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L-(+)-Bornesitol

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Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.003 Å
R factor = 0.034
wR factor = 0.085
Data-to-parameter ratio = 8.2

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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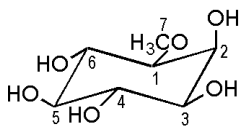
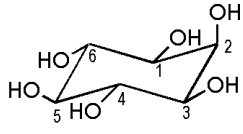
The structure of the the title compound, $C_7H_{14}O_6$, a natural *myo*-inositol derivative, has been determined. Bond distances, bond lengths and dihedral angles are similar to those of *myo*-inositol.

Comment

Bornesitol, (I), is a *myo*-inositol methyl derivative found in several plant species (Girard, 1871; Nishibe *et al.*, 2001), whose chemical structure has been previously described (Foster & Stacey, 1953; Bien & Ginsburg, 1958). *myo*-Inositol, (II), is a cyclitol which has only one axially oriented hydroxyl group (at C2) and therefore has mirror symmetry (Rabinovich & Kraut, 1964; Bonnet *et al.*, 2006).



(I)



(II)

As part of our study of plant products, we report here the crystal structure for one of the bornesitol enantiomers and assign its absolute configuration. The investigated crystal is of the dextrorotatory enantiomer, with $[\alpha]_D$ = +20.7±3.5°, a value similar to those previously described for bornesitol (Angyal & Bender, 1961). Bornesitol (Fig. 1) crystallizes in the orthorhombic space group $P2_12_12_1$. The average C—C and C—O bond lengths of (I) are not significantly different from those of *myo*-inositol, (II) (Rabinovich & Kraut, 1964; Bonnet *et al.*, 2006). The average C—C—C bond angle in the ring in bornesitol is 111.2 (7)°, and the mean value for C—C—O is 109.9 (16)°; these values are similar to those reported for *myo*-inositol.

All OH groups serve as intermolecular hydrogen-bond donors; with the exception of O5, they also act as acceptors, the atom O1 being the fifth acceptor instead (Table 1).

The absolute configuration of (+)-bornesitol is assigned on the basis of that previously reported for the title compound (Angyal & Gilham, 1957), as (1*R*)-*O*-methyl-*myo*-inositol. According to IUPAC recommendations for nomenclature of inositol derivatives, which names L-bornesitol as 1-*O*-methyl-*myo*-inositol, with clockwise numbering, (+)-bornesitol should be denoted (1*R*)-1-L-*O*-methyl-*myo*-inositol (Angyal *et al.*, 1992).

Experimental

Compound (I) was obtained from the EtOAc–MeOH (4.5:5.5) fraction of *Hancornia speciosa* leaves (Apocynaceae). The crude fraction

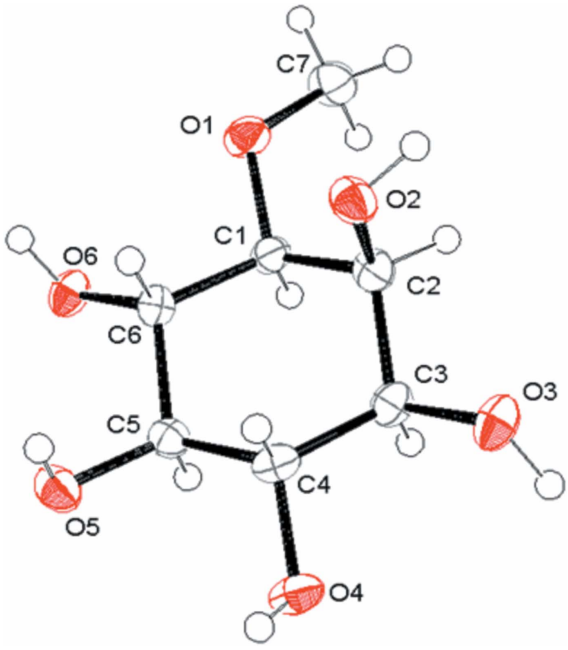


Figure 1
The molecular structure of L-(+)-bornesitol. The molecule is viewed approximately normal to the central plane of the chair-shaped cyclohexane ring; atoms C2 and C5 are below and above the plane, respectively. Displacement ellipsoids are drawn at the 50% probability level.

was dissolved in methanol–water (9:1) and the solution was kept at room temperature. Crystals of (I) grew as colourless prisms from this solution by slow evaporation. Optical rotation was determined for an aqueous solution (0.11 g per 100 ml) of compound (I), in a Perkin–Elmer polarimeter-341 at 589 nm and 293 K, using a 100 mm path length cell.

Crystal data

$C_7H_{14}O_6$
M_r = 194.19
Orthorhombic, $P2_12_12_1$
a = 6.5756 (4) Å
b = 11.0565 (7) Å
c = 11.6622 (9) Å
V = 847.88 (10) Å^3
Z = 4
D_x = 1.521 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.13 mm^{-1}
T = 150 K
Thick plate, colourless
0.48 × 0.44 × 0.23 mm

Data collection

Nonius KappaCCD diffractometer
ω scans
Absorption correction: multi-scan (Otwinowski & Minor, 1997)
T_{min} = 0.926, T_{max} = 0.972
5715 measured reflections
1151 independent reflections
974 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.085
S = 1.05
1151 reflections
140 parameters
H atoms treated by a mixture of independent and constrained refinement
$1/[\sigma^2(F_o^2) + (0.0543P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.036 (5)

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O6^{i}	0.86 (3)	1.82 (3)	2.667 (3)	170 (3)
O3—H3···O1^{ii}	0.95 (3)	1.80 (3)	2.723 (3)	162 (3)
O4—H4···O2^{iii}	0.87 (3)	1.84 (3)	2.695 (3)	167 (3)
O5—H5···O3^{iv}	0.89 (3)	2.03 (3)	2.892 (3)	163 (3)
O6—H6···O4^{v}	0.90 (3)	1.80 (3)	2.688 (3)	171 (3)

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

Hydroxyl H atoms were found in a difference map and refined freely. Other H atoms were placed in idealized positions and refined using a riding model, with C—H = 0.98 Å and U_{iso}(H) = 1.5U_{eq}(C) for the methyl group, and C—H = 1.00 Å and U_{iso}(H) = 1.2U_{eq}(C) for ring C atoms. In the absence of significant anomalous scattering, Friedel pairs were merged, and the absolute configuration was assigned from the results of Angyal & Gilham (1957).

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO/SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO/SCALEPACK*; program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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