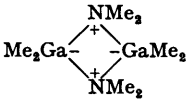
EDITORIAL REPORT ON NOMENCLATURE, 1951.*

Inorganic.

I.U.P.A.C.—An extensive report is being prepared by the Commission of Nomenclature of Inorganic Chemistry of the International Union of Pure and Applied Chemistry (I.U.P.A.C.), but details are not yet available.

Atomic Weights.—The latest (1949) I.U.P.A.C. list of Atomic Weights has been published (*J.*, 1951, 1).† For the names of elements see *J.*, 1951, 2, and the statement in the Editorial Report on Nomenclature, 1950 (*loc. cit.*).



Cyclic Compounds.—The compound of the annexed novel formula was tentatively named *cyclo*(bisdimethylammonium bisdimethylgallide) (*J.*, 1951, 2009). Two analogues were similarly named. This form of name may be useful for similar cyclic compounds.

Physical Chemistry.

Symbols, Signs, and Abbreviations.—A Report (1951) by the Symbols Committee of the Royal Society (representing the Royal Society, the Chemical Society, the Faraday Society, and the Physical Society) has been prepared to supersede the Report issued in 1937 by the Joint Committee of the Chemical Society, the Faraday Society, and the Physical Society on " Symbols for Thermodynamical and Physico-Chemical Quantities and Conventions relating to their Use."

This Report,‡ which is published in *J.*, 1951, 1677, lists the Symbols, Signs, and Abbreviations recommended for British Scientific Publications and was adopted for use forthwith in the *Journal*.

When compiling these recommendations for general use by British scientists of various disciplines, it was necessary to consider the reports of the International Union of Pure and Applied Chemistry and of the International Union of Pure and Applied Physics (cf. *Comptes rendus* of the XVth Conference of I.U.P.A.C., 1949, p. 94) and the previous customs of a variety of British scientific bodies.

The Unit of Heat.—In response to a communication from the Royal Society it has been agreed that in the Chemical Society's publications expression of quantities of heat and all other dependent concepts in both joules and calories shall be encouraged (cf. *Proc.*, 1951, 22).

Organic.

I.U.P.A.C.—At New York, in September, 1951, the I.U.P.A.C. Commission of Nomenclature of Organic Chemistry confirmed the rules proposed in 1949, after various corrections and emendations (many of them at the suggestion of the Chemical Society). The Commission revised the rule for " extra " hydrogen proposed in 1949, and certain new rules were put forward on a tentative basis. The final version of the 1949 rules and the new proposals of 1951 will be published in the *Journal* when available, and it is hoped to attach comments to them; certain changes in British practice will then be required, as the 1949 rules were approved by Council (*Proc.*, 1951, 22) subject to reconsideration of a few specified points.

This I.U.P.A.C. Commission has adopted the general procedure that its recommendations shall be first issued on a tentative basis, and shall be subject to confirmation or emendation at the following meeting after consideration of any comments which may have been received. This fully meets the condition attached by the Council of the Chemical Society to its recognition of I.U.P.A.C. nomenclature recommendations (see p. 3521).

Chromatographic Results.—The Publication Committee decided that tabulated details of chromatographic experiments, and diagrams or plates illustrating such work, shall not in future

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be published unless very exceptional conditions require it; normally, results should be expressed, briefly, in cursive text. The grade of adsorbent, and sufficient detail of dimensions and conditions, etc., should be stated to enable the work to be repeated, but it should be borne in mind that exact duplication of results is rarely possible.

A " map reference " method of reporting results of two-dimensional paper chromatography is proposed and illustrated in *J.*, 1951, 473.

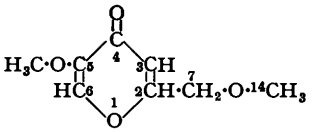
Isotopically Labelled Compounds.—The Editors to the Chemical Society and the Editorial Board of the Biochemical Society jointly prepared proposals which are believed to be applicable to the nomenclature of all isotopically labelled compounds. The proposals were unofficially circulated fairly widely for comment to British and foreign scientists working in this field. Some comments were received, generally favourable, although the Americans are known to be considering a different scheme. Copies will be supplied to any other scientists interested, on application to the Editor, The Chemical Society. This matter is under discussion between the British and the American Chemical Society and may be considered by I.U.P.A.C. Commissions.

Some principles of the British proposals, which have been tentatively used in the *Journal* and in *Biochem. J.*, are illustrated by the following examples from work published recently (*J.*, 1951, 3049, 3437, 3509).

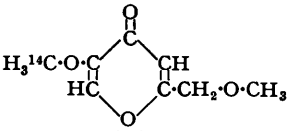
The four names below are self-explanatory :

[^{14}C]Methyl iodide	[^{14}C]Methanol
[^{14}C]Urea	[^{13}C]Formic acid

For $CH_3{\cdot}{}^{13}CO_2H$ the name is [*carboxy*-^{13}C]acetic acid.



(I)



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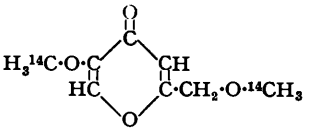


(III)

For (I) (actually prepared) the name is " kojic acid 5 : 7[$^{14}C_1$]-dimethyl ether." (II) would be named kojic acid 5[$^{14}C_1$] : 7-dimethyl ether, and (III) would be named kojic acid 5 : 7[$^{14}C_2$]-dimethyl ether.

Optically Active Isomers.—Linstead *et al.* (*J.*, 1951, 1131) have continued their use of *D* and *L* to denote the configuration of individual asymmetric atoms in organic compounds according to a precisely defined and limited extension of the Fischer convention (cf. *J.*, 1950, 3701). A general scheme has been proposed by Cahn and Ingold (*J.*, 1951, 612). Other proposals have been communicated to the Society, and a Sub-Committee has been established (cf. p. 3521) to consider all aspects of this subject and is expected to collaborate with an existing American Committee.

Amino-acids.—For I.U.P.A.C. recommendations see Appendix B (p. 3522).

Organophosphorus Compounds.—As a result of an exchange of views between Nomenclature Committees of the British and the American Chemical Society, it has been agreed that in the names of organic derivatives of phosphorus acids the terminations " ic " and " ous " shall denote quinque- and ter-valent phosphorus respectively, and that the affix " on " shall denote the larger, and the affix " in " the smaller, number of hydroxyl groups. This involves reversal of recent British practice (cf. Mitchell, " British Chemical Nomenclature," Ed. Arnold & Co., 1948, p. 64) and reversion to that used earlier; it does not affect the inorganic names phosphoric and phosphorous acid. Further, radicals attached to phosphorus by carbon shall be named as radicals, *i.e.*, the prefixes shall end in " yl "; for some compounds this involves a reversal of current American practice.

The following examples illustrate the agreed nomenclature which is now being used in the *Journal* :

H_3PO_4	phosphoric acid
H_3PO_3	phosphorous acid
$Ph{\cdot}P(O)(OH)_2$	phenylphosphonic acid
$Ph{\cdot}P(OH)_2$	phenylphosphonous acid
$Me{\cdot}PhH(O){\cdot}OH$	methylphosphinic acid
$Me_2P(O){\cdot}OH$	dimethylphosphinic acid
$Me_2P{\cdot}OH$	dimethylphosphinous acid

Et_3PO_4	triethyl phosphate
EtH_2PO_4	ethyl dihydrogen phosphate
Ag_2EtPO_4	disilver ethyl phosphate
$Ph{\cdot}P(O)(OPh)_2$	diphenyl phenylphosphonate
$Ph{\cdot}P(OH)(O{\cdot}CH_2Ph)$ ...	benzyl hydrogen phenylphosphonite
$Me_2P{\cdot}OMe$	methyl dimethylphosphinite

When a radical is attached to phosphorus by an element other than C or O, *e.g.*, when NH_2 or halogen is attached directly to phosphorus, this radical is still considered in British practice to replace hydrogen (not hydroxyl). *E.g.*,

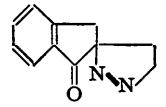
$Et{\cdot}PCl(O){\cdot}OEt$	ethyl ethylchlorophosphinate [derived from $Et{\cdot}PH(O){\cdot}OEt$]
$Ph{\cdot}P(O)(NHEt){\cdot}O{\cdot}CH_2Ph$ ...	benzyl ethylaminophenylphosphinate [derived from $Ph{\cdot}PH(O){\cdot}O{\cdot}CH_2Ph$]

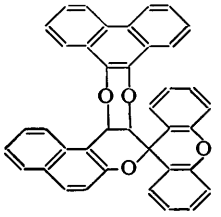
In this respect British practice still differs from American, in which these radicals are regarded as replacing hydroxyl. However, at British–American Committee discussions in New York a quite different nomenclature for such compounds was agreed. If ratified, the new proposals will be published and submitted to I.U.P.A.C.

Organoarsenic and Organoantimony Compounds.—These are now subject to the nomenclature outlined above for organophosphorus compounds.

spiro-*Compounds.*—These frequently present difficulty and there seems to be no generally accepted convention. Naming the ring-junction positions by numerals at each end of the affix *spiro* has recently proved useful. *E.g.*, (IV) was named indan-1-one-2-*spiro*-3′-$\Delta^{1'}$-pyrazoline (*J.*, 1951, 3254). A very complex case (*J.*, 1951, 1035) is presented by (V) which was named 4 : 5-(9 : 10-phenanthrylenedioxy)naphtho(2′ : 1′-2 : 3)pyran-6-*spiro*-9″-xanthen.

