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An orthorhombic polymorph of *myo*-inositol

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Key indicators

Single-crystal X-ray study
T = 180 K
Mean σ(C–C) = 0.003 Å
R factor = 0.023
wR factor = 0.048
Data-to-parameter ratio = 5.2

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

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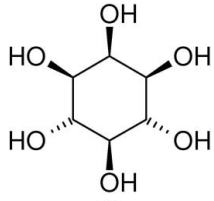
The title compound, $C_6H_{12}O_6$, has been obtained from the ethanol fraction of the aerial part of the plant *Incarvillea emodi* (Wall. ex Royle) Chatterjee, after recrystallization from ethanol/ethyl acetate (60:40). Each molecule is involved in 12 hydrogen bonds, as has been found in other reported inositol crystal structures.

Comment

The title compound, (I), which has been extracted from both plant and animal sources (Posternak, 1965), is of nutritional and medical importance and has been extensively studied for its biological applications, for example, additive effects with selective serotonin reuptake inhibitors (Seedat & Stein, 1999), anti-depressant and anti-anxiety activities (Einat *et al.*, 1999), the treatment of diabetic neuropathy (Clements *et al.*, 1979), and the side effects of medicinal lithium (Belmaker *et al.*, 1998; Wolfson *et al.*, 1998). Its crystal structure (Rabinovich & Kraut, 1964) and that of a dihydrate (Lomer *et al.*, 1963) have been reported previously. The family of inositol stereoisomers has recently received attention in the chemical literature in the context of the relationship between molecular structure, crystal structure and melting point (Simperler *et al.*, 2006). We have isolated *myo*-inositol from the ethanol fraction of the aerial part of *Incarvillea emodi* (Wall. ex Royle) Chatterjee, belonging to the Bignoniaceae family. Recrystallization of the compound from ethanol/ethyl acetate (60:40) has yielded a new orthorhombic polymorph.



(I)

The established monoclinic polymorph of (I) crystallizes in space group $P2_1/c$ with $Z' = 2$ (Rabinovich & Kraut, 1964). The orthorhombic form of (I) crystallizes in space group $Pna2_1$ with $Z' = 1$ (Fig. 1). For the monoclinic structure, Simperler *et al.* (2006) designated the independent molecules as **A** and **B**, distinguished by their hydrogen-bonding patterns. The hydrogen-bonding pattern in the orthorhombic form (Fig. 1, Table 1) is comparable to that of molecule **A** in the monoclinic form. The axial OH group (O1) forms only one O—H···O hydrogen bond in which it acts as an OH donor, and it does not accept any hydrogen bonds. The adjacent equatorial OH

group (O2) forms one hydrogen bond in which its OH group acts as a donor, and it also accepts two hydrogen bonds. All other OH groups donate one hydrogen bond and accept one hydrogen bond. Thus, there is a total of 12 O—H···O hydrogen bonds donated/accepted per molecule, in common with all other inositol crystal structures known to date (Simperler *et al.*, 2006; Day *et al.*, 2006).

Experimental

The plant *Incarvillea emodi* (Wall. ex Royle) Chatterjee was collected from the mountains of Salhad village, Abbottabad, Pakistan, and a sample was deposited at the herbarium of Quaid-i-Azam University, Pakistan. The powdered aerial part of the plant (2 kg) was extracted three times with 75% methanol (25 l). The combined extract was concentrated to a semi-solid mass and was purified by removing fatty material and carotenoids by extracting with diethyl ether. The extract was fractioned using different solvents according to their increasing polarity. The ethanol fraction was then subjected to column chromatography using silica gel (70–230 mesh Merck) eluted with a solvent system ranging from 10:90 ethanol/ethyl acetate to 90:10, followed by 100% ethanol and 100% methanol. The ethanol fraction yielded pure *myo*-inositol, which was crystallized by slow evaporation from a mixture of ethanol/ethyl acetate (60:40).

