Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.04$
$wR(F^2) = 0.11$
$S = 1.03$
1987 reflections
118 parameters
H atoms riding
$w = 1/[\sigma^2(F_o^2) + (0.043P)^2 + 0.245P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.36$ e Å^{-3}
Extinction correction: none
Scattering factors from *International Tables for Crystallography* (Vol. C)

Table 1. *Selected geometric parameters (Å, °)*

Cl1—C3	1.723 (2)	Cl2—C6	1.713 (3)
O1—C7	1.185 (3)	O3—C8	1.186 (3)
O2—C8	1.389 (3)	O2—C7	1.393 (3)
C1—C7	1.478 (3)	C2—C8	1.477 (3)
C1—C6	1.380 (3)	C2—C3	1.376 (3)
C5—C6	1.384 (4)	C3—C4	1.389 (3)
C1—C2	1.380 (3)	C4—C5	1.376 (4)
C2—C1—C6	121.1 (2)	C3—C2—C1	121.3 (2)
C1—C6—C5	117.6 (2)	C2—C3—C4	117.9 (2)
C4—C5—C6	121.5 (2)	C5—C4—C3	120.6 (2)
C2—C1—C7	107.9 (2)	C1—C2—C8	107.8 (2)
O2—C7—C1	106.8 (2)	O2—C8—C2	107.0 (2)
O1—C7—O2	120.9 (2)	O3—C8—O2	121.0 (2)
C8—O2—C7	110.5 (2)		

Data collection: *CAD-4 Operations Manual* (Enraf–Nonius, 1977). Cell refinement: *CAD-4 Operations Manual*. Data reduction: *TEXSAN* (Molecular Structure Corporation, 1985). Program(s) used to solve structure: *TEXSAN*. Program(s) used to refine structure: *SHELXTL* (Sheldrick, 1995). Molecular graphics: *SHELXTL* and *TEXSAN*.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: BK1409). Services for accessing these data are described at the back of the journal.

References

Bates, R. B. & Cutler, R. S. (1977). *Acta Cryst.* B**33**, 893–895.
Berkovitch-Yellin, Z. & Leiserowitz, L. (1984). *Acta Cryst.* B**40**, 159–165.
Bocelli, G. & Cantoni, A. (1995). *Acta Cryst.* C**51**, 2652–2654.
Britton, D. (1992). *Acta Cryst.* C**48**, 1283–1285.
Desiraju, G. R. (1991). *Acc. Chem. Res.* **24**, 290–296.
Enraf–Nonius (1977). *CAD-4 Operations Manual*. Enraf–Nonius, Delft, The Netherlands.
Molecular Structure Corporation (1985). *TEXSAN. TEXRAY Structure Analysis Package*. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Ojala, C. R., Ojala, W. H., Britton, D. & Gougoutas, J. Z. (1998). Unpublished work.
Pauling, L. (1960). *The Nature of the Chemical Bond*, 3rd ed. Ithaca: Cornell University Press.
Rudman, R. (1971). *Acta Cryst.* B**27**, 262–269.
Sheldrick, G. M. (1995). *SHELXTL*. Version 5.0. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Taylor, R. & Kennard, O. (1982). *J. Am. Chem. Soc.* **104**, 5063–5070.

Acta Cryst. (1998). C**54**, 1894–1898

17,17-Ethylenedioxyandrost-4-ene-3,6-dione and 17,17-Ethylenedioxyandrosta-1,4-diene-3,6-dione

ADDLAGATTA ANTHONY,[a] MARIUSZ JASKOLSKI,[b] ASHWINI NANGIA[a] AND GAUTAM R. DESIRAJU[a]

[a]*School of Chemistry, University of Hyderabad, Hyderabad 500 046, India, and* [b]*Institute of Bioorganic Chemistry, Polish Academy of Sciences, and Department of Crystallography, Faculty of Chemistry, A. Mickiewicz University, Poznan, Poland. E-mail: ansc@uohyd.ernet.in*

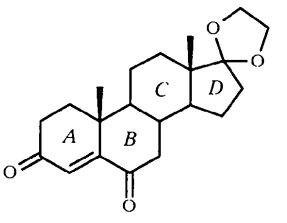
(*Received 17 March 1998; accepted 15 June 1998*)

Abstract

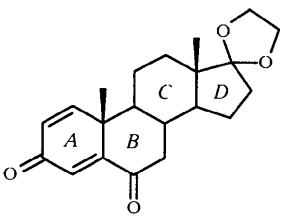
The crystal structures of 17,17-ethylenedioxyandrost-4-ene-3,6-dione, $C_{21}H_{28}O_4$, and 17,17-ethylenedioxyandrosta-1,4-diene-3,6-dione, $C_{21}H_{26}O_4$, intermediates in the synthesis of heteroandrogenic aromatase inhibitors, have been determined. Both structures are stabilized by C—H···O hydrogen bonds, highlighting the importance of weak interactions in influencing packing motifs in general and the conformation of the flexible dioxolane ring in particular.

