

crystallographically glide-related [NH₄·18C6]⁺ ions along the *a* direction in the crystal. Hydrogen-bond distances are: 3.25 (1) Å for N⁺...Cl, with an N⁺—H(c)...Cl angle of 168°, and 3.25 (1) and 3.26 (1) Å respectively for Cl⁻...OH₂ and Cl⁻...OH₂. The distance between the O atoms of the water molecules H₂O and H₂O' is 3.36 (1) Å.

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Structure of 1 α ,3 α -Trimethylene-2',5-epoxyandrostane-3 β ,17 β -diol 17-Propionate Methanol Solvate (1/0.5)

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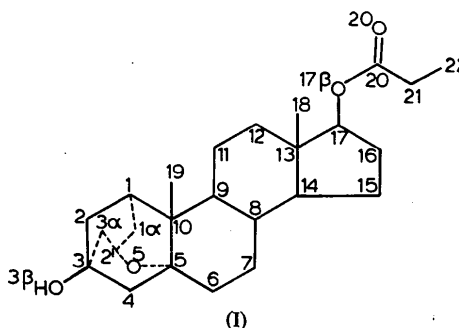
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Abstract. C₂₅H₃₈O₄·0.5CH₄O, *M_r* = 418.6, monoclinic, *P*2₁, *a* = 19.8504 (20), *b* = 7.3909 (4), *c* = 15.7998 (18) Å, β = 93.09 (2)°, *V* = 2314.7 (8) Å³, *Z* = 4, *D_x* = 1.201 Mg m⁻³, λ (Cu *K* α) = 1.54184 Å, μ = 0.604 mm⁻¹, *F*(000) = 916, *T* = 295 K, *R* = 0.056 for 4946 unique observed reflections. The crystallographic asymmetric unit contains two steroid molecules and a molecule of methanol. All six-membered rings for both molecules have chair conformations. The *D* ring has a 13 β -envelope conformation in molecule 1 and a 13 β ,14 α -half-chair conformation in molecule 2. The most significant differences between the crystallographically independent steroids are in the orientation of the H atoms of the C(3) hydroxyl groups and the conformations of the propionate side chains. When the crystallographically observed molecules are subjected to energy minimization their respective hydroxyl H-atom orientations are retained, but the *D* rings of both molecules refine to a common 13 β ,14 α -half-chair conformation and a significantly different orientation of the C(17) propionate side chain is generated. A comparison with other C(17)-ester-bearing steroids

suggests that the energy minimization fails to simulate fully all intramolecular interactions.

Introduction. The title compound (I) is a product of the Michael addition reaction of ethyl acetoacetate and 3-oxoandrosta-1,4,6-trien-17 β -yl propionate. Although UV, IR, ¹H NMR, and mass spectroscopy spectra were consistent with an oxaadamantane structure, a strained structure with a β -side addition could not be ruled out. This is the first oxaadamantane steroid for which the crystal structure has been determined.



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Experimental. A crystal (0.18 × 0.30 × 0.95 mm) was grown by slow evaporation from MeOH/H₂O and mounted in a capillary. The unit-cell parameters were determined by least-squares method from 2θ values for 25 reflections with 43 < 2θ < 58°. Data collection with 3 < 2θ < 154° (0 ≤ h ≤ 25, -9 ≤ k ≤ 0, -19 ≤ l ≤ 19), θ-2θ scan mode. Intensities of 5936 reflections measured on an Enraf-Nonius CAD-4 diffractometer using Ni-filtered Cu Kα radiation, corrected for Lp, absorption ignored. Intensities of six standard reflections (11̄8, 127̄, 12, 1̄, 1̄, 241, 625̄, 625) varied by less than 4% during the data collection, no correction applied. Direct methods using *MULTAN78* (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978) revealed positions of 33 non-H atoms. The remaining atoms were found from Fourier maps. The positional and anisotropic thermal parameters of non-H atoms were refined by full-matrix least squares using 4946 reflections for which $F_o > 3.0\sigma(F_o)$. In both molecules the 17α-propionate side chain exhibited large atomic displacement parameters. The terminal atoms C(21) and C(22) of molecule 1 were fixed in positions derived from difference Fourier maps, and the associated H atoms were placed in calculated positions. In molecule 2 the terminal methyl group C(22) was handled in the same fashion. All other H atoms were located in ΔF maps and refined with isotropic thermal parameters. Atomic scattering factors were taken from *International Tables for X-ray Crystallography* (1974). Final $R = 5.6$, $wR = 7.4\%$, $S = 2.946$ for 4946 observed reflections, $w = 1/\sigma_F^2$, $\Delta/\sigma_{\max} = 0.10$. The strongest peak in a final difference map had a density of +0.44 (-0.27) e Å⁻³. Atomic positional parameters and equivalent isotropic thermal parameters are presented in Table 1. Interatomic distances and valence angles are presented in Table 2.*

