INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

Definitive Rules for the Nomenclature of Amino Acids, Steroids, Vitamins, and Carotenoids

By the Commission on the Nomenclature of Biological Chemistry

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Introduction

There are three stages in the development of international nomenclature rules. First, experts in each field, either as individuals or as a committee, are requested to suggest the rules for naming the compounds or concepts they are working with. These suggestions or reports then are studied carefully by the Commissions of the International Union of Pure and Applied Chemistry responsible for that field, in this case the Commission on the Nomenclature of Biological Chemistry. Because nomenclature commissions have mutual problems and sometimes overlapping responsibilities it is imperative that they consult with each other when these exist. Nomenclature in biochemistry and organic chemistry is an excellent example. This Commission wishes to express its appreciation to the Commission on the Nomenclature of Organic Chemistry for its coöperation and advice. From these deliberations and with the approval of the Council of IUPAC, the so-called tentative nomenclature rules are published. After about two years, if the tentative rules prove to be satisfactory even with modest revision, they are then declared definitive. This is the third and final stage. However, definitive rules as well as tentative rules may be revised and changed as experience dictates.

This report covers the period from 1947 to 1959, inclusive. Those who have served on the Commission are: E. Cherbuliez, J. Courtois, A. H. Ennor, D. R. Fabre, W. Grassmann, Sir Charles Harington, L. Hellerman, B. C. P. Jansen, P. Karrer, W. Klyne, K. Linderstrøm-Lang,* J. Murray Luck, G. F. Marrian, P. Pratesi, G. Quagiariello, Byron Riegel, A. Rossi-Fanelli, E. C. Slater and H. B. Vickery.

* Deceased.

DEFINITIVE RULES FOR THE NOMENCLATURE OF NATURAL AMINO ACIDS AND RELATED SUBSTANCES[1]

AA-1

The configurational relationship of the asymmetric α-carbon atom of an amino acid capable of optical isomerism should be indicated by a symbol prefixed to the name; however, if a specific statement or the context makes it clear which enantiomorph is under consideration, the symbol may be omitted.

Examples: Leucine may be named without prefix if the preparation mentioned is stated to be, or is obviously the enantiomorph derived from a protein source. Leucine may be named without prefix if the preparation mentioned is stated to be synthetic and not resolved and is therefore an equimolecular mixture of the enantiomorphs. Leucine may be named without the prefix in a general statement that is true for either enantiomorph, or for any mixture of these.

AA-2

2.1.—Distinction between the enantiomorphs of the amino acids is made by a prefixed *small capital letter* D or L to denote the configurational family to which the α-carbon atom belongs. The D and L are to be pronounced dee and ell, respectively, not *dextro* and *levo*—an additional symbol to denote the direction of the rotation (*i.e.*, a plus or minus sign enclosed in parentheses) is not necessary.

Examples: L-Leucine, D-valine, L-phenylalanine, L-threonine.

2.2.—The optically inactive mixture or racemic compound of the enantiomorphs is designated by the prefix DL in *small capital letters*.

Examples: DL-Leucine, DL-valine, DL-methionine.

AA-3

3.1.—The small capital letter prefixes D and L denote that the substance name is configurationally related to the corresponding enantiomorph of glyceraldehyde. Where confusion is possible between the use of the capital letter prefix for the configuration of the α-carbon atom in amino acid nomenclature and for that of the highest numbered asymmetric carbon atom in carbohydrate nomenclature, a subscript is added to the small capital letter prefix. Where the prefix is used in the amino

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(1) *Chem. Eng. News*, **30**, 4522-6 (1952); *Biochem. J.*, **42**, 1 (1948); **52**, 1-2 (1952); *J. Biol. Chem.*, **169**, 237-245 (1947).

acid sense, the subscript s is added; where the prefix is used in the carbohydrate sense, the subscript g is added. These subscripts (lower case roman letters) refer, respectively, to serine, the fundamental substance to which amino acids that bear structural resemblance to the carbohydrates can be formally related, and to glyceraldehyde, the fundamental substance to which the configuration of the carbohydrates is formally related.

Examples: L$_s$-Threonine for which the synonym in carbohydrate nomenclature is 2-amino-2,4-dideoxy-D$_g$-threonine, D$_s$-threonine for which the synonym is 2-amino-2,4-dideoxy-L$_g$-threonic acid, L$_s$-allothreonine for which the synonym is 2-amino-2,4-dideoxy-L$_g$-erythronic acid, D$_s$-allothreonine for which the synonym is 2-amino-2,4-dideoxy-D$_g$-erythronic acid.

3.2.—Amino acids derived from amino sugars generally should be named in conformity with carbohydrate nomenclature but with the use of the subscript.

Examples: D$_g$-Glucosaminic acid for 2-amino-2-deoxy-D$_g$-gluconic acid, the α-carbon atom of which has the configuration of that in D-serine; D$_g$-mannosaminic acid for 2-amino-2-deoxy-D$_g$-mannonic acid, the α-carbon atom of which has the configuration of that in L-serine.

AA-4

Where the configurational relationship of the α-carbon atom has not been established definitively, or where it is desired to emphasize the actual direction of the rotation of an enantiomorph of known configuration, the direction of the rotation in a specified solvent, preferably of the free amino acid in water, is designated by the prefixes *dextro* or *levo* in *lower case italic letters* or alternatively by a plus or minus sign enclosed in parentheses.

Examples: *dextro*-Hydroxytryptophan, (+)-hydroxytryptophan; (+)-glutamic acid or *dextro*-glutamic acid for dextrorotatory (in water) L-glutamic acid.

AA-5

The prefix *meso* or its abbreviation *ms* in lower case italic letters is used to denote those amino acids and derivatives of amino acids that are optically inactive because of internal compensation.

Examples: *meso*-Lanthionine, *ms*-cystine.

AA-6

6.1.—Where the amino acid has two centers of asymmetry so constituted that internal compensation cannot occur, two diastereomeric forms are possible both of which possess the L$_s$ configuration at the α-carbon atom; of these forms the *first to be described* is designated the L-amino acid and its enantiomorph is designated the D-amino acid. Where the name contains one or more prefixes denoting substitution, the L- or D- is, in accordance with Rule **AA-7**, placed immediately before the part of the name (usually the trivial name of the parent amino acid) which signifies an asymmetric configuration around the α-carbon atom.