(IV)





(V)

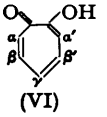
Steroids.—Rules for the nomenclature of steroids were agreed at a meeting of British, Swiss, American, and French specialists organised by CIBA Foundation in the summer of 1950. The English version of the rules was published in *Chem. and Ind.*, 1951, June 23rd, p. SN1, and is reproduced as Appendix C to this Report (p. 3527). An I.U.P.A.C. Sub-Committee has been appointed to consider these rules. Until their report is available, the CIBA rules are being used in the *Journal*. Swiss and French versions have been published and are being used in their respective countries.

Triterpenes.—The nomenclature in customary use in triterpene papers is often unsystematic and requires general clarification. Specialists should note particular usages in *J.*, 1951, 261, 1444, 2347, and 2474. In triterpene chemistry, hydroxy-ketones are customarily designated by the suffix -onol, whereas -olone was the customary form in steroid and carotenoid papers. Both forms conflict with I.U.C. rule 51, which specifies that only one group may be named as a suffix; -one having, by custom, priority over -ol as a functional group, these substances should be named with hydroxy-prefixes and -one suffixes; this systematic usage is now followed in the *Journal* for steroid papers, as well as in general nomenclature.

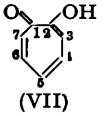
Carotenoids.—For I.U.P.A.C. recommendations, see Appendix B (p. 3525).

Vitamins.—For I.U.P.A.C. recommendations, see Appendix B (p. 3526).

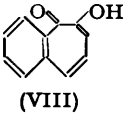
Tropolones.—The name " tropolone " is contrary to I.U.C. rule 51 (see above) and, insofar as the substance does not behave as a normal hydroxy-ketone, may be considered inappropriate; but it already has general acceptance. The position of substituents in tropolones may be indicated by Greek letters as in (VI), or by numerals as in (VII) :



(VI)



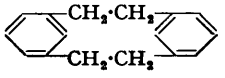
(VII)

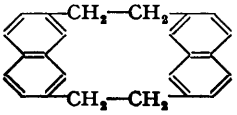


(VIII)

In the latter case, the keto-group must be assigned position 1. The benzo-derivative (VIII) (the parent of purpurogallin) may be called αβ-benzotropolone; or it may be named systematically as 4-hydroxy-1 : 2-benz*ocyclo*heptatrien-3-one (equivalent to 3-hydroxy-1 : 2-benzo-*cyclo*heptatrien-4-one). The designations *o*, *m*, and *p* may not be used in this series. Use of the name " tropone " for *cyclo*heptatrienone seems unjustified.

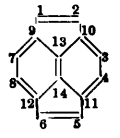
Polycyclic Compounds.—Use of Ring Index names continues to multiply (*e.g.*, *J.*, 1951, 110, 463, 787, 863, 867, 3117, 3357). However, so does the complete numbering of all atoms in the skeleton (*e.g.*, *J.*, 1951, 553, 3115); and compound (IX) was conveniently named

(IX) 

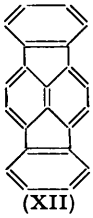
 (X)

di-*m*-xylylene (tri-*p*-xylylene was also used, for an analogous compound), and the substance (X) was called di(naphthalene-2 : 7-dimethylene) (*J.*, 1951, 201, 1114, 1118), whereas Ring Index names would have been cumbrous and less informative.

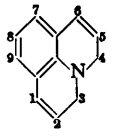
The name pyracylene has been used for (XI), with the numbering as shown (*J.*, 1951, 2391,



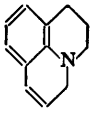
(XI)



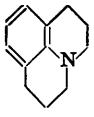
(XII)



(XIII) Juline



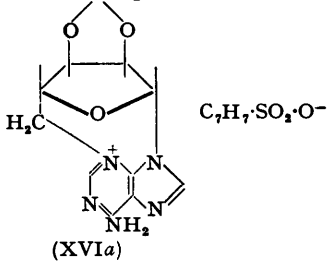
(XIV) Juloline



(XV) Julolidine

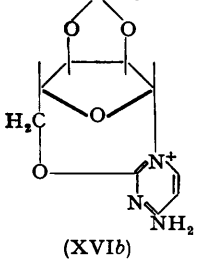
2392). The compound (XII) was then more conveniently described as 1 : 2-5 : 6-dibenzopyracylene than as a phenylenefluoranthene.

Use of the trivial names shown for (XIII)—(XV) may be noted (*J.*, 1951, 1898), and also of the generic term *cyclo*nucleoside, exemplified by (XVI*a*) and (XVI*b*) which are named 2′ : 3′-*iso*propylidene-3 : 5′-*cyclo*adenosine toluene-*p*-sulphonate and 2′ : 3′-*iso*propylidene O^2 : 5′-*cyclo*cytidine toluene-*p*-sulphonate, respectively (*J.*, 1951, 2952).



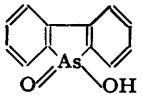
$C_7H_7\cdot SO_2\cdot O^-$

(XVI*a*)



$C_7H_7\cdot SO_2\cdot O^-$

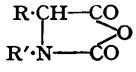
(XVI*b*)



(XVII)

Cyclic Organometallic Compounds.—An unsolved problem is involved when hetero-atoms, denoted by prefixes, are concerned as functional groups normally demanding description by suffixes. For quaternary nitrogen, the " oxa-aza " convention was extended in 1950 to use of azania as prefix (*J.*, 1950, 863, 3704). A different solution was provided by the name arsafluoreninic acid for (XVII) (*J.*, 1951, 2279).

Some Special Cases.—Oxazolid-2 : 5-diones (as XVIII) have been named as *N*-carboxyamino-acid anhydrides, this being more descriptive of their properties and mode of formation (*J.*, 1951, 213).

(XVIII) 

NH:CH·NH·CH:NH (XIX)

NH:CH·NH·CH:N·CH:NH (XX)

Compounds derived from (XIX) and (XX) have been given the class names diamidides and triamidides respectively, but individual compounds derived from (XX) have been named as tetra-azaheptatrienes (*J.*, 1951, 392).

Confusion resulting from the conflicting use of " anisyl " is exemplified in a paper by J. W. Baker (*J.*, 1951, 2506) and is also dealt with by Mitchell (*op. cit.*, p. 87). In the *Journal*, " anisyl " is no longer permitted, *p*-MeO·C_6H_4·CH_2 being termed *p*-methoxybenzyl, and *p*-MeO·C_6H_4 *p*-methoxyphenyl. The acid radical *p*-MeO·C_6H_4·CO is called *p*-anisoyl. Similar nomenclature applies to the dimethoxy- and methylenedioxy-analogues, etc., and to the bivalent (ylidene) radicals.

In polyolefinic acids having trivial names, the convention has been adopted of specifying the steric relations in order of the numbering (*J.*, 1951, 3387). *E.g.*, (XXI) is δ-methyl α-hydrogen β-methyl *cis-trans*-muconate.

$$MeO_2C\cdot CH\underset{trans}{=\!=}CH\cdot CMe\underset{cis}{=\!=}CH\cdot CO_2H \quad (XXI)$$

Nor and Homo.—The prefix nor was first used to denote replacement of two CH_3 groups (attached to oxygen) by H in transformation of opianic into noropianic acid. In terpene chemistry it commonly denotes removal of all methyl groups directly attached to the carbon skeleton. In norcodeine it denotes conversion of NMe into NH, the two methoxyl groups remaining intact. In steroid chemistry it has the well-defined meaning of stepwise replacement of CH_3 by H or by loss of CH_2 from a chain or ring (see p. 3534), and triterpene chemists tend to follow this practice. These examples do not exhaust the variations. Plainly, nor should now be used only when the resulting structure cannot possibly be in doubt. The same applies to the term homo for chain extension or ring expansion.

The " Oxa-aza " Convention in the Aliphatic Series.—The oxa-aza convention is often the simplest or clearest method of naming aliphatic compounds; recent examples (*J.*, 1951, 1929, 3508) are (XXII) 3 : 6 : 7 : 10-tetramethyl-4 : 5 : 8 : 9-tetra-azadodeca-3 : 5 : 7 : 9-tetraene-

$$(Me\cdot CO\cdot CMe{:}N\cdot N{:}CMe\cdot)_2 \quad (XXII)$$

$$HN{:}C(NH\cdot N{:}CPh\cdot N{:}NPh)_2 \quad (XXIII)$$

$$HN{:}C(NH\cdot N{:}CPh\cdot N{:}N\cdot SO_3K)_2 \quad (XXIV)$$

2 : 11-dione, (XXIII) 6-imino-1 : 3 : 9 : 11-tetraphenyl-3 : 6 : 9-tricarbaundeca-aza-1 : 3 : 8 : 10-tetraene, and (XXIV) potassium 6-imino-3 : 9-diphenyl-3 : 6 : 9-tricarbaundeca-aza-1 : 3 : 8 : 10-tetraene-1 : 11-disulphonate.

