736 (3)	147
O4—H4···O2^{iv}	0.82	1.98	2.755 (2)	158
O5—H5···O1^{iii}	0.90 (4)	1.88 (4)	2.766 (3)	170 (3)
O6—H6···O3^{v}	0.82	2.25	2.848 (3)	130

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

unit contains one molecule of L-iditol. The stereogenic carbon atoms C2, C3, C4 and C5 have *S*, *R*, *R* and *S* configurations, respectively.

In the crystal, all six hydroxy groups act as hydrogen-bond donors, forming six intermolecular O—H···O hydrogen bonds (Table 1). The donor···acceptor distances range from 2.736 (3) to 2.848 (3) Å. These interactions connect the molecules into a three-dimensional hydrogen-bonded network. The crystal packing viewed along the *a* axis is shown in Fig. 2. The intermolecular hydrogen bonding contributes to the consolidation of the crystal packing.

Synthesis and crystallization

Commercially available L-iditol (Sigma–Aldrich) 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. The absolute configuration was assigned on the basis of the known configuration of the commercially available L-iditol sample.

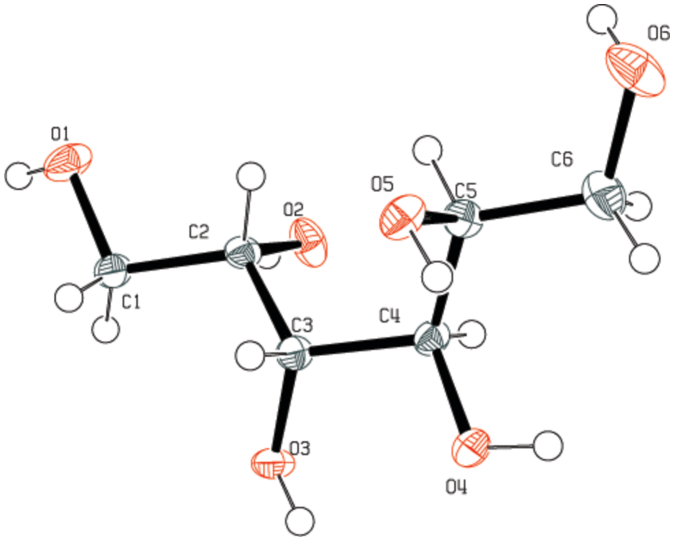


Figure 1
The molecular structure of L-iditol showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level, and hydrogen atoms are shown as spheres of arbitrary radii.

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)	5.8678 (2), 8.3869 (3), 8.1213 (3)
β (°)	93.182 (2)
V (Å^3)	399.05 (2)
Z	2
Radiation type	Cu $K\alpha$
μ (mm^{-1})	1.19
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}	0.822, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	4219, 1377, 1329
R_{int}	0.057
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.602
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.034, 0.083, 1.12
No. of reflections	1377
No. of parameters	114
No. of restraints	1
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.20, −0.20
Absolute structure	Flack x determined using 538 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	−0.24 (16)

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

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Although the refined value of the

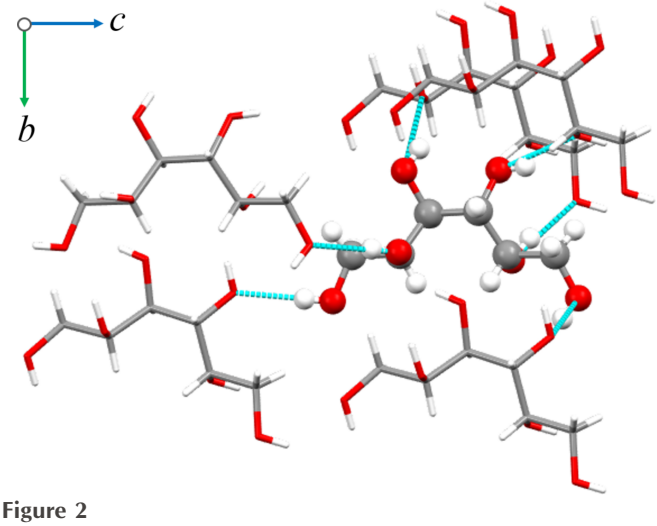


Figure 2
Crystal packing of L-iditol viewed along the *a* axis, showing the three-dimensional hydrogen-bonded network formed by O—H···O hydrogen bonds. Hydrogen bonds are shown as dashed lines, and the crystallographic *b*- and *c*-axis directions are indicated.

Flack parameter is slightly negative, it is within approximately 1.5 standard uncertainties of zero and is consistent with the absolute configuration assigned from the known configuration of the commercially available L-iditol sample.

Acknowledgements

The authors thank Professor Genta Sakane (Okayama University of Science) for insightful discussions and technical suggestions, and Kei Takeshita (FUSHIMI Pharmaceutical Co., Ltd.) for valuable advice. This work received support from the JST Support for Pioneering Research Initiated by the Next Generation (SPRING) program, Japan.

