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Steroids - Introduction

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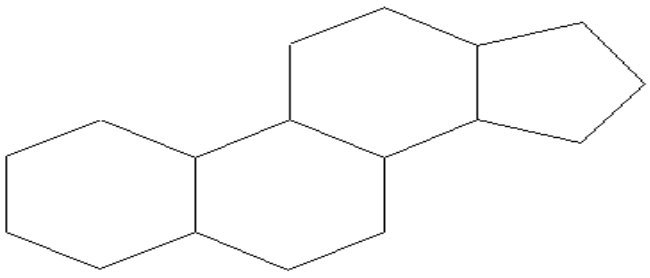
I. INTRODUCTION

(This session will have several occasions aimed at understanding structures using three-dimensional visualization. A special page lists instructions for enabling 3D structure visualization. You will need to have Chime™ plug-in on your local computer to perform this important task. If you have any questions please write or call the instructor.)

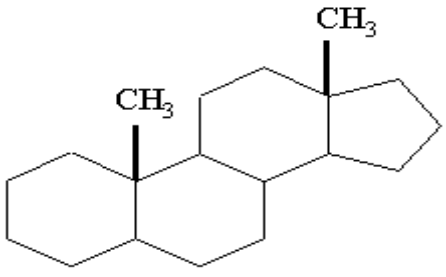
Topics of Special Interest
Handout
Structure
Numbering
Conformation
Configuration
Classes
Nomenclature
Practice Problem Set
Practice Problem Set - Key
Biosynthesis of Cholesterol

A. Structure

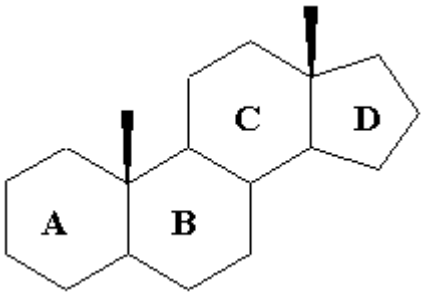
Cyclopentanoperhydrophenanthrene skeleton



Natural steroids have two methyls

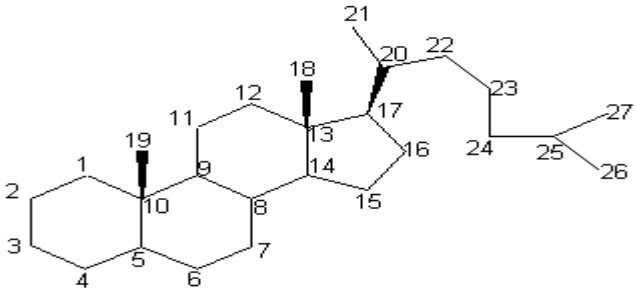


Rings are labeled A, B, C and D.



B. Numbering

Numbering of each position essentially follows a uniform pattern except for the methyls.



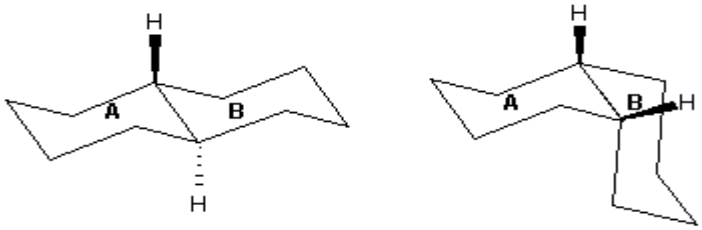
CHOLESTANE

whereas A/B rings have carbon 19, C/D rings have carbon 18. Cholesterol is an important member of the cholestane series of steroids.

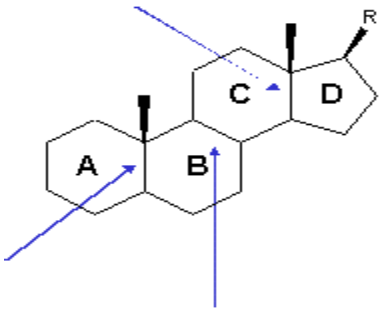
C. Conformation

There are four rings in a steroid skeleton and hence there are three fusion points. A/B, B/C and C/D rings share two carbons each (fusion). Every fusion center can either be *cis*- or *trans*-fused.

For two-ring system, the structures of cis - and trans-fused rings look like this: When the tow hydrogens are oriented opposite to each other with the ring system thought to as forming a plane, the ring fusion is called trans. When there are directed on the same side, it is called cis. To view the structures in three-dimension (using Chime™) double-click on the CIS and TRANS hyperlinks (double-click here to view individual chair and boat forms).



The three fusion centers.



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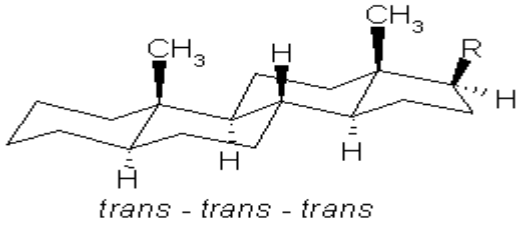
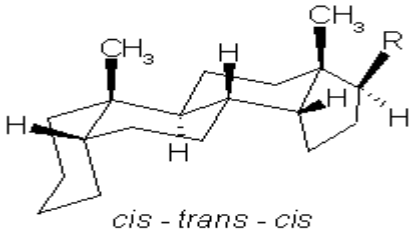
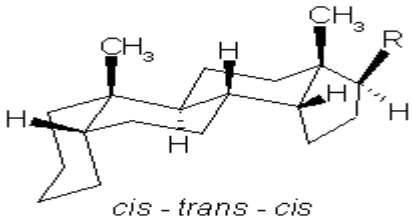
The structures most likely feasible are :
trans-trans-trans (most natural and synthetic steroids have this skeleton, e.g., 5□-dihydrotestosterone)
cis-trans-trans (some natural steroids have this skeleton, e.g., cholic acids)
cis-trans-cis (few natural steroids have this skeleton, e.g. cardiac glycosides (next semester))
The three dimensional structures of natural steroids look like this : Click on individual structures to view the structure in 3D.



trans - trans - trans



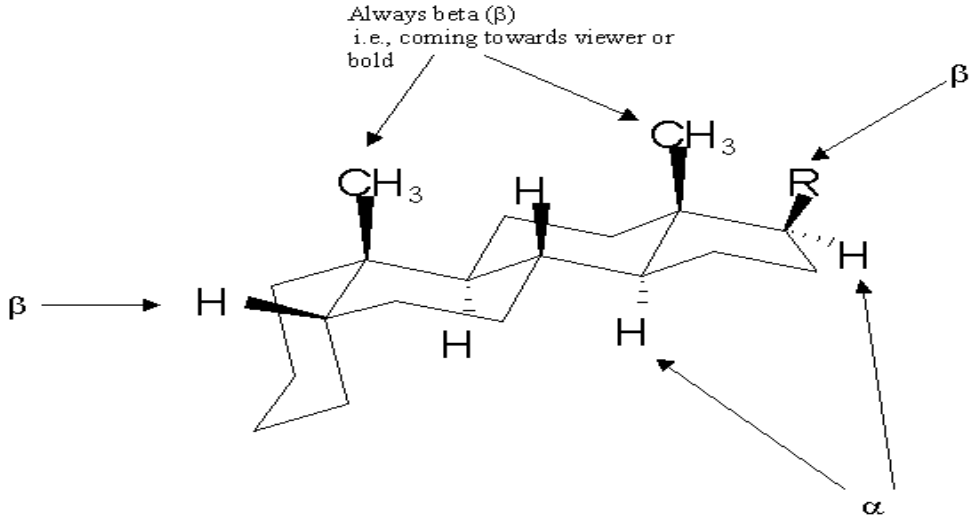
cis - trans - cis



cis - trans - cis

D. Configuration

The steroid skeleton (all carbons) with its methyls (18 and 19-CH_3) oriented as coming towards the viewer (represented as a bold line) is the reference plane in defining whether a particular hydrogen or a substituent is towards the viewer (□) or going away from the viewer (cross-hatched, □). Thus in a two-dimensional representation, with the 18- and 19-CH_3 bold, all bold substituents are □ and all cross-hatched substituents are □.



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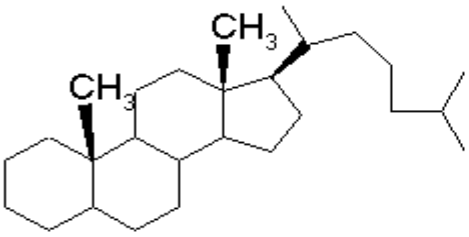
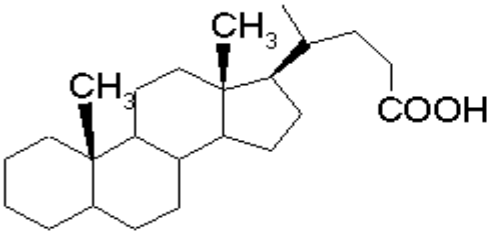
E. Classes

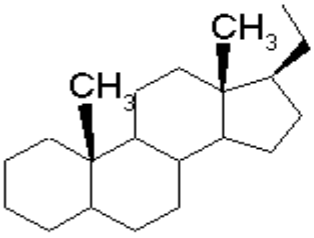
Following are the classes of steroids based on the number of nuclear carbons. Additional carbons that are not nuclear are not to be considered in classifying a steroid.



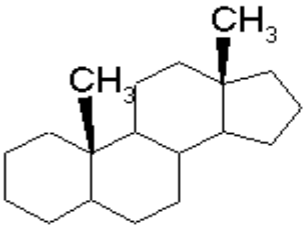
Cholestanes; 27 carbons
e.g. cholesterol



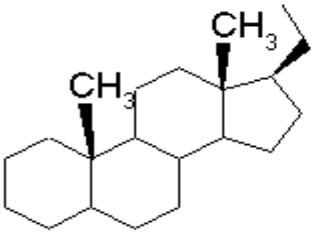
Cholic acids; 24 carbons
e.g. cholic acids



Pregnanes; 21 carbons
e.g. progesterone



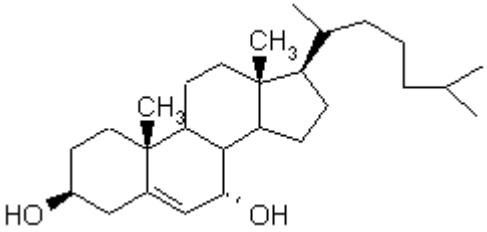
Andranes; 19 carbons
e.g. testosterone



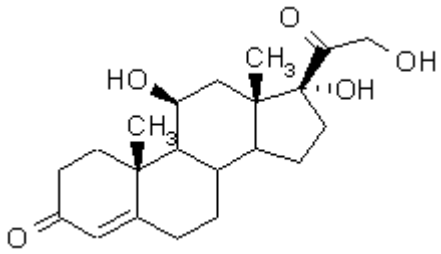
Estranes; 18 carbons
e.g. estradiol

F. Nomenclature

Study the following examples for an understanding on how the steroids are named. Use the above information on numbering, classes and configuration to deduce the name.



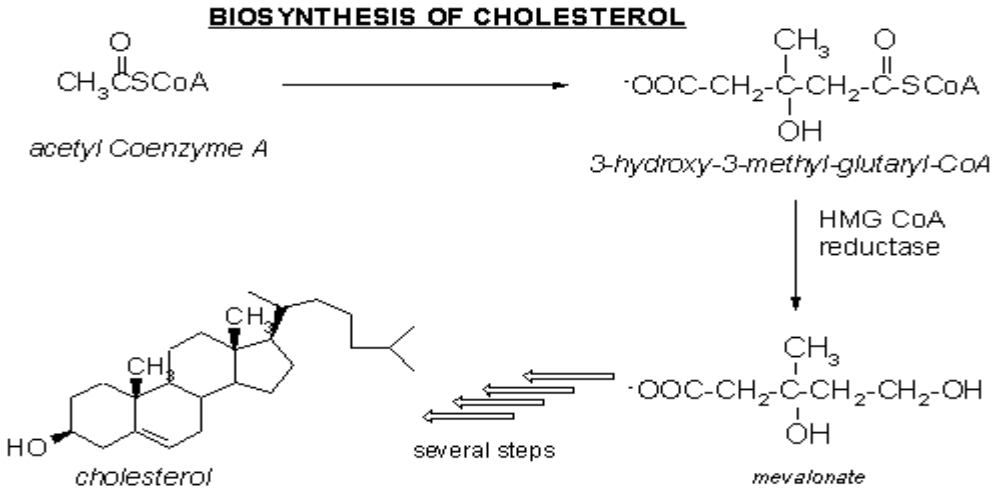
cholest-5-ene-3□,7□-diol



11□,17□,21-trihydroxy-pregn-4-en-3,20-dione

G. Biosynthesis of Cholesterol

The key step in the biosynthesis of cholesterol is the conversion of 3-hydroxy-3-methyl-glutaryl-Coenzyme A to mevalonate by HMG CoA reductase. This is the rate limiting step in cholesterol biosynthesis.



Cholesterol is the raw material for synthesis of all steroid hormones. The conversion occurs in the mitochondria of cells thus requiring the transport of cholesterol from outside cells to inside.

Cholesterol is also metabolized into cholic acid in the liver. Cholic acids are a part of bile acids that are released into the intestines.

[home] [school of pharmacy] [department of medicinal chemistry]

[links to sites of interest and download center] [instructions for downloading and installing software]

Revised: October 10, 2000

Questions or Comments : Dr. Umesh R. Desai

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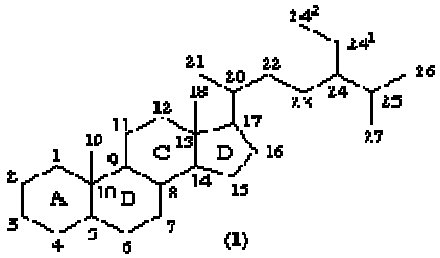
II. THE NOMENCLATURE OF STEROIDS RECOMMENDATIONS 1989 3S-1

A. 3S-1. General

1) *3S-1.0. Definition of Steroids and Sterols:* Steroids are compounds possessing the skeleton of cyclopenta[*a*]phenanthrene or a skeleton derived therefrom by one or more bond scissions or ring expansions or contractions. Methyl groups are normally present at C-10 and C-13. An alkyl side chain may also be present at C-17.Sterols are steroids carrying a hydroxyl group at C-3 and most of the skeleton of cholestane. Additional carbon atoms may be present in the side chain. *Note* This definition of sterols is rather restrictive. However, a less restrictive definition would cause difficulties, e.g. androst-16-en-3β-ol is normally not called a sterol and should not fall under the definition.

