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Structure of (17α)-Androstano[3,4-*c*][1,2,5]oxadiazole-17-ol (HS963)

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Abstract. $C_{19}H_{28}N_2O_2$, $M_r = 316$, orthorhombic, $P2_12_12_1$, $a = 10.231$ (7), $b = 11.171$ (7), $c = 14.759$ (5) Å, $V = 1687$ Å^3, $Z = 4$, $D_x = 1.24$ g cm^{-3}, λ(Cu $K\alpha$) = 1.5418 Å, $\mu = 5.57$ cm^{-1}, $F(000) = 688$, room temperature, $R = 0.055$ for 3179 observed reflections. Ring *A* is strained and rings *B* and *C* are in chair conformations. Ring *D* has an intermediate envelope–half-chair conformation. The oxadiazole ring is planar.

Introduction. Medicinal chemists have modified the structure of testosterone in various ways (Drill & Riegel, 1958) with the object of increasing the anabolic (nitrogen retention) propensity and decreasing its effect as a male hormone. This assumes that the target receptors associated with these two effects are sufficiently different to be sensitive to small changes in the structure of the drug molecule and to react accordingly. One successful approach has been to introduce different *A*-ring fused heterocycles [see, for example, Clinton *et al.* (1961), Ohta, Takegoshi, Veno & Shimizu (1965) and Kasahara, Ondera, Mogi, Oshima & Shimizu (1965)]. The title compound (HS963), depicted in Fig. 1, was prepared during the course of work on the synthesis of steroid oxadiazoles (Singh, Yadav & Jindal, 1987). We have determined the structure of HS963 in order to study the effect of the 5-en-oxadiazole system on the steroid skeleton and to clarify some conformational aspects for future structure–function studies.

Experimental. Crystallization from ethanol gave colourless needles; a specimen 0.8 × 0.2 × 0.1 mm was used for data collection. Preliminary Weissenberg photographs yielded approximate cell dimensions and showed orthorhombic (*mmm*) symmetry. Space group $P2_12_12_1$ was determined unambiguously from systematic absences ($h00$, $h = 2n + 1$; $0k0$, $k = 2n + 1$; $00l$, $l = 2n + 1$). Data were collected on an Enraf–Nonius CAD-4 automated diffractometer, with graphite monochromator, Cu $K\alpha$ radiation, ω–2θ scans [scan width $(0.85 + 0.15\tan\theta)°$], and vertical aperture 4 mm. 25 high-angle reflections ($25 < 2\theta < 28°$) were used to obtain accurate cell dimensions by least-squares fit. 3179 unique reflections ($3 < \theta < 69°$) were measured ($-12 < h < 12$, $1 < k < 8$, $0 < l < 17$). Three intensity standards (220, 200, 008) monitored at intervals of 100 measurements showed no significant variations during data collection. Intensity data were corrected for Lorentz–polarization factors. An empirical absorption correction was applied, based on φ scans for each of three reflections (North, Phillips & Mathews, 1968) for $\chi = 90°$ measured at 10° intervals from $\varphi = 0$–360°; normalized transmission factors were 0.82 to 0.91. $R_{int} = 0.027$. Structure solution was by direct methods using *SHELX*76 (Sheldrick, 1976). Refinement was by full-matrix least squares with

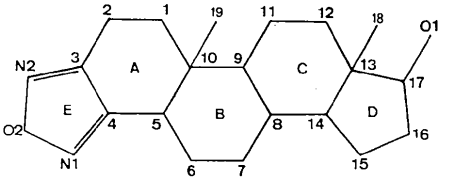

Fig. 1. Structural formula and numbering scheme. The numbers refer to C atoms unless otherwise indicated.

