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L-(+)-Bornesitol

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Abstract

The structure of the title compound, $C_7H_{14}O_6$, one natural *myo*-inositol derivative has been determinaded. Average atom distances, bond lengths and dihedral angles are similar to *myo*-inositol.

Comment

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

As part of our study of plant products, we report here the absolute structure for one of bornesitol enantiomers. The analyzed crystal belongs to the dextrorotatory enantiomer, with $[\alpha]_D$= +20.7 ± 3.5°, a value similar to those previously described for bornesitol (Angyal & Bender, 1961). Bornesitol crystallizes in the orthorhombic space group $P2_12_12_1$. The dimension of (I) is similar to *myo*-inositol (II) (Rabinowitz & Kraut, 1964), but it has non-centrosymmetric structures (Fig. 1). The intermolecular O···H distances range from 1.78 to 2.03 Å (Table 1) and are less than the intramolecular O···O distances (from 2.67 to 2.89 Å), in contrast to other cyclitols that present similar values (Rabinowitz & Kraut, 1964; Hosomi *et al.*, 2000, Bonnet *et al.*, 2006). The angle between O3—H3···O1 is *ca* 10° less than O6—H6···O4, and a minor difference is noted between O2—H2···O6 and O4—H4···H2 (Table 1).

The absolute structure of (+)-bornesitol was estimated based on the known absolute configuration of the title compound (Angyal; Gilman, 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 denominated (1*R*)-1-*L*-*O*-methyl-*myo*-inositol (Angyal *et al.*, 1992).

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Data collection: Collect (Nonius, 1998); cell refinement: *DENZO/SCALEPACK* (Otwinowski & Minor, 1996); data reduction: *DENZO/SCALEPACK* (Otwinowski & Minor, 1996); program(s) used to solve structure: Direct methods (*SIR2004*, Burla *et al.*, 2005); program(s) used to refine structure: *SHELX97* (Sheldrick, 1997); molecular graphics: *ORTEP* (Johnson, 1976) *PLATON* (Spek, 1997); software used to prepare material for publication: *SHELX97*(Sheldrick, 1997) and local programs.

Experimental

Compound (I) was obtained from the EtOAc:MeOH (4.5:5.5) fraction of *Hancornia speciosa* leaves (Apocynaceae). The crude fraction 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 a water solution (0.11 g/100 ml) of compound (I), in a Perkin Elmer polarimeter-341 at 589 nm and 20° C, using a 100 mm path length cell.

Crystal data	
$C_7H_{14}O_6$	D_x = 1.521 Mg m^{-3}
M_r = 194.19	Mo - $K\alpha$ radiation
Orthorhombic, $P2_12_12_1$	Cell parameters from 5715 reflections
a = 6.5756 (4) Å	θ = 3–27°
b = 11.0565 (7) Å	μ = 0.13 mm^{-1}
c = 11.6622 (9) Å	T = 150 K
V = 847.88 (10) Å^3	Plate, colourless
Z = 4	0.48 × 0.44 × 0.23 mm
Data collection	
Nonius KappaCCD diffractometer	1151 independent reflections
ω scans	974 reflections with > 2.0σ(I)
Absorption correction: multi-scan (Otowinwski & Minor, 1997)	R_{int} = 0.035
T_{min} = 0.926, T_{max} = 0.972	θ_{max} = 27.5°
5715 measured reflections	
Refinement	
Refinement on F^2	$1/[\sigma^2(F_o^2) + (0.0543P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.034	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.085	$\Delta\rho_{max}$ = 0.19 e Å^{-3}
S = 1.05	$\Delta\rho_{min}$ = −0.20 e Å^{-3}
1151 reflections	Extinction correction: SHELXL97 (Sheldrick 1997)
140 parameters	Extinction coefficient: 0.036 (5)
H atoms treated by a mixture of independent and constrained refinement	

The structure was solved by direct methods using *SIR2004* (Burla *et al.*, 2005). The remaining atoms were located in succeeding difference Fourier syntheses. Hydrogen atoms were included in the structure factor calculation in idealized positions using the riding model but they were not refined. The structure was refined in full-matrix least-squares where the function minimized was ©w($|F_o|^2$-|Fc|^2)^2 and the weight w is defined as 1/[$\int^2(F_o^2)$+(0.0461P)^2+0.0000P] where P=(F_o^2+2Fc^2)/3. Scattering factors were taken from the “International Tables for Crystallography”.

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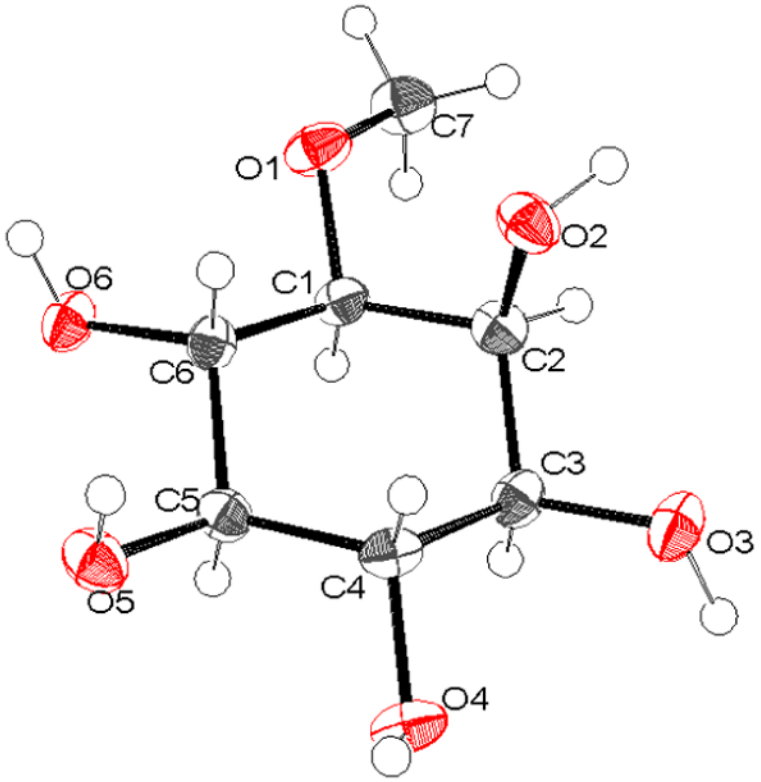
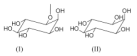


Figure 1.
ORTEP plot of *L*-(+)-bornesitol, showing atomic notation and thermal ellipsoids. The molecule is viewed approximately normal to the center plane of the chair-shaped cyclohexane ring: C2 and C5 are below and above the plane, respectively. Thermal ellipsoids are shown at the 50% probability level for non-H atoms.

Compounds



(I) (II)

Table 1

Hydrogen-bond geometry (A% , °)

D	H	A	D-H	A-H	D-A	D-H-A
O2	H2	O6	0.86 (3)	1.82 (2)	2.667 (3)	170 (3)
O3	H3	O1	0.95 (3)	1.80 (3)	2.723 (3)	162 (3)
O4	H4	O2	0.87 (3)	1.84 (3)	2.695 (3)	167 (3)
O5	H5	O3	0.89 (3)	2.03 (3)	2.892 (3)	163 (3)
O6	H6	O4	0.90 (3)	1.80 (3)	2.688 (2)	171 (3)

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