2) *3S-1.1. Numbering and Ring Letters:* Steroids are numbered and rings are lettered as in formula 1. If one of the two methyl groups attached to C-25 is substituted it is assigned the lower number (26); if both are substituted, that carrying the substituent cited first in the alphabetical order is assigned the lower number. For trimethyl steroids see Recommendation 3S-2.4, Note 2.

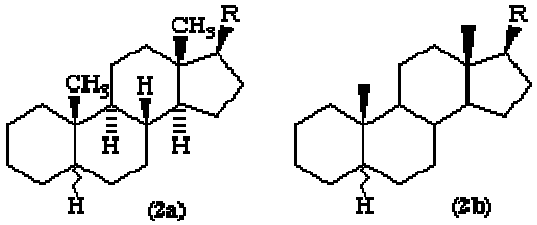


Note The numbers 28, 29 and 30 are now assigned to the additional methyl groups at C-4 and C-14 in triterpenoids, e.g. lanosterol (see 3S-2.4, Note 2). Therefore, the carbon atoms at the methyl or ethyl groups at C-24 had to be renumbered. The system adopted here allows also numbering of other carbon atoms attached to the steroid skeleton. If two side chains are attached to the same carbon atom, the shorter one receives primed numbers, e.g. $17^{1'}$ (see 3S-2.7, 3S-2.8 and addenda).

3) *3S-1.2. Absent Carbon Atoms:* If one or more of the carbon atoms shown in **1** is not present and a steroid name is used, the numbering of the remainder is undisturbed.

4) *3S-1.3. Absolute Configuration:* The absolute stereochemistry of a steroid is defined by the parent name for some chiral centres (see 3S-1.5) and by α, β, *R* or *S* for other centres (see 3S-1.4 and 3S-1.6). When the configuration at one or more centres is not known, this is indicated by the Greek letter(s) ξ(xi) prefixed by the appropriate locant(s).

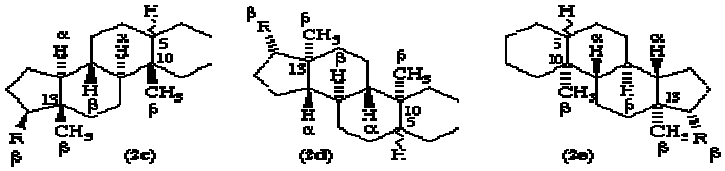
5) *3S-1.4. Orientation of Projection Formulae:* When the rings of a steroid are denoted as projections onto the plane of the paper, the formula is normally to be oriented as in **2a**. An atom or group attached to a ring depicted as in the orientation **2a** is termed α(alpha) if it lies below the plane of the paper or β(beta) if it lies above the plane of the paper. In formulae, bonds to atoms or groups lying below the plane of the paper (α) are shown as broken lines(--- or |||||||), and bonds to atoms or groups lying above the plane of the paper (β) are shown as solid lines (preferably thickened ▬ or ▬). Bonds to atoms or groups whose configuration is not known are denoted by wavy lines(∿∿∿).



Notes

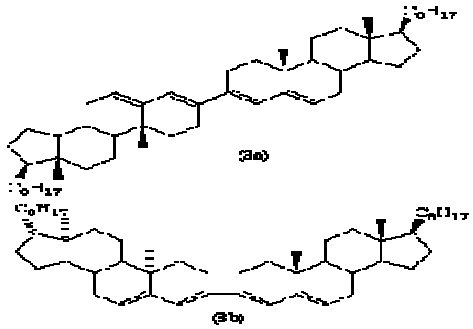
(1) In the formula **2a** given above, all angular methyl groups and H atoms have been written out explicitly. However, when there is no ambiguity, methyl groups may also be indicated by a bond without lettering as in **2b**, a practice followed in other fields. Likewise, the hydrogen atoms at the bridgehead C-8, C-9 and C-14 may be omitted if there is no ambiguity, i.e. if they are oriented 8β,9α,14α. If one of the hydrogen atoms is replaced, e.g. by a fluorine atom, care must be taken in the correct use of broken (α) and bold (β) lines. The bond to a bridgehead hydrogen atom should never be drawn without the H.

(2) Projections of steroid formulae should not be oriented as in formulae **2c**, **2d** or **2e** unless circumstances make it obligatory, e.g.in dimers formed photochemically [4].

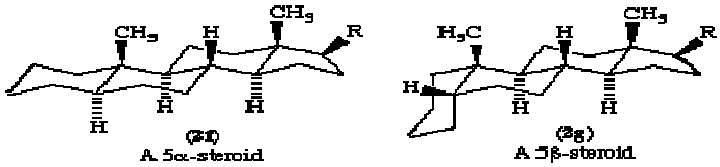


(3) With the preferred orientation **2a**, and with **2c**, which is only rotated in the plane of the paper, α-bonds appear as broken lines and β-bonds as solid (thickened) lines. The reverse is true for **2d** and **2e**; therefore, orientation **2c** is preferred over **2d** or **2e** if there is a choice. Wavy lines denote ξ-bonds for all orientations of the formula.

Example: 3,3'-Bicholesta-3,5-diene should be represented as **3a** but not as **3b**.



(4) A perspective representation of the stereochemistry of formula **2** as in **2f** or **2g** may also be used:



When steroid formulae are drawn in this way, bonds pointing upwards are, by convention, drawn bold and bonds pointing downwards are drawn broken; these representations correspond to the β- and α-bonds of projection formulae such as **2a** and do not conform to the general practice that bold and broken lines denote bonds projecting respectively above and below the plane of the paper. Note, however, that the general practice is followed with chair and boat forms of spirostans (see Recommendation 3S-3.3).

(5) To save space and to emphasise the relevant portion of the steroid formula a brace may be used. For example **2h** only shows ring D and the side chain at C-17 but in this context the portion to the left of the brace may be assumed to be the rest of an androstane ring system as in formulae **2a-g**. In other contexts, for example, it might represent the rest of an estrane ring system, including any substituents, and double bonds present in that portion.

6) *3S-1.5. Stereochemistry of ring junctions and side-chain attachment:* Unless implied or stated to the contrary (see Recommendations 3S-3, 3S-4.1 and 3S-5), use of a steroid name implies that atoms or groups attached at the bridgehead positions 8, 9, 10, 13 and 14 are oriented as shown in formula **2a** (i.e. 8β,9α,10β,13β,14α), and a side chain attached at position 17 is assumed to be β-oriented (see notes below). The configuration of hydrogen (or a substituent) at the bridgehead position 5 is always to be designated by adding α, β or ξ after the numeral 5, this numeral and letter being placed immediately before the stem name. The stereochemistry of substituents attached to the tetracyclic systemA-D is stated by adding α, β or ξ after the respective numerals denoting their position.

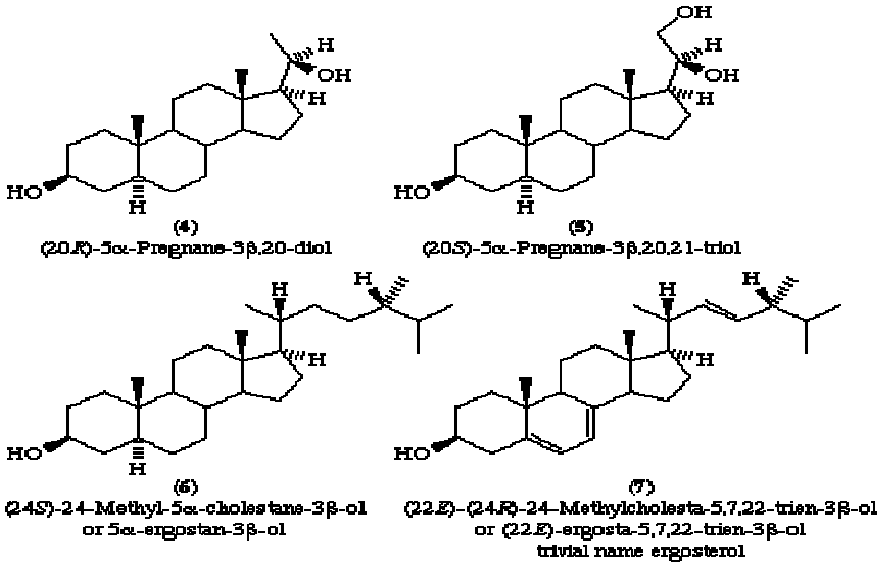
Notes

(1) If one of the bridgehead hydrogen atoms is replaced it may be desirable (although not necessary) to restate the stereochemistry, e.g.9α-fluoro-5α-pregnane instead of 9-fluoro-5α-pregnane.

(2) For the purpose of this Recommendation, a carboxyl group at position 17 is treated as a substituent (see Recommendation 3S-4.1).

(3) If two carbon chains are attached at position 17, see Recommendations 3S-2.7 and 3S-2.8.

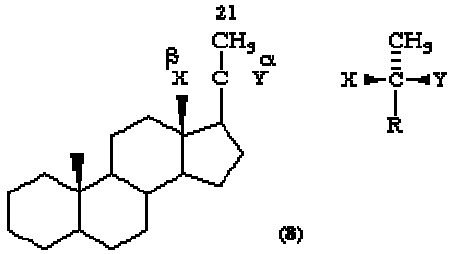
7) 3S-1.6. Stereochemistry of substituents in the side chain: The stereochemistry of substituents on the steroid side chain is described by the sequence rule procedure (see [3], section E), unless implied by the name (see 3S-2.4 and Table 1). Examples:



Notes

(1) The backbone of a side chain at C-17 is best denoted as in the plane of the paper (lines of ordinary thickness), the 17-20 bond being similarly denoted.Stereochemistry due to substituents on the chain is then indicated by the customary thick or broken lines denoting bonds that project, respectively, above and below the plane of the paper. In formulae the representation of the side chain is drawn as in examples **6** and **7** in preference to those used in the previous edition of this document [1].

(2) In the pregnane series, the stereochemistry at C-20 was formerly designatedas 20α or 20β. This convention was based on a Fischer projectionwith the highest number at the top, as given in formula **8**. Thisnomenclature is now discouraged for specific compounds in favour of the *R,S* system, which can be generally used for all chiral centres in the side chain(s). However, as α and β are independent of substituents at neighbouring atoms they are retained for the corresponding enzyme names, e.g. 20α-hydroxysteroid dehydrogenase.



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1. IUPAC Commission on the Nomenclature of Organic Chemistry (CNOC) and IUPAC-IUB Commission on Biochemical Nomenclature (CBN). The Nomenclature of Steroids, Revised tentative rules, 1967. *Arch. Biochem. Biophys.* **136**, 13-35 (1970), amended **147**, 4-7 (1971); *Biochem. J.* **113**, 5-28 (1969), amended **127**, 613-616 (1972); *Biochemistry*, **8**, 2227-2242 (1969), amended **10**, 4994-4995 (1971); *Biochim. Biophys. Acta*, **164**, 453-486 (1968), amended **248**, 387-390 (1971); *Eur. J. Biochem.* **10**, 1-19 (1969), amended **25**, 1-3 (1972); *Pure Appl. Chem.* **31**, 285-322 (1972), with amendments incorporated; also pp. 133-153 of [2], with amendments included.

2. International Union of Biochemistry (1978) *Biochemical nomenclature and related documents*, The Biochemical Society, London.

4. A. Butenandt and L. Poschmann, *Ber. Dtsch. Chem. Ges.* **73**, 893-897 (1940); cf. also A. Butenandt, L. Karlson-Poschmann, G. Failer, U. Schiedt and E. Bilkert, *Liebigs Ann. Chem.* **575**, 123-144 (1951).

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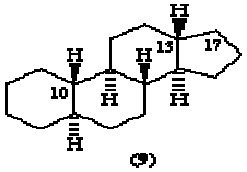
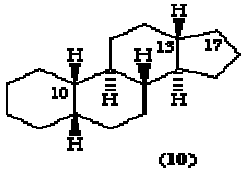
III. THE NOMENCLATURE OF STEROIDS RECOMMENDATIONS 1989 3S-2.1 TO 3S-2.4

A. 3S-2. Fundamental Carbocycles, Unsaturation and ALKYL Substitution AT C-17

1) 3S-2.1. Gonane: The parent tetracyclic hydrocarbon without methyl groups at C-10 and C-13 and without a side chain at C-17 is named gonane; see formulae **9** and **10**.

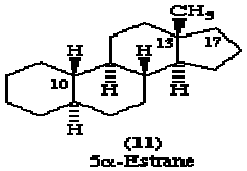


(9)
5α-Gonane

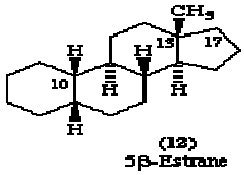


(10)
5β-Gonane

2) 3S-2.2. Estrane (oestrane): The hydrocarbon with a methyl group at C-13 but without a methyl group at C-10 and without a side chain at C-17 is named estrane (alternative spelling: oestrane), as shown in **11** and **12**. (See addendum for pronunciation of estrene.)

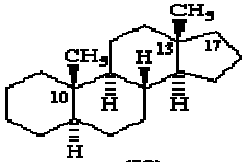


(11)
5α-Estrane

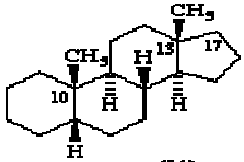


(12)
5β-Estrane

3) 3S-2.3. Androstane: The hydrocarbon with methyl groups at C-10 and C-13 but without a side chain at C-17 is named androstane **13** and **14**.



