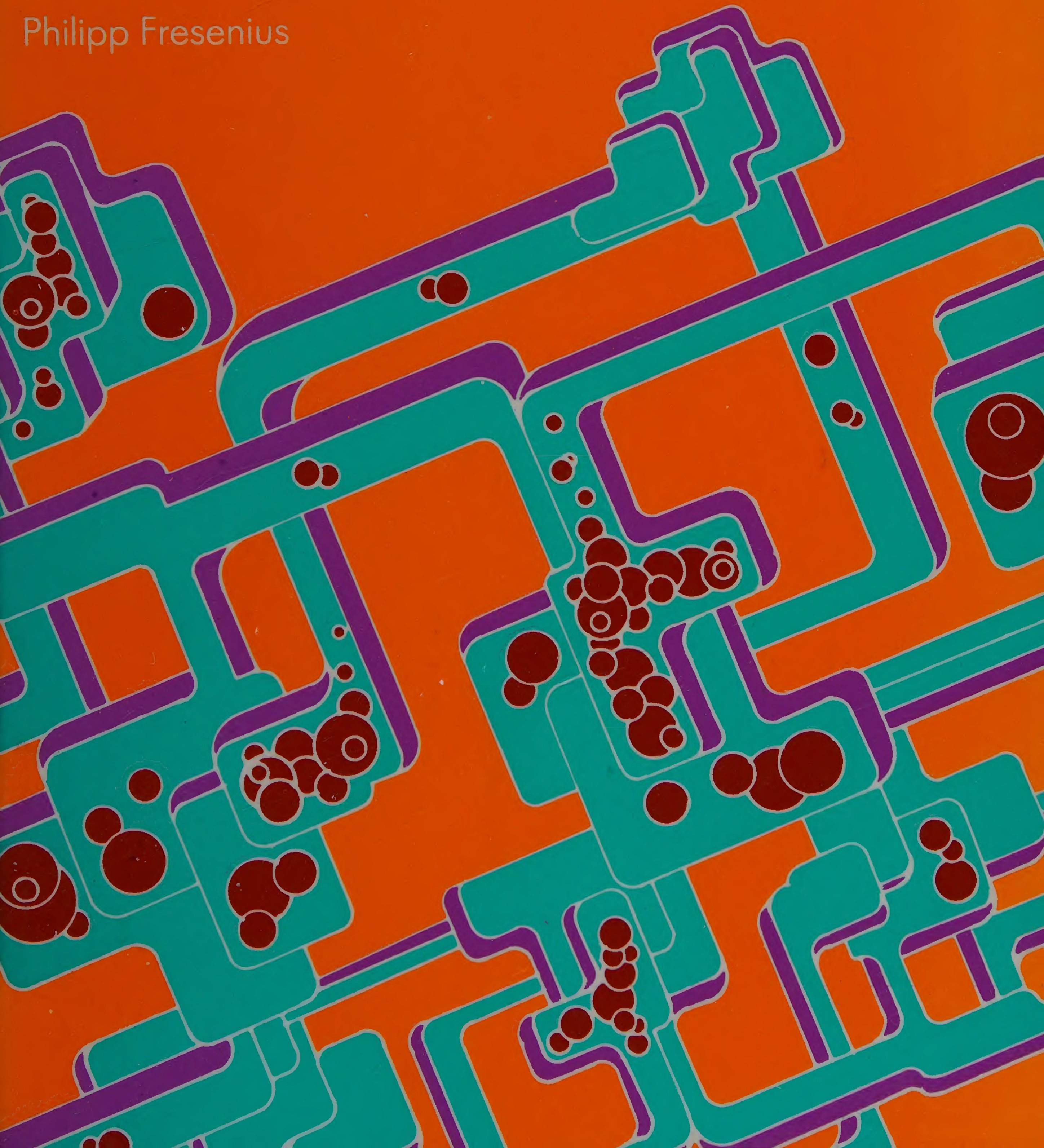
Ellis Horwood Series in ORGANIC CHEMISTRY

ORGANIC CHEMICAL NOMENCLATURE

introduction to the basic principles

Philipp Fresenius



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ORGANIC CHEMICAL NOMENCLATURE:
Introduction to the Basic Principles

PHILIPP FRESENIUS, formerly Lecturer in Pharmacy and Pharmaceutical Law, Karlsruhe University, and Director of the Government Pharmacy, Federal Republic of Germany, in collaboration with Professor Dr KLAUS GORLITZER, Professor of Pharmaceutical Chemistry, Technical University of Braunschweig, Federal Republic of Germany
Translator: A. J. DUNSDON, Laboratory of the Government Chemist, London
Translation Editor: E. W. GODLY, Laboratory of the Government Chemist, London

The second German edition of this distinguished work on systematic organic nomenclature has been extensively revised and up-dated by the author for the production of its first English edition. It considers all relevant current nomenclature systems and explains the general principles and the application of the IUPAC Rules and compares the naming of particular examples by alternative systems in current use. With many examples, the naming of organic chemicals, including natural products such as steroids, carbohydrates and carotenoids and various macromolecules is illustrated and comparison is made of IUPAC names with such names as those used by the WHO, ISO, Chemical Abstracts, European Pharmacopoeia and Beilstein.

The scope and authority of the book's scholarship is further widened by its coverage. Examples illustrating the areas of pesticide, pharmaceutical, biochemical, polymer, food and industrial chemicals, are given. The enormous task of arranging and presenting all this material has been carried out in this logical and easily accessible work of lasting reference value.

Readership: Manufacturers and workers in chemicals, biochemicals, pharmaceuticals, pesticides, fungicides; organic chemists, microbiologists, industrial chemists, pharmaceutical chemists.

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Preface to the English edition

For the English translation, the text of the second German edition has been revised. Formulae have been modified in a few cases. In the names of fused ring compounds, the lower case lettering in square brackets are italicised, in conformity with IUPAC rules.

The text has been augmented by:

(1) inclusion of basic instructions on nucleosides, nucelotides, and nucleic acids;
(2) expansion of Chapter III with a new version of the 'phane' nomenclature instructions; and
(3) the bringing together of the most important instructions on steric designations.

New in this edition is Chapter VII, an etymological glossary of chemical terms.

We have been fortunate to obtain the services of Dr Klaus Görlitzer, Professor of Pharmaceutical Chemistry at the Technical University of Braunschweig, whose cooperation has ensured that the book is cognizant of the latest developments in chemistry, and that it meets current educational needs.

Karlsruhe, Spring 1988 Philipp Fresenius

Preface to the second (German) edition

The approval which greeted the first edition, in 1981, of *Instructions in the principles of organic chemistry nomenclature*, has already made a second, improved, and significantly expanded edition necessary. The contents have been changed only so far as important corrections or rule changes have made necessary. The changes have been carried out while retaining the structure of the book.

Karlsruhe, Spring 1983 Philipp Fresenius

Preface to the first (German) edition

'Nomenclature' in organic chemistry signifies 'the study of scientific names' as well as the names themselves. The concept is also concerned in a wider sense with non-scientific (trivial) names. Nomenclature is not concerned with a fixed natural state, but seeks to express the existing order of the structural elements in a compound by means of a systematic (rational) description. 'Nomenclature' is thus seen to be system-dependent, and tied to conventions. 'Nomenclature' exists in various systems and, with the differences between these systems, is itself variable. If one nomenclature for a compound differs from another, it need not be incorrect, but may be the product of some other system. Different authors have been concerned with certain compounds, approaching them from contrasting standpoints, which has resulted in many compounds having a number of quite different names.

Between systematic and trivial names, there lie the so called semi-trivial (semi-rational) names, exhibiting a combination of trivial and systematic components. For example:

trivial: benzoic acid	*semi-trivial*: aminobenzoic acid (semi-rational)
trivial stem: prop *systematic ending*: ane	*semi-trivial*; propane

Many names, through decades of frequent use, have become practically systematic names, for example: aniline. A special kind of trivial name is provided by the international, non-proprietary, short names for individual pharmaceutical products, of the

World Health Organisation: *International non-proprietary names* (INN). These have been created for the purpose of easier, and also international, communication and for goods customs declaration purposes, for which the often long and complicated systematic names might not be suited. INN gives due consideration to the scope of the product groups and also to individual structural aspects of the specific compound.

The scientific names given for establishing the identity of materials (WHO/INN) generally follow the principles of the USA documentation journal, *Chemical Abstracts* (CA).

Thus, German (pharmaceutical) chemists, pharmacists, doctors, producers of pharmaceuticals, health authorities, and other interested parties are confronted today with scientific names which derive from the (not always identical) nomenclature principles of at least two great handbooks (Beilstein and CA). To these are added other possible names, based on neither of these sets of rules, or on none at all. Thereby nomenclature, expressed in any case in a synthetic language, becomes yet more complex, harder to communicate, and even harder to follow than it is intrinsically.

Efforts toward the creation of an international unified nomenclature, originating from the International Union of Pure and Applied Chemistry (IUPAC) have already achieved considerable success in moving toward a unified list. Such rules, however, have always been – and will always be – altered and adapted to developments. Many rules have also been discarded. Nomenclature has thus not settled into a stable condition but is, like any living language, in a state of continuous flux. Its significance increases along with the growing importance of synthetic organic compounds for many areas of life (health, medicines, cosmetics, poisons, environment, toxic substances, foodstuffs, preservatives, technology, agriculture, pest control, industry, worker-protection, etc.).

For any chemical compound, national and international institutions, work areas, and individuals concerned, a specific, unique, and universally recognised scientific name must be available by which to establish the certain identity of the material, whether it is a raw material, a finished or trade product for use in or on the body, or a waste product/pollutant.

Despite the inevitable complexity, the scientific names must be as simple as possible, correct, unambiguous, and not misleading. It must also permit recognition of the structure, and, as far as possible, it must reflect the structure faithfully. It is practically inevitable that, faced with scientific names, the non-chemist or non-expert will seek to make the nomenclature less daunting and more usable by means of simpler designations such as number codes or short-name systems.

An important step in the field of health services has been the substantial adaptation of the German edition of the European Pharmacopoeia (EP III) and of the German Pharmacopoeia 8, (DAB 8, Deutsche Artzneibuch 8) along the IUPAC guidelines. It is important, for the purposes of international alignment, that nomenclature creation and development is not to be confined to the sphere of influence of such handbooks†. There is also a nomenclature that develops from professional practice, and which must be taken into consideration.

† Formerly, as far as Germany is concerned, this was carried out by the *Chemische Zentralblatt* (Central Journal of Chemistry).

Thus, guidelines arising from the joint revision, by the IUB (International Union of Biochemistry) and IUPAC, are distinct from the IUPAC *Rules on organic chemistry*. This fact must be constantly restated.

The present introduction to the principles of organic chemistry nomenclature seeks to establish the balanced picture arising from all these circumstances. In essential matters, the notations in which it is expressed conform to IUPAC. These notations are generally not given special references. Special references, and 'divergent' notations, are given only where there is a particular reason, (e.g. CA, WHO, IUB, DAB 8). Many examples are provided with INN names, especially to meet the needs of those concerned with pharmaceutical chemistry. For the pure chemist, however, the examples are of interest in themselves. In some cases, reference only to the INN has been given (e.g. 'cf. INN'). This is the case where the chemical name under consideration concerns only part of the molecule which the INN covers. Individual simple nomenclature examples have not been checked as to whether or not the compound described is known. That would not affect the correctness of the nomenclature.

The 'Introduction' consists of chapters

I Hydrocarbons
II Heterocyclics
III Nomenclature procedure.

There is some disagreement in nomenclature circles with regard to the systematic nomenclature of compound classes with functional groups, therefore discussion of that system has been dispensed with. That type of compound will be cited in chapter III, but only to illustrate the nomenclature procedure under consideration there.

The material presented here, as well as being informative, is intended to promote appreciation of nomenclature problems, the correct recognition of a scientific name, and the ability to establish the name from the formula and vice versa. The student of nomenclature should not try to learn it by heart, but by reflection on, and understanding of the subject, to achieve independent facility in nomenclature. I hope that teachers and lecturers will find the necessary stimulus in this exposition.

Spelling is according to IUPAC: ethyl (not aethyl); ether (not aether); estrone (not oestrone). This is in accordance with 1979 usage.

Note that the aromatic rings in the formulae are, on principle, drawn with conjugated double bonds, and not with a circle representing the π or pi electron sextet. This is because the individual bonds with their numbering are needed for the name derivation, (e.g. 3,4-dihydro). Formulae are generally presented as projection formulae. Formulae and footnotes are separately numbered for each chapter, so that both begin with number 1, 2 . . . in each chapter.

My thanks go to Dr B. Langhammer of the Beilstein Institute for his friendly response to several enquiries on the Beilstein Handbook.

Karlsruhe, Spring 1981 Philipp Fresenius

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I

Hydrocarbons

1. ACYCLIC HYDROCARBONS

1.1 Saturated C_nH_{2n+2} (alkanes)

1.1.1 Unbranched

The first four members of the series have semi-trivial names

1	CH_4	Methane
2	H_3C-CH_3	Ethane
3	$H_3C-CH_2-CH_3$	Propane
4	$H_3C-CH_2-CH_2-CH_3$	Butane

The names are formed by combining a trivial part (meth-, eth-) and a systematic part (the ending -ane, indicating that the compound is saturated). Following members of the series are given systematic names. In these names, the ending -ane is combined with the Greek (sometimes also the Latin) numerical term for the number of C-atoms, in the chain.

5	C_5H_{12}	Pentane (EP) (European Pharmacopeia)
6	C_6H_{14}	Hexane
7	C_7H_{16}	Heptane
8	C_8H_{18}	Octane
9	C_9H_{20}	Nonane

10	$C_{10}H_{22}$	Decane
11	$C_{11}H_{24}$	Undecane
12	$C_{14}H_{30}$	Tetradecane
13	$C_{16}H_{34}$	Hexadecane
14	$C_{20}H_{42}$	Icosane [1](Eicosane?)
15	$C_{21}H_{44}$	Henicosane (Heneicosane?)
16	$C_{22}H_{46}$	Docosane
17	$C_{30}H_{62}$	Triacontane
18	$C_{33}H_{68}$	Tritriacontane
19	$C_{50}H_{102}$	Pentacontane
20	$C_{90}H_{182}$	Nonacontane
21	$C_{100}H_{202}$	Hectane

1.1.1.1 C_nH_{2n+1} *radicals (alkyls)*

In naming univalent radicals of these hydrocarbons, the 'ane' ending is replaced by 'yl'[2]

22 CH_4 Methane $CH_3\cdot$ Methyl

As a 'free radical', this carries an unpaired electron

23 $CH_3\cdot \,\hat{=}\, CH_3-$ (as a substituent, often written with a hyphen)

The 'yl' position (C- atom with the free valency) is given the locant 1, in numbering the chain.[3,4]

24 $\underset{4}{H_3C}-\underset{3}{CH_2}-\underset{2}{CH_2}-\underset{1}{CH_2}-$ Butyl

1.1.1.2 C_nH_{2n} *radicals (alkylidenes, alkylenes)*

The removal of one H-atom from the 'yl', that C-atom with a free valency, gives rise to a second free valency there. The divalent radical so produced is indicated by adding 'idene' to the 'yl' ending, so giving the ending 'ylidene'

25 $H_3C-CH=$ Ethylidene

26 $H_3C-CH_2-CH=$ Propylidene

1. The English spelling, with an I, was introduced in the IUPAC rules A (1979), and alignment on this spelling is followed in the German text.
2. In conjunction with [4], the use of a radical designation such as '2-Butanyl' (cf. formula 49) may be considered. The 'yl' position would be displaced thereby. (see formula 44, ref. IUPAC 1979 D-4.14)
3. Locant: in the nomenclature context, numbers or letters indicating the position of atoms or bonds in a molecule.
4. The possibility of allotting to other locants in the chain the 'yl' position is not yet decided.

Exception

27 $H_2C{=}$ Methylene

A divalent radical with two terminal 'yl' positions is indicated by the 'ylene' ending. The names

28 $-CH_2-$ Methylene

29 $-CH_2-CH_2-$ Ethylene

are used. However, for higher members of the series a multiplying prefix on the basis of methylene is used.

30 $-CH_2-CH_2-CH_2-$ Trimethylene

31 $-CH_2-CH_2-CH_2-CH_2-$ Tetramethylene and so on.

32 $H_3C-\underset{|}{C}H-CH_2-$ Propylene

This is retained, for the methyl-substituted ethylene radical (≡ methylethylene)

1.1.1.3 C_nH_{2n-1} *radicals (alkylidynes)*

A terminal trivalent radical is given the 'idyne' ending after 'yl':

33 $HC{\equiv}$ Methylidyne[5]

34 $H_3C-CH_2-C{\equiv}$ Propylidyne

1.1.1.4 Radicals of higher valency

Radicals of higher valencies, with free valencies at end or middle position C-atoms in a chain, are given corresponding endings with multiplying prefixes as necessary.

35 $H_3\overset{4}{C}-\underset{|}{\overset{3}{C}}H-\underset{|}{\overset{2}{C}}H-\overset{1}{C}H_2-$ 1,2,3-Butanetriyl

36 $H_3C-\underset{|}{C}H-\underset{\|}{C}-CH_2-$ 1,3-Butanediyl-2-ylidene

37 ${\equiv}C-CH_2-CH_2-C{\equiv}$ Butanediylidyne

1.1.2 Branched

In naming branched chains, the major chain is chosen by the following criteria:

(a) Longest chain.
(b) Chain with the greatest number of side chains.
(c) Chain with the lowest numbered locants for the side chains.

5 =C– 'methine group' replaces the obselete methenyl.

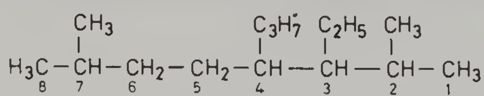
(d) Chain with the most C-atoms in the smaller side chains, that is to say that comparing the lists of side chains in ascending order, for each of the possibilities, the chain at the first point of difference is decisive.

(e) Chain with the smallest possible number of branched side chains.

The major chain will be consecutively numbered from one end to the other such that the branchings have the lowest locants possible.

The side chains designated as substituents (radicals), are put before the name of the main chain, in alphabetical order and following the appropriate locant number of the branch position. For several identical simple substituents, the multiplying prefixes (di, tri, tetra, penta, etc.; or, for identical composite substituents, bis, tris, tetrakis) are used. However, these prefixes are ignored in establishing the alphabetical order.

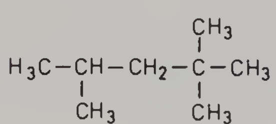
Composite radicals are arranged in order according to the first letter of the compounded name, e.g. dimethylpentyl under d.

38  3-Ethyl-2,7-dimethyl-4-propyloctane

The side chains have locants 2, 3, 4, 7. In the other direction they would have been 2, 5, 6, 7.

Retained trivial names for hydrocarbons (unsubstituted only):

39	$(H_3C)_2CH-CH_3$	Isobutane
40	$(H_3C)_2CH-CH_2-CH_3$	Isopentane

41  Isooctane (EP)
systematic: 2,2,4-Trimethylpentane

These names from the EP are of value as special pharmacopaeia designations.

42	$(H_3C)_4C$	Neopentane
43	$(H_3C)_2CH-(CH_2)_2-CH_3$	Isohexane

Retained trivial names for radicals (unsubstituted only)

44	$(H_3C)_2CH-$	Isopropyl (without locants, also 2-propanyl; syst.: 1-Methylethyl)
45	$(H_3C)_2C=$	Isopropylidene[6] (syst.: 1-methylethylidene)
46	$(H_3C)_2CH-CH_2-$	Isobutyl[6]
47	$(H_3C)_2CH-CH_2-CH_2-$	Isopentyl
48	$(H_3C)_2CH-CH_2-CH_2-CH_2-$	Isohexyl

6 alphabetic under I

49	$H_3C-CH_2-\underset{\displaystyle CH_3}{\underset{\vert}{CH}}-$	*sec*-Butyl[7] (2-Butanyl; syst.: 1-Methylpropyl (*sec*: secondary)
50	$(H_3C)_3C-$	*tert*-Butyl[7] (syst.: 1,1-Dimethylethyl) (*tert*: tertiary)
51	$H_3C-CH_2-\overset{\displaystyle CH_3}{\overset{\vert}{\underset{\displaystyle CH_3}{\underset{\vert}{C}}}}-$	*tert*-Pentyl[8] (syst.: 1,1-Dimethylpropyl)
52	$(H_3C)_3C-CH_2-$	Neopentyl[9] (syst.: 2,2-Dimethylpropyl)

1.2 Unsaturated[10]

1.2.1 C_nH_{2n} *Alkenes (Alkadienes etc.)*
C_nH_{2n-2} *Alkynes (Alkadiynes etc.)*

In naming unsaturated chains, the ‘ane’ ending of the corresponding saturated chain is changed to ‘ene’ (for 1 double bond), to ‘yne’ (for one triple bond). Further similar unsaturated molecules are named using ‘adiene’, ‘atriene’ etc. or ‘adiyne’, ‘atriyne’ etc. Where both kinds of unsaturation occur, these endings are combined in such a way that ‘ene’ precedes ‘yne’ in the name.

