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# Hiroyuki Hosomi *et al.*

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# (–)-*epi*-Inosose-2[1]

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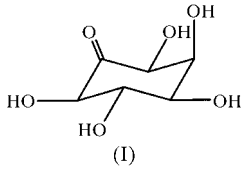
The structure of the title compound, $C_6H_{10}O_6$, was determined to confirm the position of the keto group in the molecule prepared enantioselectively by a bioconversion from *myo*-inositol. There are two independent molecules showing similar geometry.

## Comment

*myo*-Inositol has only one axial hydroxyl group and has essentially mirror symmetry. Crystal structures have been reported for *myo*-inositol (Rabinowitz & Kraut, 1964), *myo*-inositol dihydrate (Lomer *et al.*, 1963), *myo*-inositol tetraaquamagnesium dichloride (Blank, 1973) and *myo*-inositol calcium bromide pentahydrate (Cook & Bugg, 1973). The crystal structure and molecular dynamics analysis of an optically active *myo*-inositol derivative have been reported recently (Dillen *et al.*, 2000).

The title compound, (I), was prepared enantioselectively by a bioconversion from *myo*-inositol (Takahashi *et al.*, 2000).




(I)

## Experimental

Crystals of (I) were grown from an aqueous ethanol solution.

*Crystal data*

$C_6H_{10}O_6$
$M_r$ = 178.14
Monoclinic, $P2_1$
$a$ = 11.197 (2) Å
$b$ = 8.932 (2) Å
$c$ = 6.976 (2) Å
$\beta$ = 90.21 (2)°
$V$ = 697.7 (3) Å$^3$
$Z$ = 4
$D_x$ = 1.696 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta$ = 13.9–15.0°
$\mu$ = 0.155 mm$^{-1}$
$T$ = 298 (1) K
Prism, colourless
0.7 × 0.4 × 0.15 mm

*Data collection*

Rigaku AFC-7*R* diffractometer
$\theta$–$2\theta$ scans
2250 measured reflections
2151 independent reflections
2086 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.005
$\theta_{max}$ = 30°
$h = 0 \rightarrow 16$
$k = 0 \rightarrow 13$
$l = -10 \rightarrow 10$
3 standard reflections
every 150 reflections
intensity decay: none

*Refinement*

Refinement on $F^2$
$R(F)$ = 0.024
$wR(F^2)$ = 0.068
$S$ = 1.13
2151 reflections
298 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0417P)^2 + 0.0965P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.30 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.16 e Å$^{-3}$
Extinction correction: *SHELXL*97 (Sheldrick, 1997)
Extinction coefficient: 0.027 (5)

**Table 1**
Selected geometric parameters (Å).

| | | | |
|---|---|---|---|
| O1—C7 | 1.205 (2) | O51—C57 | 1.207 (2) |
| O2—C8 | 1.419 (2) | O52—C58 | 1.401 (2) |
| O3—C9 | 1.425 (2) | O53—C59 | 1.440 (2) |
| O4—C10 | 1.428 (2) | O54—C60 | 1.427 (2) |
| O5—C11 | 1.424 (2) | O55—C61 | 1.424 (2) |
| O6—C12 | 1.418 (2) | O56—C62 | 1.414 (2) |

**Table 2**
Hydrogen-bonding geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O2—H2···O53$^{i}$ | 0.76 (3) | 2.09 (3) | 2.856 (2) | 177 (3) |
| O3—H3···O54$^{i}$ | 0.84 (3) | 1.96 (3) | 2.786 (2) | 166 (3) |
| O4—H4···O53$^{ii}$ | 0.73 (3) | 2.49 (3) | 3.123 (2) | 145 (3) |
| O5—H5···O56$^{iii}$ | 0.82 (3) | 1.97 (3) | 2.785 (2) | 173 (4) |
| O6—H6···O4$^{iv}$ | 0.76 (3) | 2.10 (3) | 2.828 (2) | 163 (3) |
| O52—H52···O3$^{v}$ | 0.85 (4) | 2.04 (4) | 2.856 (2) | 161 (3) |
| O53—H53···O51$^{v}$ | 0.81 (3) | 2.06 (3) | 2.845 (2) | 164 (3) |
| O54—H54···O55$^{vi}$ | 0.83 (3) | 1.94 (3) | 2.767 (2) | 172 (2) |
| O55—H55···O6$^{vii}$ | 0.81 (3) | 1.98 (3) | 2.782 (2) | 170 (3) |
| O56—H56···O2 | 0.89 (4) | 2.06 (4) | 2.938 (2) | 170 (3) |

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

All H atoms were located from difference syntheses and refined isotropically; the O—H and C—H lengths are 0.73 (3)–0.85 (4) and 0.91 (2)–1.01 (2) Å, respectively. The absolute structure was assumed based on the known absolute configuration of the title compound (Posternak, 1946).

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1993); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1999); program(s) used to solve struc-

[1] Systematic name: (−)-2L-2,3,4,6/5-pentahydroxycyclohexanone.

ture: *SIR*92 (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); software used to prepare material for publication: *TEXSAN*.

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