Discussion. Comparison of bond lengths and bond angles of the two molecules with the average values for 5α-saturated steroids (Griffin, Duax & Weeks, 1984) revealed good overall agreement. Fig. 1 shows an *ORTEP* drawing (Johnson, 1965) of molecule 1. The overall conformations of the two molecules were compared by a least-squares superposition of atoms from the A, B, C and D rings (Fig. 2). The only significant differences in the two molecules are in the orientations of the H atoms of the hydroxyl group at the C(3) position, and of the propionate side chains at the C(17) position.

The molecules in the crystal are connected by three hydrogen bonds with the geometric features described

* Lists of structure factors, H-atom parameters, stereopacking diagrams, anisotropic thermal parameters and torsion angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44879 (32 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. Fractional atomic coordinates (×10⁵) and equivalent isotropic thermal parameters (Å² × 10) with e.s.d.'s in parentheses

$$B_{eq} = \frac{1}{3} \sum_i \sum_j \beta_{ij} a_i \cdot a_j$$

	x	y	z	B _{eq}
Molecule 1				
C(1)	64975 (10)	3569 (39)	-8577 (13)	34 (1)
C(2)	62108 (11)	8366 (42)	-17587 (13)	38 (1)
C(3)	57372 (11)	24564 (42)	-17267 (13)	38 (1)
C(4)	61189 (12)	40628 (42)	-13314 (14)	38 (1)
C(5)	63985 (11)	35867	-4371 (13)	34 (1)
C(6)	67063 (13)	52278 (41)	156 (15)	42 (1)
C(7)	69971 (13)	48042 (44)	9066 (15)	42 (1)
C(8)	74990 (11)	32195 (41)	9226 (13)	36 (1)
C(9)	71521 (10)	15506 (41)	4876 (13)	34 (1)
C(10)	69017 (10)	19674 (39)	-4502 (13)	33 (1)
C(11)	75826 (13)	-1779 (44)	5794 (16)	44 (1)
C(12)	78107 (13)	-5609 (44)	15033 (17)	46 (1)
C(13)	81851 (11)	10579 (44)	18944 (14)	40 (1)
C(14)	77253 (11)	27241 (44)	18272 (14)	39 (1)
C(15)	81018 (13)	41298 (49)	23950 (16)	48 (1)
C(16)	84489 (14)	29802 (57)	31178 (17)	51 (1)
C(17)	83126 (12)	10129 (51)	28617 (16)	46 (1)
C(18)	88560 (11)	13458 (51)	14752 (15)	47 (1)
C(19)	75165 (11)	23856 (45)	-9786 (14)	42 (1)
C(20)	89128 (18)	-8862 (62)	38747 (20)	63 (1)
C(21)	95077	-20849	39579	100 (2)
C(22)	96594	-29175	47965	160 (3)
C(1a)	59007 (10)	-1089 (41)	-3231 (14)	36 (1)