53	$\underset{5}{H_3C}-\underset{4}{CH_2}-\underset{3}{CH}=\underset{2}{CH}-\underset{1}{CH_3}$	2-Pentene
54	$\underset{5}{H_3C}-\underset{4}{CH}=\underset{3}{CH}-\underset{2}{CH}=\underset{1}{CH_2}$	1,3-Pentadiene
55	$\underset{6}{H_3C}-\underset{5}{CH_2}-\underset{4}{CH_2}-\underset{3}{C}\equiv\underset{2}{C}-\underset{1}{CH_3}$	2-Hexyne
56	$\underset{6}{H_3C}-\underset{5}{C}\equiv\underset{4}{C}-\underset{3}{CH_2}-\underset{2}{CH}=\underset{1}{CH_2}$	1-Hexen-4-yne

The numbering is so chosen that the C-atoms sharing the double bond are given the lowest locants possible. Double bonds, as far as is possible, lower than triple bonds. Only the lower of the two locants for the C-atoms of an unsaturated bond is cited.

57	$(\overset{8}{H_3C})_2\overset{7}{C}=\overset{6}{CH}-\overset{5}{CH_2}-\overset{4}{CH_2}-\overset{3}{\underset{\displaystyle CH_3}{\underset{\vert}{CH}}}-\overset{2}{CH}=\overset{1}{CH_2}$	3,7-Dimethyl-1,6-octadiene
58	$(\overset{16}{H_3C})_2\overset{15}{CH}-\overset{14-12}{(CH_2)_3}-\overset{11}{\underset{\displaystyle CH_3}{\underset{\vert}{CH}}}-\overset{10-8}{(CH_2)_3}-\overset{7}{\underset{\displaystyle CH_3}{\underset{\vert}{CH}}}-\overset{6-4}{(CH_2)_3}-\overset{3}{\underset{\displaystyle CH_3}{\underset{\vert}{C}}}=\overset{2}{CH}-\overset{1}{CH_3}$	3,7,11,15-Tetramethyl-2-hexadecene

7 alphabetic under B
8 alphabetic under P
9 alphabetic under N
10 cf. section 7. Carotenes

Retained trivial names are:

59	$H_2C{=}CH_2$	Ethylene (systematic: Ethene)
60	$H_2C{=}C{=}CH_2$	Allene (systematic: Propadiene)
61	$H_2C{=}CH{-}\overset{CH_3}{\overset{\mid}{C}}{=}CH_2$	Isoprene (systematic: 2-Methyl-1,3-butadiene)
62	$HC{\equiv}CH$	Acetylene (systematic: Ethyne)

1.2.2 Radicals

63	$CH_3{-}CH{=}\overset{2}{C}H{-}\overset{1}{C}H_2{-}$	2-Butenyl
64	${-}\overset{4}{C}H_2{-}\overset{3}{C}{\equiv}\overset{2}{C}{-}\overset{1}{C}H_2{-}$	2-Butyne-1,4-diyl, 2-Butynylene

The following trivial names for radicals are retained

65	$H_2C{=}\overset{1}{C}H{-}$	Vinyl (systematic: Ethenyl)
66	$H_2C{=}CH{-}\overset{1}{C}H_2{-}$	Allyl (systematic: 2-Propenyl)
67	$H_2C{=}\underset{CH_3}{\underset{\mid}{C}}{-}$	Isopropenyl (systematic: 1-Methyl-ethenyl) (unsubstituted only)
68	$H_2C{=}C{=}$	Vinylidene
69	$H_2C{=}CH{-}CH{=}$	Allylidene

From 'Isoprene' come

70	$H_3C{-}\overset{CH_3}{\overset{\mid}{C}}{=}CH{-}CH_2{-}$	Prenyl (systematic: 3-methyl-2-butenyl)
71	$H(H_2C{-}\overset{CH_3}{\overset{\mid}{C}}{=}CH{-}CH_2)_n{-}$	Multiprenyl (unspecific)
72	$H{-}(H_2C{-}\overset{CH_3}{\overset{\mid}{C}}H{-}CH_2{-}CH_2)_3{-}CH_2{-}\overset{CH_3}{\overset{\mid}{C}}{=}CH{-}CH_2{-}$ 8 7 6 5 4 3 2 1 12 11 10 9 16 15 14 13	Hexahydrotetraprenyl (= Phytyl)

The systematic name for the phytyl radical is (2*E*)–(7*R*,11*R*)–3,7,11,15-tetramethyl-2-hexadecenyl (cf. Phytol S p. 165)

2 CYCLIC HYDROCARBONS

2.1 Monocyclic [11]hydrocarbons

In naming saturated monocyclics (alicyclics, cycloalkanes) the name of the saturated acyclic hydrocarbon with the same number of C atoms is given the prefix 'cyclo'.

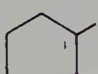
73
Cyclopropane

74
Cyclobutane

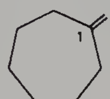
75
Cyclohexane (E.P.)

76
Cyclooctane

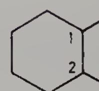
The procedure in naming radicals is analogous to that of section 1.



77
Cyclopentyl



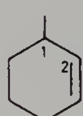
78
Cycloheptylidene



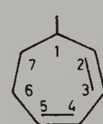
79
1,2-Cyclohexylene

For unsaturated monocyclics the corresponding procedure is followed. The 'yl-position' takes the locant 1 when numbering, and so the saturation locants precede the name.

80
Cyclopentene



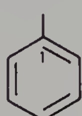
81
2-Cyclohexenyl



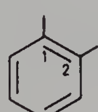
82
2,4-Cycloheptadienyl

The names derived from aromatic[12] groups (arenes) are retained:

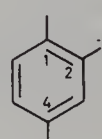
83
Benzene (EP)



84
Phenyl



85
o-Phenylene[13] (*m*-, *p*-)



86
1,2,4-Benzenetriyl

11 Polycyclics will be dealt with separately, see sections 2.2 Fused rings, 3 Bridges, 4 Spiro compounds, 8 Steroids, 9 Terpenes.

12 further, see under section 6.

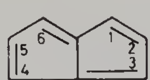
13 1,2-; 1,3-; and 1,4- positions on the benzene ring are designated *o*-(ortho), *m*-(meta) and *p*-(para) respectively; see also under sections 6 and 9.

2.2 Ortho-fused (condensed) hydrocarbons

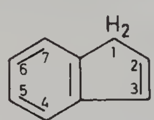
2.2.1 Trivial or semi-trivial names

2.2.1.1 The MNC systems (see p. 34)

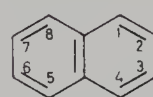
1) Pentalene (**87**)	2) Indene (**88**)	3) Naphthalene (**89**)
4) Azulene (**90**)	5) Heptalene (**91**)	6) Biphenylene (**92**)
7) *as*-Indacene (**93**)	8) *s*-Indacene (**94**)	9) Acenaphthylene (**95**)
10) Fluorene (**96**)	11) Phenalene (**97**)	12) Phenanthrene (**98**)
13) Anthracene (**99**)	14) Fluoranthene (**100**)	15) Acephenanthrylene
16) Aceanthrylene	17) Triphenylene (**101**)	18) Pyrene (**102**)
19) Chrysene (**103**)	20) Naphthacene (**104**)	21) Pleiadene
22) Picene (**105**)	23) Perylene (**106**)	24) Pentaphene (**107**)
25) Pentacene	26) Tetraphenylene	27) Hexaphene
28) Hexacene (**108**)	29) Rubicene	30) Coronene
31) Trinaphthylene	32) Heptaphene	33) Heptacene
34) Pyranthrene	35) Ovalene	



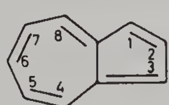
87
1. Pentalene



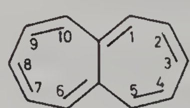
88
2. Indene (1*H*-Indene)



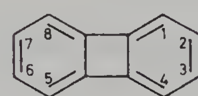
89
3. Naphthalene



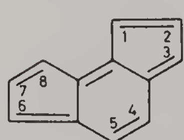
90
4. Azulene



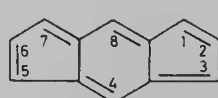
91
5. Heptalene



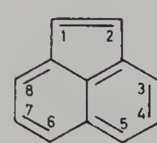
92
6. Biphenylene



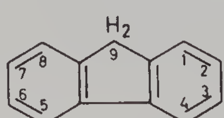
93
7. *as*-Indacene
(*as*- signifies 'asymmetric' contrast, *s*- symmetric cf. formula **94**)



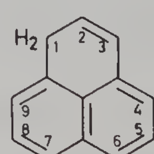
94
8. *s*-Indacene
(*s*- signifies 'symmetric' contrast *as*- asymmetric cf. formula **93**)



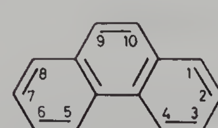
95
9. Acenaphthylene



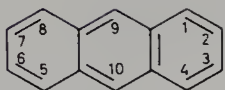
96
10. Fluorene(9*H*-Fluorene)



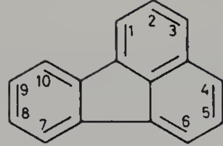
97
11. Phenalene



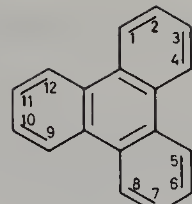
98
12. Phenanthrene



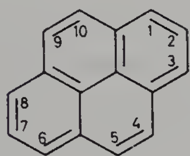
99
13. Anthracene



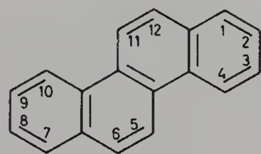
100
14. Fluoranthene



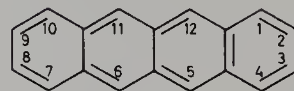
101
17. Triphenylene



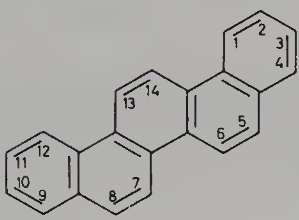
102
18. Pyrene



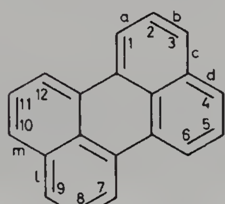
103
19. Chrysene



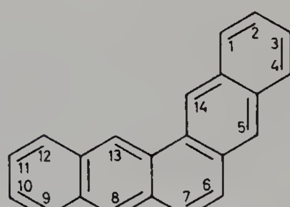
104
20. Naphthacene



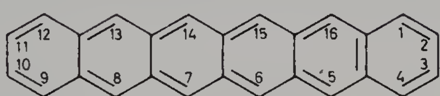
105
22. Picene



106
23 Perylene



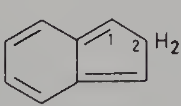
107
24. Pentaphene



108
28. Hexacene

The names end in 'ane' and indicate thereby that these hydrocarbons have the maximum number of non-cumulative[14] double bonds. Hydrocarbons which are straight, linear systems with 5 or more fused benzene rings take the ending 'acene' (25, 28, 33 of the list in 2.2.1.1) after the numerical indicator for the number of benzene rings. The ending 'aphene' occurs only with angular fused systems.

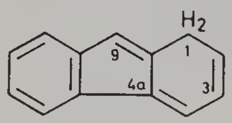
Instead of indene, the name 1*H*-indene is expressly used, to distinguish it from 2*H*-indene:



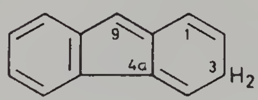
109
2*H*-Indene

14 Double bonds are differentiated as: cumulative $-HC=C=C=CH-$
conjugated $-HC=CH-CH=CH-$
isolated $-CH=CH-CH-CH=$

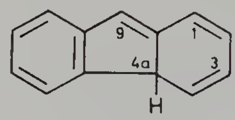
The corresponding isomers of fluorene, other than 9*H*-fluorene (**96**) are 1*H*-fluorene (**110**) and so on.



110
1*H*-Fluorene



111
3*H*-Fluorene



112
4a*H*-Fluorene

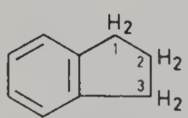
Some numerical prefixes need clarification. Biphenylene (**92**) is a three-ring system. The central four-member ring, which is not expressed in the trivial name, arises from the coming together of two (bi) *o*-phenylene radicals. In the four-ring system 'triphenylene' (**101**), three *o*-phenylene radicals form a central six-membered ring. In 'tetraphenylene' (number 26 of the list 2.2.1.1) four *o*-phenylene radicals form a central eight-membered ring.

In 'trinaphthylene' (number 31 of the list at 2.2.1.1) three 2,3-naphthylene radicals form a central six-membered ring.

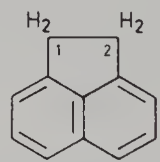
Anthracene (**99**), and phenanthrene (**98**) have individual numbering systems, which do not follow the rules for systematic allocation of locants ((compare anthracene (**99**) with naphthacene (**104**) and phenanthrene (**98**) with picene (**105**)).

2.2.1.2 Partly hydrogenated and hydrogenated hydrocarbons

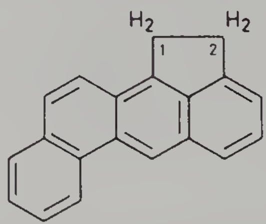
The following trivial names for partly hydrogenated hydrocarbons are used, for example:



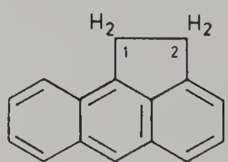
113
Indan



114
Acenaphthene



115
Cholanthrene

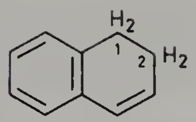


116
Aceanthrene

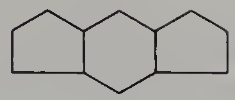
In the case of other hydrogenated hydrocarbons, hydro-prefixes are combined with the names of the hydrocarbons having the maximum number of non-cumulative double bonds:

1,2,-Dihydronaphthalene (**117**).

The method of numbering is chosen, from all the possibilities, which gives the lowest numbers for the hydrogenated bond. Compare, however the radical (**131**).



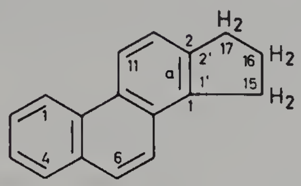
117



118

Perhydro-*s*-indacene (also Dodecahydro-*s*-indacene)

Full hydrogenation can be expressed by the prefix 'perhydro-'.



119

16,17-Dihydro-15*H*-cyclopenta[*a*] phenanthrene

or

1,2-Cyclopentenophenanthrene

In the first of these names the complete system is numbered with its own (1–17) numbering system. (Compare steroid hydrocarbons, section 2.8.) By this system, the ring position with the 'indicated H' (cf. p. 36) is given the smallest possible locant (in this case 15).

In the second name, the internal numbering for the whole system is not used; both partners are separately numbered (with and without primes). However, in the example, no further locants are required.

2.2.2 Systematic nomenclature

2.2.2.1 General principles

Where there is no acceptable trivial name for an ortho-fused or ortho- and peri-fused ring-system, the name is derived from the name of a component ring or ring-system (the base component) with prefixes designating the other components (attached components). If there is more than one prefix, the prefixes are arranged in alphabetical order before the base component name.

Prefix names are formed by changing the 'ene' ending of an hydrocarbon to 'eno' ending for an attached component.

The following exceptions are recognised:

Benzene: Benzo[15]
Acenaphthylene: Acenaphtho[15]
Phenanthrene: Phenanthro
Naphthalene: Naphtho[15]
Anthracene: Anthra
Perylene: Perylo[15]

15 Prefixes for attached components ending in 'a' (such as cyclopenta- etc.) or 'o', in the four cases noted, elide the final letter before base component names beginning with a vowel, (and also before a heterocyclic). This does not apply to a letter in square brackets coming after the prefix and designating a side. (see p. 35) (cf. footnote 4 page 74).

The base component should contain as many rings as possible, and should be as far as possible from the beginning of the list of names, number 1–35 (p. 30). The attached components should be as simple as possible.

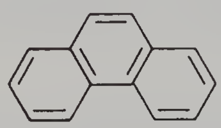
A fused ring-system must have at least 2 rings, each having at least 5 members including the shared atoms.

A fused ring-system of 2 rings with 2 shared atoms, or a system of several rings each sharing 2 atoms with the next ring, is an 'ortho-fused' system. The sum of the shared atoms in the system is then twice the number of shared sides.

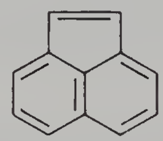
If a ring in a fused system shares two or more atoms with each of two or more rings of a series of neighbouring rings, then the system is 'ortho- and peri-fused', and the sum of shared atoms is less than double the sum of shared sides.

Prefix names for monocycles, other than Benzene, are 'cyclopenta-' 'cyclohepta-', 'cycloocta-' etc., each representing the attached component with the maximum number of non-cumulative double bonds (MNC).

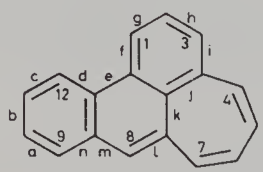
The ending 'ene' for a fused polycyclic system signifies the maximum number of non-cumulative double bonds in the system, comprising these rings. The ending 'ene', therefore, does not indicate simply 1 double bond.



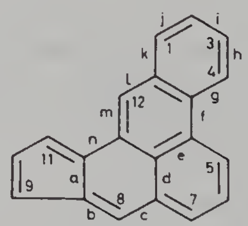
120
Phenanthrene ortho-fused
4 shared atoms
2 shared sides



121
Acenaphthylene: ortho- and peri-fused
4 shared atoms
3 shared sides



122
Cyclohepta[*jk*]phenanthrene
complete system numbering
on the inside

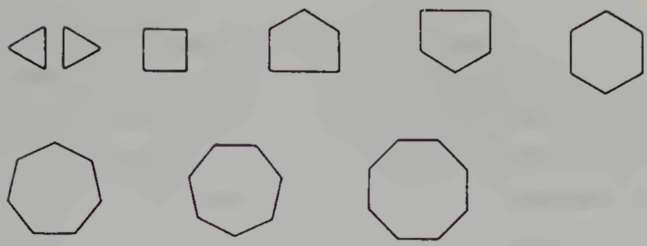


123
Benzo[*de*]cyclopent[*a*]anthracene
Attached components in alphabetical order; complete system numbering on the inside, (Anthracene 1,2=*a*;4a, 10=*e*; 5,6=*h*)

2.2.2.2 Designation of a fused system

(a) *Representation and arrangement*

The component rings of a fused polycyclic system are, for the purposes of nomenclature procedure, normally drawn as follows:



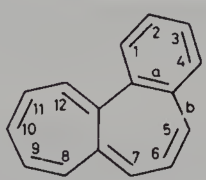
The fused ring system is so arranged that (1) as many rings as possible are in the horizontal row, and then (2) as many rings as possible are in the upper right quadrant

124

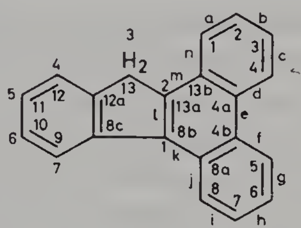
In the lower left quadrant there should be as few rings as possible.