Examples: L-Threonine, L-isoleucine, for the amino acids of protein origin which have trivial names; D-threonine, D-isoleucine for their enantiomorphs. Where there is a prefix denoting substitution, the names take the form hydroxy-L-proline, hydroxy-DL-glutamic acid, 5-hydroxy-L-lysine.

6.2.—The other diastereomer which possesses the L$_s$ configuration at the α-carbon atom is distinguished by the prefix allo in addition to the prefix L. Its enantiomorph is denoted by the prefix allo and the prefix D. Where the name is wholly trivial, the L or D is placed before the prefix allo, which is, in turn, attached to the parent name; but in names which contain one or more prefixes denoting substitution, the allo is placed before this prefix and the L- or D- is placed as stated in section **AA-6.1.**

Examples: L-Allothreonine, D-allothreonine, L-alloisoleucine, D-alloisoleucine for the pairs of enantiomorphs of the diastereomers of the amino acids of protein origin which have trivial names; allohydroxy-L-proline, allohydroxy-D-proline, allohydroxy-L-lysine, allohydroxy-D-lysine, and similarly for the enantiomorph of the diastereomers named as derivatives of amino acids which have trivial names. Where the position of the substituent group is designated, the names take the form allo-4-hydroxy-L-proline, allo-5-hydroxy-L-lysine. Systematic names take the form allo-3-hydroxy-L-2-aminobutyric acid (for L-allothreonine), allo-4-hydroxy-L-2-pyrrolidinecarboxylic acid (for allohydroxy-L-proline).

6.3.—For diastereomeric α-amino acids which have structures not encountered in nature but which are named as derivatives of naturally occurring amino acids with trivial names, choice between the prefixes L and D is made, (1) from the results of direct correlation with substances of known configuration, or, (2) tentatively, from the results of studies of biological properties, or of the change in optical rotation with change in the conditions of observation, or both. The assignment of the prefix allo to the pair of enantiomorphs of one of the diastereomers is made tentatively, if possible, in accordance with the principle in section **AA-6.1.** The prefixes are placed as stated in section **AA-6.1.**

Examples: Of the four theoretically possible optically active isomers of hydroxyaspartic acid, two should yield L-aspartic acid on reduction and are accordingly hydroxy-L-aspartic acid and allohydroxy-L-aspartic acid, the choice of these designations being made tentatively as specified. The respective enantiomorphs are named with the prefix D.

AA-7

Salts and derivatives of amino acids including peptides are designated with the use of a *small capital letter* to denote the configurational family of the α-carbon atom or atoms, this letter being placed immediately before the name of the parent acid or its radical. The customary rules of nomenclature otherwise are observed.

Examples: L-Histidine monohydrochloride monohydrate, copper L-aspartate, D-ornithine dihydrochloride, acetyl-L-tryptophan, diethyl D-glutamate, 3-hydroxy-DL-glutamic acid, L-leucyl-L-valine, glycyl-DL-leucine. Names in which prefixes involve amino acid configurations are treated similarly; thus, *S*-(D-2-amino-2-carboxyethyl)-D-homocysteine for D-cystathionine.

Where the name contains one or more prefixes denoting substitution and where specification both of configuration and of position of substitution is required, this rule should be applied, the form taken being as in the names of these naturally occurring substances: 3-phenyl-L-alanine, 4-hydroxy-L-proline, 3,5-diiodo-L-tyrosine, 3,5-dibromo-L-tyrosine, 5-hydroxy-L-lysine. However, in general biochemical writing the names of these four substances, the position of substitution of which is well understood, are admissible as exceptions: L-phenylalanine, L-hydroxyproline, L-diiodotyrosine, and L-hydroxylysine.

AA-8

Where a trivial name is applied to a compound that contains two α-amino carboxylic acid groupings attached to dissimilar carbon chains, the configurational designation is that of the α-carbon atom of the smaller of the two chains.

Examples: D-cystathionine for *S*-(D-2-amino-2-carboxyethyl)-D-homocysteine, L-allocystathionine for *S*-(L-2-amino-2-carboxyethyl)-D-homocysteine.

However, the introduction of new trivial names should be avoided in the absence of compelling reasons.

AA-9

The word inactive or the prefix (±) shall be used for inactive amino acids and their derivatives when two or more asymmetric centers are present but the steric cause of the inactivity is unknown and for the inactive form of an amino acid of which an active form of uncertain configurational relationship has been described.

Examples: Inactive 3-hydroxyglutamic acid, (±)-hydroxytryptophan.

AA-10

Amino acid radicals shall be named in conformity with the Definitive Report of the Commission on the Nomenclature of Organic Chemistry.[1]

