Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

allo-Inositol

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Key indicators

Single-crystal X-ray study
T = 180 K
Mean σ(C–C) = 0.002 Å
R factor = 0.036
wR factor = 0.102
Data-to-parameter ratio = 12.5

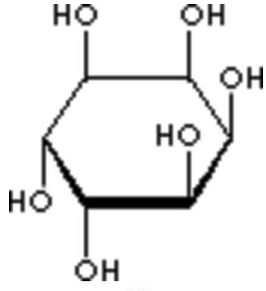
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 22 May 2006
Accepted 26 May 2006

In the crystal structure of the title compound, $C_6H_{12}O_6$, molecules adopt a chair conformation. The H atoms were located and their positions refined satisfactorily. The molecules form one intramolecular and 12 intermolecular hydrogen bonds; all hydroxyl groups act as hydrogen-bond donors and acceptors.

Comment

Inositols are isomers of pyranose sugars ($C_6H_{12}O_6$), and are present in nature and in biological systems (Podeschwa *et al.*, 2003). We have reported elsewhere on the hydrogen bonds in crystal structures of some cyclohexanol derivatives (Bonnet *et al.*, 2005), and a study of the Cambridge Structural Database (Version 5.27; Allen, 2002) reveals that the crystal structures of only five of the nine isomeric inositols have been reported. Here we report the crystal structure of *allo*-inositol (Fig. 1). Fig. 2 provides a view along the *a* axis, showing each molecule linked to eight neighbouring molecules by hydrogen bonds.



(I)

Experimental

allo-Inositol (97%) was obtained from Sigma–Aldrich UK as a crystalline powder, and its purity was confirmed by solution NMR and elemental analysis. Suitable single crystals were obtained by vapour diffusion of acetone into an aqueous solution of the inositol, after a week at room temperature. Elemental analysis gave C 40.10, H 6.66, O 53.24%; expected: C 40.00, H 6.71, O 53.28%. The onset melting temperature was determined using differential scanning calorimetry, and gave a value of 454 K with reproducibility [literature: 583 K, with decomposition (Tschamber *et al.*, 1992)].

Crystal data

$C_6H_{12}O_6$
M_r = 180.16
Monoclinic, $P2_1/n$
a = 4.9520 (2) Å
b = 11.3145 (6) Å
c = 12.7326 (6) Å
β = 91.142 (3)°
V = 713.26 (6) Å^3
Z = 4
D_x = 1.678 Mg m^{-3}
Mo *Kα* radiation
μ = 0.15 mm^{-1}
T = 180 (2) K
Block, colourless
0.23 × 0.18 × 0.18 mm

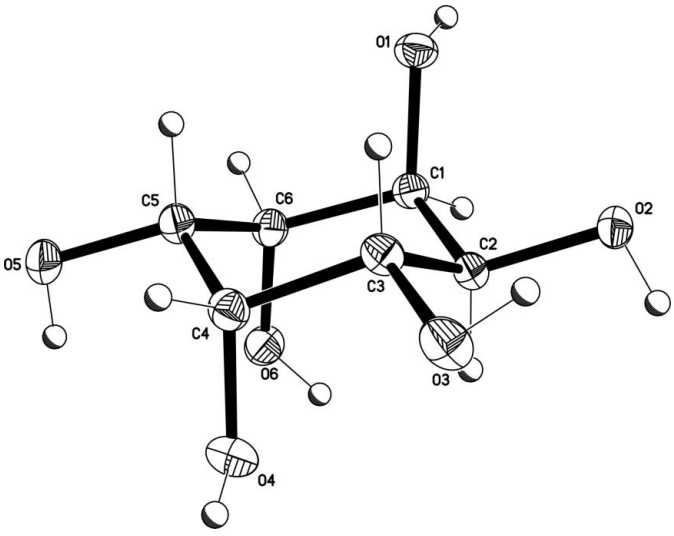


Figure 1
The molecular structure of *allo*-inositol. Displacement ellipsoids are drawn at the 50% probability level.

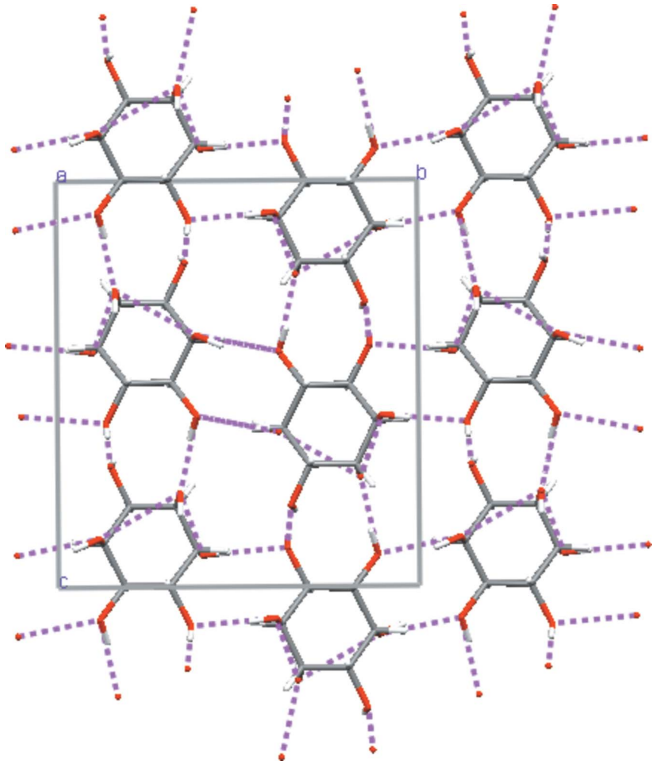


Figure 2
Packing diagram for *allo*-inositol, viewed along the *a* axis. The dashed lines show O···O contacts for hydrogen bonds.

Data collection

Nonius KappaCCD diffractometer
thin–slice ω and φ scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.896, T_{max} = 0.975
5743 measured reflections
1627 independent reflections
1387 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 27.4°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.102
S = 1.06
1627 reflections
130 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0508P)^2 + 0.2778P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.004
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2^{i}	0.82 (2)	1.95 (2)	2.7695 (14)	174 (2)
O2—H2···O5^{ii}	0.82 (2)	1.91 (2)	2.7289 (14)	179 (2)
O3—H3···O6^{iii}	0.85 (2)	1.90 (2)	2.7423 (13)	171 (2)
O4—H4···O3^{iv}	0.84 (2)	1.93 (2)	2.7461 (14)	164 (2)
O5—H5···O2^{v}	0.86 (2)	2.12 (2)	2.9014 (14)	152 (2)
O6—H6···O1^{vi}	0.82 (2)	2.05 (2)	2.8248 (13)	158 (2)

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

The O-bound H atoms were all located in a difference map and refined with a common isotropic displacement parameter [0.041 (2) Å^2]; O—H distances were restrained to a target value of 0.83 (1) Å. The C-bound H atoms were placed in calculated positions, with C—H = 1.00 Å, and refined as riding with a common isotropic displacement parameter [0.016 (2) Å^2]

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *MERCURY* (Version 1.4; Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXL97*.

The authors are grateful to Dr John Davies (Department of Chemistry, University of Cambridge) for determining the crystal structure, and Drs A. Trask and L. Fabian for help with CIF preparation. The Pfizer Institute for Pharmaceutical Materials Science is acknowledged for funding the work.

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