The following notice appeared in *Proc.*, 1951, 144 :

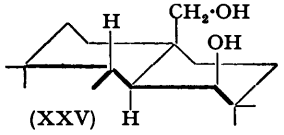
> The use of syllables ending in " a " such as oxa, aza, thia, etc., for indicating substitution by a hetero-atom into a ring skeleton has become well established; *e.g.*, a name such as 2 : 7 : 9-triazaphenanthrene is now generally understood. This usage is the subject of I.U.C. rule 16 (cf. *J.*, 1931, 1610). A more modern version of this rule was evolved by the Commission of Nomenclature of Organic Chemistry of the International Union of Pure and Applied Chemistry at its meetings in New York, in September, 1951, and will shortly be published on a tentative basis.
>
> The new rule, like the present rule 16, is confined to heterocyclic systems. The Organic Commission also considered extension of this principle to aliphatic compounds in which the main chain of atoms contains a preponderance of hetero-atoms; for instance, the compound HO·CH_2·O·CH_2·CH_2·O·CH_2·OH might be named 2 : 5-dioxahexane-1 : 6-diol; the compound CH_3·O·CH_2·O·CH_2·O·CH_2·CH_2·CO_2H might be named 2 : 4 : 6-trioxanonan-9-oic acid; the compound H_2N·CH_2·NH·NH·CH_2·NH·NH·NH_2 might be named 2 : 5-dicarbaoctazane. However, several alternatives arose when details of the rule(s) necessary for aliphatic application were discussed, and the need was felt for as wide a knowledge as possible of actual compounds to which this nomenclature could usefully be applied.
>
> The Commission would be grateful to be told of relevant examples; but it is emphasized that these should be compounds actually prepared (whether published or not) or in an advanced stage of preparation; purely theoretical compounds are not of interest as the desire is to discover the field of practical use to be covered.
>
> Silicon compounds are excluded from this request as they are covered by I.U.P.A.C. rules 70.1 to 70.20.
>
> Those (in Great Britain and kindred countries) who are willing to help are invited to send formulæ of relevant compounds to the Editor, The Chemical Society.

It may be well here to indicate some of the problems contained in the above few examples. When should the fundamental chain be based on carbon, as in 2 : 5-dioxahexane, and when on the hetero-atom, as in 2 : 5-dicarbaoctazane or 3 : 6 : 9-tricarbaundeca-aza-1 : 3 : 8 : 10-tetraene? Should the hetero-atoms of the chain have priority for lowest numbers over

functional groups (cf. 2 : 4 : 6-trioxanonan-9-oic acid with CO_2H = 9), or, if not, what functional groups have priority? Should terminal functional groups be excluded from the chain, *e.g.*, should the O of hydroxyl and carboxyl groups be excluded from the chain, as in the diol and acid examples above? and if so, what other groups should be excluded (cf. NH_2 and $NH{\cdot}NH{\cdot}NH_2$ in the octazane example)?

These and other points require answer before precise rules can be formulated. There is little primary logic applicable to the problem. The I.U.P.A.C. wishes its rules to be those best suited to the needs of practical chemists; for this the needs must be ascertained and further examples will be gratefully received by the Editor and considered by I.U.P.A.C.

Equatorial and Polar Bonds.—Formula (XXV) shows how, in some cases, equatorial and polar bonds (cf. *J.*, 1951, 1048; *J. Amer. Chem. Soc.*, 1947, **69**, 2488) can be set in type without too great distortion of the valency angles, by use only of bonds at 90° and 45°. Expensive illustrations can thus be avoided. The Editor is indebted to Dr. D. H. R. Barton for this suggestion.



(XXV)

General Policy.

The year 1951 has been notable for declarations of policy, and for international consultations, on nomenclature, but relatively few of the changes envisaged for the near future have yet materialised in practices in the Chemical Society's publications.

The previous Editorial Report on Nomenclature (*J.*, 1950, 3699) was the first fruit of a decision by the Society that its actions in matters of nomenclature should be stated openly for the benefit of Fellows; the medium of publicity being normally the *Journal* or *Proceedings*. A further outcome of this decision was publication (*Proc.*, 1951, 100) of the following explanation of the way in which nomenclature decisions are reached :

> Chemical nomenclature used in the Society's publications is decided by the Publication Committee, the Editors being considered as expert advisers and acting as executive officers of the Committee in day-to-day administration of the nomenclature policy. When major decisions on nomenclature require to be taken, the Publication Committee appoints Sub-Committees to study the problems and tender advice; these are *ad hoc* Sub-Committees which, having reported, are then disbanded. There are no Standing Committees, and the life of a Sub-Committee varies greatly according to the nature of the questions under consideration.
>
> All questions referring to nomenclature or to the Sub-Committees should be addressed to the Editor.

The membership of the Sub-Committees and Joint Committees, organised by the Chemical Society, which are still active, is given in Appendix A (p. 3521) to this Report. Some of these, and earlier, Sub-Committees were recorded in *Proc.*, 1951, 100.

The following quotation (*Proc.*, 1951, 144) explains how Fellows may take part in shaping the nomenclature used by the Society :

> Fellows wishing to submit extensive nomenclature proposals should send them to the Publication Committee for consideration. If adopted, the proposals will be published, with acknowledgments to the author, in the annual Editorial Report on Nomenclature.

In amplification, it may be stated that less extensive proposals will normally be negotiated between the author and the Editor, and that a desire to submit proposals to the Publication Committee will not hamper the use of any novel nomenclature in individual papers.

Full advantage was taken of the presence of many British chemists, including two of the Editors, at the 75th Anniversary Meeting of the American Chemical Society and at the XIIth Congress of the International Union of Pure and Applied Chemistry in New York in September 1951.

Dr. Mitchell and Dr. Cahn presented the Society's views at meetings of the I.U.P.A.C. Commission on Nomenclature of Organic Chemistry, the former as a member, the latter as consultant; and many other British chemists participated in the work of I.U.P.A.C. Commissions (a full list is not yet available). Dr. Mitchell and Dr. Cahn also read a paper on "Chemical Nomenclature in Britain Today" to the Division of Chemical Literature of the American Chemical Society (this may be published later in America; it is not being published by the Chemical Society).

The decisions of I.U.P.A.C. Commissions will be published in the *Comptes rendus* of the Conference and will thereafter be reproduced in the *Journal*. Through the courtesy of Professor Murray Luck, Chairman of the Commission of Nomenclature of Biological Chemistry, we are privileged to publish an advance English version of the decisions of that Commission (see Appendix B, p. 3522). The work of other Commissions has been referred to briefly where appropriate below.

The attitude of the Chemical Society to I.U.P.A.C. nomenclature decisions is set out in the following statement by Council (*Proc.*, 1951, 22) :

> The view was accepted by Council that international differences of nomenclature frequently form a real and serious barrier to the understanding of, and progress in, chemistry; that nomenclature, like grammar, has as its object the accurate and intelligible conveyance of information from one scientist to another; that no prestige or absolute value should attach to nomenclature apart from this object; and that, in consequence, conformity with internationally agreed nomenclature is most desirable even when the nomenclature so agreed may not seem to British chemists the best possible in particular cases.
>
> It was decided that all feasible steps should be taken to foster international collaboration and to present British views for international consideration.

Within the framework of international collaboration, the maximum amount of British–American agreement is desirable because of the common language. This was expressed in *Proc.*, 1951, 101 :

> With recurrence of more normal scientific conditions after the war, consultation between our Society's Editors and the staff of *Chemical Abstracts* has been resumed on a continually increasing scale (cf. *J.*, 1950, 3705). There is, too, growing collaboration between Nomenclature Committees of the American Chemical Society and of our Society. It is considered that adherence, so far as possible, to international decisions is most desirable (cf. *Proc.*, 1951, 21) and that British–American agreement on broad policy is an essential preliminary to international agreement. The Publication Committee of the Chemical Society and the Board of Directors of the American Chemical Society have therefore agreed to consult with each other before major changes in nomenclature are made, thus giving formal sanction to the practice of informal consultation.
>
> The Editor is responsible for organising the British participation in both the international and the American consultations, and all questions should be referred to him in the first place.

At the New York meetings, there were formal conferences between American Committees and representatives of their opposite-number British Committees on the nomenclature of carbohydrates and on that of organophosphorus compounds. In these two fields British and American differences were wide and well-embedded in the literature, causing considerable scientific difficulties; during the previous twelve months there had been extensive exchange of views in writing; the New York meetings resulted most gratifyingly in complete agreement on all the matters discussed in detail. These agreements will in due course be published in both countries and then submitted to I.U.P.A.C. for international consideration. Many other nomenclature proposals were discussed informally.

APPENDIX A

Sub-Committee on Carbohydrate Nomenclature. Professor S. Peat (Chairman), Professor W. Baker, Professor H. Burton, Professor E. L. Hirst, Dr. J. Honeyman, Professor C. K. Ingold, Professor W. H. Linnell, Professor M. Stacey, Professor A. R. Todd, Dr. B. Lythgoe, the Editors. Representatives of the Biochemical Society : Dr. D. J. Bell, Dr. W. Klyne, Dr. T. S. Work.