AMINO ACID RADICALS

Amino Acid	Radical Name	Formula
Alanine	Alanyl	$\mathrm{CH_3CH(NH_2)CO}$—
Arginine	Arginyl	$\mathrm{H_2NC(:NH)NH(CH_2)_3CH(NH_2)CO}$—
Asparagine	Asparaginyl	$\mathrm{H_2NCOCH_2CH(NH_2)CO}$—
Aspartic acid	Aspartoyl	—$\mathrm{COCH_2CH(NH_2)CO}$—
Aspartic acid	Aspartyl[a]	$\mathrm{HOOCCH_2CH(NH_2)CO}$—
Cysteine	Cysteinyl	$\mathrm{HSCH_2CH(NH_2)CO}$—
Cystine	Cystyl	—$\mathrm{COCH(NH_2)CH_2SSCH_2CH(NH_2)CO}$—
Glutamine	Glutaminyl	$\mathrm{H_2NCOCH_2CH_2CH(NH_2)CO}$—
Glutamic acid	Glutamoyl	—$\mathrm{COCH_2CH_2CH(NH_2)CO}$—
Glutamic acid	Glutamyl[b]	$\mathrm{HOOCCH_2CH_2CH(NH_2)CO}$—
Glycine	Glycyl	$\mathrm{H_2NCH_2CO}$—
Histidine	Histidyl	$\mathrm{N_2C_3H_3CH_2CH(NH_2)CO}$—
Isoleucine	Isoleucyl	$\mathrm{CH_3CH_2CH(CH_3)CH(NH_2)CO}$—
Leucine	Leucyl	$\mathrm{(CH_3)_2CHCH_2CH(NH_2)CO}$—
Lysine	Lysyl	$\mathrm{H_2N(CH_2)_4CH(NH_2)CO}$—
Methionine	Methionyl	$\mathrm{CH_3SCH_2CH_2CH(NH_2)CO}$—
Norleucine	Norleucyl	$\mathrm{CH_3(CH_2)_3CH(NH_2)CO}$—
Ornithine	Ornithyl	$\mathrm{H_2NCH_2(CH_2)_2CH(NH_2)CO}$—
Proline	Prolyl	$\mathrm{\overline{NH.CH_2.CH_2.CH_2.C}HCO}$—
Serine	Seryl	$\mathrm{HOCH_2CH(NH_2)CO}$—
Taurine	Tauryl	$\mathrm{H_2NCH_2CH_2SO_2}$—
Threonine	Threonyl	$\mathrm{CH_3CH(OH)CH(NH_2)CO}$—
Thyronine	Thyronyl	p-(p-$\mathrm{HOC_6H_4O)C_6H_4CH_2CH(NH_2)CO}$—
Tryptophan	Tryptophyl	$\mathrm{C_8H_6NCH_2CH(NH_2)CO}$—
Tyrosine	Tyrosyl	p-$\mathrm{HOC_6H_4CH_2CH(NH_2)CO}$—
Valine	Valyl	$\mathrm{(CH_3)_2CHCH(NH_2)CO}$—

[a] *Chemical Abstracts* uses α-aspartyl for $\mathrm{HOOCCH_2CH(NH_2)CO}$— and β-aspartyl for $\mathrm{HOOCCH(NH_2)CH_2CO}$—.
[b] *Chemical Abstracts* uses α-glutamyl for $\mathrm{HOOCCH_2CH_2CH(NH)_2CO}$— and γ-glutamyl for $\mathrm{HOOCCH(NH_2)CH_2CH_2CO}$—.

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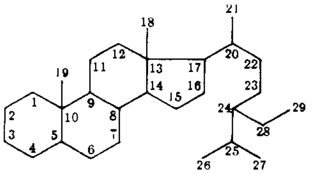
(1) *IUPAC Camptes rendus*, 15th Conference (Amsterdam, 1949) pp. 124-5.

DEFINITIVE RULES FOR NOMENCLATURE OF STEROIDS

S-1

Steroids shall be numbered as in formula (I). If one or more of the carbon atoms shown in (I) is not present and a steroid name is used, the numbering of the remainder shall remain undisturbed.



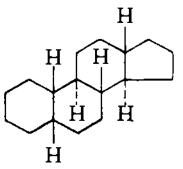
(I)

S-2

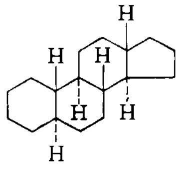
All names shall connote a specific stereochemical configuration wherever possible. The methyl group at position 10 lies in front of the general plane of the tetracyclic system (*i.e.*, above the plane of the paper) when the molecule is oriented as in formula (I). In formulas, a dotted or broken line is used to denote the α-configuration for the attachment of atoms or groups to the nucleus, *i.e.*, the atom or group lies behind the general plane of the ring system. A solid line denotes the β-configuration where the atom or group lies in front of the plane. When the configuration at one or more centers is unknown, this shall be indicated by means of the Greek letter(s) ξ (xi) prefixed by the appropriate numeral(s) and in formulas by wavy lines (see examples under Rule **S-3.4**).

S-3

3.1.—The parent hydrocarbon without methyl groups at C–10 and C–13 shall be named "gonane."

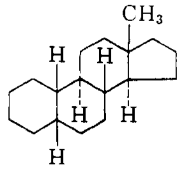


5β-Gonane

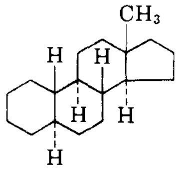


5α-Gonane

3.2.—The hydrocarbon with a methyl group at C-13 shall be named "estrane."

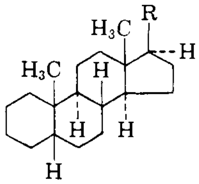


5β-Estrane

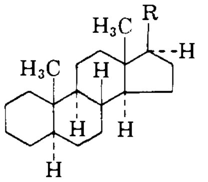


5α-Estrane

3.3.—These names shall be used for the hydrocarbons (II) and (III).



(II)

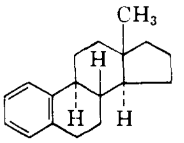


(III)

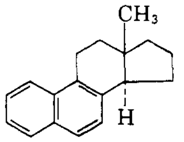
R	5β-Series	5α-Series
H	5β-Androstane	5α-Androstane
C_2H_5	5β-Pregnane	5α-Pregnane
$CH(CH_3)CH_2CH_2CH_3$	5β-Cholane	5α-Cholane
$CH(CH_3)CH_2CH_2CH_2$-$CH(CH_3)_2$	5β-Cholestane	5α-Cholestane

3.4.—Names for partly unsaturated or aromatic steroids are derived from the names of the saturated compounds by means of the systematic terminations denoting unsaturation, namely, "-ene" and "-yne."

