Table 2. *Bond distances* (Å) *and angles* (°)

Si(1)–C(3)	1·891 (3)	C(1)–C(6)	1·384 (5)
Si(1)–C(9)	1·875 (6)	C(1)–C(7)	1·526 (5)
Si(1)–C(10)	1·854 (8)	C(2)–C(3)	1·421 (5)
Si(1)–C(11)	1·878 (5)	C(3)–C(4)	1·426 (5)
Si(2)–C(4)	1·897 (3)	C(4)–C(5)	1·415 (5)
Si(2)–C(12)	1·864 (7)	C(5)–C(6)	1·387 (5)
Si(2)–C(13)	1·886 (5)	C(6)–C(8)	1·520 (5)
Si(2)–C(14)	1·869 (7)	C(7)–C(8)	1·568 (6)
C(1)–C(2)	1·376 (5)		

C(3)–Si(1)–C(9)	109·9 (2)	C(6)–C(1)–C(7)	93·3 (3)
C(3)–Si(1)–C(10)	113·7 (2)	C(3)–C(2)–C(1)	119·0 (3)
C(3)–Si(1)–C(11)	110·1 (2)	C(4)–C(3)–Si(1)	127·3 (3)
C(9)–Si(1)–C(10)	112·4 (3)	C(4)–C(3)–C(2)	119·3 (3)
C(9)–Si(1)–C(11)	104·6 (2)	Si(1)–C(3)–C(2)	113·3 (2)
C(10)–Si(1)–C(11)	105·7 (3)	C(5)–C(4)–Si(2)	111·9 (3)
C(4)–Si(2)–C(12)	109·2 (2)	C(5)–C(4)–C(3)	119·8 (3)
C(4)–Si(2)–C(13)	109·1 (2)	Si(2)–C(4)–C(3)	128·1 (3)
C(4)–Si(2)–C(14)	116·4 (2)	C(6)–C(5)–C(4)	119·0 (3)
C(12)–Si(2)–C(13)	107·7 (3)	C(8)–C(6)–C(1)	93·6 (3)
C(12)–Si(2)–C(14)	110·2 (3)	C(8)–C(6)–C(5)	145·5 (3)
C(13)–Si(2)–C(14)	103·8 (3)	C(1)–C(6)–C(5)	120·9 (3)
C(2)–C(1)–C(6)	121·9 (3)	C(8)–C(7)–C(1)	86·4 (3)
C(2)–C(1)–C(7)	144·7 (4)	C(6)–C(8)–C(7)	86·6 (3)

observable in the Si(1)–C(3)–C(4)–Si(2) torsion angle of 10·7°. The disposition of the methyl groups on the Si atoms is such that steric interactions are minimized. No strong intermolecular forces are observed.

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17β-Hydroxy-17α-methyl-4,9,11-estratrien-3-one

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Abstract. $C_{19}H_{24}O_2$, $M_r = 284$, monoclinic, $P2_1$, $Z = 4$, $a = 7{\cdot}533$ (1), $b = 19{\cdot}043$ (3), $c = 10{\cdot}891$ (1) Å, $\beta = 93{\cdot}07$ (9)°, $V = 1560{\cdot}1$ Å^3, $d_x = 1{\cdot}21$ Mg m^{-3}. The final R value is 0·03 for 2011 independent reflexions measured on a Siemens diffractometer using the five-points method. The conformations of the two independent molecules are very different, particularly on the A side of the steroid.

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Introduction. The title compound is one of the molecules which present a very pronounced affinity for androgen (Raynaud, Ojasoo, Bouton & Philibert, 1979) and progestin receptors (Ojasoo & Raynaud, 1978).

A single crystal for the present investigation (pale yellow, 0·3 × 0·3 × 0·6 mm) was grown by slow evaporation of a methanol solution. Data were collected at room temperature with a Siemens diffractometer using Cu $K\alpha$ radiation. 21 reflexions ($10 < \theta < 40°$) were refined by least squares and gave the final crystal parameters.

The structure was solved by direct methods using triplets and negative quartets (Giacovazzo, 1977; Busetta, 1978) and refined by the block-diagonal least-squares method with anisotropic thermal parameters for all non-hydrogen atoms. H atoms were located on difference Fourier maps and refined using an isotropic approximation for thermal parameters. The final R value is 0·03. The diffusion factors used are from *International Tables for X-ray Crystallography* (1974) for C, N and O and from Stewart, Davidson & Simpson (1965) for H.

Discussion. The conformations of the two independent molecules are shown in Fig. 1 and atomic coordinates are listed in Table 1.* Although the distances and valence angles are not significantly different, the torsion angles and the general conformation of the molecule are. This is clearly shown in Fig. 2, where molecules I and II are projected on the C(13)–C(17)–C(18) plane.