Sub-Committee on Organophosphorus Nomenclature. Professor A. R. Todd (Chairman), Dr. F. Bergel, Dr. H. Coates, Professor E. D. Hughes, Dr. F. G. Mann, Dr. H. N. Rydon, Dr. B. C. Saunders, Mr. L. T. D. Williams, the Editors.

Sub-Committee on Designation of Stereoisomers. Dr. D. H. R. Barton, Professor H. Burton, Professor M. Stacey, Professor E. E. Turner. Representatives of the Biochemical Society : Dr. A. Neuberger, Dr. T. S. Work. Secretary : Dr. L. C. Cross.

Joint Committee on Infra-red Absorption Data. Chemical Society: Professor E. D. Hughes, Dr. A. E. Martin, Dr. R. S. Cahn. Royal Society and Chemical Society: Dr. H. W. Thompson (Chairman). Physical Society: Dr. A. C. Menzies. Faraday Society: Dr. N. Sheppard. Institute of Petroleum: Dr. H. Powell. Co-opted: Dr. W. C. Price.

Joint Committee on Analytical Definitions. Chemical Society: Dr. H. M. N. H. Irving, Dr. R. S. Cahn. Government Chemist's Department: Mr. B. A. Ellis. Royal Institute of Chemistry: Dr. J. Haslam. Biochemical Society: Dr. W. Klyne. Society of Public Analysts: Mr. C. J. Regan. A.E.R.E., Harwell: Mr. A. A. Smales. Department of Scientific and Industrial Research: Mr. A. F. Williams.

APPENDIX B

International Union of Pure and Applied Chemistry, Commission of Nomenclature of Biological Chemistry.

Rules for the Nomenclature of Natural Amino-acids and Related Substances.

[Rules 1—5, 8, and 9, and the Appendix, were published in *Comptes rendus* of the XVth Conference in Amsterdam (1949) and were confirmed at the meeting in New York (1951). Rules 6, 7, and 10 were passed, and the Appendix was amended (to the version below), at the meeting in New York (1951), and are published in virtue of advance copy received through the courtesy of Professor D. Murray Luck.]

Rule 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 prefix in a general statement that is true for either enantiomorph, or for any mixture of these.

Rule 2.—(*a*) 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 *lævo*. An additional symbol to denote the direction of the rotation (*i.e.*, a plus or a minus sign enclosed in parentheses) is not necessary.

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

(*b*) 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.

Rule 3.—(*a*) The small capital letter prefixes D and L denote that the substance named is configurationally related to the corresponding enantiomorph of glyceraldehyde. Where confusion is possible between the use of the small 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-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-threonic acid, D_s-threonine for which the synonym is 2-amino-2 : 4-dideoxy-L_g-threonic acid, L_s-*allo*threonine for which the synonym is 2-amino-2 : 4-dideoxy-L_g-erythronic acid, D_s-*allo*threonine for which the synonym is 2-amino-2 : 4-dideoxy-D_g-erythronic acid.

(*b*) Amino-acids derived from amino-sugars should generally 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.

Rule 4.—Where the configurational relationship of the α-carbon atom has not been definitely established, or where it is desired to emphasise 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 designed by prefixes *dextro* or *lævo in lower case italic letters* or alternatively by a plus or a minus sign enclosed in parentheses.

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

Rule 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.

Rule 6.—(*a*) Where the amino-acid has two centres 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 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-*iso*leucine, for the amino-acids of protein origin which have trivial names; D-threonine, D-*iso*leucine for their enantiomorphs. Where there is a prefix denoting substitution, the names take the form hydroxy-L-proline, hydroxy-DL-glutamic acid, hydroxy-L-lysine, or, with specification of position of substitution, 4-hydroxy-L-proline, β-hydroxy-DL-glutamic acid, δ-hydroxy-L-lysine.

(*b*) 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 (*a*).

Examples : L-*allo*threonine, D-*allo*threonine, L-*alloiso*leucine, D-*alloiso*leucine for the pairs of enantiomorphs of the diastereomers of the amino-acids of protein origin which have trivial names; *allo*hydroxy-L-proline, *allo*hydroxy-D-proline, *allo*hydroxy-L-lysine, *allo*hydroxy-D-lysine, and similarly for the enantiomorphs 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*-δ-hydroxy-L-lysine. Systematic names take the form *allo*-β-hydroxy-L-α-aminobutyric acid (for L-*allo*threonine), *allo*-4-hydroxy-L-pyrrolidine-2-carboxylic acid (for *allo*hydroxy-L-proline).

(*c*) 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 observations, or both (1) and (2). 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 (*a*). The prefixes are placed as stated in section (*a*).

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 *allo*hydroxy-L-aspartic acid, the choice of these designations being made tentatively as specified. The respective enantiomorphs are named with the prefix D.

Rule 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 are otherwise observed.

Examples : L-histidine monohydrochloride monohydrate, copper L-aspartate, D-ornithine dihydrochloride, acetyl-L-tryptophan, diethyl D-glutamate, β-hydroxy-DL-glutamic acid, L-leucyl-L-valine, glycyl-DL-leucine. Names in which the 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 the following naturally occurring substances; β-phenyl-L-alanine, 4-hydroxy-L-proline, 3 : 5-di-iodo-L-tyrosine, 3 : 5-dibromo-L-tyrosine, δ-hydroxy-L-lysine. However, in general biochemical writing, the names of the following four substances, the position of substitution of which is well understood, are admissible as exceptions : L-phenylalanine, L-hydroxyproline, L-di-iodotyrosine, and L-hydroxylysine.

Rule 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-*allo*-cystathionine for *S*-(L-2-amino-2-carboxyethyl)-D-homocysteine.

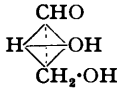
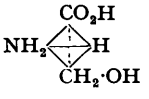
However, the introduction of new trivial names should be avoided in the absence of compelling reasons.

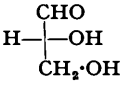
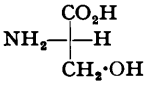
Rule 9.—The word, "inactive" or the prefix (±) shall be used for inactive amino-acids and their derivatives, (*a*) when two or more asymmetric centres are present but the steric cause of the inactivity is unknown, and (*b*) for the inactive form of an amino-acid of which an active form of uncertain configurational relationship has been described.

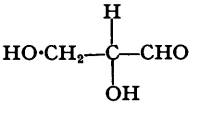
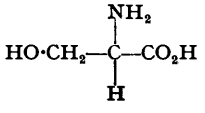
Examples : (*a*) inactive β-hydroxyglutamic acid; (*b*) (±)-hydroxytryptophan.

Rule 10.—Amino-acid radicals shall be named in conformity with rules 58.3 and 58.5 of the Report of the Commission on Nomenclature of Organic Chemistry (1949).

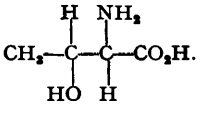
Appendix.—Representation of the configurational relationships in two dimensions may be made where desired by the use of the projection formula conventions of Emil Fischer.

D-Glyceraldehyde is  and L-serine is 

These may also be written  and 

or, by rotation of the depicting plane,  and 

According to this last system, the formula of L-threonine is written



However, when making a configurational interpretation of formulæ so written it is necessary to rotate the plane of depiction so that the α-carboxyl or α-aldehyde group is at the top.

Derivatives of *meso*-amino-acids, such that internal compensation is no longer complete, exist in enantiomorphous forms and can be specifically named under Rule 7. Thus, one of the possible monobenzoyl derivatives of *meso*cystine would be *S*-(D-2-benzamido-2-carboxyethylthio)-L-cysteine.

Rules of Nomenclature of the Carotenoids.

(These rules were agreed jointly by the Commissions of Nomenclature of Organic Chemistry and of Biological Chemistry, and were published, in French, in the *Comptes rendus* of the XIVth Conference of I.U.P.A.C., London, 1947, pp. 142—143; the original rules 1 and 6 were revised at the XVth Conference, New York, 1951. The revised text of rules 1 and 6, which has been substituted below for the rejected rules, became available through the courtesy of Professor J. Murray Luck, Chairman of the Commission of Nomenclature of Biological Chemistry. The translation and footnotes below are by R. S. Cahn.)

Rule 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 centre or near the centre of the molecule are separated by six carbon atoms, the other methyl groups being separated by five carbon atoms.

Rule 2.—" Carotene " is the name of the group of carotenoid hydrocarbons. Substitution products of carotenes are named " derivatives of carotenes."

Rule 3.—A new carotene shall be characterised 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.

Rule 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 following example :

If the carotene molecule is asymmetric the following 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

Rule 5.—The carotenoid alcohols, ketones, aldehydes, and acids are characterised by the suffixes " ol," " one," " al," and " oic," or by prefixes " hydroxy," " keto," " aldo," [a] and " carboxy," all following as closely as possible the rules of the Definitive Report [b] of the Commission on Nomenclature of Organic Chemistry.

Rule 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.

Rule 7.—For new oxygen-containing carotenoids, the structure of which is not yet known, names may be chosen which have the ending " xanthin " or, better, " xanthinne " [c] and, by their prefix, express the origin or some property of the colouring matter.