C(2)	54540 (10)	15531 (43)	-2838 (13)	37 (1)
C(3a)	51542 (10)	20171 (44)	-11707 (14)	38 (1)
O(3β)	54980 (9)	28351 (38)	-25829 (10)	47 (1)
O(5)	58319 (7)	30642 (34)	589 (9)	36 (1)
O(17β)	88618 (10)	-2101 (44)	30860 (12)	58 (1)
O(20)	85348 (15)	-3965 (66)	44070 (16)	95 (1)
Molecule 2				
C(1)	37802 (13)	28632 (47)	-48858 (15)	44 (1)
C(2)	44294 (13)	21215 (53)	-44326 (16)	50 (1)
C(3)	42664 (12)	6058 (46)	-38253 (15)	44 (1)
C(4)	38970 (13)	-8927 (46)	-43059 (15)	44 (1)
C(5)	32487 (11)	-1510 (43)	-47528 (14)	38 (1)
C(6)	28224 (15)	-16754 (46)	-51461 (17)	49 (1)
C(7)	21757 (14)	-10061 (48)	-56015 (18)	51 (1)
C(8)	23028 (12)	4643 (46)	-62497 (15)	42 (1)
C(9)	27153 (11)	20264 (43)	-58244 (13)	38 (1)
C(10)	33994 (11)	13604 (45)	-54062 (13)	38 (1)
C(11)	27898 (15)	36505 (49)	-64168 (17)	51 (1)
C(12)	21101 (16)	43131 (49)	-68063 (16)	52 (1)
C(13)	17274 (12)	27947 (49)	-72608 (14)	44 (1)
C(14)	16447 (12)	12275 (51)	-66361 (16)	47 (1)
C(15)	11450 (17)	-477 (66)	-71084 (23)	71 (1)
C(16)	6542 (18)	12994 (83)	-75784 (25)	84 (1)
C(17)	9827 (15)	31299 (62)	-74827 (18)	59 (1)
C(18)	20754 (15)	22075 (56)	-80604 (16)	54 (1)
C(19)	38486 (13)	6613 (60)	-60996 (16)	55 (1)
C(20)	3357 (16)	52005 (58)	-83392 (20)	58 (1)
C(21)	3061 (22)	62757 (70)	-91477 (25)	80 (1)
C(22)	-3940	64451	-95376	106 (2)
C(1a)	33291 (16)	36046 (44)	-42096 (16)	48 (1)
C(2)	31644 (14)	20405 (46)	-36332 (14)	44 (1)
C(3a)	38016 (14)	13320 (47)	-31685 (14)	47 (1)
O(3β)	48717 (9)	-1649 (41)	-34279 (12)	55 (1)
O(5)	28361 (8)	6093 (36)	-41124 (9)	41 (1)
O(17β)	8895 (11)	42421 (48)	-82442 (12)	67 (1)
O(20)	-1013 (13)	51925 (56)	-78432 (17)	84 (1)
Methanol molecule				
C(Me)	56900 (17)	15269 (62)	21393 (18)	64 (1)
O(Me)	51651 (11)	12846 (45)	26775 (14)	68 (1)

in Table 3. An infinite chain of hydrogen bonds extends parallel to the *b* axis. The methanol molecule accepts a hydrogen bond from steroid molecule 1 and donates a hydrogen bond to steroid molecule 2, and the 3-hydroxyl of steroid molecule 2 is the donor in a hydrogen bond to the 3-hydroxyl of steroid molecule 1.

In general, the H atom of a hydroxyl substituted on a tetrahedrally coordinated C atom has freedom of rotation about the C-O bond. However, not all