In the molecule I, rings B and C have diplanar forms and ring D has a half-chair form. In molecule II, rings B and C have half-chair forms and ring D is close to a β envelope. The general bend of the molecules is quite different. The superimposition of these two conformations with that of 17β-hydroxy-4,9,11-estratrien-3-one (Precigoux, Barrans & Hospital, 1979) shows the great flexibility of the steroid skeleton. The O(3) atom can be displaced significantly (1·5–5 Å) from the horizontal line defined in Fig. 2 and can occupy the best position for interaction with androgenic receptors (Precigoux, 1978). If we try to explain the second biological behaviour (affinity for progestin receptors), there are at least two important points: the flexibility of the molecule can allow binding to take place on two different sites [the distance between the O(3) atoms for the two conformers is about 3·5 Å] and the A ring can change its conformation (Fig. 3).

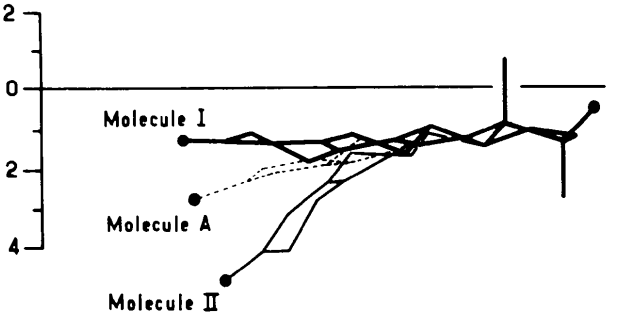
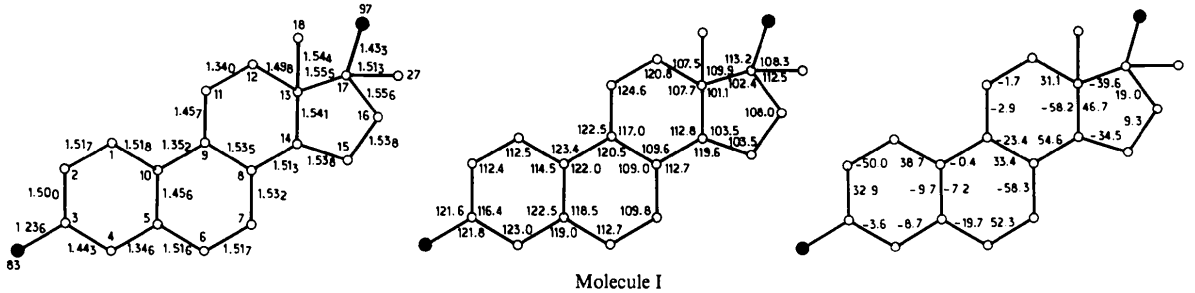


Fig. 2. Projections on the C(13)–C(17)–C(18) plane; molecules I and II: title compound; molecule A: 17β-hydroxy-4,9,11-estratrien-3-one.



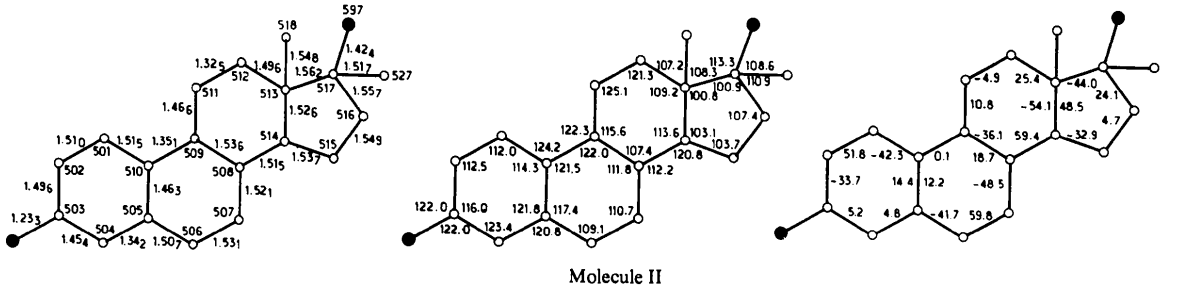


Fig. 1. Bond lengths (Å), angles (°) and dihedral angles (°) for molecules I and II. E.s.d.'s are 0·005 Å, 0·3 and 0·8° respectively.

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 35677 (23 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Final atomic parameters for the non-hydrogen atoms with e.s.d.'s in parentheses and equivalent thermal parameters* (Å²)

$$B_{eq} = \tfrac{4}{3} \Sigma_i \Sigma_j \beta_{ij} \mathbf{a}_i . \mathbf{a}_j .$$