Comment

The presence of a 4-ene-3,6-dione moiety in the *A*/*B* rings of a steroid skeleton is known to enhance the biological activity of such steroids, notably as aromatase inhibitors for the treatment of estrogen-dependent breast cancer (Numazawa *et al.*, 1993). The title compounds, 17,17-ethylenedioxyandrost-4-ene-3,6-dione, (I), and 17,17-ethylenedioxyandrosta-1,4-diene-3,6-dione, (II), were synthesised for elaboration to more complex *A*/*B*/*D* ring androgens and *A*-ring heteroandrogens (Nangia & Anthony, 1996, 1997). The conjugation in the enone (or enedione) portion of the molecule plays an important role in determining the stability of various *A*-ring conformations and in turn is able to influence the steroid–receptor interactions that control hormonal responses (Duax *et al.*, 1994).



(I)



(II)

In compound (I) (Fig. 1), ring *A* adopts the 1-α sofa conformation, ring *B* adopts a half-chair conformation,

while rings *C* and *D* are in chair and envelope conformations, respectively. In ring *A*, the C4=C5 double bond is polarized towards the C3 carbonyl rather than towards the C6 carbonyl atom [C3—O3 1.214 (3), C3—C4 1.469 (4), C4—C5 1.330 (4), C5—C6 1.502 (4) and C6—O6 1.197 (3) Å]. In ring *D*, C13 is 0.674 (4) Å above the plane containing the four remaining atoms (C14–C17). The dioxolane ring is in an envelope conformation, with C21 lying 0.548 (5) Å away from the plane containing the other four atoms (O20, C17, O23 and C22).

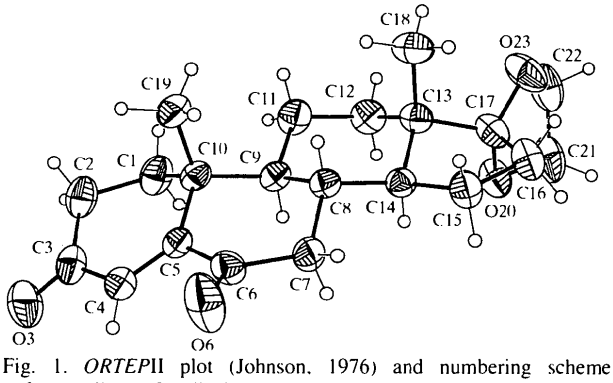


Fig. 1. *ORTEP*II plot (Johnson, 1976) and numbering scheme for enedione (I); displacement ellipsoids are drawn at the 50% probability level for non-H atoms.

In compound (II) (Fig. 2), ring *A* adopts a planar conformation with the weighted average absolute torsion angle being 1.3 (6)°. The conformations of rings *B*, *C* and *D* in (II) are similar to those in (I). In (II), atoms C13 and C21 are located 0.686 (6) and 0.208 (11) Å away from the planes of the four remaining atoms of the *D* and dioxolane rings, respectively. In contrast to (I), the C4=C5 double bond in (II) is polarized towards the C6 carbonyl atom, while the C1=C2 double bond is polarized towards the C3 carbonyl atom [C1—C2 1.313 (5), C2—C3 1.444 (6), C3—O3 1.220 (5), C3—C4 1.466 (6), C4—C5 1.331 (5), C5—C6 1.491 (5) and C6—O6 1.207 (5) Å]. The angle formed by the mean plane of ring *A* with the mean plane passing through rings *B*, *C* and *D* is 34.95 (9)° in (II), while it is 20.75 (9)° in (I), suggesting that the molecular skeleton is more bent in (II) than in (I).