Rule 8.—Modification of the ending " xanthin " to " xanthol," " xanthone," etc., to indicate the nature of the atom or atoms of oxygen, is not permitted.

Rule 9.—Degradation products of carotenoids having aldehydic, ketonic, or acidic properties shall be characterised 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*."

[a] The prefix " aldo " to denote an aldehyde group is not recognised for general use in specific names by the Organic Commission on Nomenclature of Organic Chemistry of I.U.P.A.C., but only for use in generic names. This Commission specifies that the prefix for a CHO group is formyl.

[b] The Definitive Report (1930) has been expanded and to some extent superseded by the Report in *Comptes rendus* of the XVth Conference of I.U.P.A.C. (1949).

[c] The French text has " ' xanthine ' ou mieux ' xanthinne,' " but the terminal " e " is not used for xanthin in Chemical Society publications because, according to I.U.C. rule 33, the termination " ine " is reserved exclusively for nitrogenous bases. It may have been consideration of this I.U.C. rule which led in the French text to the preference expressed for " xanthinne."

Rule 10.—In naming epoxides of carotenoids, the numbers of the carbon atoms bound to the oxidic oxygen shall be indicated (*e.g.*, 5 : 6-epoxylutein).

Rule 11.—The prefix " neo " shall be used for unstable carotenoids which may be converted into, and obtained from, their isomers.[d]

Vitamins.

[At the meeting in New York (1951) the following names were adopted. We are indebted to Professor D. Murray Luck for this advance information.]

Customary designation hitherto	Name adopted
Vitamin D_2	Ergocalciferol
Calciferol	
Vitamin D_3	Cholecalciferol
Other D vitamins derived from 7-dehydro-steroids...	To be named analogously, as above
Vitamins E	α-, β-, and γ-Tocopherol
Vitamin B_1	Thiamine
Aneurin	
Thiamine	
Vitamin B_2	Riboflavin
Riboflavin	
Vitamin PP	Nicotinamide
Niacinamide	
Nicotinamide	
Pantothenic acid	Pantothenic acid
Biotin	Biotin
p-Aminobenzoic acid	*p*-Aminobenzoic acid
Choline	Choline
Vitamins B_{12} (collectively)	Cobalamin
Vitamin B_{12} (pure substance)	Cyanocobalamin
Vitamin B_{12b}	Hydroxocobalamin
Vitamin B_{12c}	Nitrosocobalamin
Vitamin C	Ascorbic acid
Ascorbic acid	

APPENDIX C

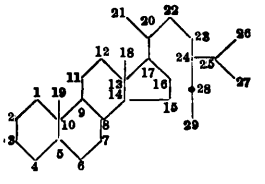
Steroid Nomenclature.

The following proposed rules for steroid nomenclature are based on agreements reached at a Conference held at the CIBA Foundation, London, on May 30th to June 1st, 1950. It is hoped to submit them for approval to the International Union of Pure and Applied Chemistry.

Numbering.

Rule 1.—Steroids shall be numbered as in formula (I). If one or more of the carbon atoms shown in (I) is not present, the numbering of the remainder shall remain undisturbed.

(I.)



Remarks. The numbering in (I) is that generally accepted in steroid chemistry, although it does not conform to that given in the " Ring Index " for cyclopenta[a]phenanthrene (No. 2561). It has been the general, but not invariable, practice to assign the number 18 to the carbon atom of the methyl group attached to $C_{(13)}$, as in (I), because this methyl group is present in *all* natural steroids whereas the methyl group (involving $C_{(19)}$) attached to $C_{(10)}$ is absent in members of the œstrogen series.

[d] The French text reads " On emploiera le préfixe ' neo ' pour des caroténoïdes instables, isomères et se laissant transformer mutuellement."

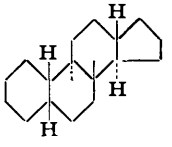
General Nomenclature.

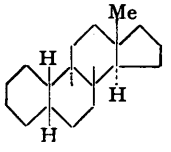
Rule 2.—All names shall connote a specific stereochemical configuration, except as provided in rule 5.2.

Remarks. Names are assigned below to a relatively few parent or fundamental compounds and each name refers to only one stereochemical configuration. All known steroids are related to these parent compounds and can be systematically named as derivatives of them. In formulæ, dotted lines denote α-configuration (bond behind the plane of the paper) and full lines denote β-configuration (bonds above the plane of the paper), according to the customary steroid convention that the methyl group at position 10 lies above the plane of the ring-system.

Parent Compounds.

Rule 3.1.—The substance (II) shall be named gonane [1] (preferred) or sterane (alternative).

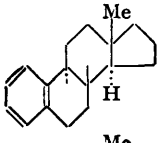
(II.) 

 (III.)

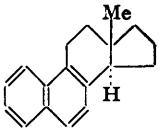
Rule 3.2.—The substance (III) shall be named œstrane.[2]

Rule 3.3.—Names for partly aromatic steroids are derived by means of standard terminations denoting unsaturation.

Examples.



Œstra-1 : 3 : 5(10)-triene.
[In German, Oestra-1,3,5 : 10-trien or Oestratrien-(1,3,5 : 10).]

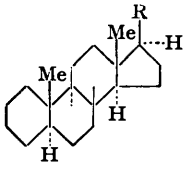


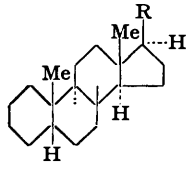
Œstra-1 : 3 : 5(10) : 6 : 8-pentaene.
[In German, Oestra-1,3,5 : 10,6,8-pentaen or Oestrapentaen-(1,3,5 : 10,6,8).]

Rule 3.4.—The following eight names shall be used for the hydrocarbons (IV) and (V) :

R.	(IV) 5α-Series.*	(V) 5β-Series.*
H	ANDROSTANE	Testane
Et	*allo*Pregnane	PREGNANE
$CHMe{\cdot}CH_2{\cdot}CH_2{\cdot}CH_3$	*allo*Cholane	CHOLANE
$CHMe{\cdot}CH_2{\cdot}CH_2{\cdot}CH_2{\cdot}CH(CH_3)_2$	CHOLESTANE	Coprostane

* For the designations 5α and 5β see rule 5.1.

(IV.) 

 (V.)

Remarks. Of the above eight names, seven are well-established and adequate. The new name testane is recommended to eliminate the practice of using " ætiocholane " and " ætiocholanic acid " for compounds of different carbon content.

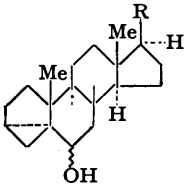
[1] In German, the terminal " e " is omitted from this and other names of hydrocarbons.
[2] In America, estrane; in German, Oestran.

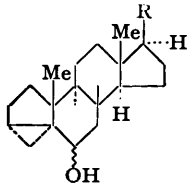
Rule 3.5.—Preference shall be given to the name printed in capital letters in rule 3.4 when naming derivatives in which $C_{(5)}$ is not asymmetric.

Example. Cholest-4-en-3-one, not " coprost-4-en-3-one."

Rule 3.6.—Names of steroids containing a three-membered ring by virtue of the presence of a link between $C_{(3)}$ and $C_{(5)}$ shall be prefixed by 3 : 5-*cyclo*.

Examples. 3 : 5-*cyclo*Steroids (generic name).





(R = ·CHMe·[CH$_2$]$_3$·CH$<^{CH_3}_{CH_3}$)

3 : 5-*cyclo*Cholestan-6-ol. 3 : 5-*cyclo*Coprostan-6-ol.

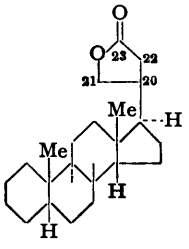
Remarks. This nomenclature was proposed by Petit (*Bull. Soc. chim.*, 1949, [v], **16**, 545) and Shoppee (Internat. Res. Colloquium, Montpellier, 1950). As in general nomenclature (*e.g.*, *cyclo*hexane) the prefix *cyclo* implies the elimination of two hydrogen atoms; it is introduced to replace *i*- and *iso*-prefixes previously used to describe such compounds, because *i* has been used to denote optical inactivity, and *iso* to denote an inversion of configuration at a particular asymmetric centre. The configuration at $C_{(5)}$ need not be stated as it is implied in the name of the fundamental nucleus. For configuration at $C_{(6)}$ ξ may be used (see rule 5.2).

Rule 3.7.—The prefix *allo* shall be used to denote a change of configuration solely at $C_{(5)}$ and then only the change of 5β into 5α.

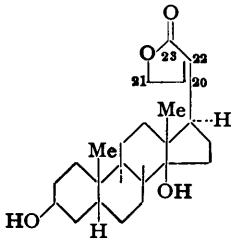
Remarks. This rule is restrictive, not permissive; *i.e.*, it limits the use of *allo* in the senses stated, but it does not over-ride rule 3.4 according to which androstane is used and not " *allo*testane," and cholestane is used and not " *allo*coprostane." See also rule 4.4. Rule 3.7 necessitates that the name " *allo*solanidane " shall disappear and be replaced by 5β-solanidane, and that the term " *allo*aglycone " (*e.g.*, " *allo*strophanthidin ") shall disappear and be replaced by 17α-aglycone (*e.g.*, 17α-strophanthidin).