(b) *Naming*

For unambiguous naming of a fused ring-system, and to distinguish between isomers, the peripheral sides of the base component are designated with lower case italic letters[16], in such a way that side 1 → 2 of the established numbering is designated *a*, the following side *b*[17], then *c*, and so forth. The attached components are given their customary numbering, and the characteristics of a side common to both attached and base components are shown by both indicators in square brackets, between the prefix and the base component name. The square brackets indicate that the figures enclosed refer not to the system numbering, but to the numbering of the components.



125
Benzo[*a*]heptalene



126
13*H*-Indeno[1,2-*l*]phenanthrene
(complete system numbering on the side)

Side *a* of the phenanthrene component of the system, as explained, corresponds to side 1 → 2 of the phenanthrene numbering. Coincidentally, this is also side *a*, side 1 → 2, in the complete system numbering. Side *l* in the direction *k-l-m*, is fused to side 1 → 2 of the indene attached component. Letters and numbers are chosen, in accordance with the methods for base component and attached component, to be as low as possible. The

16 IUPAC sets this in italics, without any corresponding rule-text.
17 The regular counting sequence; for others see, for example, anthracene. (see formulae 99 and 123)

fact that position 13 in the complete system numbering is at the same time the position of the indicated *H*, does not mean that this position in the indene component must be numbered locant 1 (cf. formula **88**).

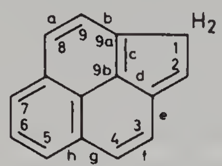
A second letter indicator of a side of the base component is not separated by comma within the square brackets if it refers to the same attached component (cf. formulae **123, 127**).

(c) *Numbering (complete system numbering, Patterson ring-numbering, autonomous numbering)*

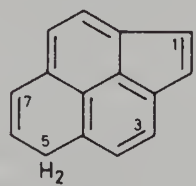
The correct orientation having been established, numbering begins at the C-atom (excluding atoms engaged in ring-fusion) which is in the furthest left position (next to a point of ring-fusion), of the furthest right ring in the upper right quadrant. From this number 1, all ring atoms not engaged in ring-fusion are numbered consecutively clockwise.

C-atoms engaged in ring-fusion take the number of the preceding peripheral C-atom with the addition of a lower case letter for each of these C-atoms as they arise in unbroken sequence.

C-atoms in the interior of the system take the number of the highest numbered periphery C-atom which they follow, with the addition of a letter.



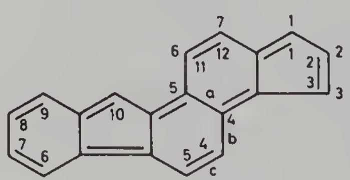
127
1*H*-Cyclopenta[*cd*]phenalene



128
5*H*-Cyclopenta[*cd*]phenalene

Isomeric condensed ring hydrocarbons having the maximum number of non-cumulative double bonds, can often be distinguished from one another by the position of *H*-atoms in the structure (indicated *H*, put in italic script; added-*H*). The *H* follows the relevant locant, and precedes the name of the parent ring system.

In the preceding examples, the ring-fusion sites are such that the numbering (not cited in the name) of the attached component and the letter designations of the base component, proceed in the same direction. Frequently however they proceed in opposite directions. This is indicated by inverse sequence of the numbers in square brackets.

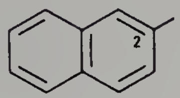


129
Indeno[5,4-*a*]fluorene

Side a (→ b) coincides not with side 4 → 5, but with side 5 → 4. Inside: the numbering of the complete system.

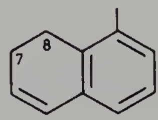
2.2.2.3 Radicals

Radical names take the normal endings (-yl, -ylene, ylidene) added onto the name of the hydrocarbon, after elision of the final 'e' of the 'ene'. The following contractions are permitted:



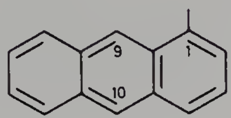
130

e.g. 2-Naphthyl from naphthalene



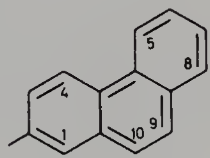
131

7,8-Dihydro-1-naphthyl (lowest possible locant for the 'yl' position) (compare however the same compound without a free valency, formula **117**)



132

e.g. 1-Anthryl from anthracene



133

e.g 2-Phenanthryl from phenanthrene (Compare formula **150**)

Normal radical name formation gives, for example:

x-Fluorenyl (from fluorene)
x-Naphthacenyl (from naphthacene)
x,y-Pentalenylene (from pentalene)
(here and in similar cases, di- radical designation 'diyl' is allowed instead of 'ylene')
1-Indenylidene (from indene)
x,y,z-Chrysenetriyl (from Chrysene)

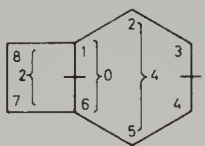
3 BRIDGED HYDROCARBONS[18]

The carbon atom skeleton of a bridged hydrocarbon consists of 2 single-atom bridge-heads, and of three or more bridges, each bridge having zero or more members.

3.1 Saturated hydrocarbons

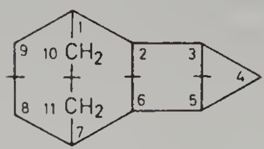
Bridge systems are differentiated into bicyclic or polycyclic systems according to the number of rings. The number of rings is established in each case by the number of scissions required to convert that ring-system into an open chain compound. The name of the ring-system consists of the name of the open chain compound with the same number of C-atoms, preceded by the appropriate numerical prefix with 'cyclo', for example, 'tetracyclo-'.

18 see also section I.9, p. 59.

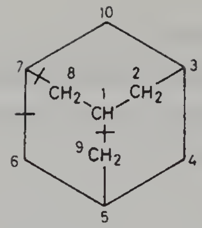


134
Bicyclo[4.2.0] octane

– 2 scissions
(4 members: 2,3,4,5;
2 members: 7,8
bridgeheads: 1,6)



135
Tetracyclo[$5.2.2.0^{2,6}.0^{3,5}$]
-undecane
– 4 scissions
(5 members: 2,3,4,5,6;
2 members: 8,9; 10, 11
bridgeheads: 1,7)



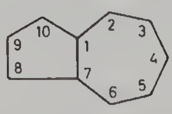
136
Tricyclo[$3.3.1.1^{3,7}$]
-decane = Adamantane
– 3 scissions
(3 members: 2,3,4;
6,7,8; 1 member 9;
10 bridgeheads: 1,5)

The numbers of bridge members, excluding the bridgehead atoms, are given in square brackets between the numeric-cyclo prefix and the stem name. A polycyclic system is first determined and numbered as a bicyclic system (the three largest bridges between the bridgeheads). The two largest bridges form 'the main ring' and the third largest 'the main bridge'. The secondary (that its, the further or supplementary) bridges follow, the locants[19] for each of these bridges are shown as superscripts, in ascending order, of the characterised bridge atoms of the bicyclic system which they join. The lowest possible numbering for the locants is chosen. The sum of the numbers on the baseline in the square brackets is equal to the number of bridge atoms, and this sum plus two (for the bridgeheads of the bicyclic system) is equal to the total number of C-atoms in the stem name of the bridged hydrocarbon.

In the square brackets, the figures for bridge members are separated by full stops, being treated as numbers and not locants. The superscript figures for the secondary bridges are locants and are separated by commas.

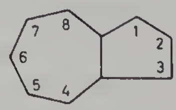
The system-numbering begins at one bridgehead with number 1, and proceeds through the largest bridge to the second bridgehead, and from there back through the second largest bridge to the first bridgehead again. From there, the numbering continues through the third largest bridge, the 'main bridge', to the second bridgehead again. Thereby the bicyclic system is established. The numbering then goes to the secondary bridges; the bridge atom next to the highest numbered ring atom takes the next higher available locant. The locants therefore for each bridge are numbered in increasing order, in the direction from the higher to the lower ring-atom encountered. The secondary bridges are considered in the order of their decreasing size.

It must be noted that the numbering of one and the same ring system is different according to whether it is considered as a bridged ring-system, or a fused ring-system.



137
Bicyclo[5.3.0] decane

or



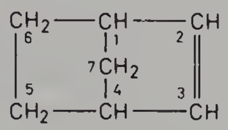
138
Perhydroazulene

19 see III.2.4, p. 99.

Radicals of saturated bridged hydrocarbons are named according to the usual procedures (see under I.1. and I.2.). The ring atom with the free valency takes the lowest possible number within the framework of the estabilished numbering of the system.

3.2 Unsaturated hydrocarbons

Unsaturation positions in bridged hydrocarbons are indicated by the appropriate endings (see under I.1.2). The unsaturated bond is given the lowest possible number.



139
Bicyclo[2.2.1.] hept-2-ene

In radicals of unsaturated bridged hydrocarbons, the ring C-atom with the free valence is given the lowest possible number within the framework of the established numbering of the system.

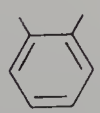
Bicyclo[2.2.2.] hept-5-en-2-yl (cf. **139**, however)

3.3 Fused ring-systems with additional bridges

When fused ring-systems (cf. I.2.2.) have additional bridges, these are added to the ring-system name by means of special 'bridge prefixes'. The bridge prefixes are formed by replacement of the final 'e' of the name of the corresponding hydrocarbon with 'o'.

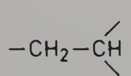
140	$-CH_2-$	Methano	**141**	$-CH=$	Metheno
142	$-CH_2-CH_2-$	Ethano	**143**	$-CH=CH-$	Etheno
144	$-CH_2-CH_2-CH_2-$	Propano	**145**	$-CH_2-CH=CH-CH_2-$	[2] Buteno

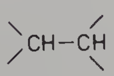
Note:
Benzeno (*o*-, *m*-, *p*-,)[20]



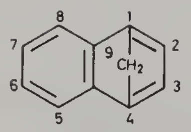
146
o-Benzeno (not *o*-Phenylene)

In some cases the 'yl' -names also are used for bridges.

147  Ethanylylidene

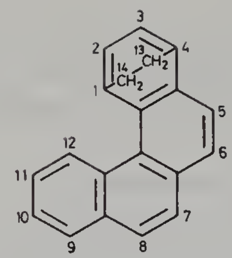
148  Ethanediylidene

20 see under I.2. page 29 and page 45.



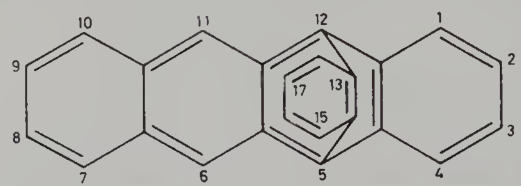
149

1,4-Methanonaphthalene
(radical . . . .naphthalen-x-yl)



150

1,4-Ethanobenzo[*c*]phenanthrene
(radical . . .phenanthren-x-yl)



151

5,12-*o*-Benzenonaphthacene
(radical . . . .naphthacen-x-yl)

The bridge is numbered by following on the numbering of the fused ring-system, such that the bridge atom nearer the ring-atom with the higher number has the lowest number of all the bridge atoms. If there are a number of bridges in the same hydrocarbon, they are cited in alphabetical order. Bridge prefixes are not separated from the stem name.

4 SPIRO-HYDROCARBONS

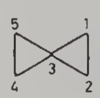
Spiro-hydrocarbons are polycyclic hydrocarbons in which one or more ring-pairs have just one C-atom in common, which is designated the 'spiro atom', (free spiro union).

If the spiro atom forms part of a further ring-system, the rules for ortho-, or ortho- and peri- fused polycyclics apply.

4.1 Spiro- prefix

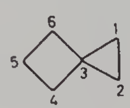
4.1.1 Simple spiro- (mono-spiro) hydrocarbons

The first part of the name (spiro prefix = 1 C-atom) is followed by the numbers of the other carbon atoms in each ring (each ring −1 for the spiro atom) in square brackets, in ascending order. Following the brackets is the hydrocarbon name appropriate for the sum of C-atoms in both rings, the spiro atom included.



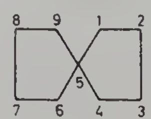
152

Spiropentane



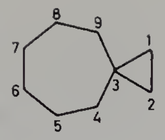
153

Spirohexane

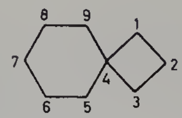


154

Spiro[4.4]nonane



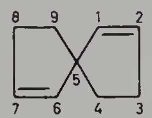
155
Spiro[2.6]nonane



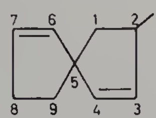
156
Spiro[3.5]nonane

In both the first examples, more details of the ring composition in square brackets would be redundant, since no isomeric spiro structures are possible.

Numbering is begun in the smaller ring, next to the spiro atom clockwise, including the spiro atom, without changing direction. Unsaturated bonds are given the lowest possible number. With radical numbering, the direction of counting is so chosen as to give the unsaturated bonds the lowest possible locants after the lowest free valence locant has been assigned.

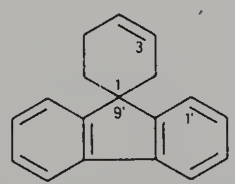


157
Spiro[4.4]nona-1,6-diene



158
Spiro[4.4]nona-3,6-dien-2-yl

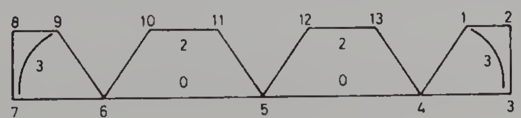
If, instead of a monocyclic, a polycyclic compound is one of the spiro partners, then the names of the two partners are put in the square brackets in alphabetical order. The established number-order of each partner is retained. The second partner is numbered with primes.



159
Spiro[3-cyclohexene-1,9′-fluorene]

4.1.2 Multi-spiro compounds (Di-, Tri-. . . .spiro compounds)

The names are prefixed with 'X-spiro' with the number of C-atoms in the individual sectors, combined with the appropriate hydrocarbon name corresponding to the combined C-total (sector numbers + spiro atoms).

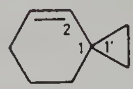


160
Trispiro[3.0.0.3.2.2]tridecane

4.2 Spiro-infix

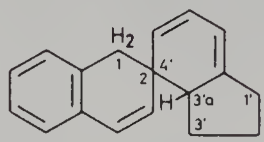
4.2.1 Simple spiro compounds

'Spiro' is put between the names of the two components, with the larger component first.



161
2-Cyclohexenespirocyclopropane

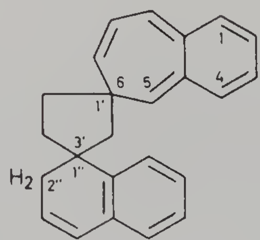
When necessary, the position of the spiro atom is established by the locants of each partner with reference to the shared spiro atom being included, before and after 'spiro'.



162
Naphthalene-2(1*H*)-spiro-4′(3′a*H*)indane[21]
1,2-Dihydronaphthalene-2-spiro-4′-(3′a,4′-dihydroindan)

4.2.2 Multi-spiro compounds

The procedure is applicable also for more than 1 spiro atom, the third ring-system following and numbered with double primes. The name begins with the most senior system.



163
6*H*-Benzocycloheptene-6-spiro-1′-cyclopentane-3′-spiro-1″(2″*H*)-naphthalene[21]
6*H*-Benzocycloheptene-6-spiro-1′-cyclopentane-3′spiro-1″-(1″,2″-dihydronaphthalene)

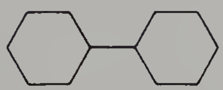
5 LINKED RINGS

5.1 Identical rings or ring-systems: 'ring-series with linking bonds' (ring assemblies, ring sequences)

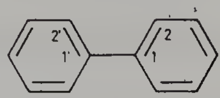
If two or more identical rings or ring-systems are directly joined by single or double bonds, according to the number of units combined the corresponding numerical prefix

21 The IUPAC rules give no example of this type and no relevant directions. The second name is permissible according to IUPAC.

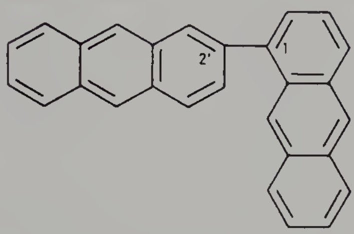
bi- (2), ter- (3), quater- (4), quinque- (5), sexi- (6), septi- (7), octi- (8), novi- (9), deci- (10) is applicable. The prefixes are put before the stem name. With the 'bi-' prefix, the stem names ending in 'ane', 'ene', or 'yl' are used. With the other prefixes, the 'yl' ending is not used except in the case of 'phenyl'.



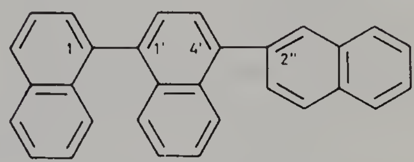
164
Bicyclohexane, Bicyclohexyl



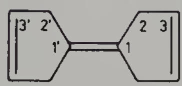
165
Biphenyl, radical: x-Biphenylyl
x,y′-Biphenylylene
3 rings e.g. 1,1′: 2′,1″-Terphenyl
= *o*-Terphenyl



166
1,2′-Bianthracene
1,2′-Bianthryl
(the lower numbered bonding position is unprimed)



167
1,1′:4′,2″-Ternaphthalene



168
a) (1,1′-)Bi-3-cyclopentenylidene
b) $\Delta^{1,1'}$-Bi-3-cyclopentenylidene[22]

(a) The double bonds in both rings having been cited as number 3, the double bond linking the rings is unambiguously 1,1′ as a reference point to the 3,3′. Citing the 1,1′ locants in the name is therefore superfluous and serves here only to illustrate the procedure.

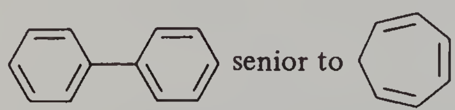
When linked cyclic systems (ring assemblies) are substituted, the substituents are, as usual, cited alphabetically (butyl, ethyl, hexyl, methyl. . .) and the lowest possible locants are chosen for the relevant ring-positions. If the same substituent is present more than once, the locants are cited in ascending order, a primed locant following immediately after an unprimed locant of the same numerical value; that is, the primed locant being considered 'higher' than the unprimed locant of the same number.

22 Δ (delta) with superscript locants symbolizes a double bond between 2 rings.

5.2 Non-identical rings or ring-systems

Where non-identical rings or ring-systems are joined by a single or double bond, one unit is treated as the parent compound, the other as its substituent. The parent compounds are ranged in order of precedence as follows (cf. III 2.3.2, p. 97):

(a) The ring-system with the most rings



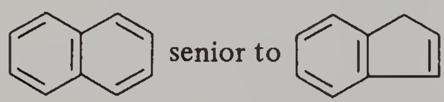
169

Biphenyl senior to Cycloheptatriene

170

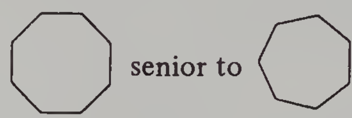
Fluorene senior to Azulene

(b) The ring-system with the largest component ring, or, between single rings, the largest.



171

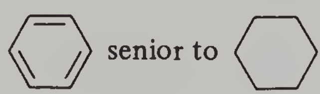
Naphthalene senior to Indene



172

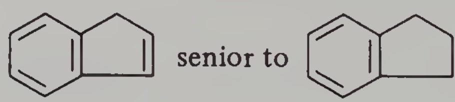
Cyclooctane senior to Cycloheptane
(Cycloheptylcyclooctane)

(c) The ring or ring-system with the highest degree of unsaturation.



173

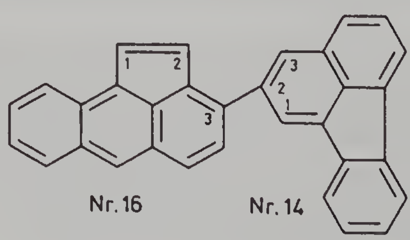
Benzene senior to Cyclohexane
(Cyclohexylbenzene)



174

Indene senior to Indane

(d) The ring-system with the higher number in the list 1–35 (see I.2.2.1, p. 30).