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Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.

full crystallographic data

IUCrData (2026). **11**, x260801 [https://doi.org/10.1107/S2414314626008011]

L-Iditol

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(2*S*,3*R*,4*R*,5*S*)-Hexane-1,2,3,4,5,6-hexol

Crystal data

$C_6H_{14}O_6$
M_r = 182.17
Monoclinic, $P2_1$
a = 5.8678 (2) Å
b = 8.3869 (3) Å
c = 8.1213 (3) Å
β = 93.182 (2)°
V = 399.05 (2) Å^3
Z = 2
$F(000)$ = 196
D_x = 1.516 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54187 Å
Cell parameters from 3800 reflections
θ = 5.3–68.3°
μ = 1.19 mm^{-1}
T = 296 K
Block, clear light colourless
0.1 × 0.1 × 0.1 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Detector resolution: 10.000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (ABSCOR; Rigaku, 1995)
T_{min} = 0.822, T_{max} = 1.000
4219 measured reflections
1377 independent reflections
1329 reflections with $I > 2\sigma(I)$
R_{int} = 0.057
θ_{max} = 68.2°, θ_{min} = 5.5°
h = −6→7
k = −10→10
l = −9→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.083
S = 1.12
1377 reflections
114 parameters
1 restraint
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.032P)^2 + 0.0743P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 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: 0.165 (10)
Absolute structure: Flack x determined using 538 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: −0.24 (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. The structure was solved using SHELXT (Sheldrick, 2015*a*) and refined on F^2 by full-matrix least-squares methods using *SHELXL* (Sheldrick, 2015*b*). All non-hydrogen atoms were refined anisotropically. The hydroxy hydrogen atom H5 was located in a difference-Fourier map and refined freely. All other hydrogen atoms were placed in geometrically calculated positions and refined using constrained models. The final refinement gave $R_1 = 0.0337$ for reflections with $I > 2\sigma(I)$ and w$R_2 = 0.0829$ for all data. The maximum and minimum residual electron densities were 0.20 and -0.20 e Å^{-3}, respectively. The Flack parameter was -0.24 (16), determined using 538 quotients of the type $[(I^+) - (I^-)]/[(I^+) + (I^-)]$ (Parsons *et al.*, 2013). Although the refined value is slightly negative, it is within approximately 1.5 standard uncertainties of zero and is consistent with the absolute configuration assigned from the known configuration of the commercially available *L*-iditol sample.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.4782 (4)	0.8448 (2)	0.4118 (2)	0.0308 (6)
H1	0.503187	0.855873	0.511527	0.037*
O2	0.0813 (3)	0.6622 (2)	0.2718 (2)	0.0251 (5)
H2	0.078439	0.670204	0.372303	0.030*
O3	0.3411 (3)	0.3703 (2)	0.2584 (2)	0.0198 (5)
H3	0.365277	0.284701	0.213852	0.024*
O4	0.2410 (3)	0.3107 (2)	−0.0653 (2)	0.0230 (5)
H4	0.152240	0.286824	−0.142921	0.028*
O5	0.4315 (3)	0.5928 (2)	−0.2005 (2)	0.0216 (5)
H5	0.466 (6)	0.505 (5)	−0.258 (4)	0.044 (11)*
O6	0.0239 (4)	0.7005 (3)	−0.3950 (2)	0.0334 (6)
H6	−0.004973	0.782453	−0.345233	0.040*
C1	0.4802 (5)	0.6794 (3)	0.3717 (3)	0.0194 (6)
H1A	0.436997	0.616425	0.465156	0.023*
H1B	0.631996	0.647182	0.343478	0.023*
C2	0.3120 (4)	0.6535 (3)	0.2265 (3)	0.0168 (6)
H2A	0.335094	0.739105	0.146973	0.020*
C3	0.3538 (4)	0.4961 (3)	0.1405 (3)	0.0158 (6)
H3A	0.508825	0.497853	0.101329	0.019*
C4	0.1871 (4)	0.4652 (3)	−0.0076 (3)	0.0159 (6)
H4A	0.030915	0.464981	0.029349	0.019*
C5	0.2062 (5)	0.5907 (3)	−0.1429 (3)	0.0176 (6)
H5A	0.179351	0.694965	−0.093078	0.021*
C6	0.0294 (5)	0.5697 (4)	−0.2842 (3)	0.0257 (7)
H6A	0.062713	0.473021	−0.343878	0.031*
H6B	−0.119857	0.557352	−0.240093	0.031*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0586 (14)	0.0176 (11)	0.0153 (9)	−0.0104 (10)	−0.0058 (9)	−0.0010 (8)
O2	0.0237 (10)	0.0349 (12)	0.0161 (8)	0.0088 (9)	−0.0028 (7)	−0.0053 (8)
O3	0.0318 (10)	0.0126 (9)	0.0150 (9)	0.0036 (7)	0.0005 (7)	0.0004 (7)
O4	0.0313 (11)	0.0153 (9)	0.0214 (9)	0.0014 (8)	−0.0066 (7)	−0.0058 (8)
O5	0.0233 (10)	0.0194 (9)	0.0224 (10)	−0.0052 (8)	0.0047 (8)	−0.0020 (8)
O6	0.0435 (13)	0.0402 (13)	0.0168 (10)	0.0142 (10)	0.0035 (9)	0.0063 (10)