(13)
5α-Androstane



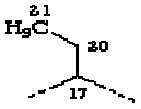
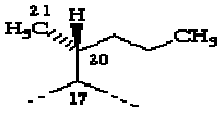
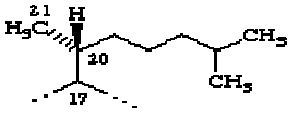
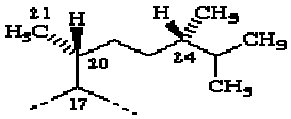
(14)
5β-Androstane

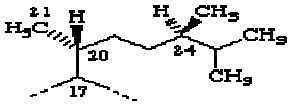
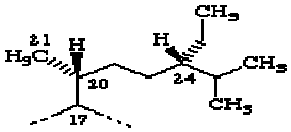
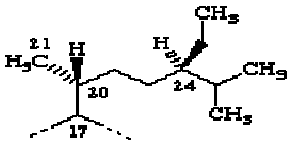
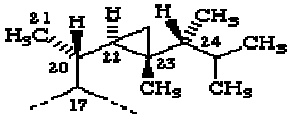
Note For the names of hydrocarbons having a methyl group attached to C-10 and a hydrogen atom attached to C-13, or compounds where an ethyl group replaces a methyl group, see 3S-6. Ring expansion or contraction is covered by 3S-7.

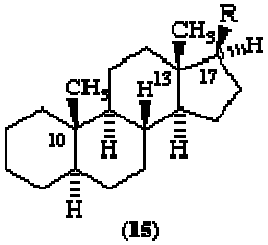
4) 3S-2.4. Parent hydrocarbons with side chain at C-17: The names used for the hydrocarbons **15** and **16** with methyl groups at both C-10 and C-13 and a side chain R are listed in Table 1. (See addendum for pronunciation of pregnene.)

Click here for "table free" view if the table below is faulty.

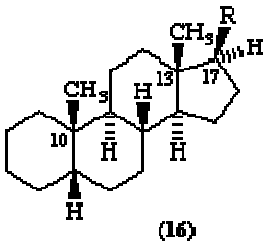
Table 1. Hydrocarbons with side chain at C-17

Side chain	Configuration	5α-Series (15)	5β-Series (16)
	-	5α-pregnane (not allopregnane)	5β-pregnane
	20*R*	5α-cholane (not allocholane)	5β-cholane
	20*R*	5α-cholestane	5β-cholestane (not coprostane)
	20*R*,24*S*	5α-ergostane	5β-ergostane

	20*R*,24*R*	5α-campestane	5β-campestane
	20*R*,24*S*	5α-poriferastane	5β-poriferastane
	20*R*,24*R*	5α-stigmastane	5β-stigmastane
	20*S*,22*R*,23*R*,24*R*	5α-gorgostane	5β-gorgostane



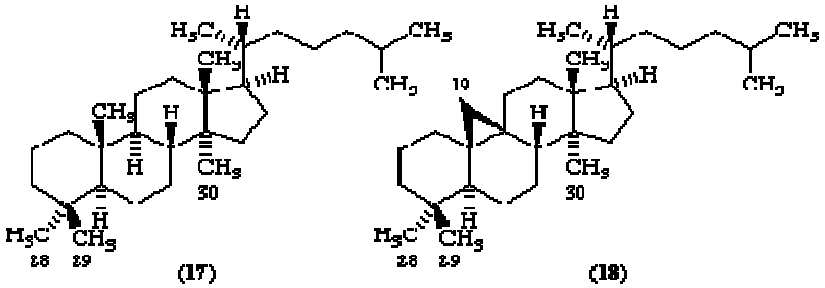
(15)



(16)

Notes

(1) The names of the hydrocarbons given in Table 1 imply the configuration at the chiral centres in the side chain as given in the second column. The conventions of the sequence rule, however, mean that *R* may change to *S* without a change at the relevant atom when there is a change in the substitution or unsaturation, e.g. compare **6** and **7**.(2) Some tetracyclic triterpenoids may be regarded as trimethyl steroids, the three additional methyl groups being numbered 28 (attached to C-4 with α-configuration), 29 (attached to C-4 with β-configuration) and 30 (attached to C-14); this numbering corresponds to that used for the triterpenoids. This type of nomenclature is especially useful for the parent hydrocarbons of biogenetic precursors of steroids. For example, lanostane **17** is 4,4,14-trimethyl-5α-cholestane, the former name implying the 5α,8β,9α,10β,13β,14α,17β,20*R* configuration. The change of configuration at C-9 in cycloartane **18** is implied in the name, although it must be specified if called 4,4,14-trimethyl-9,19-cyclo-5α,9β-cholestane. (See also addendum)



(17)
4,4,14-Trimethyl-5α-cholestane
or lanostane

(18)
4,4,14-Trimethyl-9,19-cyclo-5α,9β-cholestane
or cycloartane

(3) For the names of hydrocarbons that are related to those given in Table 1 by the addition or removal of one or more carbon atoms, see 3S-6. For ring expansion or contraction see 3S-7.

Continued in 3S-2.5 to 3S-2.10 unsaturation etc.
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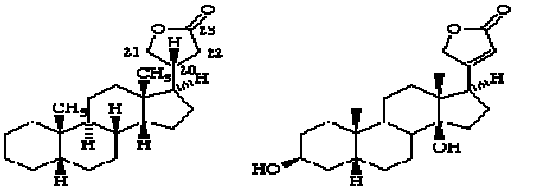
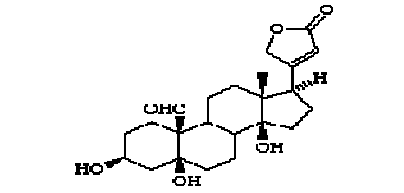
IV. THE NOMENCLATURE OF STEROIDS RECOMMENDATIONS 1989 3S-3

A. 3S-3. Steroids with Heterocyclic Rings in the Side Chain

1) *3S-3.0. General Definitions:* Many important naturally occurring steroids contain one or more additional heterocyclic ring(s), fused or attached to ring D, formed by modifications of the side chain. These steroids can be grouped into the following families: (a) cardanolides, (b) bufanolides, (c) spirostans, (d) furostans, (e) steroid alkaloids.

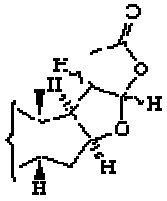
2) *3S-3.1. Cardanolides:* The name cardanolide is used for the compound of structure **33**, i.e. the parent compound of digitaloid lactones with the configuration illustrated. The 14β-configuration as well as the 20*R*-configuration are implied in the name. Examples:





Names such as card-20(22)-enolide are used for the naturally occurring unsaturated lactones of this type. The names 14,21- and 16,21-epoxycardanolide are used for the compounds containing a 14,21- or a 16,21-oxygen bridge respectively, as shown in **36**.

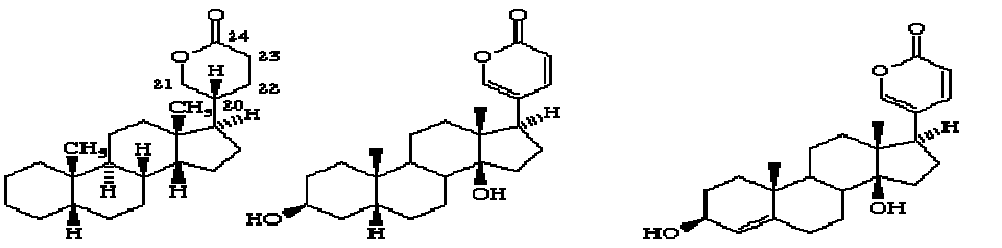
Note The former recommendation that the configuration at C-14 must always be stated as an affix is abandoned; 14β is implied unless otherwise stated. See also note 1 to 3S-1.5.



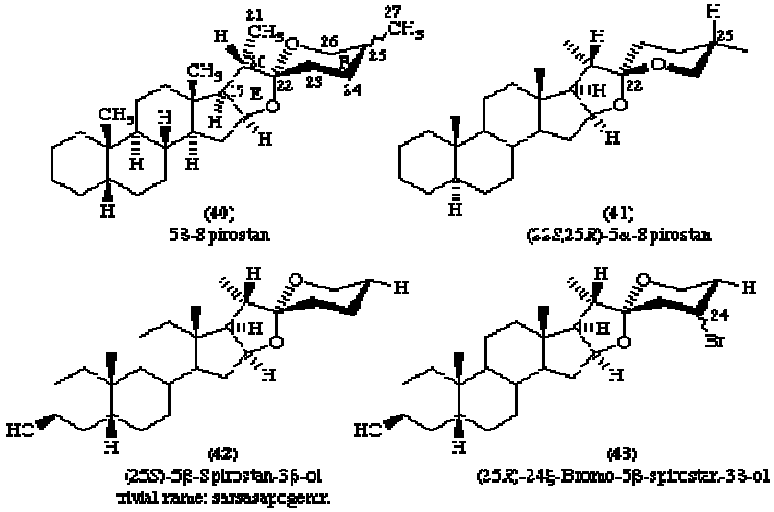
3) *3S-3.2. Bufanolides:* The name bufanolide is used for the compound of structure **37**, the parent compound of the squill-toad poison group of lactones, with the configurations 14β,20*R* as shown implied in the name. Unsaturated derivatives are named by replacing the suffix -anolide by -enolide, -adienolide, etc.; thus the name bufa-20,22-dienolide is used for the naturally occurring doubly unsaturated lactones.

Note As with cardanolides, the recommendation to always state the configuration at C-14 is abandoned. See also note (1) to 3S-1.5.

Examples:



4) 3S-3.3. Spirostans: The name spirostan is used for compounds of structure **40** (this is a 16,22:22,26-diepoxycholestane); this name specifies the configuration shown for all the asymmetric centres except positions 5 and 25. A prefix 5α- or 5β- is added in the usual way (see Recommendation 3S-1.5). Configurations at C-16 and C-17, if different from those shown in formula **40**, are designated by 16β(H) and 17β(H). Configurations at C-20 and C-22, if different from those shown in formula **40**, are designated by the sequence-rule procedure (see Section E in [3]) or, if unknown, by ξ. Steric relations of substituents at C-23, C-24 or C-26 are in all cases designated by the sequence-rule procedure or, if unknown, by ξ. Examples:



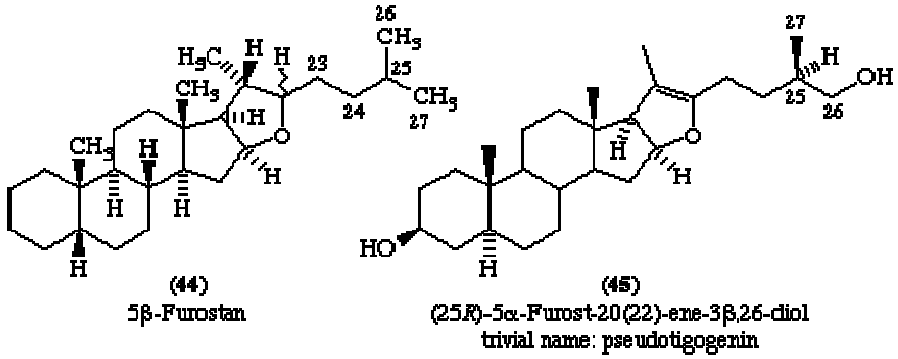
Notes

(1) Although ring E, like rings α, β, C and D, can conveniently be shown by projection on to the plane of the paper, ring F cannot be adequately represented in this way since C-23, C-24 and C-26 and the oxygen atom lie in a plane that is perpendicular to the plane of the paper. Ring F is conveniently drawn as in formulae **40-43**; in formula **40**, for instance, the broken line from C-22 to oxygen denotes that the oxygen atom and C-26 of ring F lie behind the plane of the paper and that consequently C-23 and C-24 lie in front of the plane of the paper (configuration *R* at C-22). In formula **41** the configuration at C-22 is reversed and must be stated in the name as 22*S*. It is conventional to draw ring F as a chair, but this conformation is not implied in the name spirostan. Whatever the conformation of ring F, C-27 and the 25-hydrogen atom may be considered to lie in the plane of the paper and so cannot be denoted by broken or thickened lines. In **42** the methyl group is axial (above the general plane of ring F), and in 41 it is equatorial (in the general plane of ring F).

(2) The *R,S* specification may also be affected by substituents attached to ring F or C-27, as in compound **43** (cf. **42**).

5) 3S-3.4. Furostans: The name furostan is used for the compound of structure **44** (16,22-epoxycholestane); this name specifies the configurations at all the asymmetric centres except position 5, 22 and (if position 26 is substituted) also 25. Configuration at C-5 is designated by use of α or β in the usual way (see Recommendation 3S-1.5), and configurations at C-22 and, if necessary, C-25 by the sequence-rule procedure, or in all these cases by ξ if unknown.

Substituents are indicated in the usual way, as in example **45**.



6) 3S-3.5. Steroid Alkaloids: If systematic names for steroid alkaloids are desired, they should be derived from pregnane, cholestane or some other parent name given in Table 1.

Trivial names for the parent saturated structures of steroid alkaloids are so chosen that they end in -anine. In the case of unsaturated compounds, this ending is changed to -enine, -adienine, etc. as appropriate.

An extensive treatment of the nomenclature of steroid alkaloids is beyond the scope of these recommendations. A special appendix to section F of ref. 3 dealing with these problems is in preparation.

REFERENCES

2. International Union of Biochemistry (1978) *Biochemical nomenclature and related documents*, The Biochemical Society, London.

3. International Union of Pure and Applied Chemistry, *Nomenclature of organic chemistry, Sections A, B, C, D, E, F and H*, 1979 Edition, Pergamon Press, Oxford, 1979. Section E appeared also in pp. 1-18 of [2], and section F in pp. 19-26 of [2] and in *Eur. J. Biochem.* **86**, 1-8 (1978).