Table 2. Bond lengths (Å) and bond angles (°) with *e.s.d.*'s in parentheses

Molecule			Molecule		
	1	2	1	2	
C(1)—C(1a)	1.531 (3)	1.532 (4)	C(1a)—C(1)—C(2)	107.6 (2)	108.0 (2)
C(1)—C(2)	1.546 (3)	1.541 (4)	C(1a)—C(1)—C(10)	109.9 (2)	109.8 (2)
C(1)—C(10)	1.555 (4)	1.554 (4)	C(2)—C(1)—C(10)	111.2 (2)	111.3 (2)
C(2)—C(3)	1.525 (4)	1.521 (5)	C(1)—C(2)—C(3)	110.3 (2)	110.7 (2)
C(3)—C(3a)	1.525 (3)	1.523 (4)	C(2)—C(3)—C(3a)	109.9 (2)	109.1 (2)
C(3)—C(4)	1.524 (4)	1.510 (4)	C(2)—C(3)—C(4)	109.4 (2)	109.7 (2)
C(3)—O(3β)	1.437 (3)	1.443 (3)	C(2)—C(3)—O(3β)	107.1 (2)	111.4 (2)
C(4)—C(5)	1.531 (3)	1.535 (4)	C(3a)—C(3)—C(4)	107.8 (2)	107.8 (2)
C(5)—C(6)	1.519 (3)	1.522 (4)	C(3a)—C(3)—O(3β)	111.2 (2)	111.3 (2)
C(5)—C(10)	1.560 (3)	1.561 (4)	C(4)—C(3)—O(3β)	111.5 (2)	107.4 (2)
C(5)—O(5)	1.457 (3)	1.449 (3)	C(3)—C(4)—C(5)	110.3 (2)	110.0 (2)
C(6)—C(7)	1.525 (3)	1.520 (4)	C(4)—C(5)—C(6)	111.6 (2)	110.9 (2)
C(7)—C(8)	1.537 (4)	1.524 (4)	C(4)—C(5)—C(10)	111.4 (2)	112.0 (2)
C(8)—C(9)	1.555 (4)	1.548 (4)	C(4)—C(5)—O(5)	107.8 (1)	108.0 (2)
C(8)—C(14)	1.520 (3)	1.520 (4)	C(6)—C(5)—C(10)	112.2 (2)	112.5 (2)
C(9)—C(10)	1.568 (3)	1.558 (3)	C(6)—C(5)—O(5)	105.1 (1)	104.4 (2)
C(9)—C(11)	1.539 (4)	1.534 (4)	C(10)—C(5)—O(5)	108.5 (1)	108.7 (2)
C(10)—C(19)	1.547 (3)	1.539 (4)	C(5)—C(6)—C(7)	113.2 (2)	112.9 (2)
C(11)—C(12)	1.531 (4)	1.533 (4)	C(6)—C(7)—C(8)	112.6 (2)	112.6 (2)
C(12)—C(13)	1.522 (4)	1.514 (5)	C(7)—C(8)—C(9)	109.0 (2)	110.1 (2)
C(13)—C(14)	1.533 (4)	1.536 (5)	C(7)—C(8)—C(14)	111.0 (2)	111.4 (2)
C(13)—C(17)	1.536 (3)	1.521 (4)	C(9)—C(8)—C(14)	109.0 (2)	108.7 (2)
C(13)—C(18)	1.534 (3)	1.535 (4)	C(8)—C(9)—C(10)	111.9 (2)	112.2 (2)
C(14)—C(15)	1.540 (4)	1.533 (5)	C(8)—C(9)—C(11)	112.7 (2)	112.6 (2)
C(15)—C(16)	1.554 (4)	1.554 (6)	C(10)—C(9)—C(11)	113.5 (2)	113.3 (2)
C(16)—C(17)	1.529 (5)	1.506 (7)	C(1)—C(10)—C(5)	106.0 (2)	105.5 (2)
C(17)—O(17β)	1.445 (4)	1.461 (4)	C(1)—C(10)—C(9)	111.8 (2)	112.8 (2)
C(20)—C(21)	1.477	1.503 (6)	C(1)—C(10)—C(19)	109.5 (2)	109.4 (2)
C(20)—O(17β)	1.341 (4)	1.310 (4)	C(5)—C(10)—C(9)	108.0 (2)	108.2 (2)
C(20)—O(20)	1.212 (5)	1.200 (4)	C(5)—C(10)—C(19)	112.2 (2)	111.7 (2)
C(21)—C(22)	1.477	1.495	C(9)—C(10)—C(19)	109.3 (2)	109.2 (2)
C(1a)—C(2')	1.518 (4)	1.518 (4)	C(9)—C(11)—C(12)	112.2 (2)	112.5 (2)
C(2')—C(3a)	1.531 (3)	1.521 (4)	C(11)—C(12)—C(13)	110.8 (2)	111.2 (2)
C(2')—O(5)	1.435 (3)	1.436 (4)	C(12)—C(13)—C(14)	109.1 (2)	108.8 (2)

