The title compound, C₆H₁₂O₄, exists in a chair form, with three of the four OH groups equatorially disposed. All four hydroxy groups participate in extensive intermolecular O—H⋯O hydrogen bonding.

Comment

The title compound, (1), is one of the five possible geometrical isomers of 1,2,4,5-cyclohexanetetrol. Compound (1) can be conveniently prepared from 1,4-cyclohexadiene via a selective epoxidation–hydrolysis–osmylation strategy (McCasland et al., 1963) and is the only readily obtainable configurational isomer of 1,2,4,5-cyclohexanetetrol capable of existing in two energetically different conformational isomers, (1a) and (1b).

While conformer (1a) has three of the four hydroxy groups equatorial and is capable of solely intermolecular O—H⋯O hydrogen bonding, conformer (1b), with two syn-diaxial hydroxy groups, can be stabilized through an intramolecular O—H⋯O hydrogen bond (Girling et al., 1974; Panagiotopoulos et al., 1974; James et al., 1978).

Experimentally, the hydroxy groups in (1) were found to adopt the spatial disposition present in (1a) (Fig. 1). Molecules of (1) pack in a herringbone-type arrangement in the non-centrosymmetric space group P2₁2₁2₁ (Fig. 2). Each tetrol molecule is linked to six nearest neighbors by intermolecular O—H⋯O hydrogen bonds (Table 2). The puckering parameters (Cremer & Pople, 1975) for the cyclohexane ring \([q₁ = 0.026 (2) \text{ Å}, q₂ = −0.582 (2) \text{ Å}, \varphi₂ = −17 (4)°, Q_T = 0.585 (2) \text{ Å} \text{ and } \theta₂ = 177.2 (2)°]\) describe a slightly distorted chair conformation. The total puckering amplitude \(Q_T\) is only

![Figure 1](image_url)

**Figure 1**

View of (1), with the atom-numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level.
methylmorpholine-N-oxide was obtained by slow evaporation of its solution in 1:2 dry ethyl acetate–water (50% solution in water, 0.40 ml) in 4:1 acetone–water (0.5 ml), gave suitable crystals of (1) which corresponds to a boat conformation. Therefore, the cyclohexane ring is distorted from an ideal chair conformation and is flattened at C6, allowing the C1—C6—C5 angle to increase to 112.86 (13), while the other internal ring angles remain close to the tetrahedral values. The flattening of the cyclohexane ring at C6 can be ascribed to the non-bonding (1,3-diaxial) interaction between the atom O1 and H atoms bonded to C atoms have been omitted for clarity. Dotted lines indicate hydrogen bonds.

The molecular packing of (1), viewed along the a axis. H atoms bonded to C atoms were omitted for clarity. Dotted lines indicate hydrogen bonds.

### Table 1

<table>
<thead>
<tr>
<th>Bond angles (°)</th>
<th>C1—C2—C3</th>
<th>C1—C6—C5</th>
<th>C4—C5—C6</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1—C2—C3</td>
<td>111.04 (13)</td>
<td>112.86 (13)</td>
<td>109.96 (13)</td>
</tr>
<tr>
<td>C1—C6—C5</td>
<td>112.86 (13)</td>
<td>112.86 (13)</td>
<td>109.96 (13)</td>
</tr>
<tr>
<td>C4—C5—C6</td>
<td>109.96 (13)</td>
<td>109.96 (13)</td>
<td>109.96 (13)</td>
</tr>
</tbody>
</table>

### Table 2

<table>
<thead>
<tr>
<th>Hydrogen-bond geometry (Å, °)</th>
<th>D—H—A</th>
<th>D—H—A</th>
<th>D—H—A</th>
<th>D—H—A</th>
</tr>
</thead>
<tbody>
<tr>
<td>O1—H1O—O4</td>
<td>0.82</td>
<td>1.89</td>
<td>2.705 (2)</td>
<td>172</td>
</tr>
<tr>
<td>O2—H2O—O3</td>
<td>0.82</td>
<td>2.01</td>
<td>2.765 (2)</td>
<td>153</td>
</tr>
<tr>
<td>O3—H3O—O1</td>
<td>0.82</td>
<td>1.92</td>
<td>2.742 (2)</td>
<td>176</td>
</tr>
<tr>
<td>O4—H4O—O2</td>
<td>0.82</td>
<td>1.94</td>
<td>2.752 (2)</td>
<td>169</td>
</tr>
</tbody>
</table>

Symmetry codes: (i) x, y, z; (ii) x + 1/2, y + 1/2, z + 1/2; (iii) −x + 1/2, −y + 1/2, −z + 1.

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.97–0.98 Å and Uiso(H) = 1.2Ueq(C), and O—H distances fixed at 0.82 Å and Uiso(H) = 1.5Ueq(O). Though (1) is obtained in a racemic form through synthesis, its chiral structure in the solid state appears to have resulted from a spontaneous resolution during crystallization. However, owing to the absence of any heavy atom (Z > 6) in (1), the absolute configuration could not be refined. Friedel pairs (539) were averaged prior to merging of data in P212121; the reported value of Rint corresponds to subsequent merging of equivalent reflections in this space group.

### Experimental

Compound (1) was prepared by a modification of the procedure described by McCasland et al. (1963). 1,4-Cyclohexadiene (0.5 ml, 5.3 mmol) in dichloromethane (3 ml) was treated with m-chloroperbenzoic acid (70% purity, 1.4 g) in dichloromethane (5 ml) at 273 K. The monoepoxide thus obtained was heated with a 0.2 M aqueous solution of Na2CO3 (5 ml) at 368 K to obtain trans-4-cyclohexene-1,2-diol (0.36 g) in 70% yield (Michaud & Viala, 1999). The diol (0.20 g, 1.8 mmol), upon cis-dihydroxylation with catalytic osmium tetroxide (0.5 mol%) and N-methylmorpholine-N-oxide (50% solution in water, 0.40 ml) in 4:1 acetone–water (0.5 ml), gave the tetrool (1) (0.21 g) in 80% yield. Suitable crystals of (1) were obtained by slow evaporation of its solution in 1:2 dry ethyl acetate–methanol.

### Structure Data

**Crystal data**

C3H6O4

Orthorhombic, P212121

a = 6.756 (2) Å

b = 8.783 (3) Å

c = 11.271 (4) Å

V = 668.8 (4) Å³

Z = 4

D_x = 1.471 Mg m⁻³

Mo Kα radiation

Cell parameters from 700 reflections

θ = 2.9–27.0°

μ = 0.12 mm⁻¹

T = 296 (2) K

Block, colorless

0.40 × 0.35 × 0.30 mm

**Data collection**

Bruker SMART CCD area-detector diffractometer

814 independent reflections

800 reflections with I > 2σ(I)

Rint = 0.016

Absorption correction: multi-scan

θmax = 26.4°

h = −8 → 8

k = −10 → 10

l = −14 → 13

Refinement

Refinement on F²

wR(F²) = 0.081

S = 1.18

814 reflections

95 parameters

H-atom parameters constrained

### Figures

Figure 2

The molecular packing of (1), viewed along the a axis.
al., 1993); software used to prepare material for publication: PLATON (Spek, 2003).

We thank the DST, Government of India, for the CCD facility at IISc.

References