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Table 1. *Atom coordinates and equivalent isotropic thermal parameters* (Å^2)

$U_{eq} = (U_{11}U_{22}U_{33})^{1/3}$.

	x	y	z	U_{eq}
C(1)	0.1394 (2)	0.1869 (2)	0.2618 (1)	0.0537 (4)
C(2)	0.2611 (3)	0.1097 (2)	0.2742 (1)	0.0551 (6)
C(3)	0.2676 (2)	0.0652 (2)	0.3687 (1)	0.0478 (6)
C(4)	0.1885 (2)	0.1122 (2)	0.4401 (1)	0.0457 (5)
C(5)	0.0845 (2)	0.2051 (2)	0.4277 (1)	0.0428 (5)
C(6)	0.0683 (2)	0.2843 (2)	0.5122 (1)	0.0491 (6)
C(7)	0.1864 (2)	0.3654 (2)	0.5253 (1)	0.0452 (5)
C(8)	0.2132 (2)	0.4412 (1)	0.4414 (1)	0.0341 (4)
C(9)	0.2308 (2)	0.3615 (1)	0.3561 (1)	0.0329 (4)
C(10)	0.1120 (2)	0.2778 (2)	0.3393 (1)	0.0406 (5)
C(11)	0.2700 (2)	0.4355 (2)	0.2726 (1)	0.0396 (5)
C(12)	0.3878 (2)	0.5171 (2)	0.2890 (1)	0.0390 (4)
C(13)	0.3657 (1)	0.5973 (1)	0.3710 (1)	0.0335 (4)
C(14)	0.3353 (2)	0.5174 (1)	0.4524 (1)	0.0331 (4)
C(15)	0.3473 (2)	0.6000 (2)	0.5344 (1)	0.0450 (5)
C(16)	0.4589 (2)	0.6874 (2)	0.5078 (1)	0.0485 (5)
C(17)	0.4877 (2)	0.6622 (1)	0.4067 (1)	0.0376 (4)
C(18)	0.2583 (2)	0.6900 (2)	0.3519 (1)	0.0438 (5)
C(19)	−0.0120 (2)	0.3484 (2)	0.3138 (2)	0.0562 (7)
N(1)	0.2183 (2)	0.0593 (2)	0.5164 (1)	0.0578 (6)
N(2)	0.3450 (2)	−0.0170 (2)	0.4016 (1)	0.0568 (6)
O(1)	0.5278 (1)	0.7654 (1)	0.3575 (1)	0.0508 (5)
O(2)	0.3168 (2)	−0.0222 (1)	0.4949 (1)	0.0637 (6)

anisotropic thermal factors for non-H atoms, and isotropic for H atoms which were placed in calculated positions on the corresponding C atoms (C—H = 1.08 Å), except H(1) which was identified from the difference map. The function minimized was $w(|F_o| - |F_c|)^2$, where $w = [\sigma^2(F_o) + 0.012855|F_o|^2]^{-1}$; $R = 0.055$, $wR = 0.072$, R(all data) = 0.0549, maximum (shift/σ) = 1.173. Final electron density −0.42 to 0.40 e Å^{-3}. Calculations were carried out on VAX and AMDAHL 470V/8 computers. Geometrical calculations were performed with *XANADU* (Roberts & Sheldrick, 1975) and molecular illustrations were drawn with *PLUTO* (Motherwell & Clegg, 1978).*

Discussion. The refined atomic coordinates and equivalent isotropic thermal parameters for the non-H atoms are given in Table 1. Bond distances and angles are listed in Table 2. The chemical formula with the numbering scheme of the atoms is shown in Fig. 1. Fig. 2 shows the molecular conformation.