Crystal data

$C_6H_{12}O_6$
M_r = 180.16
Orthorhombic, $Pna2_1$
a = 10.5485 (5) Å
b = 6.6177 (3) Å
c = 10.3714 (5) Å
V = 723.99 (6) Å^3
Z = 4
D_x = 1.653 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.15 mm^{-1}
T = 180 (2) K
Plate, colourless
0.20 × 0.10 × 0.05 mm

Data collection

Bruker–Nonius X8 APEX-II CCD diffractometer
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.844, T_{max} = 0.993
5306 measured reflections
695 independent reflections
582 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 25.6°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.048
S = 0.99
695 reflections
133 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0327P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O4^{i}	0.84 (3)	1.90 (3)	2.729 (2)	168 (3)
O2—H2···O5^{ii}	0.82 (3)	2.02 (3)	2.815 (3)	164 (3)
O3—H3···O2^{iii}	0.79 (4)	2.15 (4)	2.921 (3)	163 (3)
O4—H4···O6^{iv}	0.84 (3)	1.84 (3)	2.661 (2)	168 (3)
O5—H5···O3^{v}	0.82 (3)	2.04 (3)	2.852 (3)	172 (3)
O6—H6···O2^{v}	0.76 (3)	2.02 (3)	2.735 (2)	158 (3)

Symmetry codes: (i) $-x+1, -y+1, z-\frac{1}{2}$; (ii) $x+\frac{1}{2}, -y+\frac{3}{2}, z$; (iii) $-x+1, -y+2, z+\frac{1}{2}$; (iv) $-x+\frac{1}{2}, y+\frac{1}{2}, z+\frac{1}{2}$; (v) $x, y-1, z$.

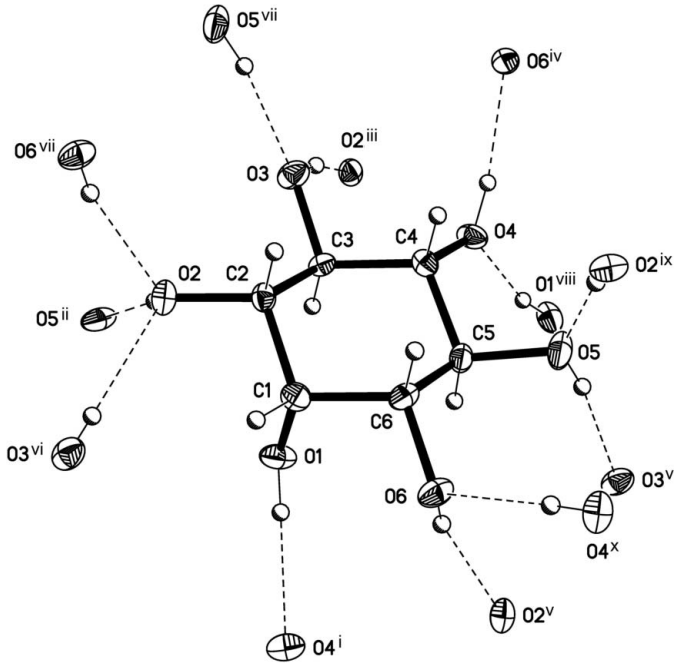


Figure 1
The molecular structure and hydrogen-bonding pattern of (I). Displacement ellipsoids are shown at the 50% probability level for non-H atoms and dashed lines indicate O—H···O hydrogen bonds. [Symmetry codes (i)–(v) are as listed in Table 1. Symmetry codes: (vi) $-x+1, -y+2, z-\frac{1}{2}$; (vii) $x, y+1, z$; (viii) $-x+1, -y+1, \frac{1}{2}+z$; (ix) $x-\frac{1}{2}, -y+\frac{3}{2}, z$; (x) $-x+\frac{1}{2}, y-\frac{1}{2}, z-\frac{1}{2}$.]

H atoms bound to C atoms were positioned geometrically with C—H = 1.00 Å and allowed to ride during subsequent refinement, with $U_{iso}(H) = 1.2\,U_{eq}(C)$. H atoms of the hydroxyl groups were located in difference Fourier maps and refined with isotropic displacement parameters, without restraint. In the absence of significant anomalous scattering, Friedel opposites (421 measured) have been merged as equivalent data.

Data collection: *APEX2* (Bruker–Nonius, 2004); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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