Continued in 3S-4.0 to 3S-4.3 functional groups.
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V. THE NOMENCLATURE OF STEROIDS RECOMMENDATIONS 1989 3S-4.0 TO 3S-4.3

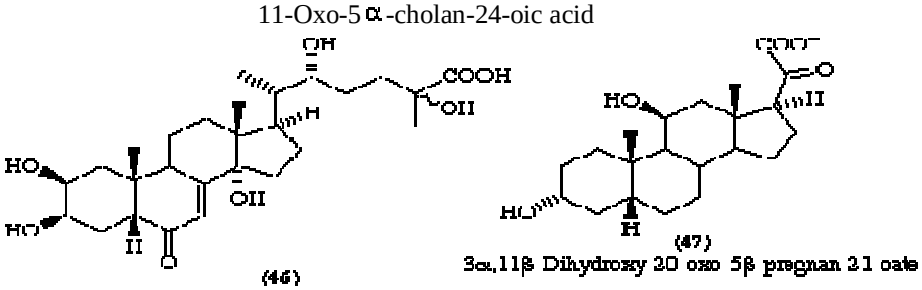
A. 3S-4. Functional Groups

1) 3S-4.0. General: Nearly all biologically important steroids are derivatives of the parent hydrocarbons (cf. Table 1) carrying various functional groups. Their nomenclature follows the general recommendations of the nomenclature of organic compounds (Sections C and D in [3]). However, there are some special problems in the application of these recommendations to natural products like steroids. Therefore, and for the benefit of the biochemist not so familiar with the recommendations of substitutive nomenclature, these are outlined and exemplified here. For full details, the reader is referred to the IUPAC Recommendations [3]. Most substituents can be designated either as suffixes or prefixes; some, however, the commonest being halogens, alkyl groups (see 3S-2.7 and 3S-2.8) and alkoxy groups, can only be designated as prefixes. Lists of these two types are given in Tables I and II respectively section C-10 of [3]. When possible, one type of substituent must be designated as suffix. When more than one type is present that could be designated as suffix only one type may be so expressed and the other types must be designated as prefixes. The choice for suffix is made according to an order of preference that is laid down in [3]; the most important part of this order, for steroids, is as follows in decreasing preferences: onium salt, acid, lactone, ester, aldehyde, ketone, alcohol, amine. Suffixes are added to the name of the saturated or unsaturated parent system (see 3S-2.5), the terminal e of -ane, -ene, -yne, -adiene etc. being elided before a vowel (presence or absence of numerals has no effect on such elisions). The following recommendations are on these principles. In this section, the formulae of examples correspond to **2b**, i.e. the methyl groups are indicated by a bond without lettering, and the hydrogen atoms at C-8, C-9 and C-14 are omitted.

2) 3S-4.1. Acids, Salts and Esters: Acids, their salts and esters are generally named by use of suffixes.

(a) If a methyl group is changed into a carboxyl group, the suffix is -oic acid; it is preceded by the appropriate locant. In biochemical papers, these compounds are often named as anions, the counter-ion being unspecified; in this case, the suffix is -oate. Examples:

11-Oxo-5α-cholan-24-oic acid



(46)

(2*R*)-2β,3β,14,22,25-Pentahydroxy-6-oxo-5α-cholest-7-en-26-oic acid
trivial name: ecdysonic acid

(47)

3α,11β Dihydroxy 20 oxo 5β pregnan 21 oate

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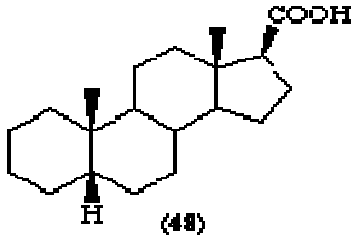
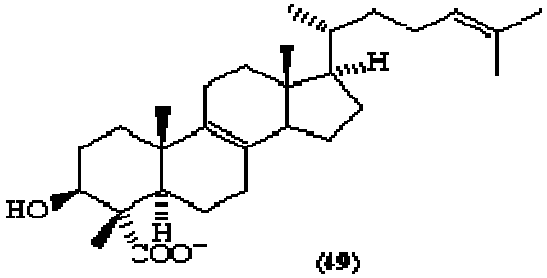
(b) If an acid is formed by substitution of a hydrogen atom in → CH, >CH_2 or -CH_3 by a carboxyl group, i.e. → C-COOH, >CH-COOH or -CH_2-COOH the suffix is -carboxylic acid or, in the ion form, -carboxylate. Note that in this case the acid contains one more carbon atom than the parent compound. Examples:

Note Compound **48** was formerly called 5β,17a(H)-etianic acid. This name, etianic acid, is now abandoned.

(c) Names of salts are formed by stating the cation and using, as a separate word, the ionic form of the name of the acid. Example:



(48)
5β-Androstane-17β-carboxylic acid

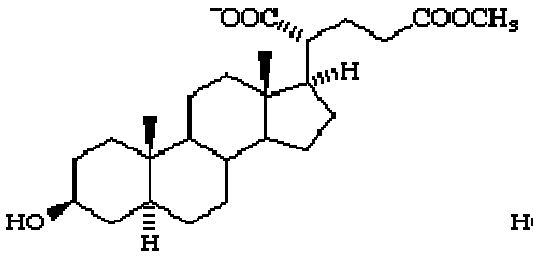


(49)
3β-Hydroxy-4β-methyl-5α-cholesta-8,24-diene-4α-carboxylate
or 3β-hydroxy-30-norlancsta-8,24-dien-28-oate

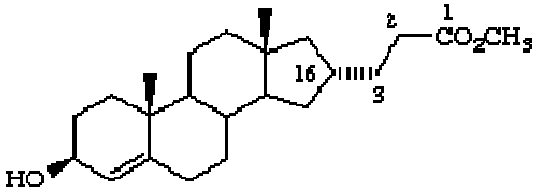
(d) Esters are conveniently named in a similar way. Examples:

Methyl 5β-androstane-17β-carboxylate

Diethyl 5α-cholane-21,24-dioate

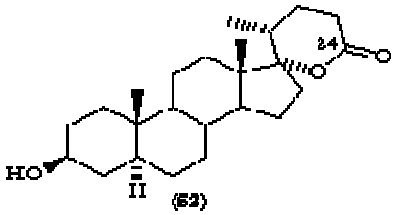


(50)
24-Methyl 3β-hydroxy-5α-cholane-21,24-dioate

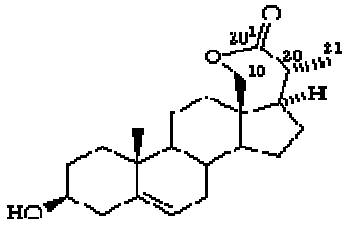


(51)
Methyl 3-(3β-hydroxyandrost-4-en-16α-yl)propanoate

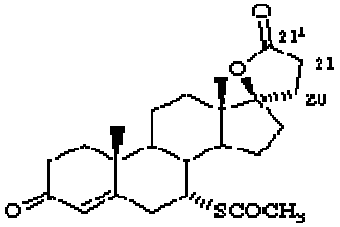
3) *3S-4.2. Lactones:* (a) Lactones, other than cardanolides and bufanolides, are named by changing the ending -ic acid or -carboxylic acid of the name of the hydroxy acid to -lactone or -carbolactone respectively, preceded by the locant of the acid group and then the locant of the hydroxyl group. The lactonised hydroxyl group is not stated separately. Examples:



(52)
3β-Hydroxy-5α-cholano-24,17-lactone



(53)
(20*R*)-3β-Hydroxypregn-5-ene-20,18-carbolactone



(54)
7β-Acetylthio-3-oxo-17α-pregn-4-ene-21,17-carbolactone
International non-proprietary name: spironolactone

Note In examples **53** and **54** the suffix carbolactone corresponds to a substituent with an additional carbon atom which is numbered accordingly (see 3S-2.7). If example **53** was called 3β-hydroxy-23,24-dinorchol-5-eno-21,18-lactone (name not recommended), then the lactone carbonyl would be C-21 (see 3S-6.2 for use of nor). Similarly, if example **54** was called 7α-acetylthio-3-oxo-21α-homo-17-pregn-4-eno-21α,17-lactone (name not recommended), then the lactone carbonyl would be C-21a (see 3S-6.1 for use of homo).

(b) Cardanolides and bufanolides. The -olide ending of these names denotes the lactone grouping, and substituents must be named as prefixes.

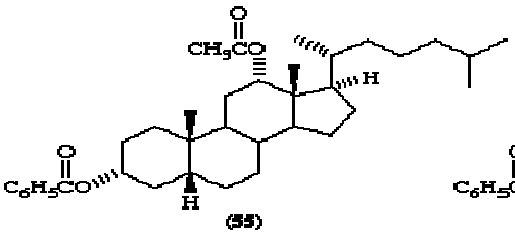
4) *3S-4.3. Esters of Steroid Alcohols:* Esters of steroid alcohols are named by the appropriate steroid substituent group followed by that of the acyloxy group in its anionic form. The steroid name is formed by replacing the terminal -e of the hydrocarbon name by -yl, -diyl, etc. and inserting this before the locant with a Greek letter to designate position and configuration. When necessary locants should be used with the anionic part of the name. Examples:

5α-Cholestan-3β-yl acetate

5β-Cholestane-3α,12α-diyl diacetate

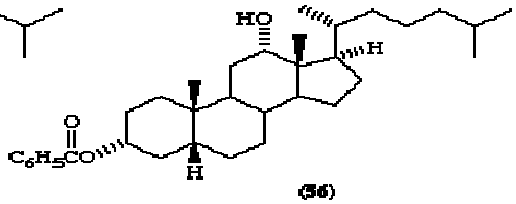
3-Oxoandrost-4-en-17β-yl acetate (trivial name testosterone acetate)

17α-Hydroxy-20-oxopregn-5-en-3α-yl sulfate



(55)

5β-Cholestane-3α,12α-diyl 12-acetate 3-benzoate



(56)

12α-Hydroxy-5β-cholestane-3α-yl benzoate

The prefix form acyloxy-, with the appropriate locants, is used if there is a preferred functional group as the suffix (e.g. an acid or lactone). Examples:

3α-Acetoxy-5β-cardanolide

3α-Benzoyloxy-11β-hydroxy-20-oxo-5β-pregnan-21-oate (monobenzoate of **47**)

3β-Acetoxy-5α-cholano-24,17-lactone (acetate of **52**)

When the steroid has a trivial name that already specifies the hydroxyl group that is esterified, the prefix must be *O*-acyl-. Examples:

3-*O*-Acetylcholic acid

17-*O*-Benzoylestradiol-17β

3-*O*-Linolenoylcholesterol

Notes

(1) If it is wanted to emphasize the unesterified form of the steroid (e.g. in an index) the polyol may be named with the ester groups indicated as in the example **55** 5β-cholestane-3α,12α-diol 12-acetate 3-benzoate. This style was recommended in the previous edition of these recommendations, but does not follow standard systematic nomenclature rules [3].

(2) In the case of simple sterols with trivial names, the substituent form of the trivial name may be used (e.g. cholesteryl linoleate). This form should not be used with polyols.

REFERENCES

2. International Union of Biochemistry (1978) *Biochemical nomenclature and related documents*, The Biochemical Society, London.

3. International Union of Pure and Applied Chemistry, *Nomenclature of organic chemistry, Sections A, B, C, D, E, F and H*, 1979 Edition, Pergamon Press, Oxford, 1979. Section E appeared also in pp. 1-18 of [2], and section F in pp. 19-26 of [2] and in *Eur. J. Biochem.* **86**, 1-8 (1978).

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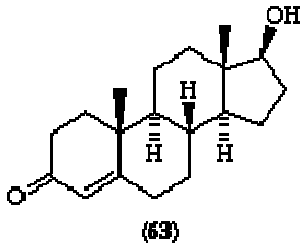
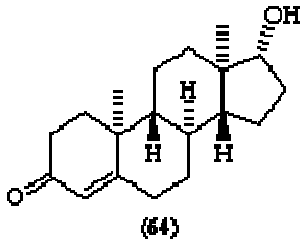
VI. THE NOMENCLATURE OF STEROIDS RECOMMENDATIONS 1989 3S-5

A. 3S-5. Stereochemical Modifications

1) 3S-5.1. Use of the prefix ent-: If, as for instance in a synthetic compound, there is stereochemical inversion at all the asymmetric centres whose configurations need not be specified in a name, the italicized prefix *ent-* (a contracted form of *enantio-*) is placed in front of the complete name of the compound. This prefix denotes inversion at all asymmetric centres (including those due to named substituents) whether these are cited separately or are implied in the name. Examples:



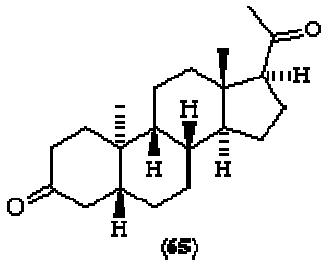
(63)
17β-Hydroxyandrost-4-en-3-one (testosterone)



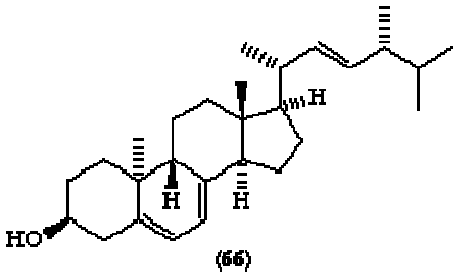
(64)
ent-17β-Hydroxyandrost-4-en-3-one (*ent*-testosterone)

Note When numerals are used to enumerate formulae, the prefix ent- may be used to indicate the enantiomer. Thus, e.g. compound **64** above may be designated ***ent*-63**.