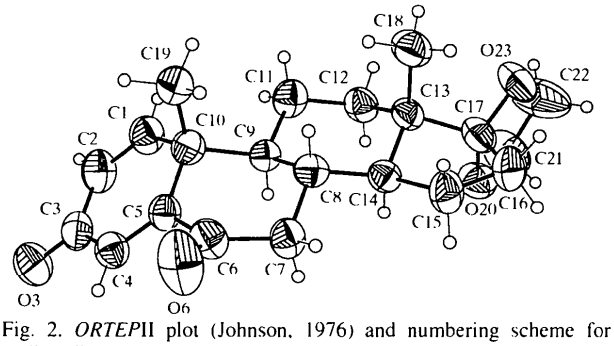


Fig. 2. *ORTEP*II plot (Johnson, 1976) and numbering scheme for dienedione (II); displacement ellipsoids are drawn at the 50% probability level for non-H atoms. Compare the larger displacement of C21 and C22 with those in Fig. 1.

There are no strong hydrogen-bonding groups in (I) and (II); the crystal structures are stabilized by weak C—H···O hydrogen bonds (Desiraju, 1996; Steiner, 1996), some of which are listed in Tables 2 and 4. The molecules in enedione (I) are oriented along [001], pack in the crystal in a head-to-tail fashion and are connected by C—H···O hydrogen bonds (Fig. 3). C4—H connects to one of the dioxolane O atoms (H···O 2.57 Å) forming a chain along [100] between screw-related molecules. Another hydrogen-bonded chain runs along [001], formed by C—H···O bonds between C2—H and O3 (H···O 2.75 Å).

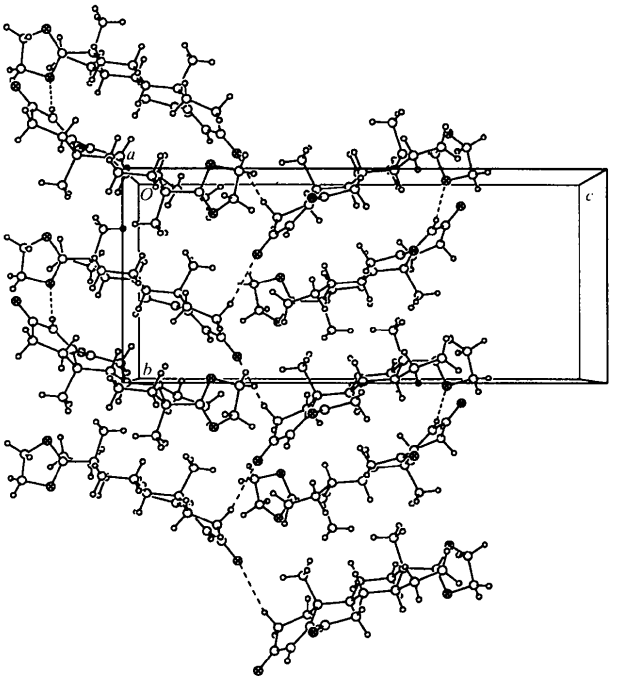


Fig. 3. Packing diagram of (I) down [100] showing the zigzag C—H···O hydrogen-bonded chain along [001]. Another C—H···O hydrogen bond (not shown) runs along [100] between the C4—H and the O23 atoms. The hydrogen bonds are shown as dashed lines.

In (II), molecules are close-packed along [100] and utilize the bent shape of the skeleton in such a way that the head and tail portions of one molecule fit into the concave cavities of adjacent screw-related molecules (Fig. 4). Molecules related by translation along [100] are connected by a chain of C—H···O hydrogen bonds between C12—H and O6 atoms (H···O 2.69 Å). In effect, the O6 atom is hydrogen bonded to ring *C* in (II), while it is bonded to the *A* and dioxolane rings in (I).

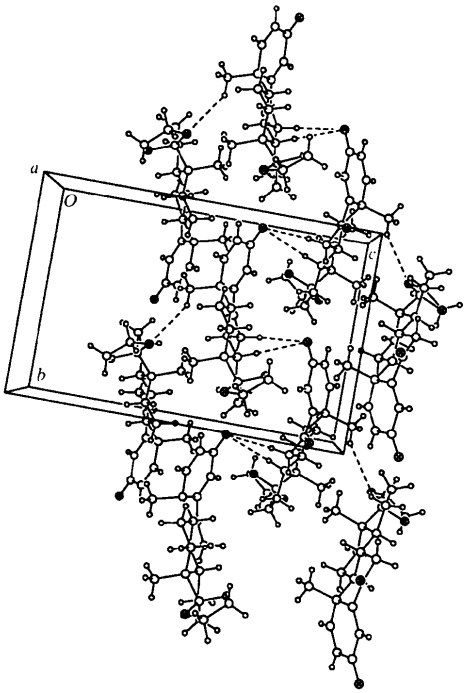


Fig. 4. Packing diagram of (II) down [100] showing the head-to-tail orientation of the bow-shaped molecules in a close-packed arrangement. C—H···O hydrogen bonds are shown as dashed lines.