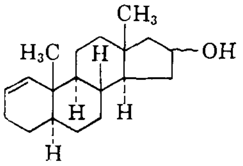
Examples:



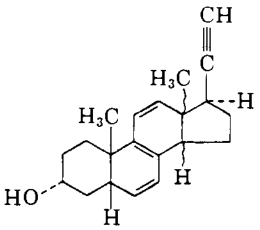
Estra-1,3,5(10)-triene



Estra-1,3,5(10),6,8-pentaene

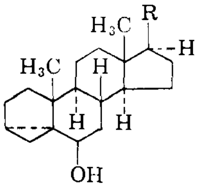


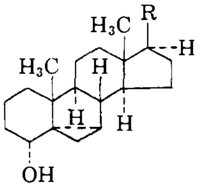
5α-Androst-1-en-16ξ-ol



5β,13ξ,14ξ-Pregna-6,8,11-trien-20-yn-3α-ol

3.5.—Names of steroids containing a three-membered ring within the nuclear structure shall be prefixed by "cyclo-" with the appropriate numerals and necessary stereochemical designations. The generic name shall be "cyclosteroids."





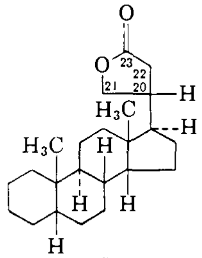
R = $CH(CH_3)CH_2CH_2CH_2CH(CH_3)_2$

3α,5-Cyclo-5α-cholestan-6β-ol

5,7α-Cyclo-5α-cholestan-4α-ol

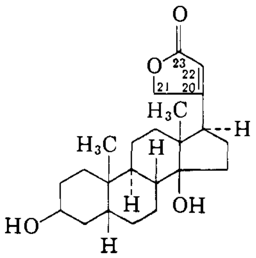
3.6.—(a) The name "cardanolide" shall be used for the fully saturated system (IV) of digitaloid lactones in which the configuration at C-20 is the same as in cholesterol (see examples to Rule **S-5.1**), *i.e.*, as shown in the Fischer projection of C-20 in (IV). (b) Names such as card-20(22)-enolide shall be used for the naturally occurring unsaturated lactones of this type. (c) The names "14,21-" and "16,21-epoxycardanolide" shall be used for the compounds containing a 14,21- and 16,21-oxygen bridge, respectively.

Examples:

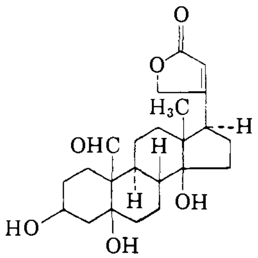


(IV)

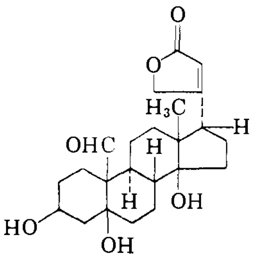
5β-Cardanolide



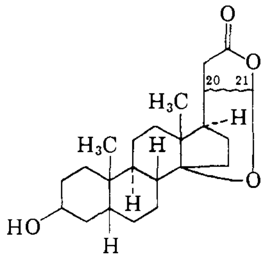
3β,14-Dihydroxy-5β-card-20(22)-enolide = Digitoxigenin*



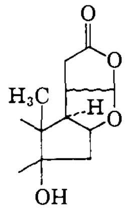
3β,5,14-Trihydroxy-19-oxo-5β-card-20(22)-enolide = Strophanthidin*



3β,5,14-Trihydroxy-19-oxo-5β,17α-card-20(22)-enolide = 17α-Strophanthidin* (also, "allostrophanthidin"†)



3β-Hydroxy-14,21-epoxy-5β,20ξ-cardanolide = "Isodigitoxigenin"(†)



16β,21-Epoxy-20ξ-cardanolide

3.7.—(a) The name "bufanolide" shall be used for the fully saturated system (V) of the squill-toad poison group of lactones, in which the configuration at C-20 is the same as in cholesterol (see examples to Rule **S-5.1**), *i.e.*, as shown in the Fischer projection of C-20 in (V). (b) Unsaturated deriva-

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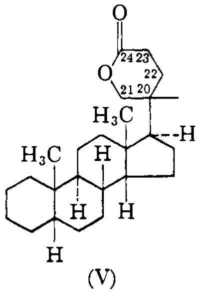
* Denotes a trivial name; the systematic name is preferred.

† "Quotation marks" denote formerly used trivial names now considered unacceptable.

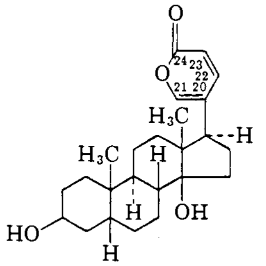
tives are named by replacing the suffix anolide by enolide, adienolide, *etc.*, thus, the name bufa-20,22-dienolide shall be used for the naturally occurring doubly unsaturated lactones.

Examples:

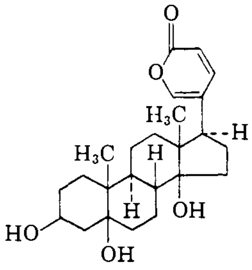


(V)

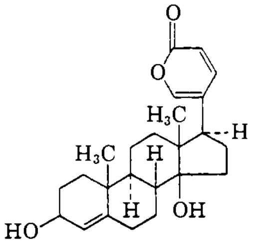
5β-Bufanolide



3β,14-Dihydroxy-5β-bufa-20,22-dienolide = Bufalin*



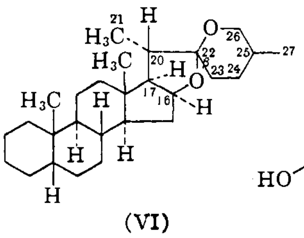
3β,5,14-Trihydroxy-5β-bufa-20,22-dienolide = Telocinobufagin*



3β,14-Dihydroxybufa-4,20,22-trienolide = Scillarenin*

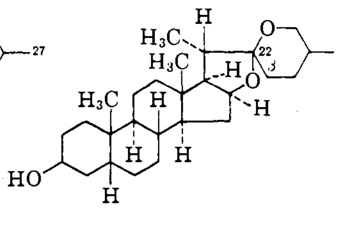
3.8.—(a) The name spirostan shall be used for the substance of structure (VI), in which the configurations at C-17 and C-20 are the same as in cholesterol, and that at C-16 is the same as that in sarsasapogenin, *i.e.*, α-H at position 17, α-CH_3 at position 20, and α-H at position 16. (b) In formulas configurations at positions 16, 17 and 20 shall be shown by dotted or solid lines in accordance with Rule **S-2.** (c) The configuration at C-22 shall be specified as α or β, this letter referring to the direction of the bond joining C-22 to C-23. (Note.—Pending further work, no rule is yet proposed for designation of asymmetry at position 25, though it should be noted that α and β cannot be used with reference to this position.)