Methanol molecule
CMe—OMe 1.392 (4)

Table 3. Hydrogen-bond geometry, *D* = donor, *A* = acceptor, 1, 2 = crystallographically independent molecules 1 and 2

<i>D</i>	<i>A</i>	<i>D</i> ... <i>A</i> (Å)	<i>D</i> — <i>H</i> (Å)	<i>A</i> ... <i>H</i> (Å)	<i>∠D</i> — <i>H</i> ... <i>A</i> (°)	Acceptor position
O ² (3)...O ¹ (3)	2.840 (4)	0.79 (4)	2.06 (4)	170 (4)		<i>x</i> , <i>y</i> , <i>z</i>
O ¹ (3)...O(Me)	2.869 (4)	0.75 (5)	2.13 (5)	166 (3)		1 - <i>x</i> , $\frac{1}{2}$ + <i>y</i> , - <i>z</i>
O(Me)...O ² (3)	2.882 (4)	0.77 (4)	2.12 (4)	171 (3)		1 - <i>x</i> , $\frac{1}{2}$ + <i>y</i> , - <i>z</i>

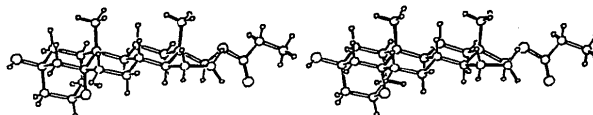
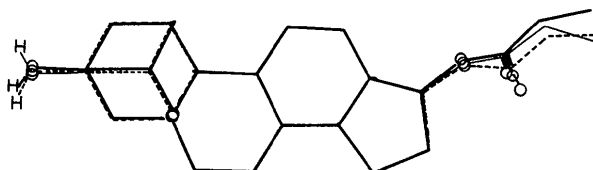


Fig. 1. ORTEP stereo drawing of molecule 1.

Fig. 2. Comparison of the two molecules obtained from X-ray data (solid lines) and the conformer calculated to be of minimum energy by molecular-mechanics calculations (dashed lines). The molecules were superimposed by a least-squares fit of the atoms of the *A*, *B*, *C* and *D* rings using the program *FITMOL* (Rohrer & Smith, 1980).

orientations of the hydroxyl H atom have equal stability and the staggered positions are energetically favored. Molecules exhibiting two of the three energetically preferred staggered conformations of the H(30) atoms are present in the crystal structure studied here. In molecule 1 the H atom is oriented *trans* to the C(2)—C(3) bond; in molecule 2 the H atom is oriented *trans* to the C(3)—C(4) bond. The crystallographically observed conformers were subjected to energy-minimization calculations using the program *MM2p* (Allinger & Yuh, 1973) in order to compare calculated with observed conformations. All positional parameters were allowed full relaxation. In the course of energy minimization the hydroxyl H atoms retained

their local minimum-energy positions. The 13β,14α-half-chair conformation of the *D* ring of molecule 2 was virtually unchanged by the energy refinement. However, during energy refinement the 13β-envelope conformation of ring *D* of molecule 1 underwent pseudorotation to a 13β,14α-half-chair conformation identical to that of molecule 2.

The 17β side chains of the independent molecules refined to a position that differed substantially from either of those observed. The observed conformations are compared with each other and with the conformation generated by the energy-minimization procedure in Fig. 2.