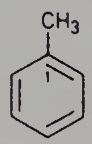


175

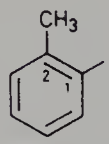
3-(2-Fluoranthenyl)aceanthrylene
No. 14 No. 16

6 RINGS WITH SIDE-CHAINS

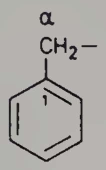
6.1 Trivial names for hydrocarbons and radicals



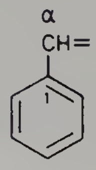
176
Toluene



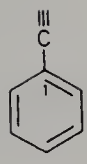
177
o-Tolyl



178
Benzyl

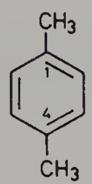


179
Benzylidene

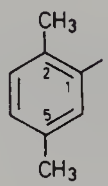


180
Benzylidyne

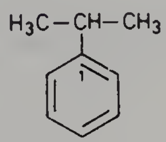
Positions 1,2 1,3 1,4 of the benzene ring can be designated *ortho*(*o*-)/*meta*(*m*-)/*para*(*p*-)[23]



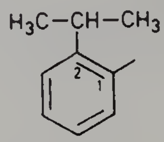
181
1,4-Xylene *p*-xylene



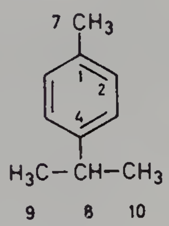
182
2,5-Xylyl



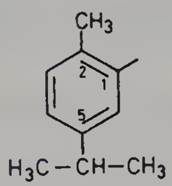
183
Cumene
isopropylbenzene



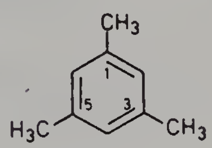
184
o-Cumenyl
2-isopropylphenyl



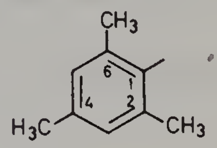
185
p-Cymene



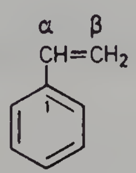
186
5-Isopropyl-
2-methylphenyl



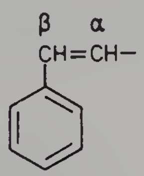
187
Mesitylene



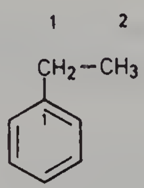
188
Mesityl
2,4,6-Trimethylphenyl



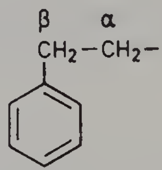
189
Styrene (locants)
Vinylbenzene
Ethenylbenzene



190
Styryl[24]
2-Phenylvinyl
2-Phenylethenyl

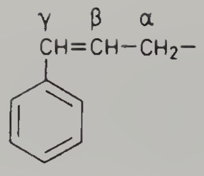


191
Ethylbenzene

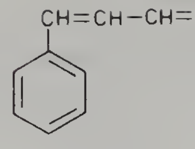


192
Phenethyl(α, β)
2-Phenylethyl

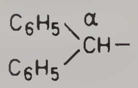
23 see also pp. 29, 39, 59.
24 Note *cis*/*trans* isomerism (*Z*) (*E*); from 189 to 190 change-over of α and β.



193
Cinnamyl[25]; 3-Phenyl-2-propenyl
3-Phenylallyl

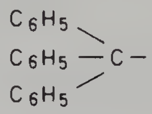


194
Cinnamylidene
3-Phenyl-2-propenylidene
3-Phenylallylidene

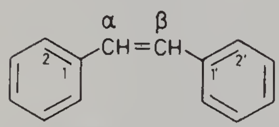


195
Benzhydryl
α-Phenylbenzyl ←(WHO)→
Diphenylmethyl

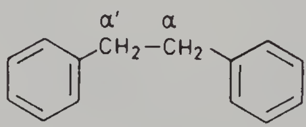
196
Benzhydrylidene
α-Phenylbenzylidene
Diphenylmethylene



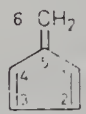
197
Trityl
Triphenylmethyl



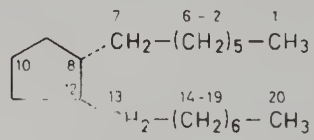
198
Stilbene[26] (locants)
1,2-Diphenylethylene



199
Bibenzyl (locants)
1,2-Diphenylethane

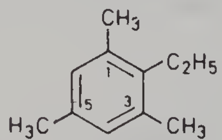


200
Fulvene (locants)
Methylenecyclopentadiene

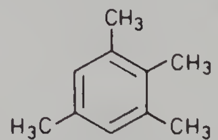


201
Prostane

If a substituted benzene ring compound, which has a trivial name, is subject to further substitution with the same substituent, the trivial name gives way to the systematic.



202
2-Ethylmesitylene but



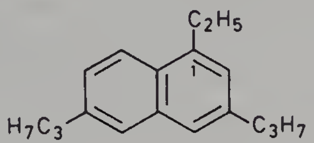
203
1,2,3,5-Tetramethylbenzene
(not Methylmesitylene)

25 IUPAC rule A 13.3 gives no indication whether a definite steric arrangement is established at the double bond β/γ in the trivially named radical.

26 Note *cis/trans* isomerism.

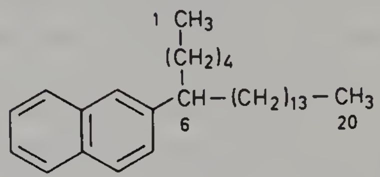
6.2 Other

Where there are no trivial names for cyclic hydrocarbons with side chains, systematic substitution names are formed. In general the procedure with rings and chains of different sizes is to choose as the base component that part with the greatest number of C-atoms, the other parts being substituents. However, one can so construct the name that the stem compound contains the greatest number of substituents. A name should be chosen which is the simplest possible which accords best with the chemical viewpoint.



204

1-Ethyl-3,6-dipropylnaphthalene
(bigger ring, small chains)



205

6-(2-Naphthyl)icosane (see p. 17)
(smaller ring, big chain)

$C_6H_5-CH=CH-CH_2-CH_2-C_6H_5$

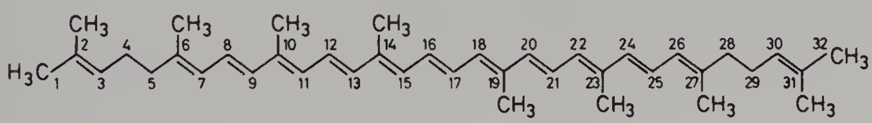
206

1,4-Diphenyl-1-butene[27]
(simplest name)

7 CAROTENOID HYDROCARBONS (CAROTENES)†

7.1 General principles

The red vegetable colour material Lycopene can be regarded as the parent substance for the carotenes.



Lycopene $C_{40}H_{56}$
(= 8 Isoprene units C)
(cf. I.1.2.2, p. 28)

207

2,6,10,14,19,23,27,31-Octamethyldotriaconta-
2,6,8,10,12,14,16,18,20,22,24,26,30-tridecaene (from I.1.2.1, p. 27)

The two middle methyl substituents (on the C-atoms 14 and 19 of the 1–32 chain) are in a 1/6 positional relationship to one another. From 14 and 19 to the ends of the chain there are 3 further methyl substituents, in 1/5 positional relationships at each end of the chain (at C-atoms 10,6,2 and 23,27,31 respectively).

The molecule therefore has 20 C-atoms in each of the two symmetrical halves. Of the 13 double bonds in the molecule, the 11 middle ones are in a conjugated row with an all-*trans*-configuration. Each end of this structure can be considered to have a group of

27 Note the *cis/trans* isomerism

† (= Tetraterpene) [*Eur. J. Biochem.* **25** 397 (1972)].

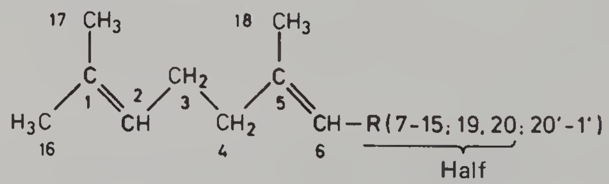
9 C-atoms (including methyl group substituents; the chain atoms 1 to 7, and 32 to 26, respectively being considered as discrete parts of the chain, each with two methyl group substituents), which in carotenes and their derivatives can be cyclised.

The special features of the structure, and the fact that many natural materials containing oxygen in various functions are derived from these hydrocarbons, led to the development of a special nomenclature in which the parent name 'Carotene' was applied to the hydrocarbons and Greek letter prefixes combined with it to indicate particular end-groups. The numbering for this special nomenclature indicates that the symmetry of the molecule is taken into account and each half of the structure is separately numbered. The numbers are therefore duplicated, and those in the right half are primed. The locant 1 in this special carotene nomenclature thus denotes not the end position C-atom in the chain shown above, but the corresponding number-2 atom in that chain. The basis for this is that C-atom 1 in the above chain is regarded as a substituent in the cyclic form of the end-group.

From this consideration, even in the open chain form, it is numbered together with the substituent CH_3-groups following on the numbering of the chain in ascending order.

In the carotene special nomenclature therefore the molecule is divided into two parts, each of which consists of an open chain or a partly cyclised chain (1 to 15, and 1′ to 15′) and 5 substituent CH_3-groups (16 to 20, and 16′ to 20′). The Greek letter prefixes appear separated for each of the two end-groups, so that 2 different or 2 similar such prefixes are given, for non-identical end-groups and for identical end-groups respectively.

7.2 End-groups with 9 C-atoms and their numbering

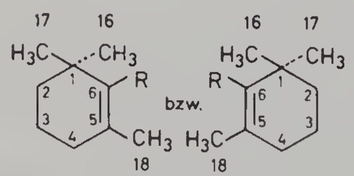


208

ψ(psi)

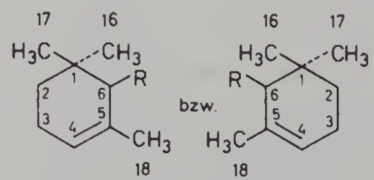
C(16) is *trans* to C(3)

C(17) is *cis* to C(3)



209

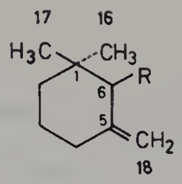
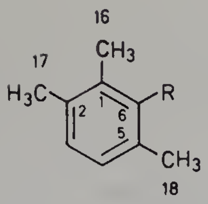
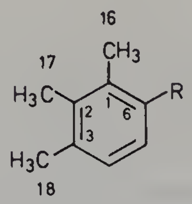
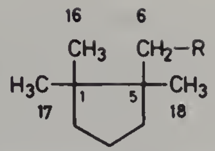
β (beta)



210

ϵ (epsilon)

The numbering of both (so-called gem(inal)) CH_3-groups at C(1), as C(16) or C(17) arises from the drawn presentation of the rings in the manner depicted.

211	212	213	214
γ (gamma)	ϕ (phi)	χ (chi)	κ (kappa)

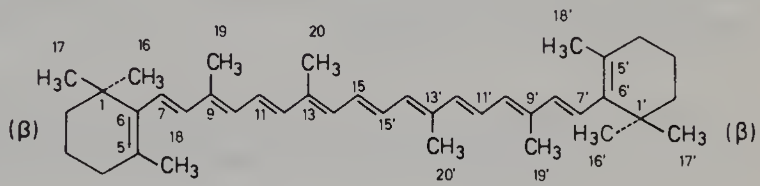
Two different prefixes would be arranged in the order of the Greek alphabet. That is β, γ, ϵ, κ, ϕ, χ, ψ.

7.3 Designations as carotenes[28]

(a) The $C_{40}H_{56}$ Lycopene discussed at I.7.1 is named ψ, ψ-Carotene in the context of the special nomenclature, both end groups being ψ-groups.

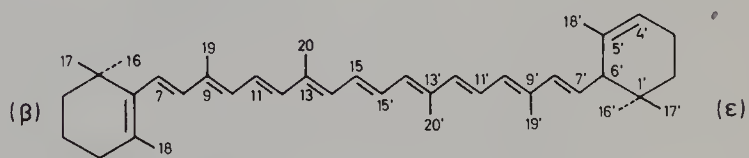
(b) Structural isomers with Lycopene are:

1. β,β-Carotene (formerly β-Carotene)



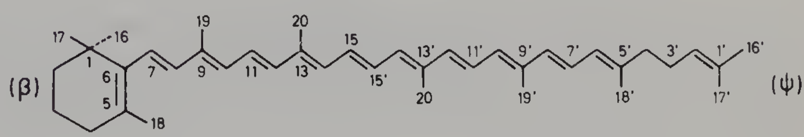
215

2. β,ϵ-Carotene (formerly α-Carotene)



216

3. β,ψ-Carotene[29] (formerly γ-Carotene)



217

4. ϵ,ψ-Carotene (formerly δ-Carotene)

28 The row of conjugated double bonds in the carotene chain (7-7′) is *trans*-configured ('all-*trans*'). In ψ,ψ-Carotene this is so for the row (5-5′) (see formula **208**). If in a particular case there is a '*cis*'-configuration, this must be expressed in the name, for example Bixin: 6′-Methyl hydrogen 9′-*cis*-6,6′-diapocarotene-6,6′-dioate.

29 The end-group ψ is for acyclic groups and not for groups with an opened ring.

(c) Further examples

3′,4′-Dihydro-β,ψ-carotene trivial: Torulene
7,8,11,12,15,7′,8′11′,12′,15′-Decahydro-ψ, ψ-carotene[30] trivial: Lycopersene

In Carotene nomenclature primed and unprimed locants are each ranged in ascending order, and then the primed are placed after the unprimed.

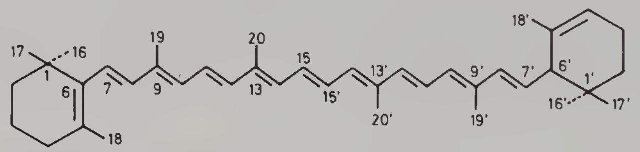
7.4 Other applicability

From the basis of the stem name 'Carotene' other alterations to the molecule can be expressed, for example, ring-opening: prefix 'seco'; demethylation (also ring-contraction): prefix 'nor' (cf. steroids I.8., terpenes I.9.).

7.5 Further special nomenclatures for carotenes

7.5.1 retro-*Nomenclature*

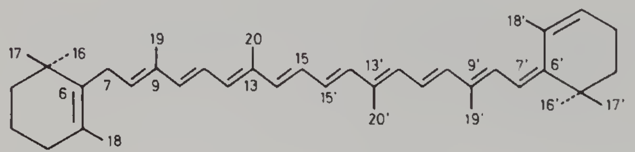
This deals with the shift, by one position, of the conjugated unsaturated system in the region delineated by two locants.



β,ε- Carotene

218

bond shift



219

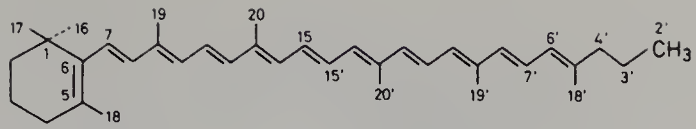
6′,7-*retro*-β,ε-Carotene

6′ gave up a proton, 7 received a proton.

7.5.2 Apo-nomenclature

This type of nomenclature allows for the case where an end part of the carotene molecule is removed, and the new end position is a saturated C-atom. The 'apo' prefix is preceded by a locant from the original molecule's numbering, indicating the C-atom which is at the end-position of the newly formed compound. If both ends of the original molecule are modified, the prefix 'diapo' is used with two locants preceding it.

30 'Hydro' prefixes in Carotenoid nomenclature are treated basically as inseparable, and thereby are not in alphabetical order, in contrast to other prefixes. (see p. 101)



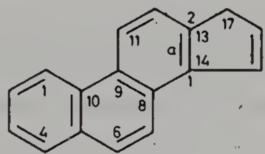
220
2′-Apo-β,ψ-carotene
(the C-atoms 1′ with 16′, 17′ of the ψ end-group are removed)
(cf. formula 217)

Greek letters are needed for the unaltered end-group but, for the shortened end-group only if the locant associated with this is 5 (or 5′) or less, in which case it can only be ψ. (cf. Retinol S. p. 166, Ionone p. 172).

8. STEROID HYDROCARBONS[31,32,†]

8.1 Unsubstituted

Steroid hydrocarbons are derived from the ring-system with the maximum number of conjugated double bonds with the ring numbering:



221
17*H*-Cyclopenta[*a*]phenanthrene

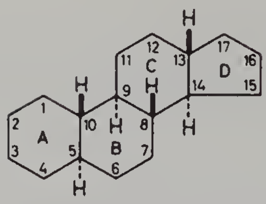
modified from the normal (cf. formula **98**, p. 30) phenanthrene numbering rule, shown here as side [*a*] (for side 1,2 outside). The complete structure numbering system (1–17 inside) also differs from the normal system, by which, for example, ring atom 17 would be locant 1. This special numbering is used for the whole group of steroid hydrocarbons derived from it.

Full hydrogenation of the above unsaturated hydrocarbon with the maximum number of conjugated double bonds is the compound

31 As an introduction to conformational formulae it would be relevant here to refer to the significance of the stereo prefixes α and β, see III.10, p.

32 Ph. Fresenius, Zur Nomenklatur der Steroide. (On the Nomenclature of Steroids) *Pharm. Ztg.* 117 682 (1792)

† *Pure Appl. Chem.* 31 285 (1972)



222

Perhydrocyclopenta[*a*]phenanthrene
trivial name: Gonane (here 5α)

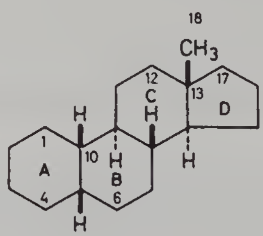
The trivial name implies the *trans*-position of rings B/C and C/D, as well as the β-position of the H-atoms at C-8, C-10, and C-13. For an adequate steric designation, it is necessary only to express the arrangement at C-5 as 5α or 5β.

Projection formulae of the group of hydrocarbons derived from gonane by substitution, should be drawn as shown in the formula. If the H-atoms at positions 8,9,10,13,14 are not designated and nothing else is indicated by a preceding name, the steric arrangement shown in the formula is assumed. The arrangement at C-5 is to be stated in any case.

8.2 With substituents

8.2.1 Substituents at C-10 and C-13

If the H-atom at C-13 of gonane is replaced by a CH_3-group, the new hydrocarbon is named 5α- or 5β-estrane (estrane). The steric arrangement of the CH_3-group is β like that of the H-atom in gonane. The C-atom of the methyl group takes the locant 18.



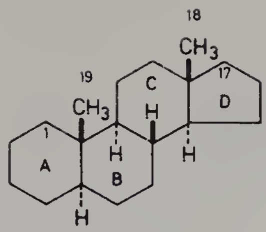
223

5β-Estrane

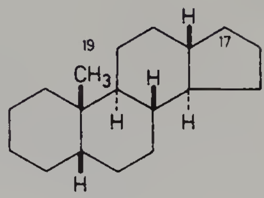
If both H-atoms at C-10 and C-13 in gonane are replaced by CH_3-groups, retaining the steric arrangement, androstane is produced. The C-atom of the methyl group at C-10 takes the locant 19 (formula 224).

If the CH_3-group at position 19 is present, but not that at position 18, the C-18 is taken out of the androstane by a special nomenclature 'nor' (= minus CH_2); there is no trivial name for this hydrocarbon.

The naming does not follow as 10-methylgonane. The prefix in this nor-nomenclature is combined with and preceded by the locant of the eliminated methyl group.

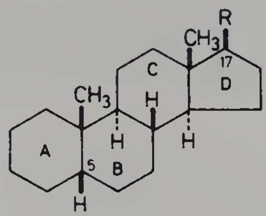


224
5*a*-Androstane



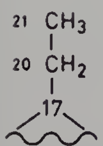
225
18-Nor-5β-androstane

8.2.2 Substituents at C-17



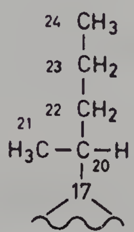
226

The following hydrocarbons are derived from substitution with various radicals at C-17 of androstane. The C-17 is itself asymmetric, and apart from the distinction between 5α and 5β-forms, there is differentiation between the 17α-position and the 17β-position. The 'normal' forms have the side chain in 17β, and 17β is assumed when nothing else is specified. If C-20 is methylated, (**228/231**) the (*R*)20-configuration is implied. In the case of ergostane (*S*)24, and of stigmastane (*R*)24, these *R*/*S* designations are implicit in the names.