Examples:



(VI)

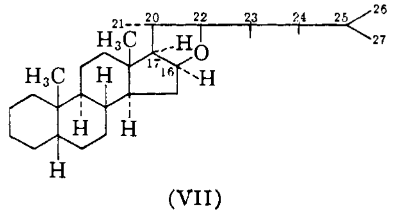
5β,22β-Spirostan



5β,22β-Spirostan-3β-ol = Sarsasapogenin*

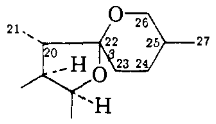
3.9.—(a) The name furostan shall be used for the substance of structure (VII), in which the configurations at C-17 and C-20 are the same as in cholesterol, *i.e.*, α-H at position 17, α-CH_3 at position 20, and α-H at position 16 according to Rule **S-2.** (b) In formulas configuration at positions 16, 17 and 20 shall be shown by dotted or solid lines in accordance with Rule **S-2.** (c) The configuration at C-22 shall be specified as α or β, this letter referring to the direction of the bond joining C-22 to C-23. (Note.—Pending further work, no rule is yet proposed for designation of asymmetry at position 25, though it should be noted that α and β cannot be used with reference to this position.)

Examples:

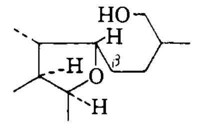


(VII)

5β-Furostan

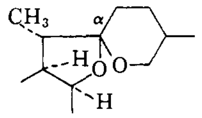


$\xrightarrow{2H}$

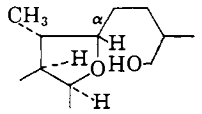


5β,22β-Spirostan-3β-ol = Sarsasapogenin*

5β,22β-Furostan-3β,26-diol = Dihydrosarsasapogenin*

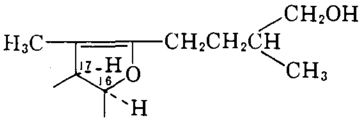


$\xrightarrow{2H}$



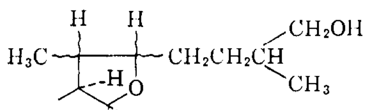
5α,22α-Spirostan-3β-ol = Tigogenin*

5α,22α-Furostan-3β,26-diol = Dihydrotigogenin*

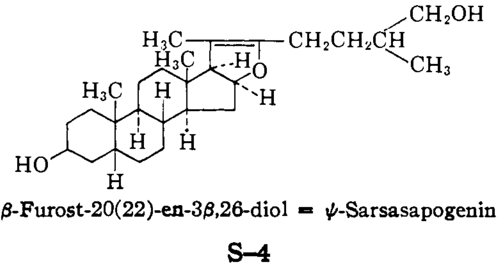


$\xrightarrow{2H}$

5α-Furost-20(22)-en-3β,26-diol = ψ-Tigogenin*



5α,20ξ,22ξ-Furostan-3β,26-diol = Dihydro-ψ-tigogenin*



5β-Furost-20(22)-en-3β,26-diol = ψ-Sarsasapogenin*

S-4

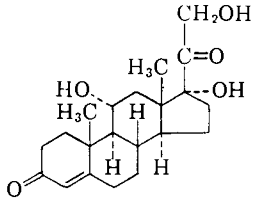
4.1.—These trivial names for steroid hormones and closely related compounds are retained: estrone, aldosterone, 17β-estradiol, 17α-estradiol,

---

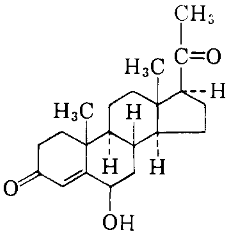
* Denotes a trivial name; the systematic name is preferred.

estriol, androsterone, testosterone, progesterone, corticosterone, deoxycorticosterone (for the 11-deoxy compound), cortisone (for the free 17,21-diol) and cortisol (for the 11β-hydroxy derivative corresponding to cortisone). If the trivial names given in this rule are used in a manuscript, the systematic name for each compound should be given at least once. These trivial names may not be used as a basis for the naming of derivatives or stereoisomers.

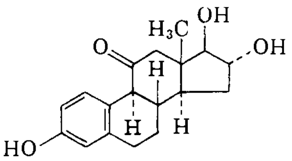
Examples:



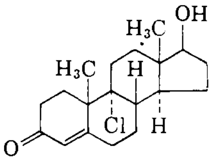
11α,17,21-Trihydroxypregn-4-ene-3,20-dione (preferred) = Epicortisol



6β-Hydroxypregn-4-ene-3,20-dione

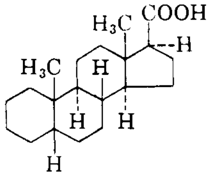


3,16α,17β-Trihydroxyestra-1,3,5(10)-trien-11-one



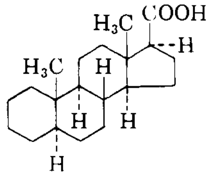
9-Chloro-17β-hydroxyandrost-4-en-3-one

4.2.—As alternatives to the preferred systematic names, the compounds (VIII) and (IX) may be called 5β-etianic acid and 5α-etianic acid, respectively.