Most of the bond lengths in HS963 are close to the expected values. The average C—C single bond lengths in rings *A*, *B*, *C* and *D* are 1.508 (3), 1.542 (3), 1.531 (3) and 1.539 (3) Å, respectively. The average value of all the C—C single bond lengths in the molecule is 1.528 (3) Å. This is in agreement with the values found in similar steroid structures, *e.g.* 17β-hydroxy-17α-methyl-5β-androstano[2,3-*c*]-[1,2,5]oxadiazole (HS804), 17β-hydroxy-17α-methyl-5α-androstano[2,3-*c*][1,2,5]oxadiazole (HS805) (El Shora, Palmer, Singh & Paul, 1984) and (20*R*)-5α-pregnano[3,4-*c*][1,2,5]oxadiazol-20-ol (HS1011) (Maes, Wyns, Lisgarten, Lisgarten & Palmer, 1992). The shortening in bond length C(2)—C(3) [1.481 (3) Å] is associated with the fusion of the oxadiazole ring with ring *A*; C(3) and C(4) both have

Table 2. *Bond lengths* (Å), *bond angles* (°) *and torsion angles* (°)

C(1)—C(2)	1.526 (3)	C(2)—C(3)	1.481 (3)
C(3)—C(4)	1.429 (3)	C(4)—C(5)	1.498 (3)
C(5)—C(6)	1.538 (3)	C(6)—C(7)	1.522 (3)
C(7)—C(8)	1.526 (2)	C(8)—C(9)	1.551 (2)
C(9)—C(10)	1.554 (2)	C(10)—C(1)	1.554 (3)
C(10)—C(5)	1.562 (2)	C(9)—C(11)	1.537 (2)
C(11)—C(12)	1.529 (2)	C(12)—C(13)	1.523 (2)
C(13)—C(14)	1.529 (2)	C(8)—C(14)	1.520 (2)
C(14)—C(15)	1.527 (2)	C(15)—C(16)	1.553 (3)
C(16)—C(17)	1.548 (2)	C(17)—C(13)	1.536 (2)
C(13)—C(18)	1.535 (2)	C(10)—C(19)	1.541 (3)
C(17)—O(1)	1.423 (2)	C(3)—N(2)	1.306 (3)
N(2)—O(2)	1.407 (3)	O(2)—N(1)	1.395 (3)
N(1)—C(4)	1.308 (3)		

C(1)—C(2)—C(3)	109.5 (1)	C(2)—C(3)—C(4)	123.1 (2)
C(3)—C(4)—C(5)	124.5 (2)	C(4)—C(5)—C(10)	109.5 (1)
C(10)—C(1)—C(2)	115.3 (2)	C(2)—C(3)—N(2)	127.8 (2)
C(3)—N(2)—C(2)	105.6 (2)	C(2)—N(2)—N(1)	110.2 (2)
O(2)—C(1)—C(4)	105.4 (2)	O(1)—C(4)—C(3)	109.7 (2)
C(4)—C(3)—N(2)	109.1 (2)	N(1)—C(4)—C(5)	125.7 (2)
C(10)—C(5)—C(6)	113.5 (1)	C(4)—C(5)—C(6)	112.0 (2)
C(5)—C(6)—C(7)	111.1 (1)	C(6)—C(7)—C(8)	111.7 (2)
C(7)—C(8)—C(9)	111.2 (1)	C(8)—C(9)—C(10)	112.6 (1)
C(9)—C(10)—C(5)	108.7 (1)	C(9)—C(10)—C(19)	112.0 (1)
C(19)—C(10)—C(1)	107.6 (2)	C(19)—C(10)—C(5)	108.7 (2)
C(1)—C(10)—C(5)	107.9 (1)	C(9)—C(8)—C(14)	108.2 (1)
C(8)—C(14)—C(13)	114.2 (1)	C(7)—C(8)—C(14)	111.8 (1)
C(14)—C(13)—C(12)	108.1 (1)	C(13)—C(12)—C(11)	111.0 (1)
C(12)—C(11)—C(9)	113.6 (1)	C(11)—C(9)—C(10)	113.6 (1)
C(11)—C(9)—C(8)	111.9 (1)	C(9)—C(10)—C(1)	111.7 (1)
C(8)—C(14)—C(15)	119.3 (1)	C(14)—C(15)—C(16)	103.9 (1)
C(15)—C(16)—C(17)	105.6 (1)	C(16)—C(17)—C(13)	105.2 (1)
C(17)—C(13)—C(14)	99.9 (1)	C(17)—C(13)—C(12)	115.4 (1)
C(13)—C(14)—C(15)	104.6 (1)	C(18)—C(13)—C(14)	113.1 (1)
C(16)—C(17)—O(1)	113.6 (1)	O(1)—C(17)—C(13)	116.2 (1)
C(17)—C(13)—C(18)	109.0 (1)	C(18)—C(13)—C(12)	110.9 (1)