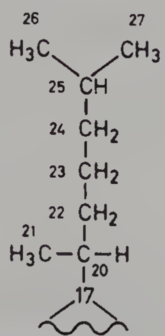
227
Ethyl

Pregnane
$C_{21}H_{36}$



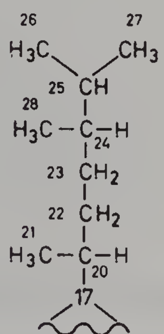
228
1-Methyl-butyl

Cholane
$C_{24}H_{42}$



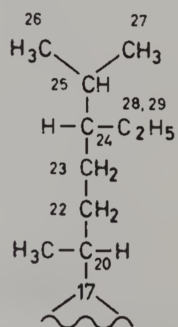
229
1,5-Dimethyl hexyl

Cholestane
$C_{27}H_{48}$



230
1,4,5-Trimethyl-hexyl

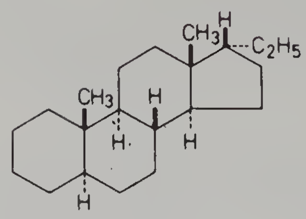
Ergostane
$C_{28}H_{50}$



231
4-Ethyl-1,5-dimethylhexyl

Stigmastane
$C_{29}H_{52}$

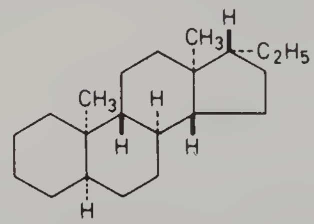
8.2.3 Steric rearrangement



232

5α,17α-Pregnane

If steric change takes place at all the asymmetric centres that need not be specified in a name, the same name can be used, with the prefix '*ent*'. However, as this prefix (from 'enantiomer') applies to all asymmetric centres, steric configurations remaining unchanged must be denoted by alteration of the previous special configuration indicators (which have been affected by the application of '*ent*' and must be brought back former to the configuration).



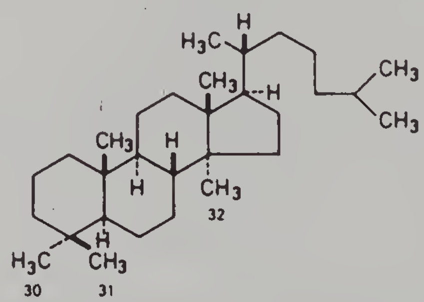
233

ent-5β,17β-Pregnane

8.3 Additional substituents

As examples of further semi-trivial names are cited:

(a)

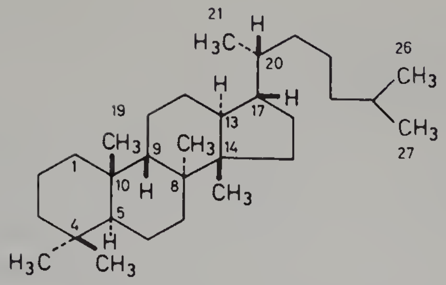


234

4,4,14α-Trimethyl-5α-cholestane [≡5α-Lanostane (numbering)]

Numbering of the three methyl groups not present in the cholestane structure does not follow on in consecutive sequence to the number 27, the highest in cholestane, but to the highest in the steroid system framework, the number 29 already assigned in Stigmastane. The 4α-group therefore takes number 30, the 4β-group number 31, the 14-substituted CH_3-group number 32.

(b)



235

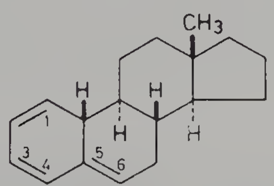
(20R)-4,4,8,14-Tetramethyl-18-nor-5α, 8α, 9β, 13α, 14β, 17β(H)-cholestane, [5a-Protostane]

In this scientific name the steric configurations at 8,9,13,14, and 17 are specified, because inversion takes place there, compared to those in 'normal' cholestane. The steric configuration at 5 must be given separately. That at 10, compared to cholestane, remains unchanged. (20R) is certainly also unchanged by reference to cholestane but is specified in these circumstances because of the introduction of a new semi-trivial name and the inversion at 17.

The depiction of the side chain at C-17 corresponds to the IUPAC recommendation, by which the 17–20 bond is not to be shown thickened or broken. In this light, the fact that C-20 is depicted in the same way should not give rise to any confusion. The 17–20 bond is therefore printed in a non-emphatic, normal manner and style. The fact that in this case it is in an 'α' position to the plane of the paper can be understood in relationship to a ring-system in that the 17-substituted H is indicated usually as 17β-.

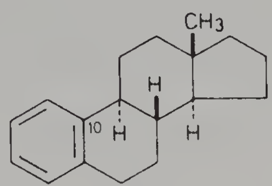
8.4 Unsaturation

Unsaturated steroid hydrocarbons are denoted in the usual manner by the modification of the ending 'ane' to 'ene', 'adiene', 'yne' etc.



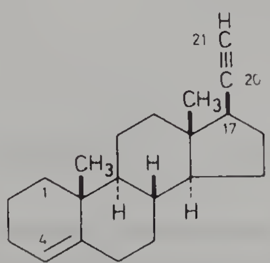
236

Estra-1,3,5-triene



237

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



238

Pregn-4-en-20-yne

8.5 Alterations at the side chain

8.5.1 Alterations at the C-17 side chain

(a)

20 21 22 23 24
17–CH(CH$_3$)–CH$_2$–CH$_2$–CH$_3$

239
Cholane

(b)

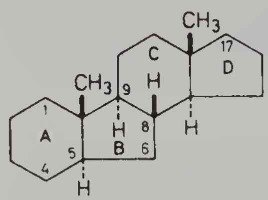
20 21 22 23
17–CH(CH$_3$)–CH$_2$–CH$_3$

240
24-Norcholane

The side-chain at (b) is shortened by one CH_2-group compared to (a). More precisely, the CH_3- end-group 24 is eliminated and replaced with an H-atom, so that a CH_3-group again stands there. Such a shortening by one ($-CH_2$) chain-member is expressed by the prefix 'nor'. The prefix is combined each time with the highest possible locant for the eliminated C-atom. Clearly, only 24 is a candidate in this case rather than 23 or 22. Were 23 also eliminated, the hydrocarbon with 22 of these C-atoms remaining but with C-22 changed to a methyl group would be presented. This would be designated as 23,24-dinor-cholane.

8.5.2 Alterations to the rings

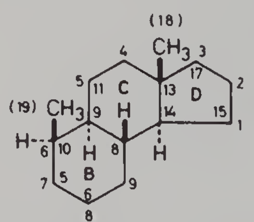
8.5.2.1 Ring-contraction



The numbering drops the highest possible locant in the 'nor'-contracted ring B in this case 7.

241
B-Nor-5*α*androstane

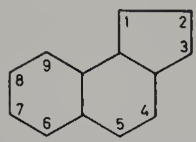
8.5.2.2 Elimination of an end-position ring



The free bonds generated by the elimination of the 1, 2, 3, 4 atoms of the androstane are taken up by hydrogen atoms.

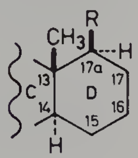
242
Des-A-androstane (steroid numbering inside)

Designation as a condensed hydrocarbon in accordance with I.2.2.2.2 is of course possible: perhydro-3aβ, 6β-dimethyl-5aα, 9aβ, 9bα-cyclopenta[*a*]naphthalene (numbering outside). The clockwise counting direction can proceed after rotating the formula into the prescribed position (see formula **124**):



243

8.5.2.3 Ring-expansion

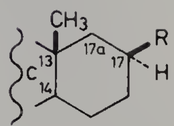


244

(a) D-Homocholane

R (see under I.8.2.2.2)

but



245

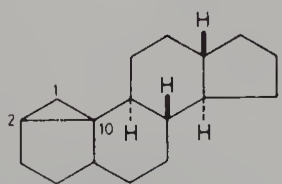
(b) 17β-(1-Methylbutyl)-D-homo-5α (or β)-androstane

Here, only designation (a) can be used, if the substituent at 17 of Cholane retains its position next to ring C, and therefore occupies position 17a in the D-Homocholane. If the substituent in the 'homo' compound is at C-17, it is moved away from the C ring and a systematic designation for the side chain must be chosen. The additional C-atom entering into a ring with the prefix 'homo' takes the highest number in that ring with the addition of 'a'.

8.5.2.4 Ring-expansion by 2 C-atoms

For a ring expansion by 2 C-atoms (for example 17a, 17b) the prefix 'dihomo' is used. If one ring of a steroid system is expanded and another is contracted, the prefixes 'homo' and 'nor' can be used together in a name, in alphabetical order. Generally this form of nomenclature is used only for the modification of up to two rings.

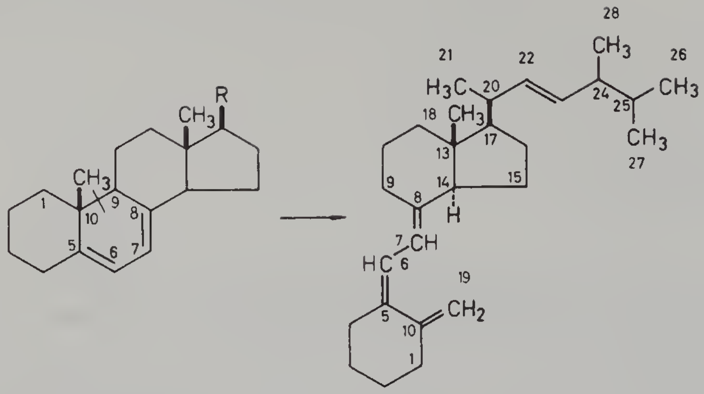
8.5.2.5 New bondings



246
2,10-Cyclogonane

The presence of a new ring formed by a new bond between two ring members is denoted by the prefix 'cyclo'. The numbers of the newly bonded atoms precede the prefix.

8.5.2.6 Ring-opening



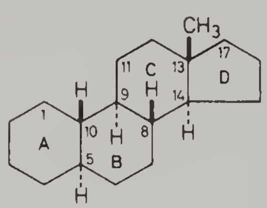
247
Ergosta-5,7,22-triene

248
9,10-Secoergosta-5,7,10(19),22-tetraene
(cf. Ergocalciferol INN, *EP*)

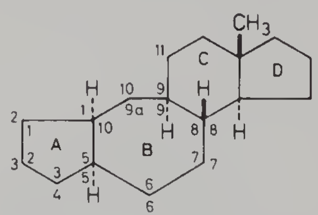
Ring-opening of a steroid system is, retaining the numbering, denoted by the prefix 'seco'[33]. This is placed after the two locants of the ring atoms between which the ring opening occurs. The free valences so formed ('cut positions') are taken up by hydrogen. The prefix 'seco' can also be used for other natural materials on the same principle, for denoting ring opening at a single bond.

8.5.2.7 Bond migration, abeo-*nomenclature*[34]

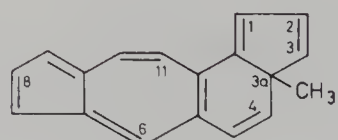
(a) *Migration of bond 5-10 to 5-1*



249
5α-Estrane



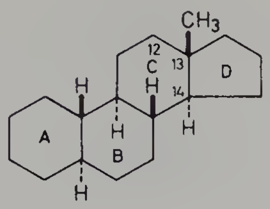
250
5-(10→1)*abeo*-1α(*H*),5α
Estrane (outer numbering) or
B(9a)-Homo-A-nor-5α,10α-
estrane (inner numbering)



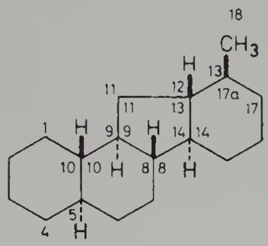
251
3a-Methyl-3a*H*
indeno[5,4-*f*] azulene
Ring-system with maximum
non-cumulative double bonds

33 From the Latin: *secare*, to cut
34 From the Latin: *abire*, to go away

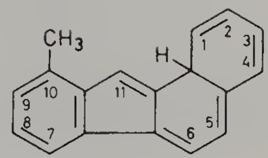
(b) *Migration of the bond 14-13 to 14-12*



252
5α-Estrane



253
14(13→12)*abeo*-5α,12β(*H*)-Estrane (outer numbering) or 17*a*β-Methyl-D-homo-C-nor-5α-gonane (inner numbering)



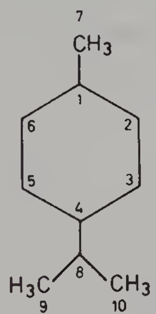
254
10-Methyl-11b*H*-benzo[*a*]fluorene
Ring-system with maximum number of non-cumulative double bonds

8.5.2.8 Several non-separable prefixes coming together (see III.2.5)
If a number of the four prefixes cyclo, homo, nor, seco come together in a name they are put in alphabetical order.

9 CYCLIC TERPENE HYDROCARBONS

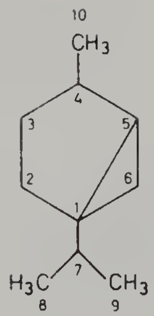
Mono-and bicyclic hydrocarbons of the following formulae: $C_{10}H_{18}$ and $C_{10}H_{20}$ (monoterpenes) are the parent compounds of this group. The bicyclics can be taken back even further to an unsubstituted C_7H_{12} hydrocarbon. Larger molecules are found in the sesquiterpenes (sesqui = 1½; 15 C-atoms) diterpenes (20 C-atoms), triterpenes (30 C-atoms) etc. For tetraterpenes, see Carotenes at I.7.

$C_{10}H_{20}$:

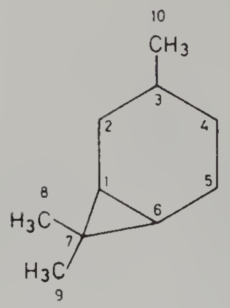


255
p-(*ara*)-Menthane (locants
[systematic: in alphabetical order 1-Isopropyl-4-methylcyclohexane (hexahydro-*p*-cymene, Cymene with locants as 255 see formula 185)

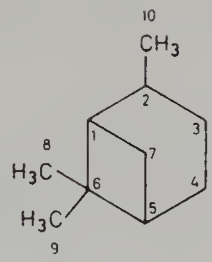
The 1,4-arrangement is denoted by *p*(*ara*), as in the case of Benzene, and correspondingly, 1,3- as *m*(*eta*) and 1,2- as *o*(*rtho*).



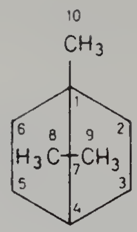
256
Thujane



257
Carane



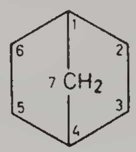
258
Pinane



259
Bornane

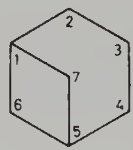
all $C_{10}H_{18}$

The independent numbering system of the $C_{10}H_{18}$ hydrocarbons corresponds to that of the bicyclic systems (cf. I.3, p. 37)



260
8,9,10-Trinorbornane[35]
Bicyclo[2.2.1]heptane

all C_7H_{12}



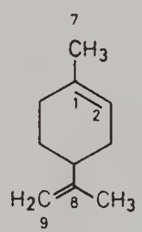
261
8,9,10-Trinorpinane
Bicyclo[3.1.1]heptane

8,9,10-Trinorcarane (Bicyclo[4.1.0]heptane)

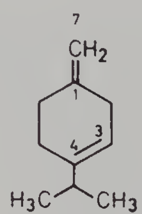
9.1 Monoterpene hydrocarbons (10 C)

9.1.1 Monocyclic $C_{10}H_{16}$

These hydrocarbons are derived from the nine named parent compounds by the introduction of double bonds. These are denoted in the normal manner by the modification of 'ane' to 'ene', and so forth.

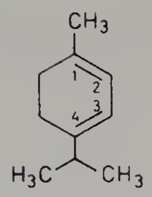


262
Limonene
1,8-*p*-Methadiene



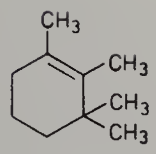
263
β-Terpinene
1(7),3-*p*-Menthadiene

35 It will be observed with regard to the C_7H_{12} hydrocarbons that, in the more recent procedure for the 'nor' prefix (= demethyl), it refers to 1 CH_3-group, so that the exchange of 3 CH_3-groups for H, is denoted by the prefix 'trinor'. Designations of the WHO (for example for Noreximide INN and Taglutimide INN) take no account of this, and use the old name norbornane (ene) for its parent compound from which tree methyl groups are missing. In this they run counter to IUPAC.



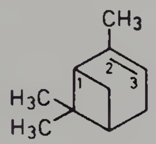
264
α-Terpinene
1,3-*p*-Menthadiene

But $C_{10}H_{18}$ with modified structure and substituent positions

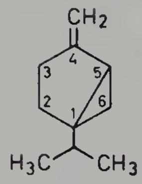


265
1,2,3,3-Tetramethylcyclohexene

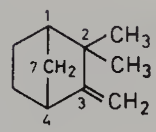
9.1.2 *Bicyclic* $C_{10}H_{16}$



266
2-Pinene
(α-Pinene)



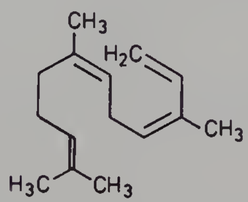
267
Sabinene
(4(10)-Thujene)



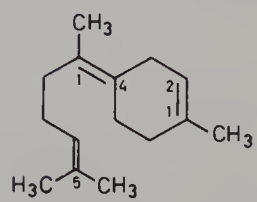
268
Camphene
[2,2-Dimethyl-3-methylene-norbornane] 2,2-Dimethyl-3-methylene-8,9,10-tribornane; 2,2-Dimethyl-3-methylene-bicyclo[2.2.1.]heptane

9.2 Sesquiterpenes

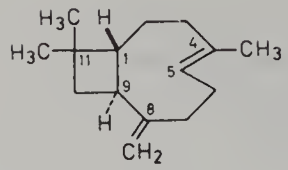
9.2.1 *General formula* $C_{15}H_{24}$



269
α-Farnesene
3,7,11-Trimethyl-1,3,6,10-dodecatetraene (open chain) (cf. I.1.2)

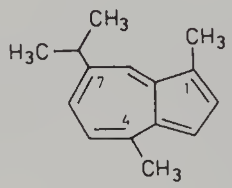


270
Bisabolene
4-(1,5-Dimethyl-4-hexenylidene)-1-methyl-1-cyclohexene (monocyclic)[36]



271
Caryophyllene
(*E*)-(1*R*,9*S*)-4,11,11-Trimethyl-8-methylenebicyclo[7.2.0.]undec-4-ene[37]

9.2.2 *Terpenes of higher unsaturation*



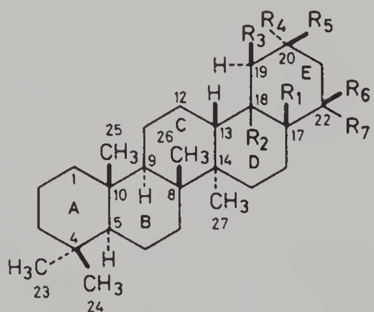
272
Guiazulene $C_{15}H_{18}$
7-Isopropyl-1,4-dimethylazulene

9.3 Triterpene hydrocarbons

Cyclic triterpene hydrocarbons include substituted, hydrogenated pentacyclic ring-systems, for example those deriving from Perhydropicene or from Perhydrocyclopenta-[*a*]chrysene. As with the steroid hydrocarbons, the established semi-trivial names are associated with fixed steric configurations. The systematic IUPAC numbering of perhydropicene is like that of picene (see formula **105**). A special numbering system is used after the introduction of 8 methyl substituents, to include the methyl groups.

9.3.1 *General formula* $C_{30}H_{52}$

(a) Perhydropicene derivatives



273
(special numbering)

37 (*E*) denotes the *cis*/*trans*-isomerism at the double bond 4=5. (*R*) and (*S*) are configuration symbols from the sequence rules of Cahn, Ingold, and Prelog, *Angew. Chem. intern. Edit.* 5 385 (1966) (III 10 p. 129)

Semi-trivial names	to 17β	to 18	to 19	to 20		to 22	
	R1	R2	R3	R4	R5	R6	R7
Oleanane	CH_3 (28)	βH	H	CH_3 (29)	CH_3 (30)	H	H
Ursane	CH_3 (28)	βH	CH_3 (29)	CH_3 (30)	H	H	H
Gammacerane	H	αCH_3 (28)	H	H	H	CH_3 (29)	CH_3 (30)

( ) Numbering

†	ring positions A : B	B : C	C : D	D : E
Oleanane	*t*	*t*	*t*	*c*
Ursane	*t*	*t*	*t*	*c*
Gammacerane	*t*	*t*	*t*	*t*

t = *trans*, *c* = cis

The systematic naming of Oleanane is as follows:

(4a*R*)-2,2,4a,6a,6b,9,9,12a-Octamethyl-
(4a*r*,6a*t*,6b*c*,8a*t*,12a*c*,12b*t*,14a*c*,14b*c*)-docosahydropicene

(4a*R*): The angular C-atom 4a has (*R*)-configuration from the sequence rules. Thereby a known configuration for the free substituents at 4a is produced.