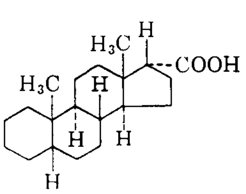
(VIII)

5β-Androstane-17β-carboxylic acid (systematic) or 5β-Etianic acid (trivial)

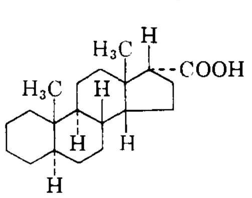


(IX)

5α-Androstane-17β-carboxylic acid (systematic) or 5α-Etianic acid (trivial)



5β-Androstane-17α-carboxylic acid (systematic) or 5β,17α-Etianic acid (trivial)

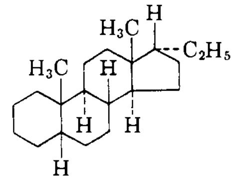


5α,14β-Androstane-17α-carboxylic acid (systematic) or 5α,14β,17α-Etianic acid (trivial)

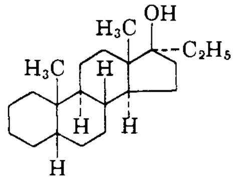
S-5

5.1.—Inversion of configuration at a ring junction and/or at position 17 of a steroid of accepted name shall be denoted by the prefix(es) α and β (see Rule S-2). The prefix(es) shall be preceded by the numeral(s) denoting the position of the carbon atom(s) at which inversion has occurred.

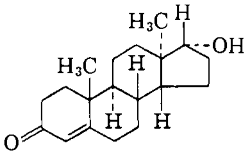
Examples:



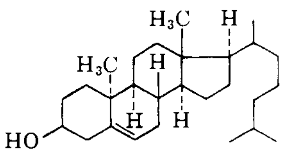
5β,17α-Pregnane



5β,17α-Pregnan-17-ol



17α-Hydroxy-13α,14β-androst-4-en-3-one

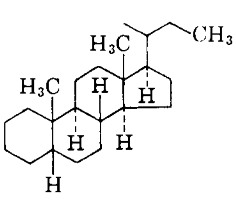


10α-Cholesterol = 10α-Cholest-5-en-3β-ol

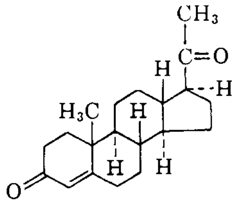
S-6

(a) Elimination of a methylene group from an alkyl group shall be indicated by the prefix "nor-." (b) The prefix "nor-" in all cases shall be preceded by the number of the carbon atom which disappears. (c) In cases of doubt the number attached to "nor" shall be the highest permissible.

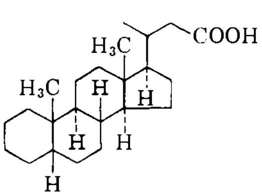
Examples:



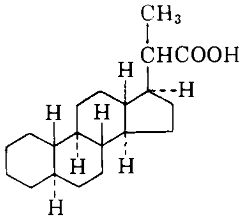
24-Nor-5β-cholane



18-Norpregn-4-ene-3,20-dione = 18-Norprogesterone



23-Nor-5β-cholanoic acid

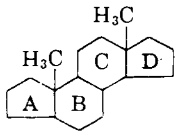


18,19-Dinor-5α-pregnane-20-carboxylic acid

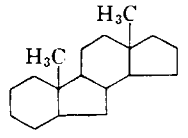
S-7

7.1.—Ring contraction and ring enlargement may be indicated by prefixes "nor-" and "homo-," respectively, preceded by a capital letter indicating the ring affected.

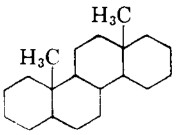
Examples:



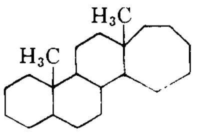
A-Nor



B-Nor



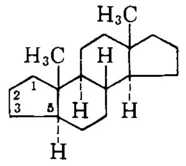
D-Homo



D-Dihomo

7.2.—On ring contraction the original steroid numbering is retained, and only the highest number(s) of the contracted ring, exclusive of ring junctions, is deleted.

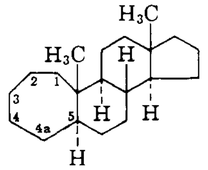
Example:



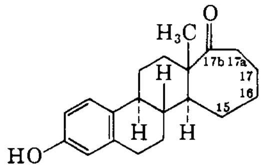
A-Nor-5α-androstane

7.3.—On ring expansion, the letter a (and b, *etc.*, as necessary) is added to the highest number in the ring enlarged, exclusive of ring junctions, and this letter and number are assigned to the last peripheral carbon atom in the order of numbering of the ring affected.

Examples:



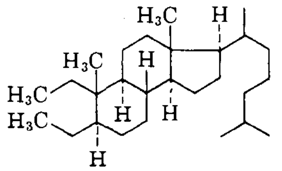
A-Homo-5α-androstane



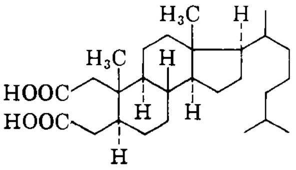
3-Hydroxy-D-dihomoestra-1,3,5(10)-trien-17b-one = D-Dihomoestrone

7.4.—Ring fission, with addition of a hydrogen atom at each terminal group thus created, is indicated by the prefix "seco," the original steroid numbering being retained.

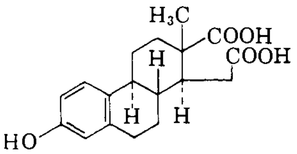
Examples:



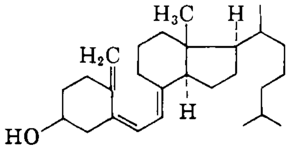
2,3-Seco-5α-cholestane



2,3-Seco-5α-cholestane-2,3-dioic acid



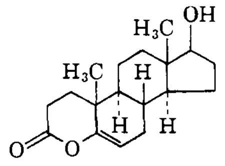
3-Hydroxy-16,17-secoestra-1,3,5(10)-triene-16,17-dioic acid = marrianolic acid*



9,10-Secocholesta-5,7,10(19)-trien-3β-ol = cholecalciferol

7.5.—If hetero atoms occur in the ring system of a steroid the "oxa-aza" system of nomenclature shall be used with steroid names and numbering.

Example:



17β-Hydroxy-4-oxaandrost-5-en-3-one

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* Denotes a trivial name; the systematic name is preferred.

DEFINITIVE RULES FOR THE NOMENCLATURE OF THE VITAMINS

V-1

1.1.—The pure substance hitherto known as vitamin A_1 or axerophthol shall be designated retinol.

1.2.—The pure substance hitherto known as retinene shall be designated retinal.