2) 3S-5.2. Use of α and β for bridgeheads: If there is stereochemical inversion at not more than half of the asymmetric centres whose configurations need not be specified in a name, the configurations of the hydrogen atoms or substituents at the affected bridgeheads, or the carbon chain (if any) at position 17, are stated by means of a prefix or prefixes α or β, each with its appropriate locant, placed before the stem name laid down in 3S-2 and 3S-3. Examples:



(65)
5β,9β,10α-Pregnane-3,20-dione

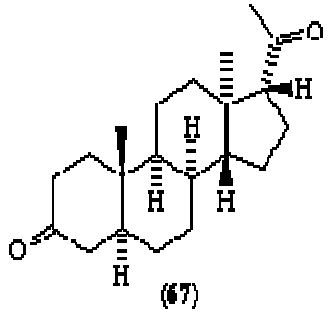


(66)
(22*E*)-9β,10α-Ergosta-5,7,22-trien-3β-ol
trivial name: lumisterol

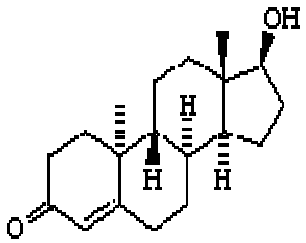
Note The prefix retro, indicating 9β,10α configuration, should not be used.

3) 3S-5.3. Use of α/β and ent-: The enantiomer of a compound designated as in Recommendation 3S-5.2 is given the same name preceded by *ent*.

Note This Recommendation covers the compounds in which there is inversion at a majority, but not all, of the asymmetric centres that need not be specified in the name. Examples:



(67)
ent-5β,9β,10α-Pregnane-3,20-dione
(not 5α,8α,13α,14β,17α-pregnane-3,2-dione)



(68)
ent-17α-Hydroxy-13α,14β-androst-4-en-3-one
(not 17β-hydroxy-8α,9β,10α-androst-4-en-3-one)

4) 3S-5.4. Use of the prefix rac-: Racemates, as for instance obtained by synthesis, are named by use of an italicized prefix *rac-* (an abbreviation of *racemo-*), placed before the complete name of the compound, the enantiomer chosen for naming being that required by Recommendations 3S-5.1 to 3S-5.3.

Example: A racemate composed of compounds **63** and **64** (= ***ent*-63**) is named *rac*-17β-hydroxyandrost-4-en-3-one or *rac*-testosterone.

Note The designation of α and β to the substituents refers to the normal series, not to the *ent*-series; the prefix *ent-* indicates that their absolute spatial orientation is inverted.

5) 3S-5.5. Use of R and S*:* When the relative, but not the absolute, configuration of two or more asymmetric centres in a steroid derivative is known, this may be indicated by *R** or *S** according to Recommendations E-4.10 and F-6.7 of [3].

REFERENCES

2. International Union of Biochemistry (1978) *Biochemical nomenclature and related documents*, The Biochemical Society, London.

3. International Union of Pure and Applied Chemistry, *Nomenclature of organic chemistry, Sections A, B, C, D, E, F and H*, 1979 Edition, Pergamon Press, Oxford, 1979. Section E appeared also in pp. 1-18 of [2], and section F in pp. 19-26 of [2] and in *Eur. J. Biochem.* **86**, 1-8 (1978).

Continued in 3S-6 homo and nor.
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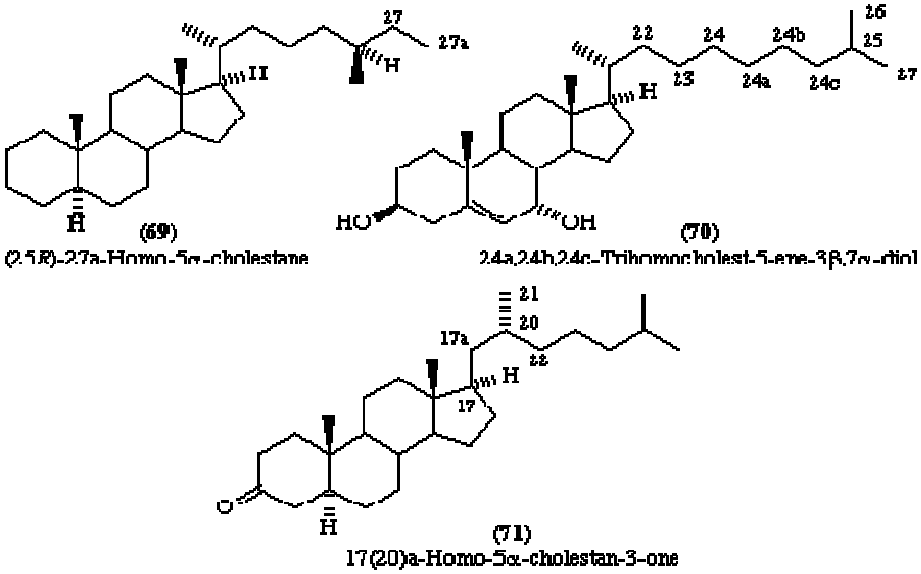
VII. THE NOMENCLATURE OF STEROIDSRECOMMENDATIONS 19893S-6

A. *3S-6. Lengthening and Shortening of Side Chains and Elimination of Methyl Groups*

1) 3S-6.1. Use of the prefix homo-: Lengthening of a side chain by insertion of one (or more) methylene groups is indicated by the prefix homo- (dihomo- etc.). The prefix is preceded by the (complex) locant(s) of the carbon atom(s) inserted. Examples:



(2*S*)-27a-Homo-5α-cholestane

24a,24b,24c-Trihomocholest-5-ene-3β,7α-diol

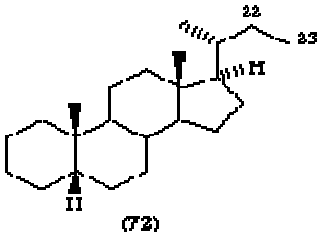
17(20)a-Homo-5α-cholestan-3-one

Notes

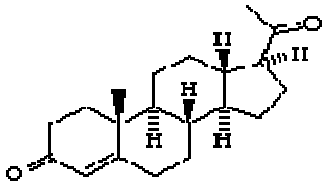
(1) If the methylene group is inserted into a methyl C-H bond or next to a methylene group the letter a (b etc.) is added to the locant of the highest numbered atom (e.g. example **69** is 27a-homo- not 26a-homo-).

(2) If the methylene group is inserted between two side-chain branch points that are directly linked, or between C-17 and a branch point at C-20 (i.e. Table 1 except pregnane) both locants are used with the letter a (b etc.) and the higher numbered locant in parenthesis. The higher number may be omitted in a structural formula but must be used in the name of the homo-steroid (e.g. 17a in compound **71**).

2) *3S-6.2. Use of the prefix nor-:* Elimination of a methylene group (-CH_2-) from a steroid side chain is indicated by the prefix nor, which in all cases is preceded by the number of the carbon atom that disappears. When alternatives are possible, the number attached to nor- is the highest permissible. Elimination of two methylene groups is indicated by the prefix dinor-. The remainder of the original steroid numbering is retained (see **73**). Examples:



(72)
24-Nor-5β-cholane

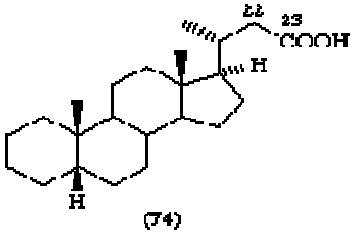


(73)
18-Norpregn-4-ene-3,20-dione

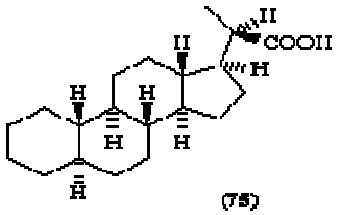
Exceptions: By recommendations 3S-2.1 and 3S-2.2 the names gonane (for 18,19-dinorandrostane) and estrane (for 19-norandrostane) constitute exceptions to the above Recommendation 3S-6.2. The names gonane and estrane are used also as parent names for their derivatives.

However, 18-nor- and 19-nor- are used with other parent and trivial names, as in 19-norpregnane, 18,19-dinorspirostan, and 18-norestrone.

The compound produced by shortening the side chain of pregnane is named 17β-methylandrostane rather than 21-norpregnane. See also Recommendation 3S-6.3. Examples:



(74)
24-Nor-5β-cholan-23-oic acid

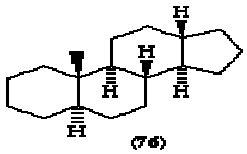


(75)
(20*R*)-10,19-Dinor-5α-pregnane-20-carboxylic acid
(not 18,19,23,24-tetranor-5α-cholan-21-oic acid)

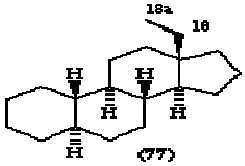
3) *3S-6.3. Preference between homo- and nor-:* A compound with a skeleton that differs from the fundamental parent systems (see 3S-2.1 to 3S-2.4 and 3S-3.1 to 3S-3.4) by changes in the side chain(s) can often be named by several different methods involving either side chain lengthening (3S-6.1) or shortening (3S-6.2) and/or alkylation (3S-4.0) and/or addition of carbon atoms associated with a functional group [3S-4.1(b), 3S-4.2(a), 3S-4.4(a)]. The preferred name is selected by the following recommendations applied in order:

(a) A name should be derived by the fewest number of modifications of the fundamental parent system. Both detachable (e.g. alkyl) and non-detachable (e.g. homo or nor) prefixes are considered as modifications. Dihomo, dinor, etc., are counted as two modifications each.

(b) Non-detachable prefixes are preferred to detachable prefixes. Examples:



(76)
18-Nor-5α-androstane
(not 10-methyl-5α-gonane)



(77)
18a-Homo-5α-estrane
(not 13-ethyl-5α-gonane or
13-ethyl-18-nor-5α-estrane)

Notes

(1) As an exception to recommendation (b) above, 17β-methyl-5α-androstane is preferred to 21-nor-5α-pregnane and 5α-androstane-17β-carboxylic acid is preferred to 21-nor-5α-pregnan-20-oic acid.

(2) Compound **77** is 13-ethyl-18-nor-5α-estrane in current Chemical Abstracts Service index nomenclature.

Continued in 3S-7 ring contraction and expansion.
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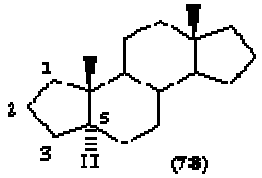
VIII. THE NOMENCLATURE OF STEROIDS RECOMMENDATIONS 1989 3S-7

A. 3S-7. Ring Contraction and Expansion

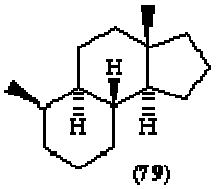
1) 3S-7.1. Use of the prefix nor-: Ring contraction by loss of an unsubstituted methylene group is indicated by the prefix nor-. For loss of two methylene groups, dinor- is used. The methylene group(s) lost is considered to include the highest numbered unsubstituted atom of the ring involved, and the locant of that lost methylene group precedes the prefix nor- in the nor-compound. The remainder of the original numbering is retained. Example:

In 4-nor-5α-androstane (**78**) C-4 is missing.



(78)

2) 3S-7.2. Use of the prefix des-: The removal of a terminal ring, with addition of a hydrogen atom at each junction atom with the adjacent ring, is indicated by the prefix des-, followed by the italic capital letter designating that ring (3S-1.1); substituents and stereochemistry implied in the trivial name remain unless otherwise stated. Example:

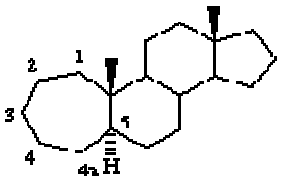


(79)
Des-*A*-androstane

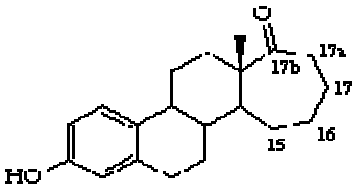
Note The prefix des- is used here, not de-, because of the ease of confusing de- with the letter D in speech.

3) 3S-7.3. Use of the prefix homo-: Ring expansion by inclusion of one methylene group is indicated by the prefix homo-, by two methylene groups by dihomo-. The prefix is preceded by the (complex) locant(s) of the carbon atom(s) inserted. These are chosen in the following way:

(a) If the methylene group is not inserted between directly linked bridgeheads or between C-13 and C-17 carrying a side chain, the letter a, b etc. is added to the locant of the highest numbered atom of the ring that is not a bridgehead. Examples:

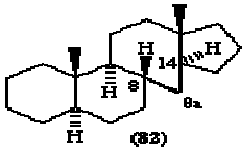


(80)
4a Homo 5α androstane

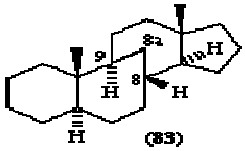


(81)
3-Hydroxy-17a,17b-dihomoestra-1,3,5(10)-trien-17b-one

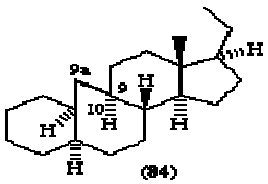
(b) If the methylene group is inserted between directly linked bridgeheads or between C-13 and C-17 carrying a side chain, the letter a (or a and b) is added to the pair of locants indicating the atoms on either side, and the higher numbered locant is placed in parentheses. Examples:



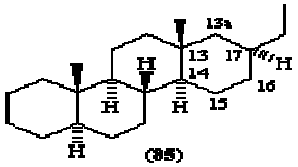
(82)
8(14)a-Homo-5α-androstane



(83)
8(9)a-Homo-5α-androstane



(84)
9(10)a-Homo-19-nor-5α,10α(H)-pregnane



(85)
13(17)a-Homo-5α-pregnane

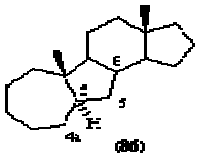
The locant(s) with the prefix homo- is placed after the prefixes required for functional groups (cf. 3S-4), before the stereodescriptor (e.g. 5^{β}) of the stem name, or if such is not required, directly before the stem name.

Notes

(1) Recommendation 3S-7.3 deviates from the former convention in 2S-8; the present recommendation is in line with the general Recommendation F-4.5 (cf. Section F in [3]).