4a*r*[38]: The free substituents at 4a serves as reference substituent *r*.

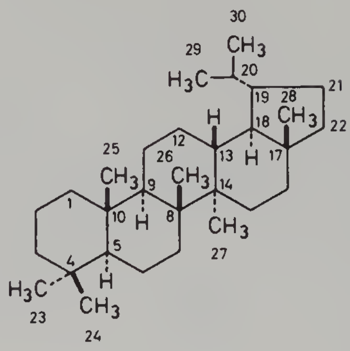
6a*t*, 6b*c* etc.: The free substituents or H-atoms at the other angular C-atoms are in *t*(*rans*)- or *c*(*is*)-position to the 4a-substituent.
As the (4a*R*) has a β position (above the plane of the ring), the *t*-configurations are always drawn α and the *c*-configurations always drawn β.

Comparative numbering for the Oleanane ring skeleton

IUPAC-special numbering	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22
systematic	12	11	10	9	8a	8	7	6b	12b	12a	13	14	14a	6a	6	5	4a	14b	1	2	3	4

38 As reference atom, the lowest numbered angular atom is chosen here.

(b) Perhydrocyclopenta[*a*]chrysene derivatives



274
Lupane (special numbering)

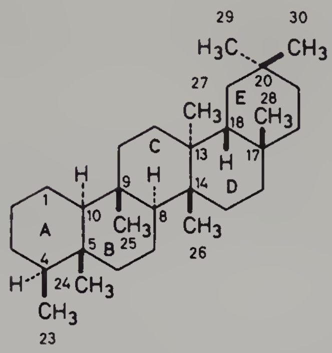
9.3.2 Friedo[39] and Neo nomenclature (not IUPAC, but CA)

9.3.2.1 Friedo- names; substituent migration and steric transfer

Oleanane	28(17β) 29(20α) 30(20β)	27(14*t*)	26(8*c*)	25(10*c*)	24(4β)	23(4*a*)
D-Friedo-oleanane	”	27: 14→13*t* 14*cH*	26: † 8*c*→8*t*	”	”	”
D:C-Friedo-oleanane	”		26: 8*t*→14*c* (8*tH*)	”	”	”
D:B-Friedo-oleanane	”		”	25: 10*c*→9*c* (10*tH*)	”	”
D:A-Friedo oleanane	”	”	”	”	24: 4β→5*c* (4βH)	23: 4*a*→4β

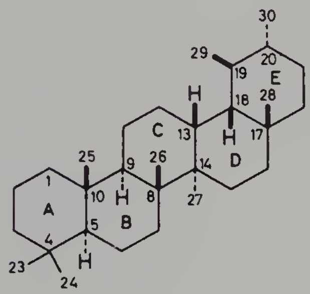
† From *CA Index Guide* 1977.

39 Named after Ch. Friedel 1832–99 Strasburg/Paris (Sorbonne).

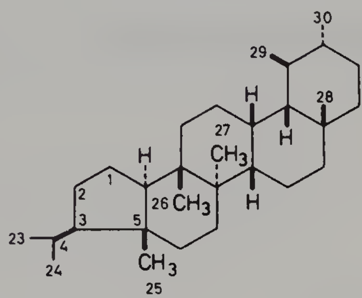


275
Friedelane, *D*:*A*-Friedo-oleanane

9.3.2.2 Neo-names; ring-contraction A, substituent migration and steric transfer



276
Ursane



277
A:*D*-Neo-ursane

Ursane†	Ring-C4 with 23,24	25 (10*c*)	26 (8*c*)	27 (14*t*)	28(17β); 29(19β) 30(20*a*)
A-Neo-ursane	Contracted ring Isopropyl side chain at 3β	”	”	”	”
A:*B*-Neo-ursane	”	25 10*c*→5*c*	” ”	” ”	” ”
A:*C*-Neo-ursane	”	”	26 8*c*→9*c* (8*tH*)	”	”
A:*D*-Neo-ursane	”	”	”	27 14*t*→8*t* (14*cH*)	”

† Reference substituent at 4a of the systematic numbering (cf. Oleanane). In this table = 17β-Methyl.

II

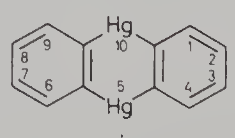
Heterocyclic systems

1 TRIVIAL NAMES

1.1 Rings with the maximum number of non-cumulative double bonds

The following list applies to heteromonocyclic compounds, and to heterocyclic systems containing two or three fused rings. The list, numbered 1–70, is so arranged that the name of a ring or a ring-system considered as a component in a name of a larger fused ring system, is taken as the base-component when combined with a name occurring earlier in the list and as the attached component when combined with one later in the list. The rings having been drawn and oriented in the normal way (see I.2.2.2.2, p. 34) the numbering begins with 1 at a hetero atom in a monocyclic compound but, in fused ring systems, 1 is a ring atom in the furthest right (upper) ring, next to a ring junction, such that clockwise numbering from that position results in the lowest possible numbers for the hetero atoms. The numberings of xanthene, purine, carbazole, and acridine do not follow this rule. Although C-atoms engaged in fusion positions take the same number as the preceding periphery C-atom, with the addition of a small letter (cf. Hydrocarbons I.2.2.2.2), heteroatoms engaged in fusion positions have their own numbers.

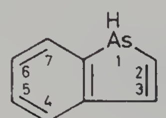
1. Phenomercurin (= 1)



1

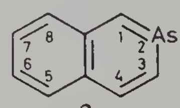
2. Isoarsindole

3. Arsindole (= 2)



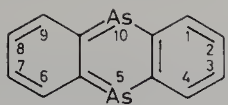
2

4. Isoarsinoline (= 3)



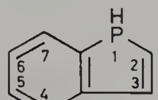
3

5. Arsinoline
6. Arsanthridine
7. Acridarsine
8. Arsanthrene (= 4)



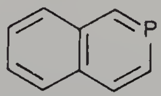
4

9. Isophosphindole
10. Phosphindole (= 5)



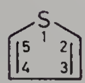
5

11. Isophosphinoline (= 6)



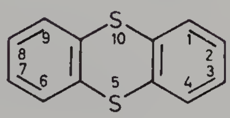
6

12. Phosphinoline
13. Phosphantrene
14. Tellurophene
15. Selenophene
16. Selenanthrene
17. Thiophene (= 7)



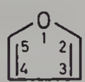
7

18. Thianthrene (= 8)



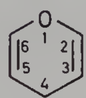
8

19. Phenothiarsine
20. Furan (= 9)



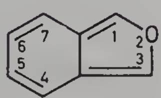
9

21. 4*H*-Pyran (= 10) (also 2*H*)[1]



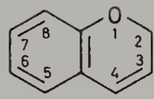
10

22. Isobenzofuran (= 11)



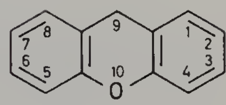
11

23. 2*H*-Chromene (= 12) (also 4*H*)[1]



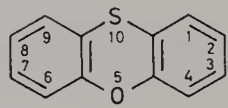
12

24. Xanthene[1] (= 13)



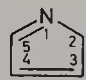
13

25. Phenoxantimonin
26. Phenoxarsine
27. Phenoxaphosphin
28. Phenoxatellurin
29. Phenoxaselenin
30. Phenoxathiin (= 14)



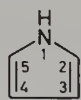
14

31. 2*H*-Pyrrole (= 15)



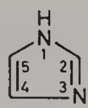
15

32. Pyrrole (= 16)



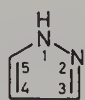
16

33. Imidazole (= 17)



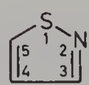
17

34. Pyrazole (= 18)



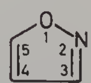
18

35. Isothiazole (= 19)



19

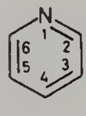
36. Isoxazole (= 20)



20

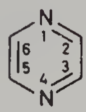
1 For thio analogues see footnote 5 of II.3.1, p. 77.

37. Pyridine (= 21)



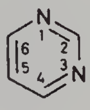
21

38. Pyrazine (= 22)



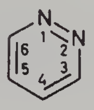
22

39. Pyrimidine (= 23)



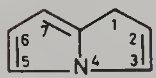
23

40. Pyridazine (= 24)



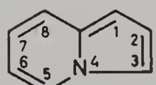
24

41. 1*H*-Pyrrolizine (= 25) (also 3*H*)



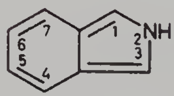
25

42. Indolizine (= 26)



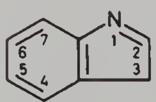
26

43. Isoindole (= 27)



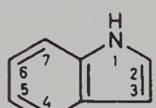
27

44. 3*H*-Indole (= 28)



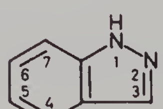
28

45. Indole (= 29)



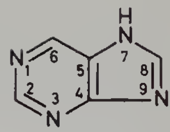
29

46. Indazole (= 30)



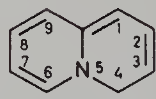
30

47. Purine (7*H*-Purine) (= 31) (also 1*H*, 3*H*, 5*H*, 6*H*, 8*H*, 9*H*)



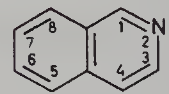
31

48. 4*H*-Quinolizine (= 32) (also 2*H*, 9a*H*)



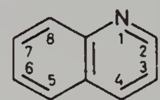
32

49. Isoquinoline (= 33)



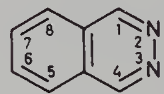
33

50. Quinoline (= 34)



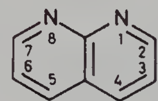
34

51. Phthalazine (= 35)



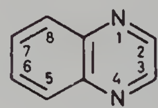
35

52. 1.8-Naphthyridine (= 36) (also 1,5; 1,6; 1,7; 2,6; 2,7)



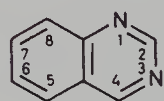
36

53. Quinoxaline (= 37)



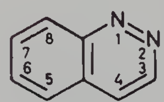
37

54. Quinazoline (= 38)



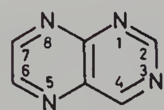
38

55. Cinnoline (= 39)



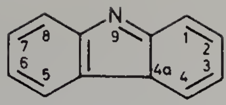
39

56. Pteridine (= 40)



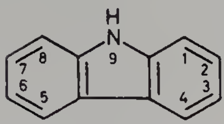
40

57. 4a*H*-Carbazole (= 41)



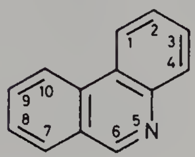
41

58. Carbazole (= 42)



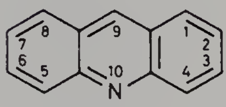
42

59. Phenanthridine (= 43)



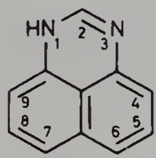
43

60. Acridine (= 44)



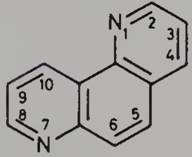
44

61. Perimidine (= 45)



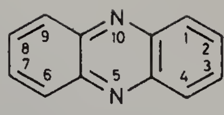
45

62. 1,7-Phenanthroline (= 46) (also 1,8; 1,10; 3,8; 4,7)



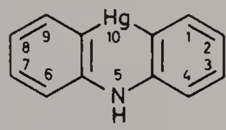
46

63. Phenazine (= 47)



47

64. Phenomercazine (= 48)

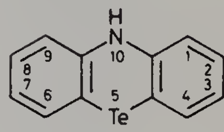


48

65. Phenarsazine

66. Phenophosphazine

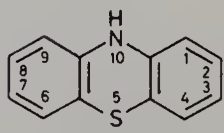
67. Phenotellurazine (= 49)



49

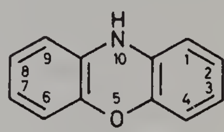
68. Phenoselenazine

69. Phenothiazine (= 50)



50

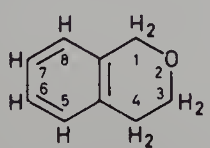
70. Phenoxazine (= 51)



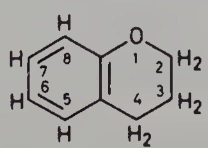
51

1.2 Saturated and partly saturated rings

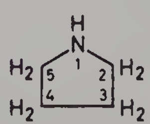
The following trivial names are not used as components in fusion-names. They can, however, be considered for naming heterocyclic spiro compounds.



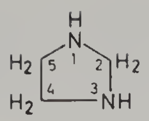
52
Isochroman



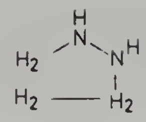
53
Chroman



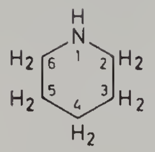
54
Pyrrolidine



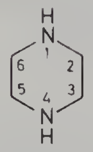
55
Imidazolidine



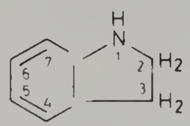
56
Pyrazolidine



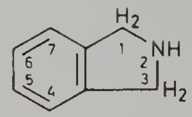
57
Piperidine



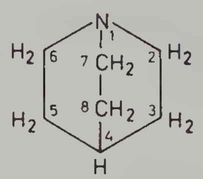
58
Piperazine



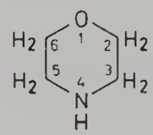
59
Indoline



60
Isoindoline



61
Quinuclidine



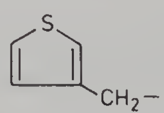
62
Morpholine (1,4-Oxazinane)

1.3 Radicals

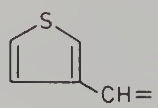
Radicals are in general, designated by adding the ending 'yl', 'diyl' etc., or 'ylidene' to the name of the parent compound (after elision of final 'e' if present). At the same time the number of the appropriate ring atom is put in front of the name. The following are valid exceptions:

Furan/furyl, pyridine/pyridyl, isoquinoline/isoquinolyl, quinoline/quinolyl, thiophene/thienyl, piperidine/piperidyl. Instead of '1-piperidyl', 'piperidino' is used; 'morpholino' is used instead of 'morpholin-4-yl'.

The '2-furylmethyl' radical is called 'furfuryl'. This name is also extended as 'furfurylidene' and 'furfurylidyne' for the higher-valent radicals. Correspondingly for 'thienylmethyl' (preceded by the locants) 'thenyl', 'thenylidene', 'thenylidyne' according to the valency of the radical.



63
3-thenyl



64
3-thenylidene

The named exceptions are not extended to cover their fused compounds; thus, for example, 'Benzofuran' and 'Isobenzofuran' (formulae 22/11) produce the radicals 'benzofuranyl' and 'isobenzofuranyl' respectively (with locants).

2 SYSTEMATIC NAMES

2.1 Hantzsch–Widman System[2]

Monocyclic compounds with 1 or more hetero atoms in a 3–10 membered ring are named by using a prefix ending in ‘a’, the ‘a’ term combined with an end term indicating the ring size and degree of hydrogenation. The most important prefixes are:

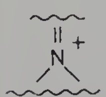
Element	Valence	Prefix	Element	Valence	Prefix
Fluorine	I	Fluora	Arsenic	III	Arsa
Chlorine	I	Chlora	Antimony	III	Stiba
Bromine	I	Broma	Bismuth	III	Bisma
Iodine	I	Ioda	Silicon	IV	Sila
Oxygen	II	Oxa	Germanium	IV	Germa
Sulphur	II	Thia	Tin	IV	Stanna
Selenium	II	Selena	Lead	IV	Plumba
Tellurium	II	Tellura	Boron	III	Bora
Nitrogen	III	Aza	Mercury	II	Mercura
Phosphorus	III	Phospha			

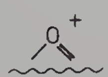
The inclusion of the halogens allows the formation of names with a halogen cation.

The following endings are for ring size and degree of saturation.

Ring members		mnc without; with N†	saturated without; with N†	derived from
10		ecine	ecane	deca
9		onine	onane	nona
8		ocine	ocane	octa
7		epine	epane	hepta
6	(B,F,Cl,Br,I,P,As,Sb)	inine	inane	
	(N, Si, Ge, Sn, Pb)		inane	
	(O,S,Se,Te,Bi,Hg)	ine	ane	
5		ole	olane;olidine†	
4		ete	etane;etidine†	tetra
3		irene, irine†	irane; iridine†	tri

mnc: maximum number of non-cumulative double bonds (the ionic forms, for example





, are not included in the mnc assessment)

2 *Pure Appl. Chem.* **55** 409 (1983)

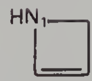
† The endings with ‘irine’, or ‘idine’ are preferred for N-containing rings.

65
Thiirine;
saturated: Thiirane

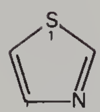
66
Azirene
saturated: Aziridine

67
Thiete (2*H*-Thiete);
saturated: Thietane

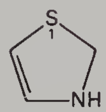
68
Azete



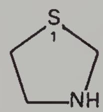
69
1,2-Dihydroazete
('o' is retained before 'a')
saturated: Azetidine



70
1,3-Thiazole

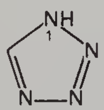


71
2,3-Dihydro-1,3-thiazole



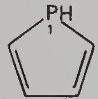
72
1,3-Thiazolidine

(The locants [1,3] are sometimes dropped in view of the trivial name 'isothiazole' used for the 1,2-isomer, but their retention avoids ambiguity.)

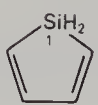


73
1*H*-Tetrazole

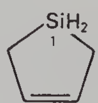
generally:
α) 'a' of a numerating prefix is elided before a vowel
β) 'a' of the 'a' term is elided before a vowel, for example Tetra/aza/ole shortened to Tetrazole



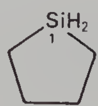
74
Phosphole;
saturated: Phospholane



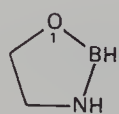
75
1*H*-Silol



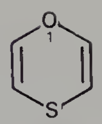
76
3,4-Didehydrosilolane;
2,5-Dihydro-1*H*-silole
(in general a 'hydro' prefix is used in preference to a 'dehydro' prefix.)



77
Sil*olane*

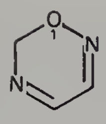


78
with N present, however 1,3,2-Oxazabor*olidine*



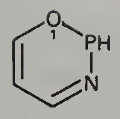
79

1,4-Oxathiine
saturated: 1,4-Oxathiane



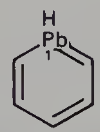
80

6*H*-1,2,5-Oxadiazine
saturated: 1,2,5-Oxadiazinane



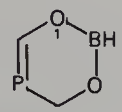
81

2*H*-1,3,2-Oxazaphosphinine
saturated: . . .inane



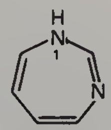
82

Plumbine
saturated: . . .inane



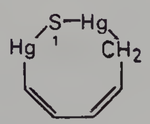
83

4*H*-1,3,5,2-Dioxaphosphaborinin;
saturated: . . .inane
(indicated H is not given for a position between two divalent ring members)



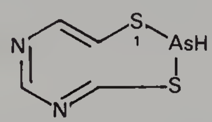
84

1*H*-1,3-Diazepine;
saturated: . . .epane



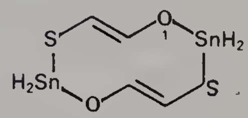
85

3*H*-1,2,8-Thiadimercurocin
saturated: . . .ocane



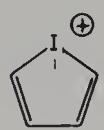
86

1,3,5,7,2-Dithiadiazarsonine
saturated: . . .onane
('a' of 2 'a' terms elided before a vowel)
(Dithia/diaza/arsa/onine: . . .diazarsonine)



87

1,6,3,8,2,7-Dioxa-dithiadistannecin
saturated: . . .ecane



88

Iodolium cation
(cf. p. 120 formula 235b)
('a' of the 'a' term elided before the vowel)

If a ring contains only 1 hetero atom, numbering begins with this as 1. Thereafter, the 'indicated-H' takes the lowest possible locant. If a ring contains more than one like hetero atom, the hetero prefix ('a' term) is preceded by a multiplying prefix, and the locants come before this. Numbering begins at whichever one of the hetero atoms gives them the lowest set of locants. If a ring contains different hetero atoms, numbering begins with 1 being nearest the beginning of the table of 'a' terms, and proceeds in the direction that results in the lowest set of locants for all the hetero atoms. If there is then any further choice, the hetero atoms are numbered so that the lowest locants are given in the order in which they appear in the name. In names, first come the locants in the order of the 'a' table, then the 'a' terms in table order, then the ending for the ring-size. Various endings are used for six-membered rings. In any particular case, the ending is used which is appropriate for the hetero atom furthest from the beginning of the table of 'a' terms.