Ring *A*

C(1)—C(2)—C(3)—C(4)	−13.6	C(2)—C(3)—C(4)—C(5)	4.2
C(3)—C(4)—C(5)—C(10)	−22.7	C(4)—C(5)—C(10)—C(1)	48.6
C(5)—C(10)—C(1)—C(2)	−63.9	C(10)—C(1)—C(2)—C(3)	44.1

Ring *B*

C(9)—C(10)—C(5)—C(6)	53.2	C(10)—C(5)—C(6)—C(7)	−55.1
C(5)—C(6)—C(7)—C(8)	55.4	C(6)—C(7)—C(8)—C(9)	−55.9
C(7)—C(8)—C(9)—C(10)	55.8	C(8)—C(9)—C(10)—C(5)	−53.2

Ring *C*

C(12)—C(11)—C(9)—C(8)	51.7	C(11)—C(9)—C(8)—C(14)	−51.7
C(9)—C(8)—C(14)—C(13)	58.4	C(8)—C(14)—C(13)—C(12)	−61.0
C(14)—C(13)—C(12)—C(11)	56.0	C(13)—C(12)—C(11)—C(9)	−54.0

Ring *D*

C(17)—C(13)—C(14)—C(15)	45.7	C(13)—C(14)—C(15)—C(16)	−34.3
C(14)—C(15)—C(16)—C(17)	9.0	C(15)—C(16)—C(17)—C(13)	19.2
C(16)—C(17)—C(13)—C(14)	−39.4		

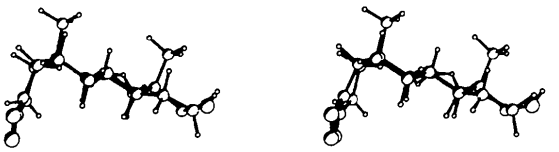

Fig. 2. Stereoview of the molecule.

* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55252 (17 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: HE0046]

C(sp^3) character. The bond length C(3)—C(4) of 1.429 (3) Å is in agreement with those found in HS804 and HS805 (El Shora *et al.*, 1984) whose values are 1.425 (4) and 1.429 (4) Å respectively. The C(3)=N(2) bond length is 1.306 (3) Å which agrees well with those quoted for HS804 and HS805. But the C(4)=N(1) bond length of 1.308 (3) Å is significantly longer than the corresponding value of 1.273 (5) Å in HS805. The shortening of bond length C(3)—C(4) may be associated with π delocalization in the system N(2)=C(3)—C(4)=N(1), similar to that found for other heterocyclic oxadiazoles [see, for example, Sagebarth & Cox (1965), Calleri, Chiari, Chesi Villa, Gaetani, Manfredotti, Guastini & Viterbo (1975), Viterbo & Serafino (1978) and El Shora *et al.* (1984)].

The N(2)—O(2) bond length of 1.407 (3) Å and the N(1)—O(2) bond length of 1.395 (3) Å are comparable to the values found in 3-amino-4-methylfurazan 1.380 (3)–1.406 (3) Å (Viterbo & Serafino, 1978), and in HS804 and HS805 [1.367 (7)–1.393 (5) Å (El Shora *et al.*, 1984), and to the average values of N—O bond lengths found in furazan [1.380 (3) Å (Sagebarth & Cox, 1965)].