A change in the *A*-ring functionality in (I) and (II) was found to have little effect on the conformation of rings *B*, *C* and *D*. The *B/C/D* ring system of the two compounds could be superimposed on each other with a very small r.m.s. deviation (0.029 Å). The conformational flexibility in the dioxolane ring portion of the molecules was examined computationally (*Cerius*[2]; Molecular Simulations, 1998). A 'systematic search' of the possible conformations in (I) and (II) was carried out by the breaking and recomposition of one bond, chosen arbitrarily, in each of the five rings (C1–C2, C6–C7, C11–C12, C15–C16 and C21–C22) (Guarna *et al.*, 1997). The overlay plots (100 conformations, $\Delta E <$ 13 kJ mol^{-1}; Fig. 5) show that the dioxolane ring has far greater flexibility in conformational space compared with the rest of the steroid skeleton. Furthermore, it appears that ring *A* can adopt more conformations in enedione (I) than in dienedione (II); this could be relevant in binding to the receptor (Duax *et al.*, 1994). That the conformations adopted by the dioxolane ring in (I) and (II) are different could be a result of the low energy barrier to conformational changes and the different packing motifs in the two structures. The atomic displacement parameters of the C20 and C21 atoms are larger in (II) compared with those in (I); this is ascribed to differences in their hydrogen-bonding patterns (Steiner, 1997). In (I), both the H atoms of C21 are hydrogen bonded to the O3 and O23 acceptor atoms of distinct screw-related molecules and, additionally, the H atom of C22 is bonded to O6 (C21—H···O3 2.78, C21—H···O23 2.77 and C22—H···O6 2.80 Å). In (II), on the other hand, there is only a very long contact between C22—H and O3 (H···O 2.99 Å). A comparison of the crystal structures of steroids (I) and (II) underscores the importance of weak hydrogen bonding in the conformation and hence the binding characteristics of these biomolecules (Wahl & Sundaralingam, 1997).

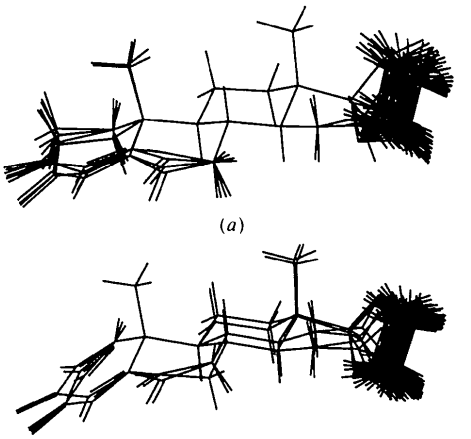


Fig. 5. Conformations of (*a*) (I) and (*b*) (II) generated through the 'systematic search' module in *Cerius*[2] (Molecular Simulations, 1998). Notice that a large number of dioxolane ring conformations are possible in both molecules.

Experimental

Compounds (I) and (II) were prepared according to the literature procedures of Nangia & Anthony (1997).

Compound (I)

Crystal data

$C_{21}H_{28}O_4$	Mo $K\alpha$ radiation
M_r = 344.43	λ = 0.71073 Å
Orthorhombic	Cell parameters from 52 reflections
$P2_12_12_1$	θ = 7.5–22.9°
a = 8.162 (2) Å	μ = 0.087 mm^{-1}
b = 9.919 (2) Å	T = 293 (2) K
c = 22.021 (4) Å	Prism
V = 1782.8 (7) Å^3	0.6 × 0.5 × 0.4 mm
Z = 4	Light yellow
D_x = 1.283 Mg m^{-3}	
D_m not measured	