(2) Although complex locants are necessary in the names of homo-steroids, simple locants may be used with structural formulae, e.g. 8a in compound **82** or 13a in compound **85** with the lower-numbered carbon atom as parent locant.

4) *3S-7.4. Use of both nor- and homo- in one Name:* The above recommendations for ring expansion and contraction may be used for modifications of two rings in the same molecule, as illustrated in example **86**.



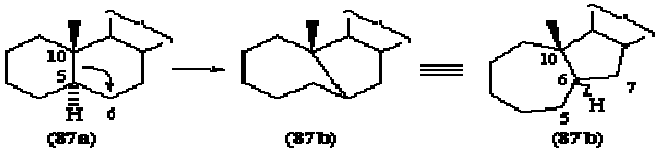
(86)
4a-Homo-7-nor-5α-androstane

Notes

(1) Names incorporating homo- and nor- are normally preferred to alternatives incorporating cyclo- and seco- (cf. examples **84** and **86**).

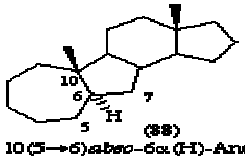
(2) A compound with excessive modification of the steroid skeleton usually is best described by a systematic name. It is recommended that no more than two of the steroid rings be altered by any combination of the prefixes homo- and nor-.

5) *3S-7.5. Use of the prefix abeo-:* As an alternative to the application of nor- and homo- to the same molecule, the abeo system may sometimes be used. A compound that may be considered to arise from a steroid by bond migration may be given the name laid down in the preceding Recommendations for the steroid in question, to which is attached a prefix of the form *x*(*y*→*z*)*abeo*-. This prefix is compiled as follows: a numeral denoting the stationary (unchanged) end of the migrating bond (*x*) is followed by parentheses enclosing (i) the number denoting the original position (*y*) from which the other end of this bond has migrated, (ii) an arrow, and (iii) the number (*z*) denoting the new position to which the bond has moved (see formulae **87a** and **87b**).

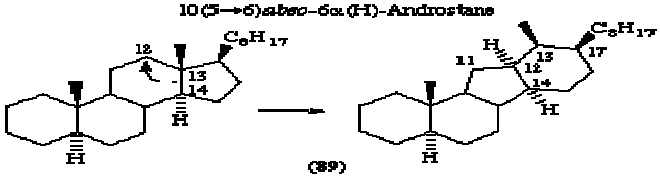


(87a) (87b) (87b)

The original numbering is retained for the new compound and is used for the numbers *x*, *y* and *z*. It is always necessary to specify the resulting stereochemistry. Examples:



(88)
10(5→6)*abeo*-5α(H)-Androstane



(89)
14(13→12)*abeo*-5α,12-α(H),13α(H)-Cholestane
(trivial name: 5α-Jervane)

Notes

(1) The *abeo* nomenclature described in this Recommendation is permissive, not compulsory. It is most suitable for use in discussions of reaction mechanism and biogenesis. For registration in a general (non-steroidal) compendium, the general systematic names, or names assigned by the homo- or nor- method, may be preferable. Thus **88** is identical with **86**.

(2) The *abeo* system has the advantage that the normal numbering of the steroid skeleton is retained. An example is **89**, the parent structure of some steroid alkaloids. Also, **84** may be named 9(10→19)*abeo*-5α,10a(H)-pregnane, C-9a remaining C-19.

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2. International Union of Biochemistry (1978) *Biochemical nomenclature and related documents*, The Biochemical Society, London.

3. International Union of Pure and Applied Chemistry, *Nomenclature of organic chemistry, Sections A, B, C, D, E, F and H*, 1979 Edition, Pergamon Press, Oxford, 1979. Section E appeared also in pp. 1-18 of [2], and section F in pp. 19-26 of [2] and in *Eur. J. Biochem.* **86**, 1-8 (1978).

Continued in 3S-8 and 3S-9 seco and viamin D.
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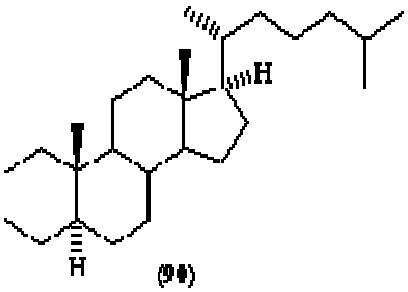
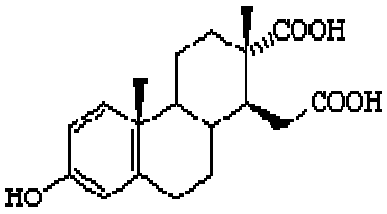
IX. THE NOMENCLATURE OF STEROIDS RECOMMENDATIONS 1989 3S-8 AND 3S-9

A. 3S-8 Ring Fission

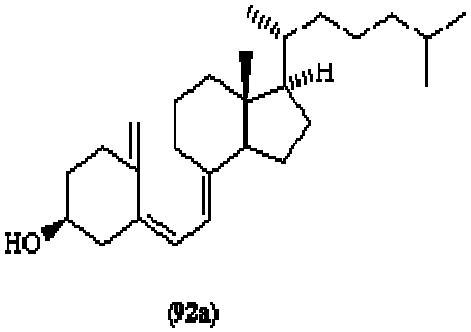
1) 3S-8.1. Use of the prefix seco-: Fission of a ring, with addition of a hydrogen atom at each terminal group thus created, is indicated by the prefix seco-, the original steroid numbering being retained. (If more than one ring is opened, general systematic nomenclature may be preferable. The principles of Note 2 to Recommendation 3S-7.4 apply also to seco-steroids.) Examples:



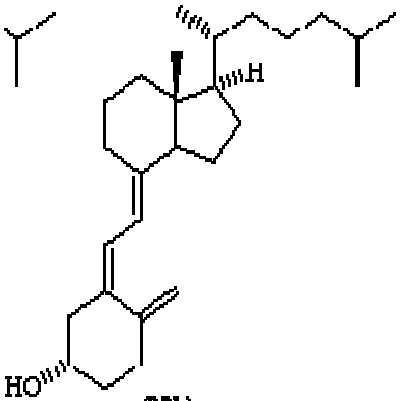
(90)
2,3-Seco-5α-cholestane



(91)
3-Hydroxy-16,17-secoestra-1,3,5(10)-triene-16,17-dioic acid



(92a)



(92b)
(5Z,7E) (3S) 9,10 Secocholesta 5,7,10 (19) trien 3 ol
trivial name: cholecalciferol or calciol

2) 3S-8.2. Use of α and β in seco-compounds: The stereochemical steroid descriptors α and β apply only when the remaining rings of a seco-compound are oriented as in the parent steroid, but not to alternative conformations (see formulae **92a** and **92b**). It is therefore recommended that after fission of ring B the stereochemistry of substituents on ring A is indicated by the *R,S* convention and α and β are restricted to rings C and D. Likewise after fission of ring C the stereochemistry of substituents on ring D is indicated by the *R,S* convention and α and β are restricted to rings A and B.

B. 3S-9. Vitamin D Group

1) 3S-9.0. General: By far the most important seco-steroids are the D vitamins and their derivatives. They can be named according to Recommendation 3S-8.1, but this results in very cumbersome names. For this reason and for the benefit of biochemists, a set of trivial names has been proposed [5], which can also be used as stem names for modified compounds. These names are permissive, not compulsory; authors may prefer to use the systematic seco-steroid names, which may indeed be more convenient for complicated structures.

Another reason for the revision of the vitamin D nomenclature is the confusion arising from the application of the steroid descriptors α and β. According to 3S-8.2, the *R,S* system should be used to describe the stereochemistry of substituents in ring A. Likewise, the geometry of the double bonds should be assigned by the *E,Z* system.

The names of the principal members of the vitamin D group are given in Table 3.

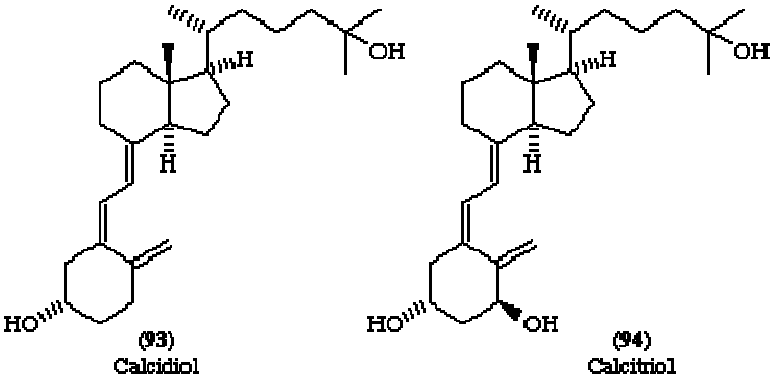
2) 3S-9.1. Trivial names: The compound **92**, also known as vitamin D_3 or cholecalciferol, is named calciol. The name implies the stereochemistry shown, which is 3*S*,5*Z*,7*E*. The name should only be used for the compound with a hydroxyl group at C-3 with the same orientation as in 3β-hydroxy steroids. Compound **93** is named calcidiol, and compound **94** is calcitriol. Some more trivial names are listed in Table 3, together with the systematic steroid names.

Click here for "table free" view if the table below is faulty.

Table 3. Nomenclature for vitamin D compounds

Current trivial name	Recommended trivial name	Systematic steroid name
Cholecalciferol	calciol or cholecalciferol (**92**)	(5*Z*,7*E*)-(3*S*)-9,10-secocholesta-5,7,10(19)-trien-3-ol
25-Hydroxycholecalciferol	calcidiol (**93**)	(5*Z*,7*E*)-(3*S*)-9,10-secocholesta-5,7,10(19)-triene-3,25-diol
1α,25-Dihydroxycholecalciferol	calcitriol (**94**)	(5*Z*,7*E*)-(1*S*,3*R*)-9,10-secocholesta-5,7,10(19)-triene-,3,25-triol
Ergocalciferol	ercalciol or ergocalciferol	(5*Z*,7*E*,22*E*)-(3*S*)-9,10-secoergosta-5,7,10(19),22-tetren-3-ol [a]
1α,25-Dihydroxyergocalciferol	ercalcitriol	(5*Z*,7*E*,22*E*)-(1*S*,3*S*)-9,10-secoergosta-5,7,10(1),22-tetraen-1,3,25-triol [b]
22,23-dihydroergocalciferol	(24*S*)-methylcalciol or 22,23-dihydroercalciol	(5*Z*,7E)-(3*S*)-9,10-secoergosta-5,7,10(19)-trien-3-ol [b]
1α,24*R*,25-Trihydroxycholecalciferol	calcitetrol	(5*Z*,7*E*)-(1*S*,3*S*,24*R*)-9,10-secocholesta-5,7,10(9)-triene-1,3,24,25-tetrol
Previtamin D_3	(6*Z*)-tacalciol	(6*Z*)-(3*S*)-9,10-secocholesta-5(10),6,8-trien-3-ol
Tachysterol$_3$	tacalciol (**95**)	(6*E*)-(3*S*)-9,10-secocholesta-5(10),6,8-trien-3-ol
Dihydrotachysterol$_3$	dihydrocalciol	(5*Z*,7*E*)-(3*S*,10*S*)-9,10-secocholesta-5,7-dien-3-ol
Isovitamin D_3	(5*E*)-isocalciol (**96**)	(5*E*,7*E*)-(3*S*)-9,10-secocholesta-1(10),5,7-trien-3-ol

[a] 24*R*-configuration
[b] 24*S*-configuration



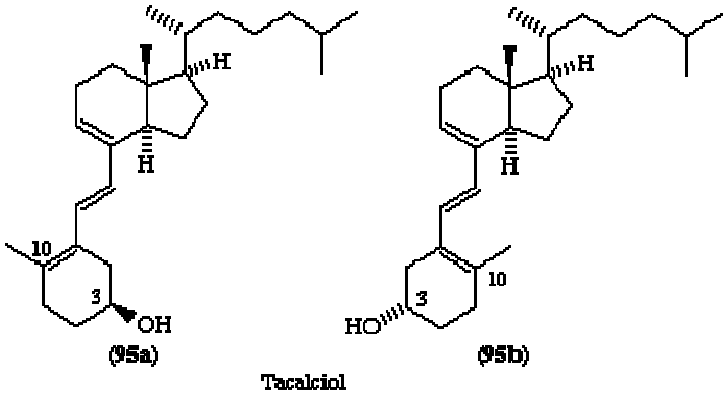
Notes

(1) The names calciol, calcidiol, calcitriol imply not only the stereochemistry but also the location of the hydroxyl group(s). Compounds with hydroxyl groups in other positions must be named either according to 3S-9.4 (below), or in the usual semisystematic way applying Recommendation 3S-8.1.

(2) The trivial names cholecalciferol and ergocalciferol are retained. They should, however, not be used for naming metabolites.

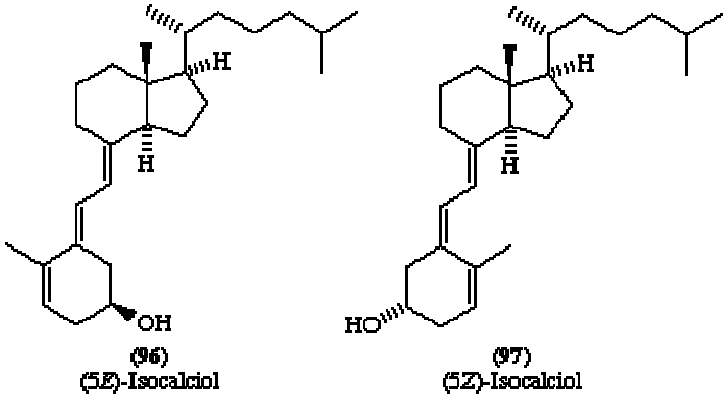
(3) Because of the nature of the sequence rule, it is not possible to transfer *R* or *S* from one compound to its derivatives. Calciol is a 3*S* compound but calcitriol is a 3*R* compound though the absolute configuration of the hydroxyl group at C-3 is not changed.