	x	y	z	B_{eq}
C(1)	−0·0169 (5)	−0·2473 (2)	0·4741 (4)	4·3 (1)
C(2)	−0·0311 (5)	−0·2133 (2)	0·3480 (4)	4·9 (1)
C(3)	0·1106 (5)	−0·1592 (2)	0·3321 (4)	4·5 (1)
C(4)	0·2806 (5)	−0·1723 (2)	0·3952 (4)	4·2 (1)
C(5)	0·3111 (5)	−0·2274 (2)	0·4708 (3)	3·7 (1)
C(6)	0·5003 (5)	−0·2431 (2)	0·5172 (4)	4·6 (1)
C(7)	0·5092 (5)	−0·2896 (2)	0·6304 (4)	4·4 (1)
C(8)	0·3958 (4)	−0·3555 (2)	0·6063 (3)	3·5 (1)
C(9)	0·2037 (4)	−0·3333 (2)	0·5720 (3)	3·3 (1)
C(10)	0·1696 (4)	−0·2734 (2)	0·5084 (3)	3·6 (1)
C(11)	0·0631 (4)	−0·3798 (2)	0·6099 (3)	3·8 (1)
C(12)	0·0907 (5)	−0·4413 (2)	0·6676 (3)	3·8 (1)
C(13)	0·2753 (4)	−0·4684 (2)	0·6948 (3)	3·4 (1)
C(14)	0·3989 (4)	−0·4045 (2)	0·7156 (3)	3·6 (1)
C(15)	0·5759 (5)	−0·4375 (2)	0·7631 (4)	4·8 (1)
C(16)	0·5176 (5)	−0·5006 (2)	0·8394 (4)	4·9 (2)
C(17)	0·3133 (5)	−0·5098 (2)	0·8164 (3)	4·1 (1)
C(18)	0·3257 (5)	−0·5135 (2)	0·5841 (4)	4·5 (1)
C(27)	0·2102 (6)	−0·4815 (3)	0·9211 (4)	5·7 (2)
O(83)	0·0856 (4)	−0·1081 (2)	0·2633 (3)	6·4 (1)
O(97)	0·2771 (4)	−0·5835 (1)	0·8045 (3)	4·9 (1)
C(501)	1·5361 (5)	−0·2109 (2)	1·0026 (4)	4·2 (1)
C(502)	1·5166 (5)	−0·2359 (2)	1·1328 (4)	4·7 (1)
C(503)	1·3869 (5)	−0·2950 (2)	1·1399 (4)	4·5 (1)
C(504)	1·2368 (5)	−0·2937 (2)	1·0501 (4)	4·4 (1)
C(505)	1·2189 (5)	−0·2461 (2)	0·9594 (3)	3·8 (1)
C(506)	1·0525 (5)	−0·2435 (2)	0·8763 (4)	4·8 (1)
C(507)	0·9982 (5)	−0·1668 (2)	0·8557 (4)	4·5 (1)
C(508)	1·1449 (4)	−0·1261 (2)	0·7966 (3)	3·7 (1)
C(509)	1·3271 (4)	−0·1390 (2)	0·8627 (3)	3·4 (1)
C(510)	1·3580 (4)	−0·1947 (2)	0·9376 (3)	3·5 (1)
C(511)	1·4629 (4)	−0·0857 (2)	0·8426 (4)	4·1 (1)
C(512)	1·4326 (5)	−0·0241 (2)	0·7891 (4)	4·0 (1)
C(513)	1·2527 (4)	−0·0053 (2)	0·7337 (3)	3·4 (1)
C(514)	1·1119 (4)	−0·0476 (2)	0·7972 (3)	3·4 (1)
C(515)	0·9364 (5)	−0·0169 (2)	0·7423 (4)	4·4 (1)
C(516)	0·9812 (5)	0·0613 (2)	0·7199 (4)	4·7 (1)
C(517)	1·1835 (5)	0·0711 (2)	0·7522 (3)	4·0 (1)
C(518)	1·2552 (6)	−0·0198 (2)	0·5939 (3)	4·8 (1)
C(527)	1·2157 (6)	0·0979 (2)	0·8827 (4)	4·9 (2)
O(583)	1·4016 (4)	−0·3403 (2)	1·2207 (3)	5·6 (1)
O(597)	1·2548 (4)	0·1206 (2)	0·6701 (3)	4·9 (1)

If we compare two steroids with almost the same relative positions for the O(3) and O(17) atoms, *e.g.* testosterone and 19-nortestosterone (Precigoux, Hospital & Van den Bosche, 1973; Precigoux, Busetta, Courseille & Hospital, 1975), only the latter has any affinity for progestin receptors and it is also the only one that has two conformations for the *A* ring (quasi-*cis* and quasi-*trans*).

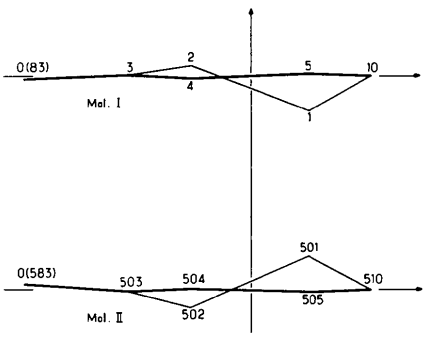


Fig. 3. Projections of the *A* rings of molecules I and II perpendicular to the mean planes defined by C(3)–C(4)–C(5)–C(10) and C(503)–C(504)–C(505)–C(510) respectively.

The flexibility of the molecule and the two possible conformations for the *A* ring should be important points in the explanation of the affinity of the title compound for both androgen and progestin receptors.

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