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2,2,6,6-Tetrakis(hydroxymethyl)cyclohexanol

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Key indicators

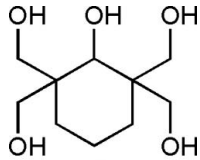
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.027
wR factor = 0.069
Data-to-parameter ratio = 6.6

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

In the title compound, $C_{10}H_{20}O_5$, the six-membered ring adopts a slightly twisted chair conformation. The crystal packing is stabilized by intermolecular O—H···O interactions.

Comment

The title compound, (I), is the key intermediate in the synthesis of Nicomol which is a hypolipidemic drug (Roach & Wittcoff, 1951).



(I)

The six-membered ring adopts a slightly twisted chair conformation. There is an intramolecular O—H···O bond (Fig. 1). In the crystal structure of (I), intermolecular O—H···O hydrogen bonds link molecules into a three-dimensional array (Fig. 2 and Table 1).

Experimental

Compound (I) was synthesized according to the procedure of Wittcoff (1950, 1951). Crystals suitable for X-ray analysis were grown by slow evaporation of a solution in absolute ethanol at room temperature over a period of 12 d.

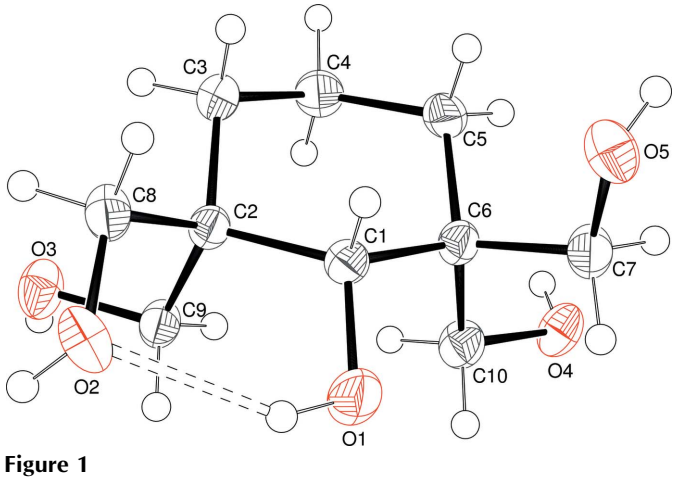


Figure 1
The molecular structure of (I), shown with 30% probability displacement ellipsoids (arbitrary spheres for H atoms). The hydrogen bond is shown as a double dashed line.

Crystal data

$C_{10}H_{20}O_5$
M_r = 220.26
Orthorhombic, $Pna2_1$
a = 12.181 (3) Å
b = 6.0387 (16) Å
c = 14.606 (4) Å
V = 1074.4 (5) Å^3
Z = 4
D_x = 1.362 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 294 (2) K
Block, colourless
0.28 × 0.20 × 0.10 mm

Data collection

Bruker SMART 1000 CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.970, T_{max} = 0.989
5104 measured reflections
990 independent reflections
930 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.069
S = 1.12
990 reflections
151 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0378P)^2 + 0.1306P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2	0.88 (3)	2.06 (3)	2.806 (2)	143 (2)
O2—H2···O4^{i}	0.85 (3)	1.89 (3)	2.719 (2)	166 (3)
O3—H3···O2^{ii}	0.85 (3)	1.98 (3)	2.795 (2)	161 (3)
O4—H4···O5^{ii}	0.85 (3)	1.91 (3)	2.749 (3)	170 (3)
O5—H5···O3^{iii}	0.81 (3)	2.02 (3)	2.834 (3)	175 (3)

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

The C-bound H atoms were positioned geometrically (C—H = 0.97–0.98) and refined as riding. The O-bound H atoms were located in a difference map and their positions were freely refined. The constraint U_{iso}(H) = 1.2$_{eq}$(C) or 1.5U_{eq}(O) was applied. In the absence of significant anomalous scattering effects, Friedel pairs were merged.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

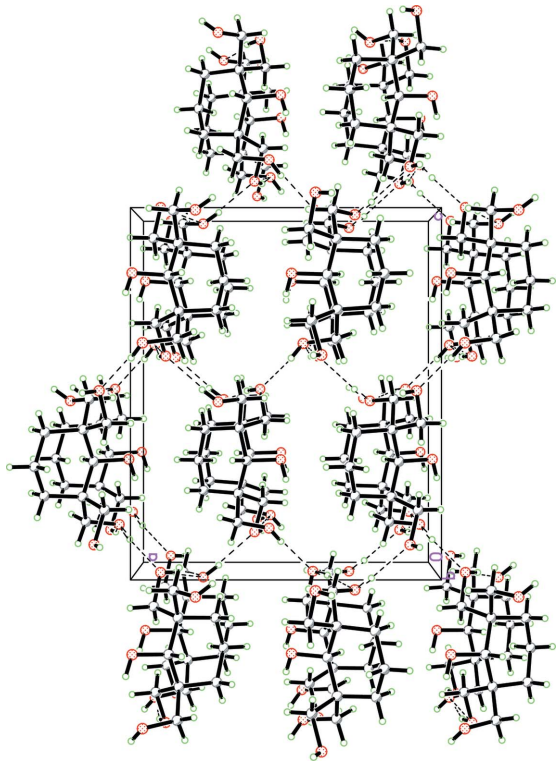


Figure 2
Part of the crystal structure of (I), with hydrogen bonds shown as dashed lines.

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