3) *3S-9.2. Modifications of the Triene System:* The prefix ta- (derived from tachysterol) indicates a change of the triene system from (5*Z*,7*E*)-5,7,10(19) to (6*E*)-5(10),6,8 as in tacalciol **95a** and **95b**.

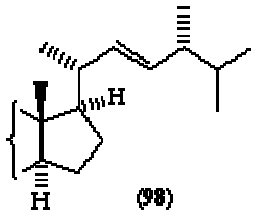


Tacalciol

The prefix iso- (derived from isovitamin D) when applied to calciol changes the location of the triene system to 1(10),5,7 with 7*E* configuration implied; the geometry at position 5, when known, must be specified by 5*E* **96** or 5*Z* **97**.



4) *3S-9.3. Modification of the Side Chain:* The prefix er- (derived from ergosterol) is used to indicate the side chain of the vitamin D_2 or ergocalciferol. This prefix implies the 22*E*,24*R* configuration as given in formula 98 unless otherwise specified.



(98)

5) *3S-9.4. Additional Hydroxyl Groups:* Additional hydroxyl groups cannot be indicated by modification of the suffix -ol, -diol, -triol, -tetrol, since these have definite meanings (see Table 3). They can, however, be added as prefix, e.g. (1*S*)-1-hydroxycalciol, 16β-hydroxycalciol. If possible, the full stereochemistry should be given, e.g. (25*R*)-26-hydroxycalciol. For other modifications and more detailed discussion of the nomenclature problems in the vitamin D field, the reader is referred to the original document [5].

REFERENCE

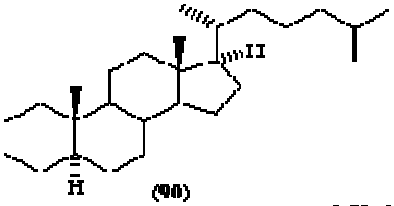
5. IUPAC-IUB Joint Commission on Biochemical Nomenclature (JCBN), Nomenclature of vitamin D. Recommendations 1981. *Arch. Biochem. Biophys.* **218**, 342-346 (1982); *Endokrinol. Inform.* 1982(2), 53-62; *Eur. J. Biochem.* **124**, 223-227 (1982); *Mol. Cell. Biochem.* **49**, 177-181 (1982); *Pure Appl. Chem.* **54**, 1511-1516 (1982).

Continued in 3S-10 Additional rings.
Return to Steroids Home Page

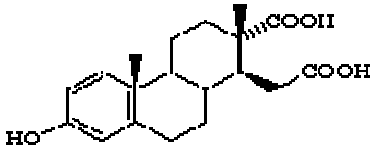
X. THE NOMENCLATURE OF STEROIDS RECOMMENDATIONS 1989 3S-8 AND 3S-9

A. 3S-8 Ring Fission

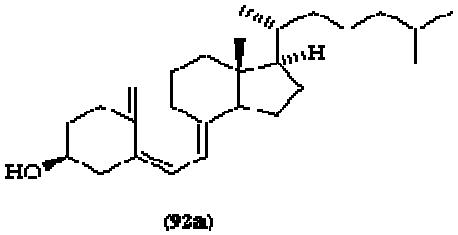
1) *3S-8.1. Use of the prefix seco-:* Fission of a ring, with addition of a hydrogen atom at each terminal group thus created, is indicated by the prefix seco-, the original steroid numbering being retained. (If more than one ring is opened, general systematic nomenclature may be preferable. The principles of Note 2 to Recommendation 3S-7.4 apply also to seco-steroids.) Examples:



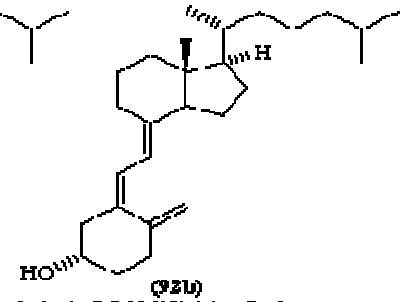
(90)
2,3-Seco-5α-cholestane



(91)
3-Hydroxy-16,17-secoestra-1,3,5(10)-triene-16,17-dioic acid



(92a)



(92b)
(5*Z*,7*E*) (3*S*) 9,10 Secocholesta 5,7,10(19) trien 3 ol
trivial name: cholecalciferol or calciol

2) *3S-8.2. Use of α and β in seco-compounds:* The stereochemical steroid descriptors α and β apply only when the remaining rings of a seco-compound are oriented as in the parent steroid, but not to alternative conformations (see formulae **92a** and **92b**). It is therefore recommended that after fission of ring B the stereochemistry of substituents on ring A is indicated by the *R,S* convention and α and β are restricted to rings C and D. Likewise after fission of ring C the stereochemistry of substituents on ring D is indicated by the *R,S* convention and α and β are restricted to rings A and B.

B. 3S-9. Vitamin D Group

1) *3S-9.0. General:* By far the most important seco-steroids are the D vitamins and their derivatives. They can be named according to Recommendation 3S-8.1, but this results in very cumbersome names. For this reason and for the benefit of biochemists, a set of trivial names has been proposed [5], which can also be used as stem names for modified compounds. These names are permissive, not compulsory; authors may prefer to use the systematic seco-steroid names, which may indeed be more convenient for complicated structures. Another reason for the revision of the vitamin D nomenclature is the confusion arising from the application of the steroid descriptors α and β. According to 3S-8.2, the *R,S* system should be used to describe the stereochemistry of substituents in ring A. Likewise, the geometry of the double bonds should be assigned by the *E,Z* system. The names of the principal members of the vitamin D group are given in Table 3.

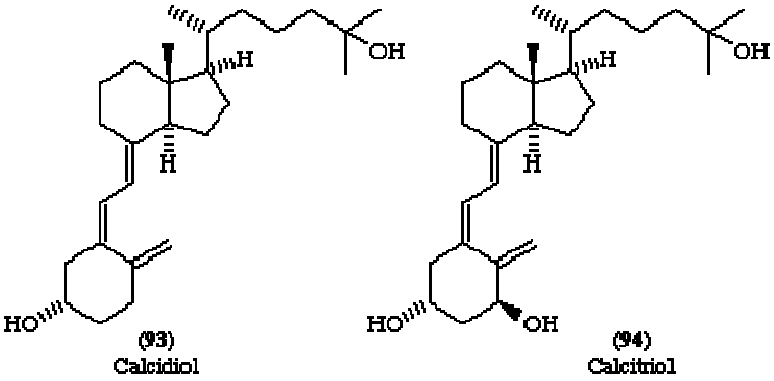
2) *3S-9.1. Trivial names:* The compound **92**, also known as vitamin D_3 or cholecalciferol, is named calciol. The name implies the stereochemistry shown, which is 3*S*,5*Z*,7*E*. The name should only be used for the compound with a hydroxyl group at C-3 with the same orientation as in 3β-hydroxy steroids. Compound **93** is named calcidiol, and compound **94** is calcitriol. Some more trivial names are listed in Table 3, together with the systematic steroid names.

Click here for "table free" view if the table below is faulty.

Table 3. Nomenclature for vitamin D compounds

Current trivial name	Recommended trivial name	Systematic steroid name
Cholecalciferol	calciol or cholecalciferol (**92**)	(5*Z*,7*E*)-(3*S*)-9,10-secocholesta-5,7,10(19)-trien-3-ol
25-Hydroxycholecalciferol	calcidiol (**93**)	(5*Z*,7*E*)-(3*S*)-9,10-secocholesta-5,7,10(19)-triene-3,25-diol
1α,25-Dihydroxycholecalciferol	calcitriol (**94**)	(5*Z*,7*E*)-(1*S*,3*R*)-9,10-secocholesta-5,7,10(19)-triene-,3,25-triol
Ergocalciferol	ercalciol or ergocalciferol	(5*Z*,7*E*,22*E*)-(3*S*)-9,10-secoergosta-5,7,10(19),22-tetren-3-ol [a]
1α,25-Dihydroxyergocalciferol	ercalcitriol	(5*Z*,7*E*,22*E*)-(1*S*,3*S*)-9,10-secoergosta-5,7,10(1),22-tetraen-1,3,25-triol [b]
22,23-dihydroergocalciferol	(24*S*)-methylcalciol or 22,23-dihydroercalciol	(5*Z*,7E)-(3*S*)-9,10-secoergosta-5,7,10(19)-trien-3-ol [b]
1α,24*R*,25-Trihydroxycholecalciferol	calcitetrol	(5*Z*,7*E*)-(1*S*,3*S*,24*R*)-9,10-secocholesta-5,7,10(9)-triene-1,3,24,25-tetrol
Previtamin D_3	(6*Z*)-tacalciol	(6*Z*)-(3*S*)-9,10-secocholesta-5(10),6,8-trien-3-ol
Tachysterol$_3$	tacalciol (**95**)	(6*E*)-(3*S*)-9,10-secocholesta-5(10),6,8-trien-3-ol
Dihydrotachysterol$_3$	dihydrocalciol	(5*Z*,7*E*)-(3*S*,10*S*)-9,10-secocholesta-5,7-dien-3-ol
Isovitamin D_3	(5*E*)-isocalciol (**96**)	(5*E*,7*E*)-(3*S*)-9,10-secocholesta-1(10),5,7-trien-3-ol

[a] 24*R*-configuration
[b] 24*S*-configuration



(93) Calcidiol (94) Calcitriol

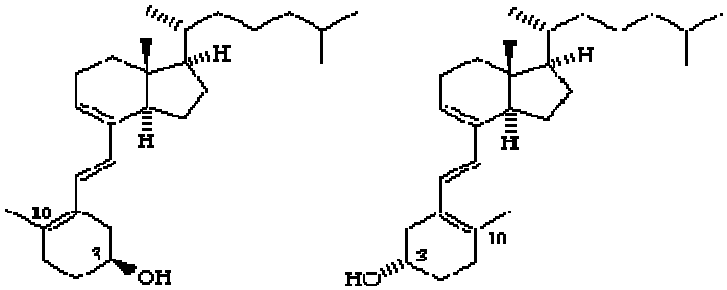
Notes

(1) The names calciol, calcidiol, calcitriol imply not only the stereochemistry but also the location of the hydroxyl group(s). Compounds with hydroxyl groups in other positions must be named either according to 3S-9.4 (below), or in the usual semisystematic way applying Recommendation 3S-8.1.

(2) The trivial names cholecalciferol and ergocalciferol are retained. They should, however, not be used for naming metabolites.

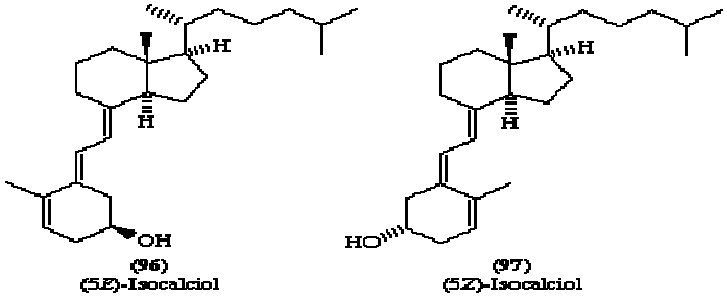
(3) Because of the nature of the sequence rule, it is not possible to transfer *R* or *S* from one compound to its derivatives. Calciol is a 3*S* compound but calcitriol is a 3*R* compound though the absolute configuration of the hydroxyl group at C-3 is not changed.

3) *3S-9.2. Modifications of the triene system:* The prefix ta- (derived from tachysterol) indicates a change of the triene system from (5*Z*,7*E*)-5,7,10(19) to (6*E*)-5(10),6,8 as in tacalciol **95a** and **95b**.

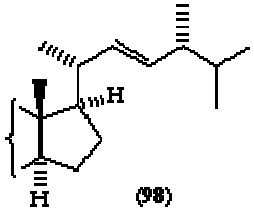


Tacalciol

The prefix iso- (derived from isovitamin D) when applied to calciol changes the location of the triene system to 1(10),5,7 with 7*E* configuration implied; the geometry at position 5, when known, must be specified by 5*E* **96** or 5*Z* **97**.



4) *3S-9.3. Modification of the side Chain:* The prefix er- (derived from ergosterol) is used to indicate the side chain of the vitamin D_2 or ergocalciferol. This prefix implies the 22*E*,24*R* configuration as given in formula **98** unless otherwise specified.



(98)

5) *3S-9.4. Additional Hydroxyl Groups:* Additional hydroxyl groups cannot be indicated by modification of the suffix -ol, -diol, -triol, -tetrol, since these have definite meanings (see Table 3). They can, however, be added as prefix, e.g. (1*S*)-1-hydroxycalciol, 16β-hydroxycalciol. If possible, the full stereochemistry should be given, e.g. (25*R*)-26-hydroxycalciol. For other modifications and more detailed discussion of the nomenclature problems in the vitamin D field, the reader is referred to the original document [5].

REFERENCE

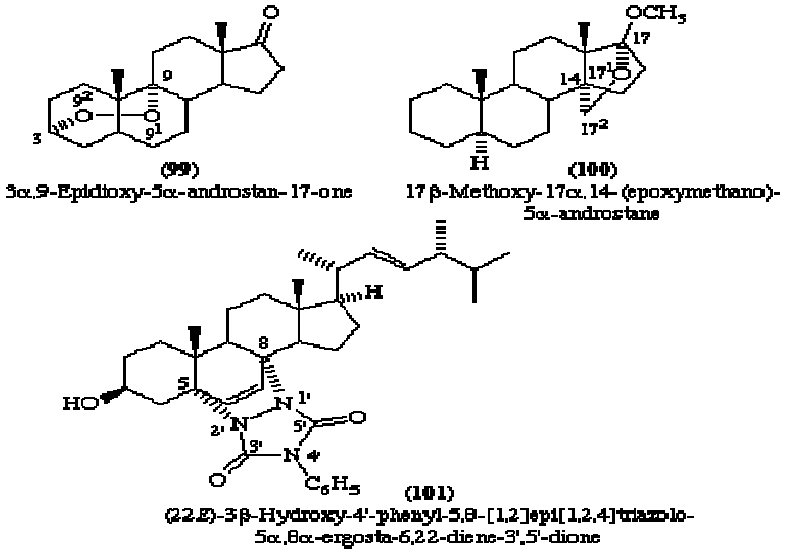
5. IUPAC-IUB Joint Commission on Biochemical Nomenclature (JCBN), Nomenclature of vitamin D. Recommendations 1981. *Arch. Biochem. Biophys.* **218**, 342-346 (1982); *Endokrinol. Inform.* 1982(2), 53-62; *Eur. J. Biochem.* **124**, 223-227 (1982); *Mol. Cell. Biochem.* **49**, 177-181 (1982); *Pure Appl. Chem.* **54**, 1511-1516 (1982).