Rule 3.8.—(*a*) The name cardanolide (preferred) or cardogenan (alternative) shall be used for the fully saturated system (VI) of digitaloid lactones in which the configuration at $C_{(20)}$ is the same as in cholesterol. (*b*) When the configuration at $C_{(20)}$ is unknown, the prefix 20ξ- must be used (see rule 5.2). (*c*) The name cardenolide (preferred) or cardogenen (alternative) shall be used for the naturally occurring unsaturated lactones. (*d*) The names 14 : 21- and 16 : 21-epoxycardanolide (or -epoxycardogenan) shall be used for the compounds containing a 14 : 21- and 16 : 21-oxygen bridge, respectively (in German, oxido shall replace epoxy).

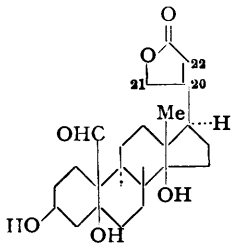
Examples.



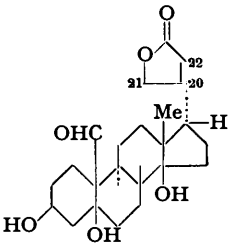
(VI.) Cardanolide (or cardogenan).



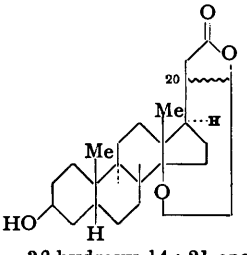
Digitoxigenin = 3β : 14-dihydroxycard-20(22)-enolide [or cardogen-20(22)-en-3β : 14-diol].



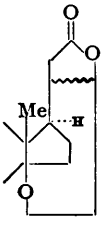
Strophanthidin = 3β : 5 : 14-trihydroxy-19-oxocard-20(22)-enolide [or 19-oxocardogen-20(22)-en-3β : 5 : 14-triol].



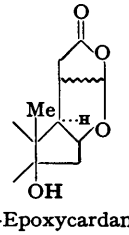
17α-Strophanthidin (formerly "*allo*strophanthidin") = 3β : 5 : 14-trihydroxy-19-oxo-17α-card-20(22)-enolide.



"*iso*Digitoxigenin" = 3β-hydroxy-14 : 21-epoxy-20ξ-cardanolide [or 14 : 21-epoxy-20ξ-cardogenan-3β-ol].



14 : 21-Epoxycardanolide.

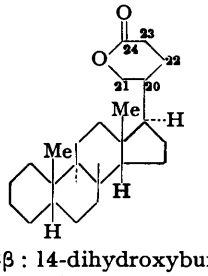


16 : 21-Epoxycardanolide.

Remarks. (*a*) A decision between cardanolide and cardogenan, etc., may be taken by the International Union of Pure and Applied Chemistry. (*b*) Oxido is preferred in German because in that language epoxy has been used more specifically for three-membered rings.

Rule 3.9.—(*a*) The name bufanolide (preferred) or bufogenan (alternative) shall be used for the fully saturated system (VII) of the squill–toad poison group of lactones, in which the configuration at $C_{(20)}$ is the same as in cholesterol. (*b*) When the configuration at $C_{(20)}$ is unknown, the prefix 20ξ- must be used (see rule 5.2). (*c*) The name bufadienolide (preferred) or bufogenadiene (alternative) shall be used for the naturally occurring doubly-unsaturated lactones.

Examples.



(VII.)
Bufanolide (or bufogenan).

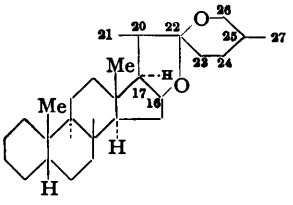
Bufalin = 3β : 14-dihydroxybufa-20 : 22-dienolide [or bufogena-20 : 22-dien-3β : 14-diol].

Telecinobufagin = 3β : 5 : 14-trihydroxybufa-20 : 22-dienolide [or bufogena-20 : 22-dien-3β : 5 : 14-triol].

Remark. The name bufadienolide was suggested by Klyne (*Nature*, 1950, **165**, 313).

Rule 3.10.—(*a*) The name spirostan shall be used for the substance of structure (VIII), 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. (*b*) The configuration at $C_{(22)}$ in this series must be specified as a or b by reference to that of sarsasapogenin which is 22b. (*c*) If configuration at any of the asymmetric centres named above is not known, the prefix ξ- (preceded by the appropriate numerals) shall be used (see rule 5.2).

Examples.



(VIII.)
Spirostan.

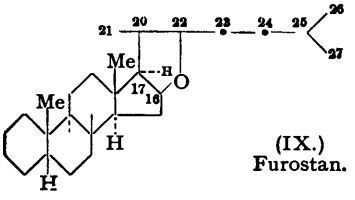
Sarsasapogenin = 22b-spirostan-3β-ol (normal = 22b-series).

Smilagenin = 22a-spirostan-3β-ol (" 22-*iso* " = 22a-series).

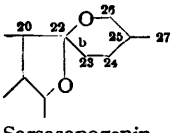
Remark. The name spirostan was suggested by Rosenkranz and Djerassi (*Nature*, 1950, **166**, 104).

Rule 3.11.—(*a*) The name furostan shall be used for the substance of structure (IX), in which the configurations at $C_{(17)}$ and $C_{(20)}$ are the same as in cholesterol. (*b*) The configuration at $C_{(22)}$ in this series must be specified as a or b by reference to that of dihydrosarsasapogenin which is 22b. (*c*) If configuration at any of the asymmetric centres named above is not known, the prefix ξ- (preceded by the appropriate numerals) shall be used (see rule 5.2).

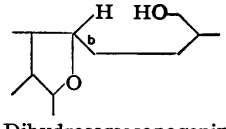
Examples.



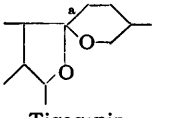
(IX.)
Furostan.



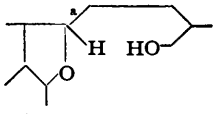
Sarsasapogenin
(= 22b-spirostan-3β-ol).



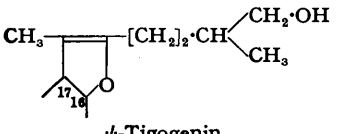
Dihydrosarsasapogenin
(= 22b-furostan-3β : 26-diol).



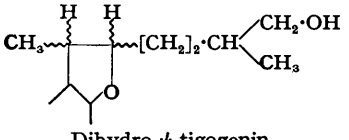
Tigogenin
(= 5α : 22a-spirostan-3β-ol).



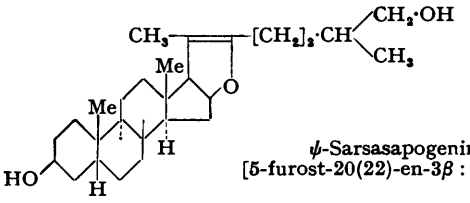
Dihydrotigogenin
(= 5α : 22a-furostan-3β-ol).



ψ-Tigogenin
[5α-furost-20(22)-en-3β : 26-diol].



Dihydro-ψ-tigogenin
[5α : 20ξ : 22ξ-furostan-3β : 26-diol].



ψ-Sarsasapogenin
[5-furost-20(22)-en-3β : 26-diol].

Remarks. The name furostan was suggested by Rosenkranz and Djerassi (*loc. cit.*). It is highly probable that in furostans configuration at $C_{(16)}$ is β, as at $C_{(17)}$; if inversion at one or other of these asymmetry centres cannot be excluded, it will be necessary to modify the name for ψ-tigogenin to 5α : 16ξ : 17ξ-furost-20(22)-ene-3β : 26-diol, and that of dihydro-ψ-tigogenin to 5α : 16ξ : 17ξ : 20ξ : 22ξ-furostan-3β : 26-diol.

It is probable, but not certain, that the conversion of sarsasapogenin into dihydrosarsasapogenin takes place without inversion of configuration at $C_{(22)}$; dihydrosarsasapogenin is therefore chosen as the reference compound.

Trivial Names.

Rule 4.1.—The following trivial names for hormones are retained : œstrone, œstradiol-17β, œstradiol-17α, œstriol, androsterone, testosterone, progesterone, corticosterone, cortisone (free 17 : 21-diol).

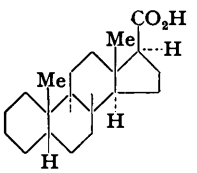
Rule 4.2.—The name cortexone may be used for 11-deoxycorticosterone.

Remark. This rule is subject to further research on trade names.

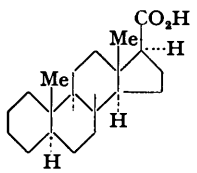
Rule 4.3.—The name coprostanol, more specifically coprostan-3β-ol, shall be used in place of " coprosterol."

Remark. Compare rule 3.4.

Rule 4.4.—The trivial name etianic acid shall be used for the acid (X), and the trivial name *allo*etianic acid for its 5α-isomer (XI), and stereoisomers shall be named as derivatives thereof.