Data collection

Kuma KM-4 diffractometer	θ_{max} = 25.54°
ω–2θ scans	h = 0 → 9
Absorption correction: none	k = 0 → 12
1929 measured reflections	l = 0 → 26
1929 independent reflections	2 standard reflections every 100 reflections
1466 reflections with $I > 2\sigma(I)$	intensity decay: <1.7%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.098$
$S = 1.064$
1926 reflections
226 parameters
H atoms fixed
$w = 1/[\sigma^2(F_o^2) + (0.043P)^2 + 0.3994P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.174$ e Å^{-3}
$\Delta\rho_{min} = -0.138$ e Å^{-3}
Extinction correction: none
Scattering factors from *International Tables for Crystallography* (Vol. C)

Table 1. *Selected geometric parameters (Å, °) for (I)*

C1—C2	1.527 (4)	C4—C5	1.330 (4)
C1—C10	1.531 (4)	C5—C6	1.502 (4)
C2—C3	1.480 (4)	C5—C10	1.514 (4)
C3—O3	1.214 (3)	C6—O6	1.197 (3)
C3—C4	1.469 (4)	C6—C7	1.488 (3)
C2—C1—C10	114.4 (2)	C5—C4—C3	122.9 (3)
C3—C2—C1	112.5 (2)	C4—C5—C6	117.8 (2)
O3—C3—C4	120.9 (3)	O6—C6—C7	121.8 (3)
O3—C3—C2	122.9 (3)	O6—C6—C5	121.0 (2)
C4—C3—C2	116.2 (2)	C7—C6—C5	117.0 (2)

Table 2. *Hydrogen-bonding geometry (Å, °) for (I)*

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H11···O6^{i}	0.97	2.71	3.345 (4)	124
C2—H21···O3^{ii}	0.97	2.75	3.681 (3)	162
C4—H41···O20^{iii}	0.93	2.57	3.480 (4)	167
C16—H161···O3^{iv}	0.97	2.88	3.682 (4)	140
C16—H162···O3^{iii}	0.97	2.79	3.603 (4)	141
C19—H193···O3^{ii}	0.96	2.87	3.607 (2)	134
C21—H211···O3^{v}	0.97	2.78	3.556 (5)	138
C21—H211···O23^{vi}	0.97	2.77	3.459 (4)	128
C22—H221···O6^{iv}	0.97	2.80	3.551 (1)	135

Symmetry codes: (i) $1+x, y, z$; (ii) $1-x, y-\frac{1}{2}, \frac{1}{2}-z$; (iii) $x-\frac{1}{2}, \frac{3}{2}-y, -z$; (iv) $\frac{1}{2}-x, 1-y, z-\frac{1}{2}$; (v) $\frac{1}{2}+x, \frac{3}{2}-y, -z$; (vi) $1-x, \frac{1}{2}+y, \frac{1}{2}-z$.

Compound (II)

Crystal data

$C_{21}H_{26}O_4$
$M_r = 342.42$
Orthorhombic
$P2_12_12_1$
$a = 9.854$ (2) Å
$b = 10.860$ (2) Å
$c = 16.524$ (3) Å
$V = 1768.3$ (6) Å^3
$Z = 4$
$D_x = 1.286$ Mg m^{-3}
D_m not measured
Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 53 reflections
$\theta = 7.5$–$21.5°$
$\mu = 0.088$ mm^{-1}
$T = 293$ (2) K
Prism
0.55 × 0.40 × 0.25 mm
Light yellow

Data collection

Kuma KM-4 diffractometer
ω–2θ scans
Absorption correction: none
1810 measured reflections
1810 independent reflections
1097 reflections with $I > 2\sigma(I)$
$\theta_{max} = 25.04°$
$h = 0 \rightarrow 11$
$k = 0 \rightarrow 12$
$l = 0 \rightarrow 19$
2 standard reflections
every 100 reflections
intensity decay: <1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.115$
$S = 1.035$
1807 reflections
226 parameters
H atoms fixed
$w = 1/[\sigma^2(F_o^2) + (0.0474P)^2 + 0.4925P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.153$ e Å^{-3}
$\Delta\rho_{min} = -0.141$ e Å^{-3}
Extinction correction: none
Scattering factors from *International Tables for Crystallography* (Vol. C)