C1	0.0285 (14)	0.0152 (15)	0.0141 (12)	−0.0017 (11)	−0.0026 (11)	0.0000 (10)
C2	0.0239 (13)	0.0149 (13)	0.0114 (11)	−0.0002 (11)	0.0003 (10)	0.0018 (10)
C3	0.0193 (12)	0.0150 (13)	0.0130 (11)	0.0000 (10)	0.0014 (9)	−0.0001 (9)
C4	0.0190 (12)	0.0142 (13)	0.0148 (12)	−0.0012 (10)	0.0015 (10)	−0.0017 (9)
C5	0.0223 (13)	0.0169 (12)	0.0136 (12)	0.0024 (11)	0.0019 (10)	−0.0018 (10)
C6	0.0276 (15)	0.0305 (17)	0.0188 (13)	0.0007 (13)	−0.0015 (11)	0.0027 (12)

Geometric parameters (Å, º)

O1—H1	0.8200	C1—H1B	0.9700
O1—C1	1.425 (3)	C1—C2	1.511 (3)
O2—H2	0.8200	C2—H2A	0.9800
O2—C2	1.424 (3)	C2—C3	1.521 (3)
O3—H3	0.8200	C3—H3A	0.9800
O3—C3	1.430 (3)	C3—C4	1.529 (3)
O4—H4	0.8200	C4—H4A	0.9800
O4—C4	1.420 (3)	C4—C5	1.530 (4)
O5—H5	0.90 (4)	C5—H5A	0.9800
O5—C5	1.427 (3)	C5—C6	1.514 (4)
O6—H6	0.8200	C6—H6A	0.9700
O6—C6	1.418 (4)	C6—H6B	0.9700
C1—H1A	0.9700		
C1—O1—H1	109.5	C2—C3—H3A	108.2
C2—O2—H2	109.5	C2—C3—C4	113.3 (2)
C3—O3—H3	109.5	C4—C3—H3A	108.2
C4—O4—H4	109.5	O4—C4—C3	105.6 (2)
C5—O5—H5	114 (2)	O4—C4—H4A	109.2
C6—O6—H6	109.5	O4—C4—C5	111.3 (2)
O1—C1—H1A	110.2	C3—C4—H4A	109.2
O1—C1—H1B	110.2	C3—C4—C5	112.3 (2)
O1—C1—C2	107.7 (2)	C5—C4—H4A	109.2
H1A—C1—H1B	108.5	O5—C5—C4	110.5 (2)
C2—C1—H1A	110.2	O5—C5—H5A	107.3
C2—C1—H1B	110.2	O5—C5—C6	111.2 (2)
O2—C2—C1	112.4 (2)	C4—C5—H5A	107.3
O2—C2—H2A	107.5	C6—C5—C4	112.9 (2)
O2—C2—C3	110.1 (2)	C6—C5—H5A	107.3
C1—C2—H2A	107.5	O6—C6—C5	112.4 (2)
C1—C2—C3	111.6 (2)	O6—C6—H6A	109.1
C3—C2—H2A	107.5	O6—C6—H6B	109.1
O3—C3—C2	108.48 (18)	C5—C6—H6A	109.1
O3—C3—H3A	108.2	C5—C6—H6B	109.1
O3—C3—C4	110.3 (2)	H6A—C6—H6B	107.8
O1—C1—C2—O2	−73.8 (3)	O5—C5—C6—O6	−64.8 (3)
O1—C1—C2—C3	162.0 (2)	C1—C2—C3—O3	57.2 (3)
O2—C2—C3—O3	−68.3 (2)	C1—C2—C3—C4	−179.9 (2)

O2—C2—C3—C4	54.6 (2)	C2—C3—C4—O4	−176.3 (2)
O3—C3—C4—O4	−54.5 (2)	C2—C3—C4—C5	62.2 (3)
O3—C3—C4—C5	−176.0 (2)	C3—C4—C5—O5	59.4 (3)
O4—C4—C5—O5	−58.8 (3)	C3—C4—C5—C6	−175.3 (2)
O4—C4—C5—C6	66.5 (3)	C4—C5—C6—O6	170.3 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O3^{i}	0.82	2.04	2.834 (3)	163
O2—H2···O6^{ii}	0.82	1.95	2.764 (3)	171
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