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(1*R*,5*R*,6*S*)-6-(2-Hydroxyethyl)-2-methyl-5-(prop-1-en-2-yl)cyclohex-2-enol

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The crystal structure determination of the title compound, $C_{12}H_{20}O_2$, is part of a model study carried out to investigate the chemistry related to our ongoing efforts toward the total synthesis of the zoanthamine alkaloids. The cyclohexene ring adopts a half-chair conformation. In the crystal structure, the molecules are linked by intermolecular O—H···O hydrogen bonds between the hydroxyl groups of neighbouring molecules, forming columns parallel to the *b* axis.

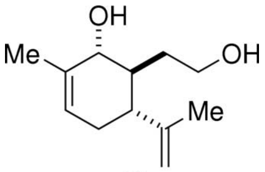
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
R factor = 0.049
wR factor = 0.134
Data-to-parameter ratio = 12.1

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

Comment

During a model study carried out in order to investigate the chemistry related to our ongoing efforts toward the total synthesis of the zoanthamine alkaloids, the title compound, (I), a diol was prepared. The structure determination established unambiguously the relative stereochemistry at the two newly formed stereocenters (Fig. 1). The bond lengths and angles are as expected for this type of compound (Allen *et al.*, 1987). The cyclohexene ring adopts a half-chair conformation with the secondary hydroxyl, the hydroxyethyl, and the isopropenyl substituents all located in a pseudo-equatorial orientation. The stereochemistry at the secondary hydroxyl is thus the result of pseudo-axial attack by the reducing agent $LiAlH_4$. No intramolecular hydrogen bonding takes place between the two hydroxyl moieties, but the crystal packing is influenced by O—H···O intermolecular hydrogen bonds (Table 1) between the hydroxyl groups of neighboring molecules, forming columns parallel to the *b* axis (Fig. 2).



(I)

Experimental

Compound (I) was prepared according to the method previously described (Juhl *et al.*, 2006). Single crystals suitable for X-ray measurements were obtained from cold (291 K) $CHCl_3$.

Crystal data

$C_{12}H_{20}O_2$
M_r = 196.28
Monoclinic, $P2_1$
a = 6.9388 (6) Å
b = 6.7185 (6) Å
c = 12.9422 (11) Å
β = 100.563 (2)°
V = 593.12 (9) Å^3
Z = 2
D_x = 1.099 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 295 (2) K
Block, colorless
0.38 × 0.33 × 0.24 mm

doi:10.1107/S1600536806056443

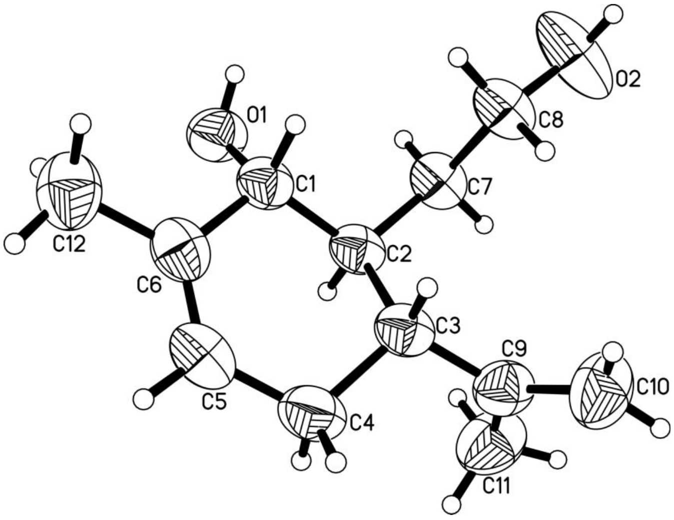


Figure 1
The molecular structure and the atom-labeling scheme of (I). Displacement ellipsoids are drawn at the 50% probability level.

Data collection

Bruker SMART 1K CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001*a*)
$T_{\min} = 0.889$, $T_{\max} = 0.992$

4218 measured reflections
1536 independent reflections
1449 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.017$
$\theta_{\max} = 28.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.134$
$S = 1.08$
1536 reflections
127 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0904P)^2 + 0.0286P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.17$ e Å^{-3}
$\Delta\rho_{\min} = -0.24$ e Å^{-3}

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O1—H11$\cdots$O2$^{\rm i}$	0.82	2.11	2.641 (3)	123
O2—H21$\cdots$O1$^{\rm ii}$	0.82	1.89	2.693 (2)	168

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

The absolute configuration of the structure could not be determined due to the lack of heavy atoms. Therefore, the Friedel pairs were merged; the absolute configuration is known from that of the starting materials. All H atoms were positioned geometrically and refined using a riding model with C—H = 0.96 Å, $U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(C) for methyl, O—H = 0.82 Å, $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(O) for OH groups and C—H = 0.93–0.98 Å, $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C) for the remaining H atoms.

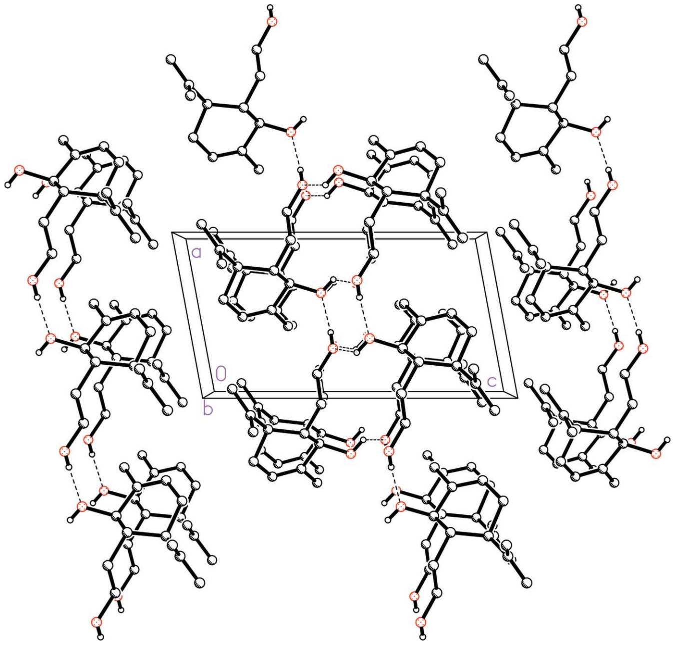


Figure 2
The molecular packing of (I) viewed down the *b* axis. The dashed lines denote the O—H$\cdots$O hydrogen bonds. The non-hydrogen-bonded H atoms have been omitted for clarity.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2001*b*); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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