If bond angles C(3) to C(4) are excluded, the average C—C—C bond angle within the steroid skeleton is 109.4°. The interior angle C(17)—C(13)—C(14) [99.9 (1)°] of ring *D* is significantly less than the same angle in similar compounds: 100.8 (3) and 101.1 (3)° in HS804 and HS805 respectively. All of the bond angles have either central CH or CH_2 substituents, while the small bond angles have either central C(10) or C(13), both bearing CH_3 groups. The average values of the bond angles in these three categories are 110.2 (central CH_2), 110.7 (central CH) and 106.2° (central C bearing CH_3 substituent). The data for the steroid oxadiazoles HS804 and HS805 (El Shora *et al.*, 1984) show a similar effect with average bond angles in these three categories of 110.5 (central CH_2), 111.8 (central CH) and 107.8° (central C bearing CH_3).

Conformational features of the molecule may be described in terms of torsion angles (Table 2) and asymmetry parameters (Table 3). The pseudo torsion angle C(19)–C(10)···C(13)—C(18) (Duax & Norton, 1975), giving a quantitative measure of the twist about the length of the molecule, has a value of 2.3° in HS963. Conformation and symmetry in the six-membered rings *A*, *B* and *D* depart, as is to be expected, from the ideal. Following Duax & Norton (1975) the magnitudes of the asymmetry parameters ΔC_s and ΔC_2 (Table 3) have been calculated to indicate the deviation (about bond directions and bond-angle bisectors) from mirror and twofold symmetry. (A true *m* plane corresponds to $\Delta C_s = 0°$, and a twofold axis to $\Delta C_2 = 0°$.) Ring *A* is an intermediate strained 10β-sofa/10β,1α-half-chair. Rings *B* and *C* have low values for both ΔC_s and ΔC_2 showing good approximation to the ideal chair conformation. Ring *D* is intermediate between 13β-envelope and 13β,14α-half-chair. The oxadiazole ring *E* is planar (r.m.s. deviation 0.0024 Å). Ring connections are *A*/*B cis*, *B*/*C trans* and *C*/*D* quasi-*trans*. The oxadiazole ring is *trans* fused to ring *A*. The hydroxyl moiety attached to the steroid skeleton at C(17) is axial (α oriented).

Table 3. *Asymmetry parameters* (°)

Ring *A*		Ring *B*	
$\Delta C_s^1 = 25.4$	$\Delta C_2^{1,2} = 47.2$	$\Delta C_s^5 = 1.8$	$\Delta C_2^{1,6} = 2.4$
$\Delta C_s^2 = 41.3$	$\Delta C_2^{2,3} = 40.3$	$\Delta C_s^6 = 2.1$	$\Delta C_2^{9,10} = 1.9$
$\Delta C_s^3 = 16.0$	$\Delta C_2^{3,4} = 7.2$	$\Delta C_s^7 = 0.5$	$\Delta C_2^{5,10} = 1.3$
Ring *C*		**Ring *D***	
$\Delta C_s^8 = 6.7$	$\Delta C_2^{11,12} = 7.3$	$\Delta C_s^{13} = 1.6$	
$\Delta C_s^{11} = 3.2$	$\Delta C_2^{9,11} = 2.3$	$\Delta C_s^{14} = 22.9$	
$\Delta C_s^9 = 3.9$	$\Delta C_2^{8,9} = 6.9$	$\Delta C_s^{16} = 8.0$	

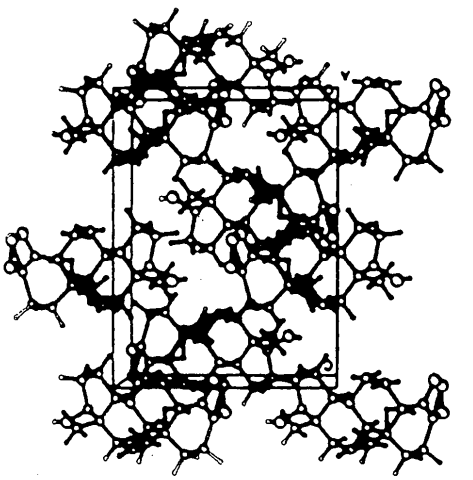

Fig. 3. View illustrating the molecular packing as seen along the *a* axis.