Table 3. *Selected geometric parameters (Å, °) for (II)*

C1—C2	1.313 (5)	C4—C5	1.331 (5)
C1—C10	1.487 (5)	C5—C6	1.491 (5)
C2—C3	1.444 (6)	C5—C10	1.507 (5)
C3—O3	1.220 (5)	C6—O6	1.207 (5)
C3—C4	1.466 (6)	C6—C7	1.488 (5)
C2—C1—C10	125.9 (4)	C2—C3—C4	116.0 (4)
C1—C2—C3	121.9 (4)	C5—C4—C3	121.6 (4)
O3—C3—C2	122.5 (4)	C4—C5—C6	119.5 (3)
O3—C3—C4	121.5 (4)	C4—C5—C10	124.3 (4)

Table 4. *Hydrogen-bonding geometry (Å, °) for (II)*

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H41···O20^{i}	0.93	2.90	3.795 (5)	161
C7—H71···O3^{ii}	0.97	2.77	3.682 (6)	157
C11—H112···O3^{iii}	0.97	2.82	3.732 (6)	156
C12—H122···O6^{iv}	0.97	2.69	3.522 (5)	144
C14—H141···O3^{ii}	0.98	2.78	3.675 (5)	153
C19—H191···O23^{v}	0.96	2.72	3.499 (5)	139
C22—H221···O3^{vi}	0.97	2.99	3.596 (8)	122

Symmetry codes: (i) $-1-x, y-\frac{1}{2}, -\frac{1}{2}-z$; (ii) $-1-x, \frac{1}{2}+y, -\frac{1}{2}-z$; (iii) $\frac{1}{2}+x, -\frac{3}{2}-y, -1-z$; (iv) $1+x, y, z$; (v) $x-\frac{1}{2}, -\frac{1}{2}-y, -1-z$; (vi) $1+x, 1+y, z$.

For both compounds, data collection: *KM-4 User's Guide* (Kuma, 1989); cell refinement: *KM-4 User's Guide*; data reduction: *KM-4 User's Guide*; program(s) used to solve structures: *SHELXS86* (Sheldrick, 1990); program(s) used to refine structures: *SHELXL93* (Sheldrick, 1993); molecular graphics: *ORTEP*II (Johnson, 1976) and *PLUTO* (Motherwell & Clegg, 1978); software used to prepare material for publication: *SHELXL93*.

AA thanks the CSIR for fellowship support. AN and GRD acknowledge financial support from the DST (SP/S1/G-25/91). This work was made possible in part by the Indo–Polish Cooperation Programme (INT/POL/POC/P-22/96). The research of MJ was supported by the HHMI.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: KA1285). Services for accessing these data are described at the back of the journal.

References

Desiraju, G. R. (1996). *Acc. Chem. Res.* **29**, 441–449.
Duax, W. L., Griffin, J. F. & Ghosh, D. (1994). In *Structure Correlation*, Vol. 2, edited by H.-B. Bürgi & J. D. Dunitz, pp. 605–633. New York: VCH.
Guarna, A., Occhianti, E. G. & Machetti, F. (1997). *J. Med. Chem.* **40**, 3466–3477.

Johnson, C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
Kuma (1989). *KM-4 User's Guide*. Version 3.1. Kuma Diffraction, Wroclaw, Poland.
Molecular Simulations (1998). *Cerius*^{2}. Version 3.5. Molecular Simulations, 9685 Scranton Road, San Diego, CA 92121-3752, USA, and 240/250 The Quorum, Barnwell Road, Cambridge CB5 8RE, England.
Motherwell, W. D. S. & Clegg, W. (1978). *PLUTO. Program for Plotting Molecular and Crystal Structures*. University of Cambridge, England.
Nangia, A. & Anthony, A. (1996). *Synth. Commun.* **26**, 225–236.
Nangia, A. & Anthony, A. (1997). *Indian J. Chem.* **36**B, 1113–1118.
Numazawa, M., Mutsumi, A., Asano, N. & Ito, Y. (1993). *Steroids*, **58**, 40–46.
Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1993). *SHELXL*93. *Program for the Refinement of Crystal Structures*. University of Göttingen, Germany.
Steiner, T. (1996). *Cryst. Rev.* **6**, 1–57.
Steiner, T. (1997). *Chem. Commun.* pp. 727–729.
Wahl, M. C. & Sundaralingam, M. (1997). *Trends Biochem. Sci.* **22**, 97–102.