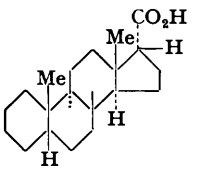


(X.) Etianic acid (systematic name, testane-17β-carboxylic acid).

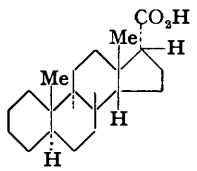


(XI.) *allo*Etianic acid (systematic name, androstane-17β-carboxylic acid).

Examples.



17α-Etianic acid (systematic name, testane-17α-carboxylic acid)

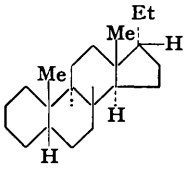


14β-17α-*allo*Etianic acid (systematic name, 14β-androstane-17α-carboxylic acid).

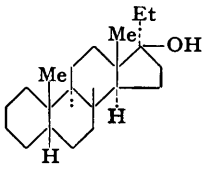
Remarks. The trivial names etianic and *allo*etianic acid replace " ætiocholanic " and " ætio-*allo*cholanic acid " (androstane-17β-carboxylic acid, also incorrectly called " 17β-androstanylcarboxylic acid " or " androstan-17β-ylcarboxylic acid "), respectively.

STEREOISOMERISM.

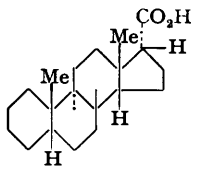
Rule 5.1.—Inversion of configuration at (i) a ring junction and/or (ii) $C_{(17)}$ of a steroid of accepted name shall be denoted by the prefix(es) α or β, denoting the orientation of the bond (i) to the methyl group or hydrogen atom attached to the ring junction and/or (ii) to the carbon side-chain attached to $C_{(17)}$, these groups being implied as present by the accepted name; and the prefix(es) shall be preceded by the numeral(s) denoting the position of the carbon atom(s) at which inversion has occurred.



17α-Pregnane.



17-Hydroxy-17α-pregnane or 17α-pregnan-17-ol.

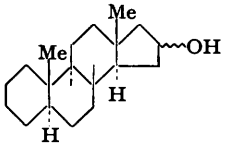


14β : 17α-Etianic acid or 14β-testane-17α-carboxylic acid

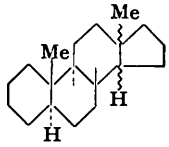
Remarks. This rule accords with the proposals by Fieser and Fieser (" Natural Products Related to Phenanthrene," Rheinhold Publ. Corp., 1949, p. vi). It will be noted that testane can be fully described as 5β-androstane, *allo*pregnane as 5α-pregnane, *allo*cholane as 5α-cholane, and coprostane as 5β-cholestane.

Rule 5.2.—When configuration at one or more centres is unknown, this shall be indicated by means of the Greek letter(s) ξ (xi) prefixed by the appropriate numeral(s), and in formulæ by a wavy line.

Examples.



Androstan-16ξ-ol.



13ξ : 14ξ-Androstane.

ξ-Androstane, for an isomer where the configurations of several asymmetric centres are unknown.

Remarks. This situation can arise with, *e.g.*, synthetic compounds.

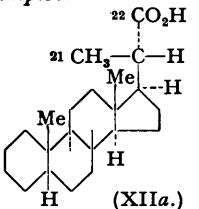
Rule 5.3.—When introduction of substituents into the nuclear skeleton creates one or more new asymmetric centres, the configuration at these centres shall be represented by appropriate numerals and prefixes α or β relating to the orientation of the bond attached to the substituent; if two substituents are present at such a peripheral position, only one of their configurational prefixes shall be cited, namely, that relating to the group chosen according to the following order of increasing preference : [H], Cl, Br, I, OH, NH_2, CH_3, C_2H_5, $CO{\cdot}CH_3$, CO_2H.

Remark. The order of preference of groups is that given in Beilstein's " Handbuch der organischen Chemie," 4th Edn., Vol. I, p. 941.

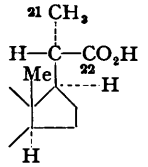
Rule 5.4.—Configuration in the side-chain shall be denoted by the method proposed by Fieser and Fieser [*Experientia*, 1949, **4**, 285; see also Appendix, section (a)] for configuration at $C_{(20)}$ of pregnane derivatives.

Rule 5.5.—Fieser and Fieser's proposals (*loc. cit.*) may be extended as suggested by Plattner in the Appendix to these Rules. When this is done, preference for the rearmost position in the model and for citation by prefix in a name shall be given to the longest carbon chain or, if the chains are of equal length, according to the order given in rule 5.3.

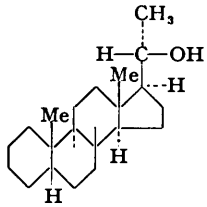
Examples.



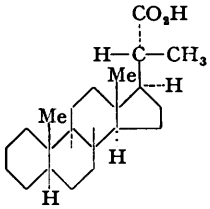
(XII*a*.)
Bisnorcholanic acid (20*β*)
(20 normal).



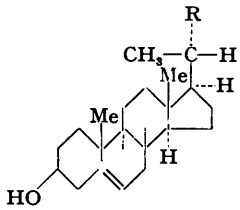
(XII*b*.)
(Unconventional, cf. Remarks.)



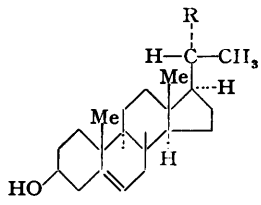
Pregnan-20*α*-ol.



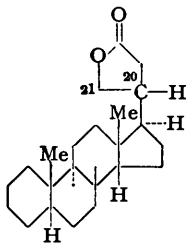
20*α*-Bisnorcholanic acid
(= 20-*iso*bisnorcholanic acid).

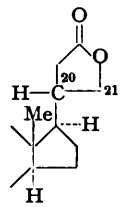


Cholesterol (20*β*).



20*α*-Cholesterol
(= 20-*iso*cholesterol).





20*α*-Cardanolide (20-*iso*).

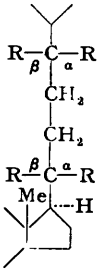
20*β*-Cardanolide [20(normal)-configuration identical with that of cholesterol].

Remarks. (*a*) When the 17-side-chain contains only the skeleton $-C\begin{smallmatrix}C\\C\end{smallmatrix}$, the order of preference will, in practice, generally assign $C_{(22)}$ to the rearmost position. (*b*) The formula (XII*a*) could be represented as (XII*b*), but this would be contrary to the rule as CO_2H has preference over CH_3 for the rearmost position. Normal bisnorcholanic acid has at $C_{(20)}$ the same configuration as pregnan-20α-ol in the sense that the carboxyl group replaces the hydroxyl group without inversion; nevertheless, if it is named as a bisnorcholanic acid the prefix must be 20β as CO_2H has preference for the rearmost position and for citation in a name. The acid could however also be correctly named as pregnane-20α-carboxylic acid (cf. XII*b*).

Rule 5.6.—The method of rule 5.5 will be capable of extension to other asymmetric centres (*e.g.*, $C_{(24)}$) in the side-chain when configuration at such centres can be correlated with that at $C_{(20)}$ or $C_{(17)}$ (cf. Appendix). Until this is possible, steroids which possess at $C_{(24)}$ the same configuration as ergosterol and stigmasterol shall be designated as 24b-steroids, and the isomerides as 24a-steroids.

Example. Campesterol is a 24a-compound.

Remark. For the proposal recommended for present use see Fieser and Fieser (*op. cit.*, p. 412). When the necessary correlation is established, configuration would be designated as in (XIII).

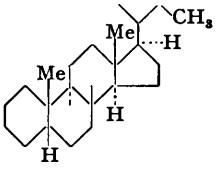


(XIII.)

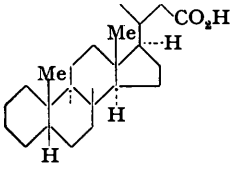
SHORTENING OF SIDE-CHAIN AND ELIMINATION OF METHYL GROUPS.

Rule 6.1.—(*a*) Elimination of a methylene group from a methyl group or from a position adjacent to a carboxyl group shall be indicated by a prefix nor. (*b*) If elimination occurs from a methyl group attached to a ring junction, the prefix shall be preceded by the number attaching to the carbon atom which disappears.

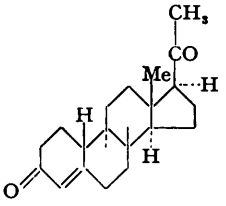
Examples.



Norcholane.



Norcholanic acid.



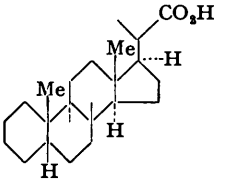
(XIV.)

19-Norprogesterone (or 19-nor-10ξ-progesterone if configuration at $C_{(10)}$ is unknown).

Remarks. (*a*) Use of the number of the atom to which the missing methyl group has been attached, *e.g.*, naming (XIV) as 10-norprogesterone, is considered to be more ambiguous and is not permitted. (*b*) Replacement of a methyl group by hydrogen does not disturb the numbering of other atoms, *e.g.*, of the side chain (see rule 1).