Rings with more than 10 members are given replacement names (cf. II.3, p. 77).

2.2 Fused ring-systems

In deciding which is the base-component, the following criteria are considered in order:

(a) the base-component is a heterocycle (rather than any carbocycle);
(b) the base-component is an N-containing component;
(c) the base-component is, in the absence of N, the component containing the hetero atom nearest the beginning of the table of 'a' terms (cf. II.2.1, p. 71);
(d) the base-component is the component with most rings;
(e) the base-component is the component with the largest single ring;
(f) the base-component is the component with the greatest number of hetero atoms of any kind;
(g) the base-component is the component with the greatest number of different kinds of hetero atom;
(h) the base-component is the component with the highest number of hetero atoms first listed in the table of heteroatoms (p. 71);
(i) the base-component is the component with the lowest locant number for the hetero atoms before fusion.

Naming and numbering follow the same principles as those by which hydrocarbons (I.2.2)[3] and the trivial names of fused heterocyclics (p. 66) have been named. The attached component takes the ending 'o'[4] joined to the name in the list at II.1.1 numbers 1–70 (after elision of final 'e', if present). For example,

Pyrazine/pyrazino-.

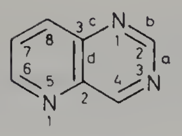
The following shortened forms are used:

Furan/furo; thiophene/thieno; imidazole/imidazo; pyridine/pyrido; pyrimidine/pyrimido; quinoline/quino; isoquinoline/isoquino.

The numbers cited, in square brackets between attached component and base-component to denote the fusion positions, are not those of the complete system numbered clockwise (1–8 inner). Those of each component are chosen so as to give, in naming order, 1. the earliest letter and 2. the lowest numbers. For example,

3 See footnote 16 (I.2.2.2.2) for the italic letter designation for the base component sides, p. 35.

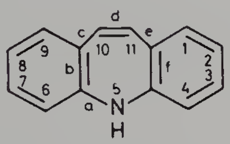
4 The 'o' as end letter of a heterocyclic attached component is retained before a vowel at the beginning of the base component name. (for example, formula 95; but see footnote 15 (I.2.2.2.1).



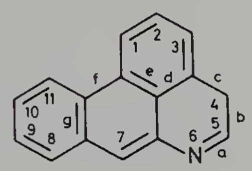
89
Pyrido[3,2-*d*] pyrimidine
not Pyrido[6,5-*e*] pyrimidine

The fused ring-systems are so numbered as to give the lowest possible numbers to the hetero-atoms. When different hetero-atoms in comparable positions in the structure are considered, the numbering system giving the lowest number to the hetero-atom nearest the beginning of the table of 'a' terms is chosen. After this, the lowest number for the C-atoms engaged in ring fusion; and after this, the lowest number for the indicated-*H*, are considered.

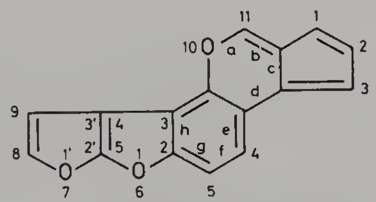
If the attached component itself consists of a base component (primary attached component) and an attached component (secondary attached component), then the secondary attached component is numbered with primes.



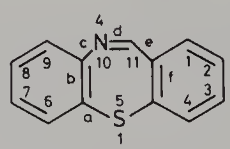
90
5*H*-Dibenz[*b, f*] azepine
(cf. Carbamazepine INN)



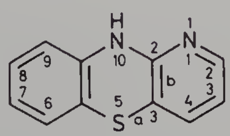
91
Dibenzo[*de,g*] quinoline
(cf. Apomorphine hydrochloride EP)



92
Cyclopenta[*c*] furo[3′,2′:4,5] furo-[2,3-*h*] [1] benzopyran
(cf. Aflatoxins)

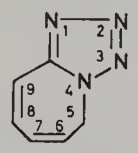


93
Dibenzo[*b,f*] [1,4] thiazepine
(cf. Clotiapin INN)

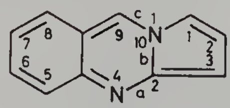


94
10*H*-Pyrido[3,2-*b*] [1,4] benzothiazine
(cf. Prothipendyl INN)

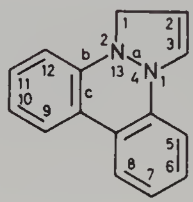
If a hetero-atom is common to two rings, the names of both components indicate this. The trivial names pyrrolizine, indolizine and quinolizine are exceptions. A hetero-atom common to two or more rings is given its own locant, in contrast to a C-atom occupying such a position.



95
5*H*-Tetrazoloazepine
(6,7,8,9-Tetrahydro-form:
Pentetrazole INN)

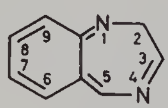


96
Pyrrolo[2,1-*b*]quinazoline
(cf. Alkaloid Vasicin)

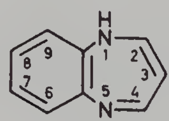


97
1*H*-Benzo[*c*]pyrazolo[1,2-*a*]cinnoline
(cf. Cinnofuradione INN)

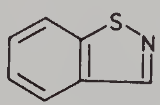
With fused ring-systems in which benzene is one component, a simplified nomenclature can be used, citing the positions of the hetero-atoms relative to the 'benzo' component and naming the fused system on that basis.



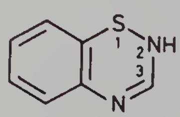
98
2*H*-1,4-Benzodiazepine
(cf. Diazepam INN for example)



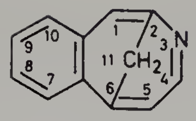
99
1*H*-1,5-Benzodiazepine
(cf. Lofendazam INN)



100
1,2-Benzothiazole
(otherwise: Benzo[*d*][1,2]thiazole,
trivial: 1,2-Benzisothiazole)
(cf. Saccharin-Sodium DAB 8)



100
2*H*-1,2,4-Benzothiadiazine
(cf. Chlorothiazide INN)



102

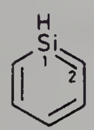
2,6-Methano-3-benzazocine
(cf. Moxazocin INN for example)

3 REPLACEMENT NAMES

(Exchange names, 'a' names[5]) (cf. also III.7, p. 116)

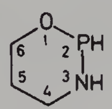
3.1 Replacement of carbon with hetero atoms[6]

Heterocyclic compounds can be named by combining 'a' terms (see II.2.1) with names of hydrocarbons. The basic concept is of exchanging a ring C-atom (($-CH_2-$) or ($-CH=$)-group) of the hydrocarbon for a hetero-atom similarly combined with hydrogen to the same degree of saturation, relative to the normal valency of the hetero-atom. The 'a' term for hetero atoms – in the case of more than one, in the order they appear in the list of 'a' terms – are cited before the hydrocarbon name. The principle can be applied to monocyclic compounds and to fused ring, and other, systems both MNC and in the (partly) hydrogenated state, for example naphthalene, indane, cyclohexane.



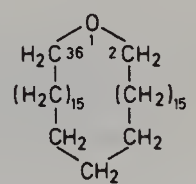
103

Silabenzene



104

1-Oxa-3-aza-2-phosphacyclohexane
(cf. formula **81** p.73)

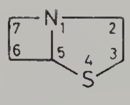


105

Oxacyclohexatriacontane
(cf. Primycin INN)

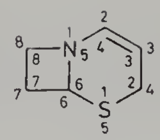
5 Replacement names belong to the so called matrix names. They can be distinguished from other matrix names which do not deal with replacement of a C- with a hetero- atom in a hydrocarbon stem compound but with (for example) sulphur taking the place of oxygen. In these cases, the hetero-prefix 'thia' would not apply, but the prefix 'thio': Thiopyran, Thiochromen, Thioxanthene (cf. the analogous oxygen compounds in the list of trivial names at II.1.1 formulae **10, 12, 13**, p. 67). Other trivial names of a similar sort are arsindole (2, As for N) and phosphindole (5, P for N).

6 The 'a' ending of 'a' prefixes here is not elided before a vowel (see formulae **104, 106, 107**; also (for example) . . triazaindene; . .oxa. . .azaicosane.



106

4-Thia-1-azabicyclo[3.2.0]heptane
(cf. Penicillin)



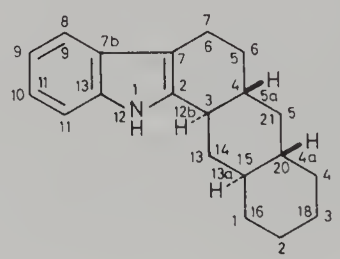
107

5-Thia-1-azabicyclo[4.2.0]oct-2-ene
(outer numbering)
[(cf. trivial: Cephem . . .8-oxo. .
(inner numbering)
see Cefaloridinium EP]

3.2 Replacement of hetero-atom by carbon

Replacement of one or more hetero-atoms of a heterocyclic compound with carbon can be indicated by giving the locant(s), then the prefix 'carba', in front of the parent heterocyclic name.

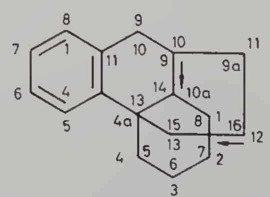
The parent heterocyclic compound numbering is retained for the C-analogue. (If a hetero-atom in the parent heterocyclic compound is not numbered, the C-atom replacing it takes the number of the lowest numbered ring-atom bound to it, with the addition of the letter 'a' (cf. formula **109**a).)



108

(a) 4β-4-Carbayohimbane (inner numbering)
(b) 4aβ,5aβ,12bα.13aα-1,2,3,4,4a,5,5a,6,7,12b,13,13a-Dodecahydro-12*H*-naphtho[2,3-*a*]carbazole (outer numbering)

Designation (a) of formula **108** is in agreement with the IUPAC F-rules for natural products. For designation (b) to correspond with rule 2.2, the formula must be turned through 180 degrees about its horizontal axis. (The steric designations are thereby changed.)



109

(a) 9a-Carbamorphinan (inner number 1–16 + 9a)
(b) 1,2,3,9,10,10a-Hexahydro-4*H*-4a,10-propanophenanthrene (outer numbering 1–13 + 10a)

For designation **109b** to accord with rule 2.2 p. 74, the formula must be turned through 45 degrees anticlockwise.

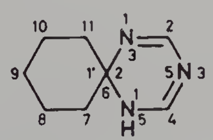
4 HETEROCYCLIC SPIRO COMPOUNDS

The name is formed in two ways:

(a) When the two components are individual rings, the name is formed by using a spiro prefix as at I.4.1.1. The hetero-atoms are introduced by 'a' terms in the spiro hydrocarbon name. The numbering is retained and the hetero-atoms within the framework of the system (examples **110, 111**).

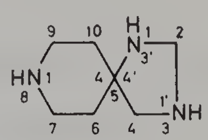
If at least one part of the spiro compound is a system of more than one ring, the trivial names of the heterocycles are combined with those of carbocycles, or the trivial names of heterocycles are combined as appropriate (examples **112, 113, 114**). A numbering system for the whole structure is not generated; the components retain their own numbering. The components are cited alphabetically, the numbers of the later-occurring component being given primes. With double spiro compounds, the third component is given double primes. If the components of a hetero–spiro compound are alike, the prefix 'spirobi' is used, following the locant for the spiro atom.

(b) The name is formed by using a spiro infix. The order of precedence for the heterocycles follows that of rule 2.2 (heterocyclic compounds). A heterocyclic component takes precedence over a carbocycle of the same size. The spiro atoms are given the lowest possible numbers within the framework of the components numbered in the normal way (examples **110, 111, 112**).



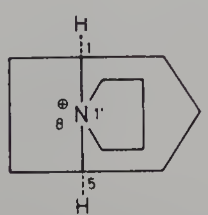
110

(a) 1,3,5-Triazaspiro[5.5]undeca-1,3-diene (outer locants)
(b) 1,2-Dihydro-1,3,5-triazine-2-spiro cyclohexane (inner locants) (cf. Spirazine INN)



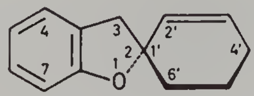
111

(a) 1,3,8-Triazaspiro[4.5]decane (outer locants)
(b) Piperidine-4-spiro-4′-imidazolidine (inner locants) (cf. Spiperone INN, Spiramide INN)



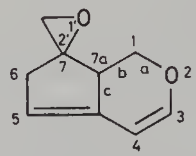
112

(a) Spiro[1a*H*,5a*H*-nortropan-8,1′-pyrrolidinium] (cation)
(b) Nortropan-8-spiro-1′-pyrrolidinium (cation) (cf. Trospium chloride INN)



113

Spiro[2,3-dihydrobenzofuran-2,1′
cyclohex-2-ene]
(but cf. Griseofulvin INN and EP)



114

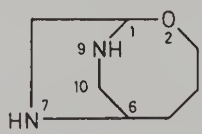
(a) Spiro[1,6,7,7a-tetrahydrocyclopenta[*c*]pyran-7,2′-oxiran] (IUPAC) (cf. Valtrate INN)

(b) 1,7a-Dihydro-spiro[cyclopenta[*c*]pyran-7(6*H*),2′-oxiran] (WHO) (CA) (not IUPAC)

5 HETEROBRIDGES

5.1 ‘a’ terms

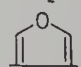
The example is taken outside those of II.3.1., because here all three bridges contain hetero atoms:



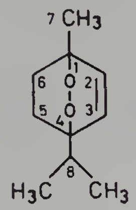
115

2-Oxa-7,9-diazabicyclo[4.2.2]decane
(cf. Bicozamycin INN)
Radical . . .[. . .]. . .dec-x-yl

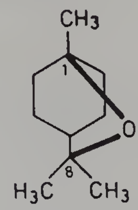
5.2 Bridge prefixes

–O–	Epoxy	–O–NH–	Epoxyimino	–N=N–	Azo
–O–O–	Epidioxy	–S–O–NH–	Epithioximino	–NH–NH–	Biimino
–S–	Epithio	–N=	Nitrilo	–NH–CH_2–CH_2–	Iminoethano
–S–S–	Epidithio	–NH–	Imino or Epimino		Furano (generally 3,4-)

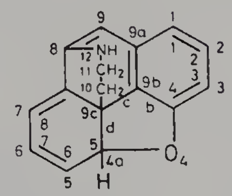
Prefixes for heterobridges can remain attached to the name of the cycle stem, but can be separately brought in (in alphabetical order of substituents). If there is more than one bridge prefix, they are cited alphabetically. Before the bridge prefix, come the locants of the stem-system ring-atoms which it links. These locants are in ascending order or in the order in which the terminal atoms of the bridge prefix arise.



116
trivial: Ascaridole
As terpine-derivative:
1,4-Epidioxy-2-*p*-menthene
(locants)
Syst.: 4-Isopropyl-1-methyl-2,3-dioxabicyclo[2.2.2]oct-5-ene



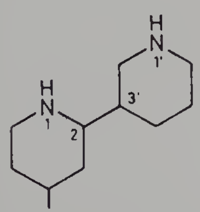
177
trivial: Cineole
As terpine-derivative:
1,8-Epoxy-*p*-menthane
(locants)
Syst.: 1,3,3-Trimethyl-2-oxabicyclo[2.2.2]octane



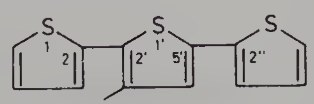
118
4a*H*-8,9c-Iminoethano-phenanthro[4,5-*bcd*]furan
(cf. Morphine etc.)
(inner 1–8 to phenanthrene)

6 RING-SERIES WITH LINKING BONDS (RING SEQUENCES, RING ASSEMBLIES)

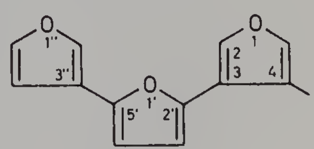
The same multiplying prefixes are used for heterocyclic ring sequences as those for the corresponding hydrocarbons (I.5).



119
2,3′-Bipiperidine
2,3′-Bipiperidyl
Radicals . . .4-yl



120
2,2′:5′,2″-Terthiophen-3′-yl

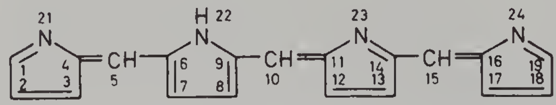


121
3,2′:5′3″-Terfuran-4-yl
(locants) or
4-[5-(3-Furyl)-2-furyl]-3-furyl

7 RING-SERIES WITH LINKING GROUPS, TETRAPYRROLES[7]

7.1 Linear ring-series

Stem system 'Bilin' (for bile pigments)



122

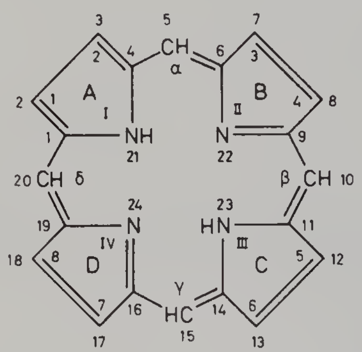
22*H*-Bilin (completely MNC system)

Because of the biosynthesis of bile pigments and the derivation of the 'Bilin stem' system from the 'Porphin' ('Porphyrin') stem system, the locant 20 in Bilin (in Porphin, the bridge linking 19 and 1) is not used.

7.2 Macrocyclic ring-series

Beilstein, CA, *Ring Index*, IUPAC–IUB.

(a)



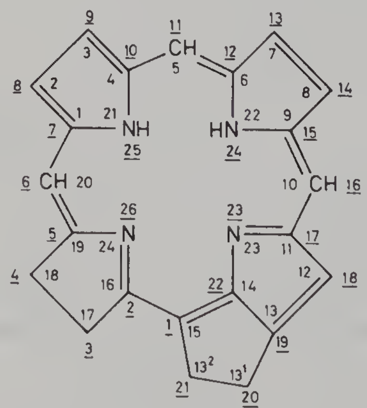
123
Porphyrin
21*H*,23*H*-Porphin

The formula can also be written in the 21*H*,22*H* form, and similarly in the 22*H*,24*H* form.

The outer locants 1–20 with rings A–D and N21–24 correspond to recent numbering.

The inner locants 1–8 with bridges α–δ and rings I–IV go back to Fischer (1927).

(b)



124
Phorbin (locants 1–26; CA 1972; *Ring Index*)

7 *Pure Appl. Chem.* **51** 2251 (1979).

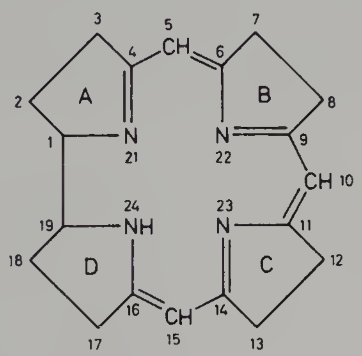
systematic: *Ring Index*:

23,24, 25,26-Tetraazahexacyclo$[15.4.2.1^{2,5}.1^{7,10}.1^{12,15}.0^{19,22}]$
hexacosa-1(22),2(26),5,7,9,11,13,15,17(23),18-decaene

The bridgeheads are C-1 and C-17. The 15-member bridge encompasses C-atoms 2–16, the 4-member bridge C-atoms 18–21 and the 2-member bridge atoms 22 and 23. The N-atoms 24–26 form three one-member secondary bridges (outer numbering 1–26).

IUPAC–IUB do not classify 'Phorbin' as representing the stem group, but relate the derivatives to the Porphyrins. Accordingly, the inner counting sequence is (1–24, 13, 13).

(c)



125
Corrin

The numbering is based on that of porphin. Thus, as the bridge 20 of porphin is missing from corrin, the locant 20 is also missing from corrin, and 21 follows directly after 19.