XI. THE NOMENCLATURE OF STEROIDS RECOMMENDATIONS 1989 3S-10

A. *3S-10. Additional Rings*

1) *3S-10.0. General:* When additional rings are formed within, or on, a steroid nucleus, it is often desirable to retain the steroid stem name, since it implies the stereochemistry of most of the chiral centres. The following recommendations show how such names can be constructed. It will be seen, however, that these names may become cumbersome with more complicated - especially substituted - structures. Recourse to general systematic nomenclature may then be preferable. The decision whether any one compound shall receive such a modified steroid name or a general systematic name is left to authors and editors in the particular circumstances of each case. Moreover, the requirements of different journals or compendia are not necessarily identical.

2) *3S-10.1. Bridged steroids:* Steroids with non-adjacent ring positions linked by a bivalent bridge such as -O-O-, -$[CH_2]_n$- (see recommendations A-34 and B-15 in [3]) are named by the appropriate name and locants to indicate its attachment and α or β to indicate stereochemistry where necessary. Examples:



(99)
5α,9-Epidioxy-5α-androstan-17-one

(100)
17β-Methoxy-17α,14-(epoxymethano)-5α-androstane

(101)
(22*E*)-3β-Hydroxy-4'-phenyl-5,8-[1,2]epi[1,2,4]triazolo-5α,8α-ergosta-6,22-diene-3',5'-dione

Notes

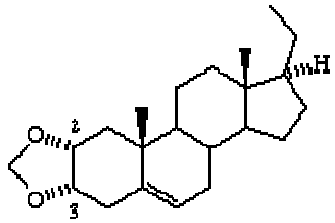
(1) In a composite bridge such as epoxymethano in compound **100** the first number of the two locants cited in front of the bridge corresponds to the first cited component of the composite bridge i.e. epoxy (recommendation B-15.2 in [3]).

(2) With linear bridges such as in compounds **99** and **100** the atoms may be labelled for identification by the superscript number starting from the higher numbered attachment position (see 3S-2.7). It is not recommended that the steroid numbering should be continued with the bridge atoms as the highest used number depends on the steroid skeleton present (recommendation A-34.2 in [3]).

(3) With a cyclic bridge, such as in compound **101**, the numbering of the ring system is retained but each number is primed if needed for identification or further substitution. The name of the bridge includes the attachment positions in front of the name.

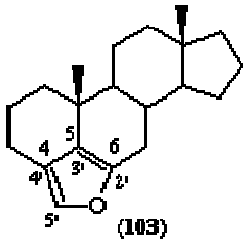
These locants and any required to name the ring are cited within square brackets without any primes (ref. 3, recommendation B-3.1). Low numbers are preferred for the attachment positions with the lower number nearer the higher numbered attachment position of the steroid.

This system should not normally be extended to adjacent positions, except for simple symmetric bridges, e.g. **102**. For other cases see 3S-10.2. Example:

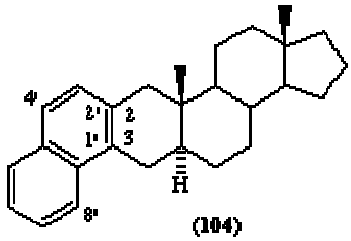


(102)
2α,3α-(Methylenedioxy)pregn-5-ene

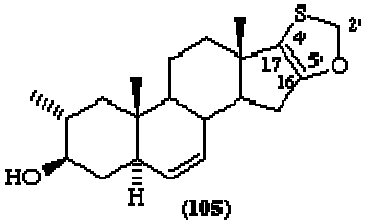
3) *3S-10.2. Additional ring(s) fused to a steroid:* Fusion of a carbocyclic or heterocyclic ring component with the maximum number of non-cumulative double bonds to a steroid may be indicated by a modification of fusion nomenclature (see recommendations A-21.3 to A-21.6, B-3.1 to B-3.3 in [3]). The preferred component is always the steroid. The name of the carbocyclic or heterocyclic attached component is modified to give its prefix form and is cited in front of the steroid name with the nature of the fusion indicated between square brackets. The numbering of the steroid moiety is retained; the atoms of the attached component are identified by primed locants. Those involved in fusion are cited in the order corresponding to those of the steroid. Examples:



(103)
Furo[4',3',2':4,5,6]androstane



(104)
Naphtho[2',1':2,3]-5α-androstane



(105)
2α-Methyl[1,3]oxathiolo[5',4':16,17]-5α-androst-6-en-3β-ol

Notes

(1) There are three changes from the previous recommendations [1], that are still used by Chemical Abstracts Service index nomenclature:

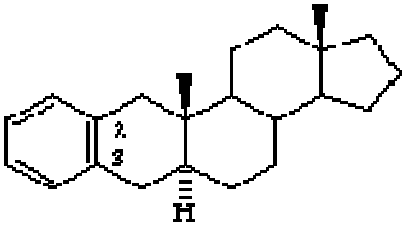
(i) the unsaturation in the steroid ring due to the fused component is not cited;

(ii) the preferred component is always the steroid;

(iii) a terminal a or o of the prefix is not elided.

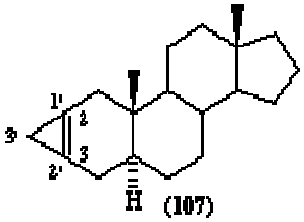
(2) The current Chemical Abstracts Service index names for **103**, **104** and **105** are androst-5-eno[6,5,4-*bc*]furan, naphth[2',1':2,3]-5α-androst-2-ene, and 2α-methyl-5α-androstα-6,16-dieno[17,16-*d*][1,3]oxathiol-β-ol respectively.

Fusion locants may be omitted if unnecessary. Example:

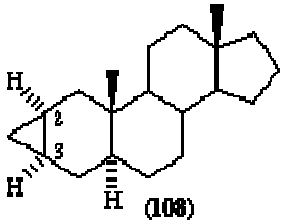


(106)
Benzo[2,3]-5α-androstane

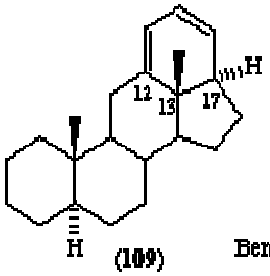
If necessary isomers are distinguished by the use of indicated hydrogen (see recommendation A-21.6 in [3]). If there is a choice of locants due to fusion the unprimed locant is used. Examples:



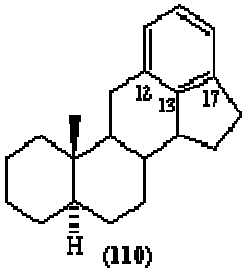
(107)
3'*H*-Cyclopropa[2,3]-5α-androstane



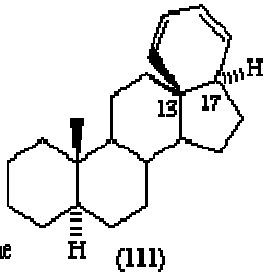
(108)
2α,3α-Dihydro-3'*H*-cyclopropa[2,3]-5α-androstane



(109)
17α*H*-Benzo[12,13,17]-5α-androstane



(110)
Benzo[12,13,17]-18-nor-5α-androstane

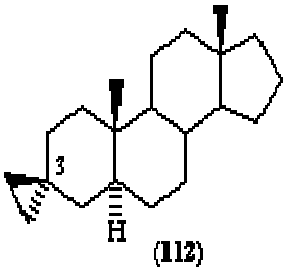


(111)
17α*H*-Benzo[13,17]-18-nor-5α-androstane

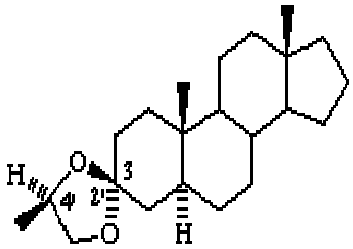
Note As shown by examples **108** and **110**, insertion of the maximum number of non-cumulative double bonds into the attached component is considered to take place after fusion.

4) 3S-10.3. Spiro Union with a Steroid: Simple spiro systems may be named in an analogous way to bridged steroids (3S-10.1). For example, compound **112** is 3,3-ethylene-5α-androstane.

In general a spiro union is cited in the normal way (see recommendations A-41.4, B-10.2 in [3]). Examples:



(112)
Spiro[5α-androstane-3,1'-cyclopropane]



(113)
(4'*R*)-4'-Methyl-(3*S*')-spiro[5α-androstane-3,2'-[1,3]dioxolane]

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[2] International Union of Biochemistry (1978) Biochemical nomenclature and related documents, The Biochemical Society, London.

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[4] A. Butenandt and L. Poschmann, Ber. Dtsch. Chem. Ges. 73, 893-897 (1940); cf. also A. Butenandt, L. Karlson-Poschmann, G. Failer, U. Schiedt and E. Bilkert, Liebigs Ann. Chem. 575, 123-144 (1951).

[5] IUPAC-IUB Joint Commission on Biochemical Nomenclature (JCBN), Nomenclature of vitamin D. Recommendations 1981. Arch. Biochem. Biophys. 218, 342-346 (1982); Endokrinol. Inform. 1982(2), 53-62; Eur. J. Biochem. 124, 223-227 (1982); Mol. Cell. Biochem. 49, 177-181 (1982); Pure Appl. Chem. 54, 1511-1516 (1982).

[6] International non-proprietary names (INN) for pharmaceutical substances, cumulative list 6, World Health Organization, 1982.

Continued in 3S appendix
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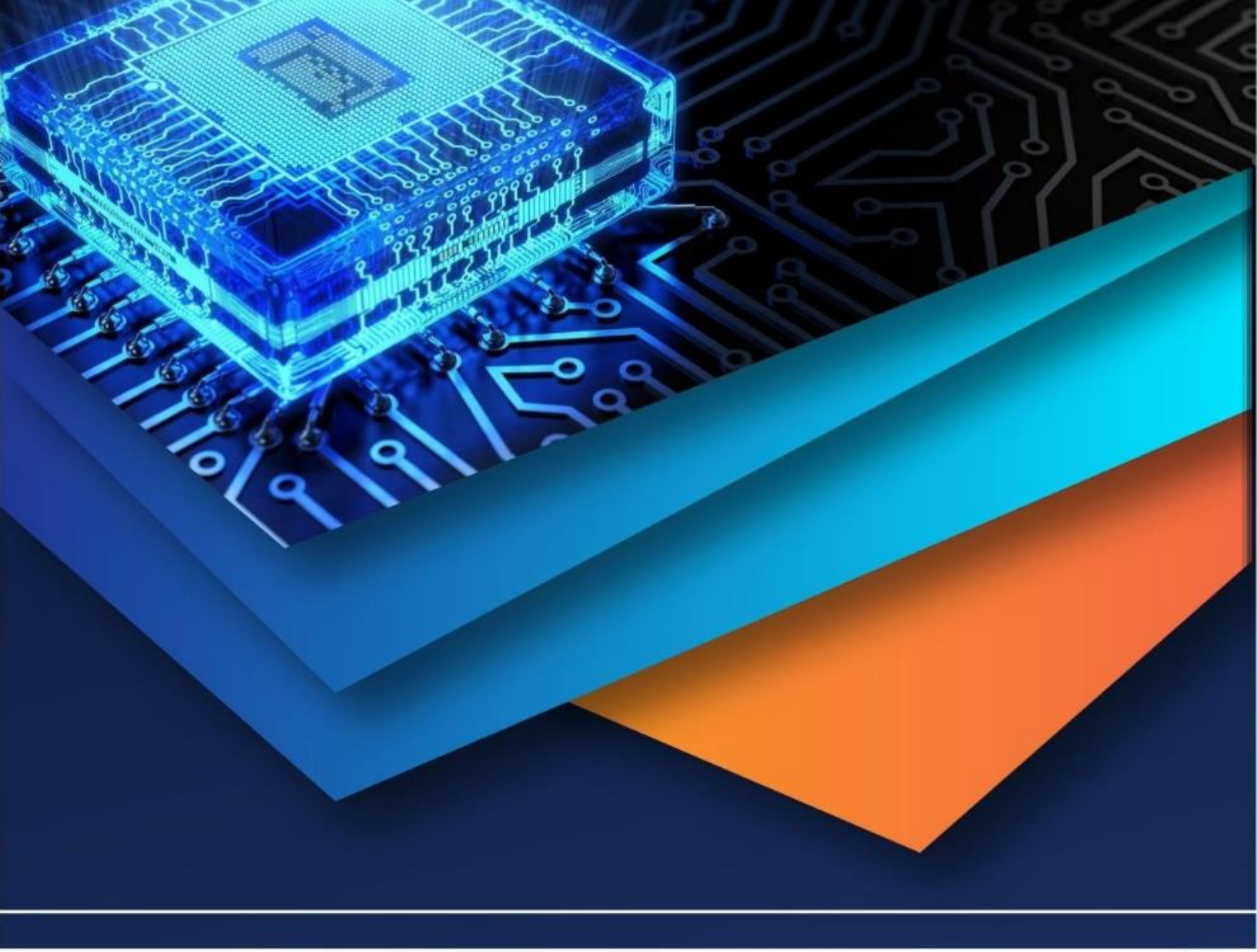

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