1.3.—The pure substance hitherto known as vitamin A acid shall be designated retinoic acid.

1.4.—The pure substance hitherto known as vitamin A_2 shall be designated 3-dehydroretinol or dehydroretinol.

1.5.—The pure substance hitherto known as retinene-2 shall be designated 3-dehydroretinal or dehydroretinal.

V-2

2.1.—The pure substance hitherto known as vitamin D_2 or calciferol shall be designated ergocalciferol.

2.2.—The pure substance hitherto known as vitamin D_3 shall be designated cholecalciferol.

These names have the advantage of permitting other D vitamins, derived from 7-dehydrosterols, to be named by analogy through use of the appropriate prefix.

V-3

The pure substances hitherto known as the vitamins E shall be designated α-tocopherol, β-tocopherol and γ-tocopherol.

V-4

4.1.—When 2-methyl-3-phytyl-1,4-naphthoquinone is designated by a trivial name, *e.g.*, in biochemical papers, that name shall be phylloquinone.

4.2.—When 2-difarnesyl-3-methyl-1,4-naphthoquinone is designated by a trivial name, *e.g.*, in biochemical papers, that name shall be farnoquinone.

V-5

The substance hitherto known as vitamin B_1, aneurin(e), or thiamine shall be designated thiamine.

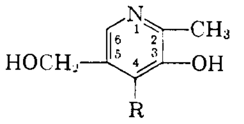
V-6

The substance hitherto known as vitamin B_2 or riboflavin shall be designated riboflavine.

V-7

The term pyridoxine may be used as a group name to designate the naturally occurring pyridine derivatives with vitamin B_6 activity.

Derivatives of 3-hydroxy-5-(hydroxymethyl)-2,4-dimethylpyridine in which one of the functional groups designated below is attached to, or replaces, the 4-methyl group shall be named: pyridoxol (CH_2OH at position 4); pyridoxal (CHO at position 4); pyridoxamine (CH_2NH_2 at position 4).



R = CH_2OH pyridoxol
R = CHO pyridoxal
R = CH_2NH_2 pyridoxamine

V-8

The pure substance hitherto known as vitamin PP, niacinamide or nicotinamide shall be designated nicotinamide.

V-9

The vitamin hitherto known as pantothenic acid shall continue to be so designated.

V-10

The vitamin hitherto known as biotin shall continue to be so designated.

V-11

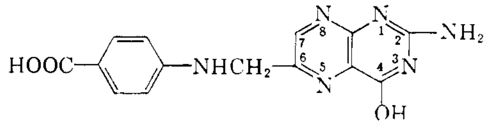
Until the nomenclature of the cyclohexitols is codified, the substance usually designated mesoinositol should continue to be called mesoinositol (or *meso*-inositol).

V-12

The vitamin hitherto known as *p*-aminobenzoic acid shall continue to be so designated.

V-13

13.1.—The name pteroic acid shall designate the compound formed by linkage of C-6 of 2-amino-4-hydroxypteridine by means of a methylene group with the nitrogen atom of *p*-aminobenzoic acid.



13.2.—The pteroylglutamic acids may be designated generically as folic acids.

13.3.—The pure substance hitherto known as folic acid, folacine or vitamin B_c shall be named pteroylmonoglutamic acid.

13.4.—Compounds analogous to pteroylmonoglutamic acid but containing several glutamic acid residues united by amide linkages may be named pteroyltriglutamic acid, pteroylheptaglutamic acid, etc.

V-14

The vitamin hitherto known as choline shall continue to be so designated.

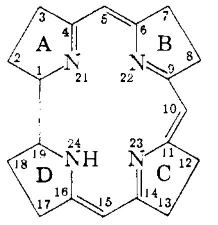
V-15

15.1.—In the vitamin B_{12} field these trivial names are used for the compounds and ions formulated:

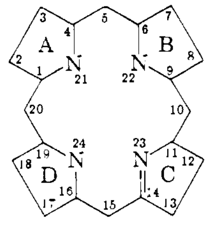
(I)	corrin	(IIIb)	cobinamide
(II)	cobyrinic acid	(IVa)	cobamic acid
(IIIa)	cobinic acid	(IVb)	cobamide

The generic name for compounds of this series containing the corrin nucleus is "corrinoids."

15.2.—The corrin nucleus and its derivatives in this field are numbered as in (I).



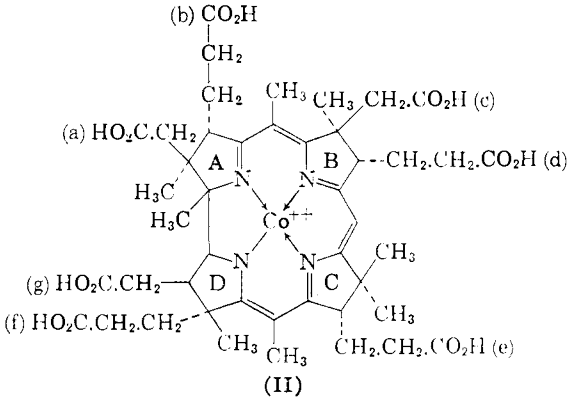
Corrin (I)



Porphyrin nucleus

The number 20 is omitted in the corrin nucleus so that the numbering system will correspond to that for the porphyrin nucleus.

15.3.—The terminal carboxyl groups or modified carboxyl groups in substances of type (II), (III), and (IV) are designated by letters *a* to *g* as shown in (II).

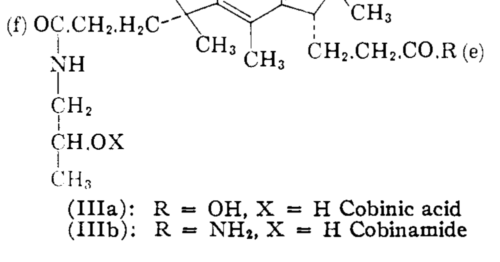


(II)
Cobyrinic acid

15.4.—For nucleotides of this series the name of the additional heterocyclic radical, ending in -yl, is prefixed to the name of the appropriate ion mentioned in Rule **V-15.1**.

