resembles more closely that in *N*-methylcytosine with its paired N—H···N interactions with one partner molecule and N—H···O with another; however, the striking non-coplanarity of hydrogen-bonded bases in *N*-methylcytosine is not evident here.

This study further strengthens the idea that 2-aminopyrimidin-4-ones are very adaptable both in their tautomeric form and in their intermolecular interactions.

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Structure of (1*S*,6*S*,8*S*,9*S*,1′*S*)-8-(1′-Hydroxyethyl)-9-hydroxymethyl-1,5,5-trimethylbicyclo[4.3.0]nonane

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Abstract. $C_{15}H_{28}O_2$, $M_r = 240{\cdot}39$, orthorhombic, $P2_12_12_1$, $a = 6{\cdot}518\,(2)$, $b = 12{\cdot}849\,(5)$, $c = 17{\cdot}796\,(7)$ Å, $V = 1490{\cdot}4\,(9)$ Å^3, $Z = 4$, $D_x = 1{\cdot}07$ Mg m^{-3}, $\lambda(\text{Mo } K\alpha) = 0{\cdot}71069$ Å, $\mu = 0{\cdot}07$ mm^{-1}, $F(000) = 536$, $R = 0{\cdot}039$ and $wR = 0{\cdot}038$ for 893 observed reflections, $T = 293$ K. The absolute configuration was not determined; stereochemistry at the 8 and 1′ positions is established. The cyclohexane and cyclopentane rings have chair and half-chair conformations, respectively, and are *trans*-fused.

Introduction. Drimenol (1) is a sesquiterpenic alcohol isolated from *Drymis winteri* Forst (Appel, Brooks & Overton, 1959). As part of a systematic study of molecule (1) in order to obtain derivatives of interest in pharmacology (Ley & Mahon, 1981) and perfumery (Brunke, 1980), the tosylated molecule (2) has been synthesized (Planas, Cortès & Bonet, 1985). The reduction of (2) with $LiAlH_4$ gives a product (35%

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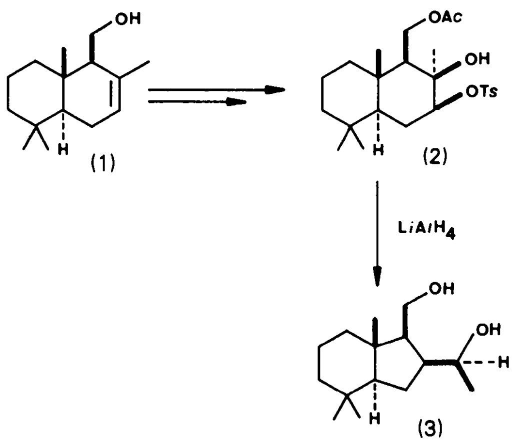
yield) whose complete structure could not be elucidated. The X-ray structural analysis was therefore undertaken to determine the structure and stereochemistry of the reduction product.



Experimental. Colourless crystals were prepared by slow evaporation from an acetone/petroleum ether solution. A suitable monocrystal of *ca* 0·4 × 0·6 × 0·6 mm was mounted on a Syntex $P2_1$ four-circle diffractometer with graphite-monochromated Mo $K\alpha$ radiation. Cell parameters from 15 reflections ($9 \leq 2\theta \leq 22°$). The intensities were measured using ω-scan technique up to $2\theta = 47°$. One standard reflection, monitored every 50 measurements, showed no significant variation. Of 1306 independent reflections measured ($0 \leq h \leq 7$, $0 \leq k \leq 14$, $0 \leq l \leq 17$), 893 were considered as observed [$I \geq 2{\cdot}5\sigma(I)$]. Data were corrected for Lorentz–polarization effects but not for absorption. The structure was solved by direct methods (*MULTAN*80: Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980); all non-H atoms found in the best-FOM E map. Full-matrix least-squares refinement on F using *SHELX* (Sheldrick, 1976). All H atoms located by difference Fourier synthesis and refined with an overall isotropic temperature factor. Final $R = 0{\cdot}039$, $wR = 0{\cdot}038$, $w = [\sigma^2(F) + 4{\cdot}6 \times 10^{-4}F^2]^{-1}$; max. shift/e.s.d. = 0·46 on positional parameters and 0·53 on thermal parameters; max. and min. heights in final difference Fourier synthesis 0·12 and −0·13 e Å^{-3}; scattering factors from *International Tables for X-ray Crystallography* (1974).

Discussion. Final atomic coordinates and equivalent isotropic temperature factors are given in Table 1.* Bond lengths and the numbering scheme are given in Figs. 1 and 2. The reduction reaction described above takes place with ring contraction giving a product with stereochemistry 8S and 13S (1′S) at the new chiral centres created in the reaction.