The orientation of the side chain relative to the *D* ring is defined by the torsion angle C(13)—C(17)—O(17β)—C(20). The value for this torsion angle in 25 17β-acetates and haloacetates studied crystallographically (Duax, Weeks & Rohrer, 1976) is observed to range in an even distribution from -85 to -178°. Conformations in this broad range must be of approximately equal energy and stabilized by subtle inter- and intramolecular interactions. It is worth noting that the values of the C(13)—C(17)—O(17β)—C(20) torsion angles in molecules 1 and 2 are nearly identical (-158.8 and -154.7° respectively) and well within the previously observed range.

Conformations of energy-minimized structures might be expected to fall in the center of the broad observed range. The values for the C(13)—C(17)—O(17β)—C(20) torsion angles in the energy-minimized structures are

−175.2 and −171.7° in molecules 1 and 2, respectively. The fact that the conformations of the energy-minimized structures are at one edge of the distribution indicates that either the distribution in the solid state is systematically skewed by packing interactions or the calculations are not accurately simulating intramolecular interaction. Since no characteristic packing interaction or patterns are discernable in the 27 structures in the sample it seems more plausible to suggest that the calculations are limited. Analysis of crystallographic observation of the progesterone side chain *versus* molecular-mechanics calculations indicates that H—C—C=O and C—C—C=O parameters in *MM2p* are not adequately defined (Duax, Griffin & Rohrer, 1981). This could account for the results observed here.

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Structure of an Antihistaminic Drug, Thonzylamine Hydrochloride

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Abstract. *N*-[(4-Methoxyphenyl)methyl]-*N'*,*N'*-dimethyl-*N*-2-pyrimidinyl-1,2-ethanediamine hydrochloride, $C_{16}H_{23}N_4O^+Cl^-$, $M_r = 322.84$, orthorhombic, *Pca*₂₁, $a = 9.916$ (3), $b = 15.722$ (3), $c = 10.840$ (8) Å, $V = 1690$ (2) Å³, $Z = 4$, $D_x = 1.27$ Mg m⁻³, $\lambda(Mo K\alpha) = 0.71073$ Å, $\mu = 0.231$ mm⁻¹, $F(000) = 688$, $T = 293$ (1) K, $R = 0.042$ for 2218 observed data with $I > 3\sigma(I)$. Both six-membered rings are individually planar and the configurations at bonds N(1)—C(9) and C(5)—C(6) are *cis* and *trans*, respectively. The cation is protonated at the terminal dimethylamino group and is hydrogen bonded to the Cl⁻ ion, $N \cdots Cl$ 3.031 (3) Å.

Introduction. Thonzylamine is an active component of some cold remedies (Witiak, 1970). Unlike tripelemamine, which is a potent antihistaminic drug widely used as a cure for hay fever and other allergies, thonzylamine has a lower toxicity and causes markedly less drowsiness than the former (Wilhelm, 1961). The crystal structure of thonzylamine hydrochloride has been determined to establish its conformation as part of a program correlating biological activity and molecular

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structures of antihistamine drugs containing an alkyldiamine group.

Experimental. Colorless crystals of thonzylamine hydrochloride (Sigma Inc.) were grown from methanol by slow evaporation at room temperature. A crystal of approximate dimensions 0.45 × 0.32 × 0.70 mm was obtained by cutting a large plate and used for data collection. Cell dimensions were determined by a least-squares refinement of the setting angles of 25 reflections with θ in the range 10–17°. Intensity data in the range $2 < \theta < 30^\circ$ were collected on an Enraf-Nonius CAD-4 diffractometer using the $\omega/2\theta$ scan technique, variable scan speed (0.72–2.35° min⁻¹) and monochromatized Mo *K* α radiation. The intensities of three standard reflections, monitored at intervals of 2 h exposure time, decreased by 4.8% (linear decay) over the period of the data collection; this decay was corrected for by appropriate scaling. 2990 intensity maxima were collected (h 0–13, k –22–0, l 0–15) and corrected for Lorentz, polarization and absorption effects (North, Phillips & Mathews, 1968); the maximum and minimum transmission factors were