Acta Cryst. (1998). C**54**, 1898–1900

5β-Androstan-3,17-dione

ADDLAGATTA ANTHONY,[a] MARIUSZ JASKOLSKI,[b] ASHWINI NANGIA[a] AND GAUTAM R. DESIRAJU[a]

[a]*School of Chemistry, University of Hyderabad, Hyderabad 500 046, India, and* [b]*Institute of Bioorganic Chemistry, Polish Academy of Sciences, and Department of Crystallography, Faculty of Chemistry, A. Mickiewicz University, Poznan, Poland. E-mail: ansc@uohyd.ernet.in*

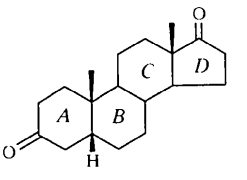
(*Received 6 April 1998; accepted 8 June 1998*)

Abstract

The title compound, $C_{19}H_{28}O_2$, has the 5β configuration and a bowing angle of 71.76 (5)° at the *A*/*B* ring junction. The crystal structure is stabilized by weak intermolecular C—H···O and van der Waals interactions.

Comment

The configuration at C5 is known to play an important role in the hormonal responses of steroids (Lawrence *et al.*, 1986). The activity of steroid analogues and their ability to bind to the receptor varies depending on whether the configuration at C5 is α or β, because of differences in the overall shape of the two epimers. The 5α steroids are flat, whereas the 5β epimers are bent at the *A*/*B* ring junction. 5α- and 5β-androstan-3,17-dione are important compounds in steroid metabolism and their biological activity has been studied extensively. In the Cambridge Structural Database (CSD; Allen & Kennard, 1993), two crystal structures of 5α-androstan-3,17-dione [CSD refcodes: ANDION10 (Coiro *et al.*, 1973) and ANDRDO (Peck *et al.*, 1974)] and the cell parameters for the 5β-epimer [CSD refcode: ZZZPDK (Norton *et al.*, 1962)] are reported. Here we report the crystal structure of 5β-androstan-3,17-dione, (I).



(I)

Ring *A* is in a half-chair conformation, rings *B* and *C* are in a chair conformation and ring *D* adopts the commonly found 14α-envelope conformation (Duax & Norton, 1975; Paixão *et al.*, 1998). The bowing angle in (I) [71.76 (5)°] is comparable to the corresponding angles found in other 5β-steroids reported recently [81.53 (9) and 81.97 (9) (Andrade *et al.*, 1997) and 58.91 (6)° (Ramos Silva *et al.*, 1996)]. There are three conformers of 5α-androstan-3,17-dione available for comparison with the 5β-epimer (I): ANDION10 and two symmetry-independent molecules of ANDRDO. The overlay plot of (I) with the three 5α-androstandione conformers shows that the *B*, *C* and *D* rings overlap with very low r.m.s. deviations (0.082, 0.059 and 0.066 Å), while the conformational flexibility in ring *A* is considerable.

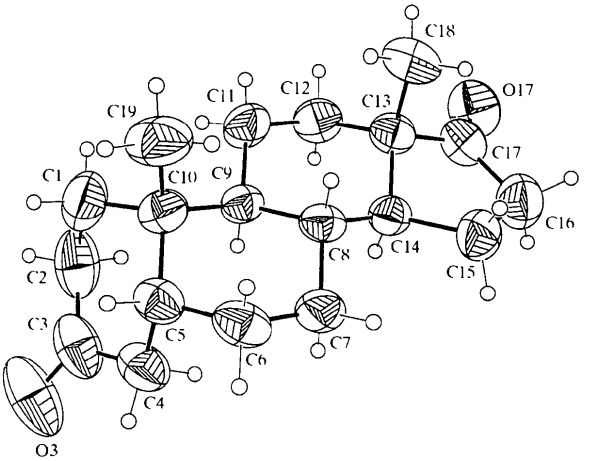


Fig. 1. *ORTEP*II (Johnson, 1976) plot of the title compound. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as spheres of an arbitrary radius.

The crystal structure of (I) (Fig. 2) is stabilized by weak C—H···O hydrogen bonds (Desiraju, 1996). A hydrogen-bonded chain runs along [010], involving C7β—H and O3 atoms (H···O 2.68 Å, C—H···O 130°) of translation-related molecules. Additionally, the C5β—H and C19—H donors are hydrogen bonded along [001] to O3 of a screw-related molecule (2.73 Å, 152°; 2.69 Å, 147°). The C3 carbonyl-O atom thus