The cyclohexane ring shows a chair conformation as in drimenol (Escobar & Wittke, 1984) with all asymmetry parameters below 5 (Duax & Norton, 1975). Mirror symmetry is dominant (approximate C_s plane through C2 and C5 with $\Delta C_s^2 = 2{\cdot}4(5)$. There is 1,3-diaxial interaction between C10 and C12;

Table 1. *Final fractional atomic coordinates* (×10^4) *and equivalent isotropic temperature factors* (Å^2), *e.s.d.'s in parentheses*

$$B_{eq} = \tfrac{8}{3}\pi^2 \textstyle\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	B_{eq}
C1	8372 (6)	7780 (3)	2421 (2)	3·70
C2	10196 (8)	7342 (5)	2859 (3)	5·07
C3	9662 (10)	7213 (5)	3684 (3)	6·04
C4	8921 (9)	8200 (5)	4057 (3)	5·41
C5	7049 (7)	8719 (4)	3665 (2)	4·35
C6	7612 (7)	8777 (3)	2816 (2)	3·55
C7	6126 (8)	9250 (4)	2257 (3)	4·14
C8	7265 (7)	9117 (3)	1492 (2)	3·51
C9	8933 (7)	8272 (3)	1651 (2)	3·46
C10	5085 (9)	8132 (6)	3837 (3)	5·73
C11	6813 (12)	9823 (5)	3962 (3)	6·48
C12	6739 (9)	6927 (4)	2320 (3)	4·95
C13	5847 (7)	8983 (3)	0812 (2)	3·78
C14	4481 (10)	9917 (4)	0700 (3)	5·62
C15	9412 (8)	7503 (4)	1025 (3)	4·48
O16	10420 (5)	8022 (3)	0402 (2)	5·17
O17	4553 (5)	8074 (3)	0883 (2)	4·06

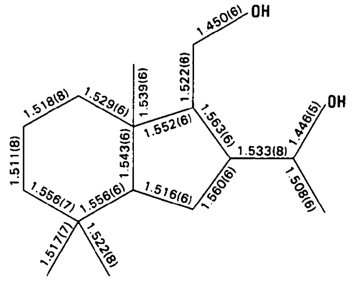


Fig. 1. Bond lengths (Å) with e.s.d.'s in parentheses.

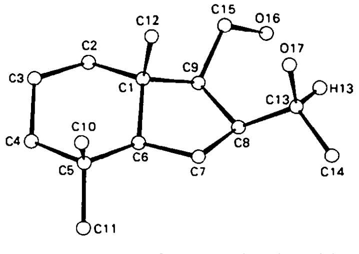


Fig. 2. A perspective view of the molecule with atom labelling (*ESTER*; Gaete, 1985).

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* Lists of structure amplitudes, anisotropic thermal parameters, H-atom parameters, bond angles and torsion angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43385 (11 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

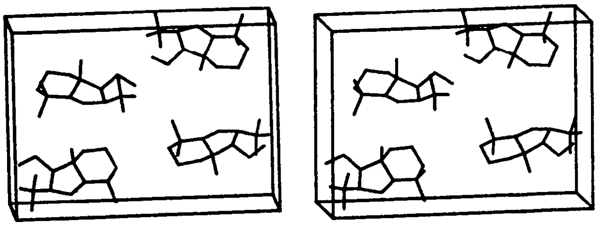

Fig. 3. Stereoscopic view of the crystal packing (*ESTER*; Gaete, 1985).

C10···C12 = 3·29 (1) Å, shorter than a normal van der Waals separation. The five-membered ring exhibits a half-chair conformation [$\Delta C_2^8 = 5{\cdot}2\,(6)$]. Both C12 and the two substituents at C8 and C9 point to the same side of the molecule. The ring junction is *trans*.* The molecules are linked by intermolecular hydrogen bonds forming infinite double chains along the x axis, O16—H···O17 ($x + 1, y, z$) and O17—H···O16 ($-\frac{1}{2} + x, 1\frac{1}{2} - y, -z$) with O···O distances of 2·827 (6) and 2·744 (6) Å.† The crystal packing is depicted in Fig. 3.

We are greatly indebted to Drs J. J. Bonet and A. Planas (Instituto Químico de Sarriá, Barcelona, Spain) and Dr M. Cortés (Pontificia Universidad Católica de Chile) for suggesting the problem and providing the sample.

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* Torsion angles C2—C1—C6—C5 and C9—C1—C6—C7 −54 and 49°, respectively.

† Details of the hydrogen bonding have been deposited. See deposition footnote.

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Structure of 1-Acetyl-2,4,5,7-tetrahydroxy-9,10-anthracenedione

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Abstract. $C_{16}H_{10}O_7$, $M_r = 314{\cdot}2$, orthorhombic, *Pbca*, $a = 15{\cdot}400\,(7)$, $b = 6{\cdot}930\,(2)$, $c = 23{\cdot}92\,(1)$ Å, $V = 2552{\cdot}8$ Å^3, $Z = 8$, $D_x = 1{\cdot}63$, $D_m = 1{\cdot}62$ Mg m^{-3}, $\lambda(\mathrm{Cu}\,K\alpha) = 1{\cdot}54178$ Å, $\mu = 1{\cdot}15$ mm^{-1}, $F(000) = 1296$, $T = 293$ K, final $R = 0{\cdot}052$ for 812 unique observed reflections. The crystal structure consists of stacks of 'dimerized' planar molecules related by the b glide plane and interlinked by a hydrogen-bond network to form a densely packed arrangement. The molecular structure is analysed in detail and results are compared with those of five other analogues reported (with comparable accuracy) earlier. There is crystallographic evidence for the existence of a significant attractive charge-transfer interaction which is probably of the n–π^* type and involves an sp^3-like lone pair of a carbonyl oxygen as n donor and the π system of the

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