Rule 6.2.—Elimination of an ethylene group from the end of the side-chain or from a position adjacent to a carboxyl group shall be indicated by the prefix bisnor, but terms such as ternor shall not be used.

Example.



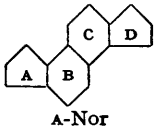
Bisnorcholanic acid.

Remark. Names such as " 19 : 22 : 23-ternorcholanic acid " (= 17β-ethylœstrane-20α-carboxylic acid) are not permitted.

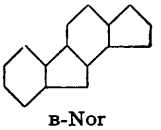
RING ENLARGEMENT, CONTRACTION, AND FISSION.

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

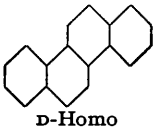
Examples.



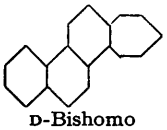
A-Nor



B-Nor



D-Homo



D-Bishomo

See also below.

Remarks. The above suggestion, by Ruzicka and Meldahl (*Helv. Chim. Acta*, 1940, **23**, 364), has been found satisfactory, but two other systems suggested at the Conference led to the following names for the above structures :

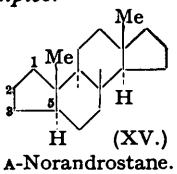
A-*cyclo*Nor	B-*cyclo*Nor	D-*cyclo*Homo	D-*cyclo*Bishomo
A-Quinqua	B-Quinqua	D-Sexa	D-Septa

Rule 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.

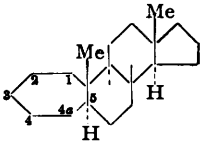
Example. As in A-norandrostane (XV).

Rule 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.

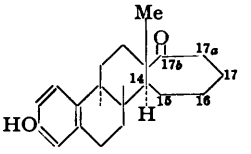
Examples.


(XV.)

A-Norandrostane.



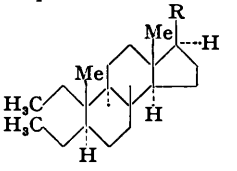
A-Homoandrostane.



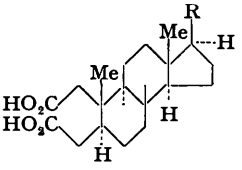
D-Bishomoœstrone.

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

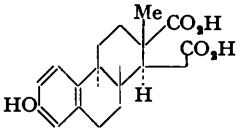
Examples.



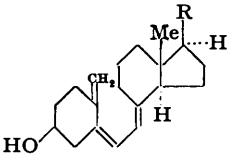
2 : 3-*seco*Cholestane.



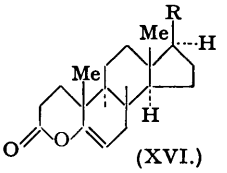
2 : 3-*seco*Cholestane-2 : 3-dioic acid.



3-Hydroxy-16 : 17-*seco*œstra-1 : 3 : 5(10)-triene-16 : 17-dioic acid (marrianolic acid).



9 : 10-*seco*Cholesta-5 : 7 : 10(19)-trien-3β-ol (vitamin D_3).


(XVI.)

5-Hydroxy-3 : 5-*seco*-A-norcholest-5-en-3-oic 3 : 5-lactone.

Remarks. The example (XVI) illustrates the simultaneous use of rules 7.1 and 7.4, and inclusion of 5-hydroxy in the name illustrates the importance of the phrase in the rule concerning addition of hydrogen.

Note.—Proposals were also made at the Conference for the nomenclature of steroid alkaloids, but after further consideration the matter is postponed for further study. Nevertheless, application of rule 3.7 to debar " *allo*solanidane " remains definite.

R. S. Cahn	(London)	A. Petit	(Paris)
R. K. Callow	(London)	Pl. A. Plattner	(Zurich)
J. W. Cook	(Glasgow)	T. Reichstein	(Basle)
E. C. Dodds	(London)	Sir Robert Robinson	(Oxford)
L. F. Fieser	(Harvard)	L. Ruzicka	(Zurich)
Mary Fieser	(Harvard)	B. Riegel	(Evanston, Ill.)
W. Klyne	(London)	C. R. Scholz	(New York)
G. F. Marrian	(Edinburgh)	C. W. Shoppee	(Swansea)
K. Miescher	(Basle)	F. S. Spring	(Glasgow)
G. Müller	(Paris)	A. Wettstein	(Basle)

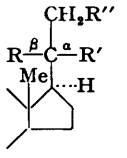
E. R. H. Jones (Manchester) (absent through indisposition has signified agreement)

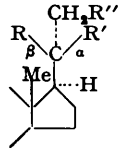
Appendix.

Description of configuration in the side-chain.

By Pl. A. Plattner.

(a) *Definition.*—The following convention for description of configuration at $C_{(20)}$ relatively to $C_{(17)}$ and so to the whole steroid ring system has been proposed by Fieser and Fieser (*Experientia*, 1948, **4**, 285; *op. cit.*, p. 412): If $C_{(21)}$ (R″ = H or OH) is made by rotation about the



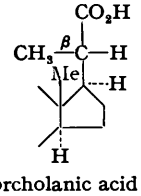


$C_{(17)}$–$C_{(20)}$ axis to occupy the rearmost position, then the substituent (R or R′) which according to the Fischer projection appears on the left is described as β-oriented. Conversely, an α-oriented substituent stands to the right of the $C_{(17)}$–$C_{(20)}$ bond axis.

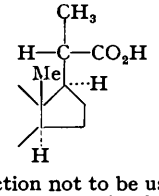
This convention can readily be applied to the $C_{(20)}$-isomeric compounds of the sterol and bile acid series. It is only necessary to state which of the two carbon atoms $C_{(21)}$ or $C_{(22)}$ has to take up the position of the $C_{(21)}$ in the above scheme. The custom in carbohydrate chemistry is always to select the longest side-chain, *i.e.*, the substituent which occupies the last position in the order of preference given by Beilstein (cf. rule 5.3); *in the steroid series this will be* $C_{(22)}$.

By such extension of Fieser and Fieser's proposal to the sterols, bile acids, and related compounds, the current nomenclature of the adreno-cortical compounds and 20-hydroxypregnane derivatives remains unaltered.

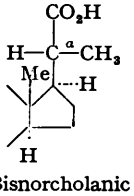
(b) *Present Situation.*—By degradation of compounds of the type of norcholan-22-one to 20-hydroxypregnanes by per-acids, Wieland and Miescher (*Helv. Chim. Acta*, 1949, **32**, 1922) have been able to relate the configuration at $C_{(20)}$ of sterols and bile acids to that at $C_{(17)}$ and so to the whole ring system. The work of Friess (*J. Amer. Chem. Soc.*, 1949, **71**, 2571), Gallagher and Kritschevsky (*ibid.*, 1950, **72**, 882), and Turner (*ibid.*, p. 878) has shown that in this degradation there is no inversion of configuration at $C_{(20)}$. The foregoing suggested extension of the Fiesers convention appears therefore to be well-founded, and leads to the following description of configuration at $C_{(20)}$ in sterols, bile acids, and related compounds. Assignment of indices α or β to the two substituents lying to the right or left in the plane of projection follows the order of preference set out in rule 5.3, whereby at $C_{(17)}$, if H and Alkyl are present, the index of the alkyl group is given although the alkyl group itself is already contained in the name:



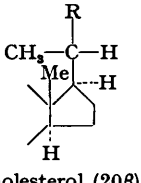
Bisnorcholanic acid (20β) (normal bisnorcholanic acid).



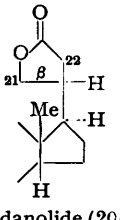
Projection not to be used for derivation of index.



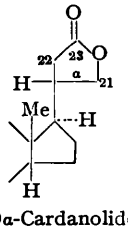
20α-Bisnorcholanic acid (20-*iso*Bisnorcholanic acid).



Cholesterol (20β) (20-*iso*cholesterol = 20α-cholesterol).



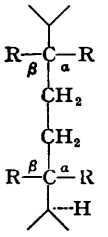
Cardanolide (20β) (20-normal).



20α-Cardanolide (20-*iso*).

(c) *Extension of Definition to* $C_{(24)}$.—Extension of the above nomenclature to $C_{(24)}$ depends on correlation of configuration at $C_{(24)}$ with that at $C_{(20)}$ or $C_{(17)}$. Because this is not yet possible, use must be made of Fieser and Fieser's provisional proposal (*op. cit.*, p. 280), whereby compounds which correspond in configuration at $C_{(24)}$ with ergosterol and stigmasterol are described as 24b-steroids whilst epimers, such as campesterol, are described as 24a-steroids.

As soon as the configuration is more accurately known, the indices α and β should be used. The carbon atoms of the side-chain, $C_{(20)}$, $C_{(22)}$, $C_{(23)}$, $C_{(24)}$, and $C_{(25)}$, form a chain with all



members drawn vertically and according to the Fischer projection (*Ber.*, 1891, **24**, 2683) whereby R–R represents the front edge of the tetrahedron, substituents to the left being designated β and to the right α. An advantage is that this readily permits extension of the convention for $C_{(20)}$ to $C_{(24)}$.