There are only two intermolecular close contacts O(1)···C(2′) = 3.387 (3) and O(1)···C(11′) = 3.402 Å (symmetry operator: $1-x$, $-0.5+y$, $0.5-z$). No evidence of any disorder was apparent. The packing of the molecules along the *a* axis is shown in Fig. 3.

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Structure of an Adenine–Hydrogen Peroxide Adduct

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Abstract. $C_5H_5N_5.H_2O_2$, $M_r = 169.14$, monoclinic, $C2/c$, $a = 8.939$ (3), $b = 10.697$ (4), $c = 14.920$ (4) Å, $\beta = 102.55$ (2)°, $V = 1392.5$ (7) Å^3, $Z = 8$, $D_x = 1.614$ g cm^{-3}, λ(Mo $K\alpha_1$) = 0.71069 Å, $\mu = 1.209$ cm^{-1}, $F(000) = 704$, $T = 293$ K, final $R = 0.047$ for 1090 observations. Each hydrogen peroxide molecule hydrogen bonds with three adjacent adenine molecules. Hydrogen bonding also occurs between N(9)—H(N9) and N(3) of an inversion related molecule. Molecules from adjacent planes are related by a non-crystallographic inversion center and exhibit strong stacking interactions along the b axis [planar separation 3.283 (3) Å].

Introduction. Hydrogen peroxide (H_2O_2) is a by-product of several metabolic pathways, including the conversion of hypoxanthine to xanthine by xanthine oxidase. H_2O_2 is also produced in the 'respiratory burst' following neutrophil phagocytosis. Significant quantities of H_2O_2 have been detected in whole human blood using a radio-isotopic exchange technique (Varma & Devamanoharan, 1991). It is likely that these concentrations represent a dynamic equilibrium between the amount of H_2O_2 produced and the amount decomposed by catalase.

H_2O_2 may generate highly reactive radicals by any or all three of the following mechanisms: the Fenton reaction, the Haber–Weiss reaction, or the reaction of H_2O_2 with ascorbic acid (Rowley & Halliwell, 1983). Free radicals generated *in vivo* may damage biomolecules, including DNA. Ten modified DNA bases have been identified after treating mammalian cells with H_2O_2 (Dizadaroglu, Nackerdien, Chao, Gajewski & Rao, 1991). Mode I killing of *Escherichia coli* strains by H_2O_2 occurs at physiologically relevant doses and DNA damage appears to be a significant factor in cell death (Cantoni, Brandi, Cerutti, Meyn & Murray, 1987). Alloxan, an agent which exhibits potent diabetogenicity, causes the production of H_2O_2 which is then believed to induce DNA strand breaks, eventually leading to diabetes (Takasu, Asawa, Komiya, Nagasawa & Yamada, 1990).

Recent findings suggest that many biological effects of H_2O_2 in aqueous solution are actually mediated by H_2O_2 adducts; hydrogen-bonded complexes of H_2O_2 and compounds found in biochemical systems (Schubert & Wilmer, 1991). H_2O_2 adducts enhance H_2O_2 stability by decreasing the rate of H_2O_2 decomposition up to several hundredfold. Neutrally charged H_2O_2 adducts appear to cross the cell membrane, thereby carrying extracellular H_2O_2 to intracellular targets. Exchange experiments between glucose, nucleic acid components and H_2O_2 strongly suggest that nucleic acids form H_2O_2 adducts (Schubert & Wilmer, 1991). The base adenine and its nucleoside adenosine appear to form the most stable adducts; however, no structural studies of such compounds have been performed prior to our work. We report here the structure of an adenine–hydrogen peroxide complex, obtained *via* crystallization of adenine from aqueous H_2O_2.

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