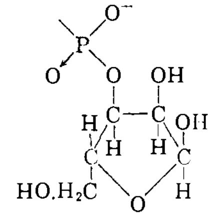
Examples:

α-(5,6-dimethylbenzimidazolyl)cobamide cyanide (Vitamin B_{12})
α-(2-methyladenyl)cobamide cyanide (Factor A)
α-(5-hydroxybenzimidazolyl)cobamide cyanide (Vitamin B_{12} III)



(IIIa): R = OH, X = H Cobinic acid
(IIIb): R = NH_2, X = H Cobinamide

(IVa): R = OH, X =



Cobamic acid

(IVb): R = NH_2, X as above Cobamide

15.5.—For molecules formed from the ions named in Rule **V-15.1,** the ligand attached to the metal is named by a method used in inorganic chemistry and not by a prefix which would denote substitution in the organic part of the molecule.

Examples:

cobamic acid dichloride
dinitritocobamic acid
α-(5,6-dimethylbenzimidazolyl)aquocobamide (Vitamin B_{12b})

15.6.—When in compounds of Type (II), (III), or (IV) the cobalt atom is replaced by that of another metal, the syllable co- is replaced by the name of the other metal followed by "o" or "i" according to the valence. When the cobalt is replaced by hydrogen, the prefix "hydrogeno" replaces "co."

Examples:

ferrobamic acid
nickelibamic acid
hydrogenobamic acid

15.7.—Other derivatives are named systematically from the largest of the compounds (I)–(IV) which is contained in that derivative.

Examples:

cobyrinic *abcdeg*-hexaamide *f*-2-hydroxyethylamide
3,8,13,17 - tetraethyl - 1,2,2,5,7,7,12,12,15,17,18-undecamethylcobalticorrin dichloride (for the dichloride of fully decarboxylated cobyrinic acid)
12,1′-carboxycobyrinic acid (for cobyrinic acid in which one of the 12-methyl groups has been replaced by CH_2CO_2H)

15.8.—Cyanocobalamin is a permissive name for vitamin B_{12}, aquocobalamin for vitamin B_{12b} and nitritocobalamin for vitamin B_{12c}; however, the term cobalamin should not be used in any other sense.

V-16

The pure substance hitherto known as vitamin C or ascorbic acid shall be designated ascorbic acid.

DEFINITIVE RULES FOR NOMENCLATURE OF CAROTENOIDS[1]

C-1

The carotenoids are chemical compounds of aliphatic or aliphatic-alicyclic structure, composed of partly dehydrogenated isoprene groups (from 3 or 4 to 8 or more).

These groups are formed into a chain in such a way that the alternate single and double bonds (conjugated double bonds) form the chromophoric system; this occurs in such a way that, in most of the carotenoids, two methyl side chains situated at the center or near the center of the molecule are separated by six carbon atoms, the other methyl groups being separated by five carbon atoms.

C-2

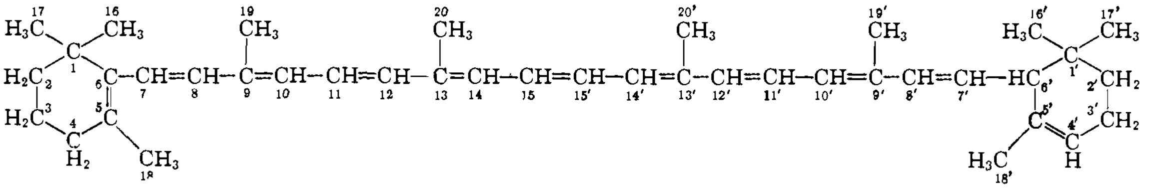
"Carotene" is the name of the group of carotenoid hydrocarbons. Substitution products of carotenes are named "derivatives of carotenes."

C-3

A new carotene shall be characterized by the word "carotene" preceded either by a Greek letter or by a prefix derived from the name of the source of the substance in question.

C-4

The carotene molecule is considered as composed of two similar parts; the corresponding carbon atoms of the two parts shall receive the same numbers, one set with and one set without "primes." The numbering shall take place according to the principle indicated in the example



If the carotene molecule is asymmetric, these rules should be observed:

The molecule contains:	Numbers not primed:
The β-ionone and the α-ionone ring........	β-Ionone ring
The β-ionone ring and the end of the chain open..............................	β-Ionone ring
The α-ionone ring and the end of the chain open..............................	α-Ionone ring

C-5

The carotenoid alcohols, ketones, aldehydes, and acids are characterized by the suffixes "-ol," "-one," "-al," and "-oic," or by prefixes "hydroxy-," "oxo-," "aldo," and "carboxy," all following as closely as possible the rules of the Definitive Report of the Commission on Nomenclature of Organic Chemistry.

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(1) *IUPAC Comptes rendus*, 14th Conference (London, 1947), pp. 142–3; 16th Conference (New York, 1951), p. 110. These rules shall be known as Carotenoid Rule 1, etc.

C-6

The name "lutein" is that which should preferably be used to designate dihydroxy-α-carotene, the principal dihydroxycarotene of leaves.

The name "xanthophyll" is a group name suitable and acceptable for naturally occurring carotene derivatives which are soluble in alcohol and non-saponifiable.

C-7

For new oxygen-containing carotenoids, the structures of which are not yet known, names may be chosen which have the ending "xanthin" with a prefix to express the origin or some property of the coloring matter.

C-8

Modification of the ending "xanthin" to "xanthol," "xanthone," *etc.*, to indicate the nature of the atom or atoms of oxygen, is not permitted.

C-9

Degradation products of carotenoids having aldehydic, ketonic, or acidic properties shall be characterized by the prefix "apo-" and the endings "-al," "-one," or "-oic," the number of the carbon atom which carries the aldehyde, ketone, or carboxylic acid group being placed in each case in front of "apo-."

C-10

In naming the epoxides of carotenoids, the numbers of the carbon atoms bound to the oxide oxygen should be indicated, *e.g.*, xanthophyll 5,6-epoxide.

C-11

The prefix "neo" will be used for carotenoids that are labile isomers mutually transformable.