Corrin $C_{19}H_{22}N_4$ is the parent structure of the corrinoids to which vitamin B_{12} belongs.

An octadehydrocorrin is named corrole $C_{19}H_{14}N_4$. This designation was previously valid for the MNC form (decadehydro) of the system (*Ring Index*).

III

Nomenclature procedures

1 GENERAL PRINCIPLES

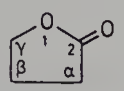
Whatever the chosen nomenclature procedure, the classes of organic compounds are put in a ranking order, which allows the principal class to be decided from among a number present in a molecule. The most important classes of compound are given below in increasing order of precedence. In each case the later class forms the main class compared to earlier ones. The classes of compound are related to characteristic groups.

1. Polysulfides, peroxides;
2. Sulfides, ethers;
3. Derivatives of inorganic acids, which do not come under 6 and 14;
4. Stibines, arsines, phosphines, azenes, azanes, hydrazines, imines, amines;
5. Hydropolysulfides, hydroperoxides;
6. Neutral esters of inorganic acids (apart from hydrogen halides) with alcohols and phenols;
7. Selenols, thiols, alcohol-phenols;[1]
8. Ketone derivatives (semicarbazones, azines, hydrazones, oximes, acetals);
9. Thioketones, ketones;
10. Aldehyde derivatives (as under 8);
11. Thioaldehydes, aldehydes;
12. Isocyanides, cyanides, nitriles;

1. The ranking difference between alcohols and phenols of the IUPAC Rules 1969/71 has not been confirmed in the 1979 rules.

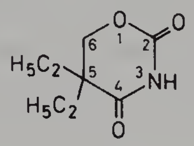
13. Derivatives of acids[2] (of 15). (amidines, imides, hydrazides, lactams, amides (*urea included*), halides, lactones, esters, anhydrides);
14. Derivatives of inorganic acids,[3] whose central atom is bound to the organic part (C-atom), through 1 or more hetero atoms and which are still acids;
15. Acids (-arsonic, -phosphinic, -sulfenic, -sulfinic, -sulfonic, thiocarboxylic, peroxy-carboxylic, -carboxylic);
16. Cations.

Generally, establishing the class of compound is not difficult. However, recognising a compound class from a name can require special considerations. Thus heterocyclic intramolecular acid amides can equally be identified as lactams, as aligned on the basis of the 'one' suffix of the ketone nomenclature in their names (5-pentanelactam = 2-piperidinone; 5-pyrazolone; 2,6-purinedione). There are corresponding possibilities with lactones.



1

γ-Butyrolactone
Tetrahydro-2-furanone



2

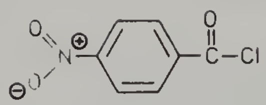
Diethadione (INN)
5,5-Diethyldihydro-2*H*-1,3-oxazine-2,4(3*H*)-dione (WHO)
5,5-Diethyl-1,3-oxazinane-2,4,-dione (IUPAC)

Here, the lactone grouping may, just as well as the lactam grouping, be conveyed in a heterocycle name.

A compound class can also be obscured by some types of nomenclature; for example if an ester group $\overset{\displaystyle O}{\overset{/\!/}{-\text{C}}}-\text{O}-\ldots$ is named according to replacement nomenclature as . . .oxo . . .oxa or . . .oxa. . .one.

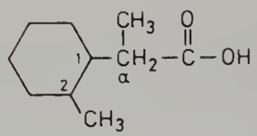
It is of particular relevance to establish the relationship of a name to a known nomenclature procedure. The question is very important in the realm of the systematology of nomenclature. Many names clearly are identifiable as proper to one nomenclature procedure, but other names come within the scope of two nomenclature procedures, for example:

2. CA lay down that the order of precedence among the acid halides and the like follow in sequence after the acids (group 15). The ranking order related to each of the acids is as given at formula 182. For amides, esters, anhydrides, a ranking order similarly follows each member of group 15.
3. It would be too much for this 'introduction' to go into detail. Those particularly interested can turn to IUPAC Rule D-1.33.



3

p-Nitrobenzoyl chloride
Substitutive -(*p*-nitro) and radicofunctional (. . . .oylchloride) nomenclature



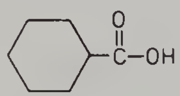
4

α,2-Dimethylcyclohexaneacetic acid
Substitutive (dimethyl) and conjuctive (cyclohexaneacetic acid) nomenclature

Even with simple names, however, there are different conceptions of the available procedure.

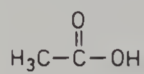
(a) 'Methylamine', for example, can be considered as substitutive (substituted ammonia which becomes an amine) (IUPAC). It can also be ascribed to radicofunctional nomenclature. In the form 'methanamine' the name is unambiguously substitutive with the main group as a suffix, clearly the reverse of 'aminomethane'.

(b) The designation of a carboxylic acid is clearly proper to substitutive nomenclature:



5

Cyclohexanecarboxylic acid
Stem compound with suffix



6

1. Ethanoic acid

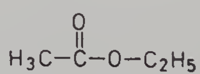
Substitution $H_3C{-}CH_3 \rightarrow H_3C{-}C(=O){-}OH$

2. [Methanecarboxylic acid]
3. Acetic acid

The trivial name 3 (unlike its German equivalent 'Essigsaeure') can be used in semi-systematic nomenclatures.

The relationships in the derivatives of carboxylic acid are more complex.

(c) Esters can be designated by using Latin or English stem words:



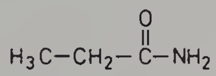
7

1. Ethyl ethanoate
2. Ethyl acetate
3. Acetic acid, ethyl ester[4]

4 The German version of the IUPAC C-Rules is still awaited. It is expected that this form will be authorized.

The designation 2 is classed among substitutive names in the IUPAC C-Rules 1979, the '. .yl . .ate' construction being provided for the suffixes. Esters are not included in radicofunctional nomenclature, even though the '. .yl. . .ate' form clearly parallels the '. .oyl . .ide' of acid chlorides such as Benzoyl chloride through the arrangement: radical-function in anion-form. The IUPAC D-Rules 1979 express inorganic ester names as radicofunctional. The German (and the English) form of name 3 can clearly be seen to be radicofunctional by virtue of the '. .yl ester' (Ger. '. .ylester') ending.

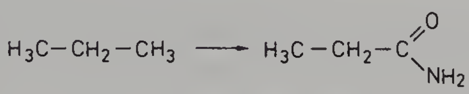
(d) Corresponding considerations apply to acid amides.



8

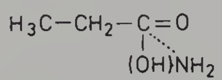
1. Propanamide
2. Propionamide

Designation 1 is clearly attributed to substitutive nomenclature. It is based on the substitution of three hydrogen atoms by: $\bar{O}$ and $H_2\bar{N}\cdot$, one oxygen atom and one amino group (radical).



9

By contrast designation 2 depicts the substance as a derivative of propionic acid. The question as to whether the name could be considered radicofunctional is left open. 'Propion' could be considered as the acyl radical with elision of the 'yl' ending and 'amide' the function in anion form.[5] There is a parallel between propionamide and benzoyl chloride in this. It would also be possible to think of the name as deriving from propionic acid,[†] with the hydroxyl group being directly replaced by an amino group.



10

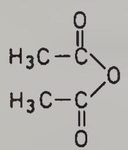
If 'propion' is interpreted as not from propionyl but from propionic acid, the name 'propion (acid) -amide' provides a direct link with the acid amide class of compounds. To

5 The anion from ammonia, NH_3, with the formula $H_2\bar{N}^-$ is called an amide (IUPAC Inorganic Rules 3.2.2.1). 'Anion form' indicates that which customarily is designated as an anion, but in this context the group is not present as an anion. Radical + anion does not give rise to a neutral molecule. Cf. III.5.2 also p. 111.

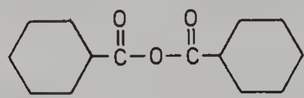
† *tr Translator's note*: The case argued by the author loses some force in translation, since 'Propionsaeure' like most German nouns is one word, whereas its English equivalent is two separate words. Propionaldehyde is an English name which could have fitted his case, except that unfortunately in that case a H-atom is replaced.

accommodate this in the nomenclature system, a widening of the definition is needed, from 'substitution (replacement) of H-atoms by radicals' to 'replacement of a radical by another'. Such a concept is supported by the systematic formulation of an acid amide using the suffix 'carboxamide'. Here, 'carboxamide' is considered as a unitary concept (like 'carboxylic acid') in suffix form; the comparison leads again to the idea of exchange of radicals.

(e) In systematic nomenclature terms, what does the name '. .acid anhydride' or 'carboxylic acid anhydride' produce?



11
Acetic anhydride
Acetic acid anhydride



12
Cyclohexane carboxylic acid anhydride

Naming acetic anhydride could be by means of a radicofunctional name (diacetyl oxide), but this would not be a customary method of dealing with organic anhydrides. In any case, these are customarily given names of the pattern: '. . . (acid) anhydride', which has nothing to do with such a nomenclature approach. A further radicofunctional method (giving acetyl acetate, analogous to benzoyl chloride) is also not customary. Naming this class of compounds, comes within the ambit of subtractive nomenclature. Subtractive prefixes such as 'anhydro' or 'dehydro' are ranged alphabetically along with substitutive prefixes, even though they are of a quite distinct character. In this way, 'anhydride' as an affix (for prefix form see footnote[6]) takes its place along with the suffixes of substitutive nomenclature. As far as nomenclature is concerned, there is thus an additive member (with subtractive connotations) which takes its place in a series along with such as 'S-S-dioxide'. Only here does the additive nomenclature also have an additive connotation. The ending 'ide' which is anionic in 'oxide' and not so in 'anhydride' implies no relationship between the two affixes. Similarly, 'anhydride' is not comparable to the hydrogen anion 'hydride'. One could also consider '. . (carboxylic) acid anhydride' as a unitary concept for a compound class and list it, like 'carboxylic acid', among the suffixes of substitutive nomenclature.

2 SUBSTITUTIVE NAMES

2.1 Overview

Substitutive nomenclature is the nomenclature system most frequently used. It is based on the formal replacement of hydrogen atoms of the parent compound by other atoms or

6 The substitutive prefix 'anhydro' refers to elimination of water between alcohol hydroxl groups and not between carboxylic acids. In the context of sugars, 'anhydride' is also used in a different relationship from that in acid anhydrides. Cf. the prefix formula **151** for identical units (p. 104).

groups of atoms, without, however, changing the function (that is, changing the functional group) by the replacement. Thus, ($-NH_2/NR_2$ is allowed, but not $-COOH/COOR$) as well as C-group radicals and hetero-group radicals, for example, H_3C-, $-\overset{O}{\overset{\|}{C}}-OH$, $-NH_2$, $-OH$, and carbocyclic or heterocyclic radicals are also considered. Insofar as it is not merely a question of hydrocarbon or heterocyclic radicals, such groups are designated 'characteristic groups' or, in appropriate cases, 'functional groups'. Such substituents may be placed in front of the parent compound name as a prefix, or after the parent compound name as a suffix. The principal compound class for the substance being decided, the relevant substituent is cited as the suffix (principal group). The other groups are cited as prefixes.

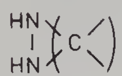
If a suffix group occurs only once in a molecule, then that part of the molecule where it occurs is chosen as the parent compound. If the suffix group occurs more than once and in different parts of the molecule, the part of the molecule in which it occurs most frequently is chosen as the parent compound. In other parts of the molecule the group is cited as a prefix.

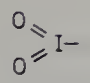
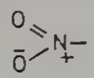
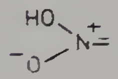
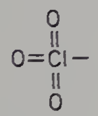
2.2 Order of characteristic groups

2.2.1 Groups which are cited only as prefixes,[7] in alphabetical order

13	$R-\underset{\|\|}{\overset{}{C}}-O-\underset{\|\|}{C}-$ (with =O on each C)	Acyloxycarbonyl: e.g. acetoxycarbonyl (corresponding. . .SO_2-. . . sulfonyl)
14	$R-O-$	Alkyloxy[8]: ethoxy, methoxy, pentyloxy etc. Aryloxy[8]: phenoxy, tolyloxy
15	$R-S-$	Alkylthio: methylthio
16	$R-Se-$	Alkylseleno
17	$R-Te-$	Alkyltelluro
18		Azi (substituent at one C-atom, forming one part of a spiro compound)
19	$\|\overset{\ominus}{\underline{N}}=\overset{\oplus}{N}=\bar{N}-$	Azido
20	$C_6H_5-N=N-(\overset{\|}{\underset{\|}{C}}-)$	Benzeneazo, Phenylazo
21	$Br-$	Bromo
22	$Br-\underset{O}{\underset{\|\|}{C}}-$	Bromoformyl

7 Only for substitution.
8 C_1-C_4 (butoxy*l*: the 'yl' ending of the alkyl radical is dropped, as with phenoxy).

23	$Cl-$	Chloro
24	$Cl-C(=O)-$	Chloroformyl
25	$Cl-S(=O)_2-$	Chlorosulfonyl
26	$O=Cl-$	Chlorosyl
27	$(O=)_2Cl-$	Chloryl
28	$(N\equiv C-)$	Cyano (see also formula 76)
29	$N\equiv C-O-$	Cyanato
30	$(H_3C-C(=O)-O)_2I-$	Diacetoxyiodo
31	Cl_2I-	Dichloroiodo
32	$-O-O-$	Dioxy, epidioxy
33	$-S-S-$	Dithio, epidithio
34	$-O-$	Epoxy, oxydi
35	$-S-$	Epithio, thiodi
36	$F-$	Fluoro
37	$F-C(=O)-$	Fluoroformyl
38		Hydrazi
39	$H-O-O-$	Hydroperoxy
40	$\overset{\ominus}{\mid C}\equiv\overset{\oplus}{N}-$	Isocyano (see also p. 107 formula 178)
41	$I-$	Iodo
42	$I-C(=O)-$	Iodoformyl
43	$O=I-$	Iodosyl

44		Iodyl
45		Nitro
46		*aci*-Nitro
47	$O=N-$	Nitroso
48		Perchloryl
49	$N\equiv C-S-$	Thiocyanato

2.2.2 Groups which can be cited as prefixes or suffixes

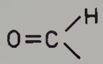
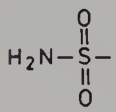
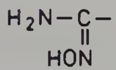
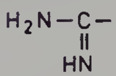
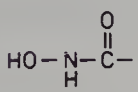
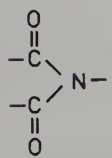
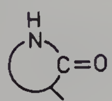
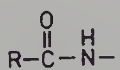
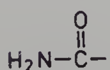
If there are different groups in a compound, which do not appear among those cited in 2.2.1, one and only one of them is cited in the name as a suffix. The others are cited as prefixes, apart from rare exceptions. The following characteristic groups are so ordered that they will be chosen as prefix with regard to any later occurring one, and as suffixes[9] over those occurring earlier (increasing order of priority as suffixes).

	Formula	Compound class groups after 1 (pp. 84, 85)	Prefix	Suffix or functional class
50	H_2As-	4	Arsino-	-arsine
51	H_2P-	4	Phosphino-	-phosphine
52	$H_2N-N=N-\overset{H}{N}-$	4	2-Tetrazeno-	-2-tetrazene
53	$H_2N-N=N-$	4	1-Triazeno-	-1-triazene
54	$H_2N-\overset{H}{N}-\overset{H}{N}-$	4	Triazano-	-triazane
55	$-\overset{H}{N}-\overset{H}{N}-$	4	Hydrazo-	[-hydrazine]
56	$H_2N-\overset{H}{N}-$	4	Hydrazino-	-hydrazine
57	$HN=$	4	Imino-	-imine(-amine)
58	H_2N-	4	Amino-	-amine

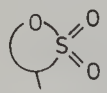
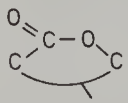
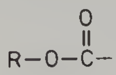
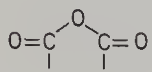
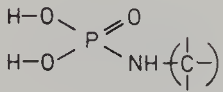
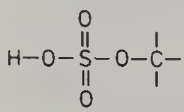
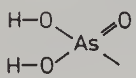
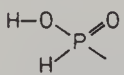
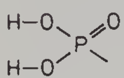
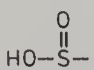
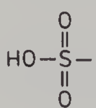
9 Only for substitutive names.

	Formula	Compound class groups after 1	Prefix	Suffix or functional class
59	$O{=}P(O{-})_3$ Alkyle	6, 14	Phosphoryltrioxy-	-phosphate[10]
60	$(O{=})_2S(O{-})_2$ Alkyle	6, 14	Sulfonyldioxy-	-sulfate
61	$H{-}Se{-}$	7	Hydroseleno-	-selenol
62	$H{-}S{-}$	7	Mercapto-	-thiol
63	$H{-}O{-}$	7	Hydroxy-	-ol
64	$H_2N{-}C({=}O){-}NH{-}N{=}$	8	Semicarbazono-	-semicarbazone
65	$=N{-}N{=}$	8	Azinodi-	-azine
66	$H_2N{-}N{=}$	8	Hydrazono-	-hydrazone
67	$HO{-}N{=}$	8	Hydroxyimino-	-oxime
68	$(RO)_2C{<}$	8	Di(alkyloxy)-	-acetal
69	$Se{=}C{<}$	9	Selenoxo-	-selone
70	$S{=}C{<}$	9	Thioxo-	-thione
71	$O{=}C{<}$	9	Oxo-	-one
	Aldehyde derivatives	10	order of precedence as 8. (ketone derivatives) (formulae 64–68)	names analogous to 8.
72	$Se{=}C({-}H){-}$	11	Selenoformyl-	-selenal
73	$S{=}C({-}H){-}$	11	Thioformyl-	-thial (C)[11] -carbothialdehyde

10 Cf. text c) to formula 7.
11 (C) signifies that the C in the characteristic group formula is not counted as within the suffix.

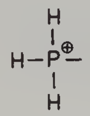
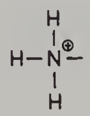
	Formula	Compound class group after 1	Prefix	Suffix or functional class
74		11	Formyl-	-al (C)[11] -carbaldehyde (Bn. IUPAC) -carboxaldehyde (CA)
75	N≡C–	12	Cyano-	-nitrile (C)[11] (see also p. 95 and 113) -carbonitrile
76		13	Sulfamoyl-	-sulfonamide
77		13	Amino (hydro-xyimino)methyl-	-(carbox)-amidoxime[12]
78		13	Amidino-	-(carbox) amidine[12]
79		13	Hydroxycarbamoyl-	-N-hydroxy . . . amide -(carbo)hydroxamic acid[12]
80		13	R-imido-	-imide (C)[11] -dicarboximide
81			Oxohetero-cycle-yl-	-lactam
82		13	-amido-	-amide
83		13	Carbamoyl-	-(carbox)amide[12]

12 When the syllables (carbo) or (carboxy) are in brackets, this indicates the form of the suffix not including the C or the carbonyl group respectively.

	Formula	Compound class group after 1	Prefix	Suffix or functional class
84		13	Hetero-cycle-yl-. . .dioxide	-sultone
85		13	Oxohetero-cycle-yl-	-olide -(carbo)lactone[12]
86		13	R-oxycarbonyl-	R-yl. . .ate R-yl. . .carboxylate
87		13	(cf. Formula **151**)	-anhydride[13]
88		14	Phosphono-amino	-ylphosphoramidic acid R-ylamidophos-phoric acid
89		14	Hydroxysulfonyloxy	-hydrogensulfate
90		15	Arsono-	-arsonic acid
91			Hydroxy-phosphinoyl-	-phosphinic acid
92		15	Phosphono-	-phosphonic acid
93	HO−S−	15	Sulfeno-	-sulfenic acid
94		15	Sulfino-	-sulfinic acid
95		15	Sulfo-	-sulfonic acid

13 Cf. text e) to formulae **11**, **12**, p. 88.

	Formula	Compound class group after 1	Prefix	Suffix or functional class
96	$H-S-C(=S)-$	15	Dithiocarboxy-	(carbo)dithioic acid (C)[11]
97	$H-S-C(=O)-$	15	Thiocarboxy- Mercaptocarbonyl	(carbo)thioic acid (carbo)thioic *S*-acid (C)[11]
98	$H-O-C(=S)-$	15	Thiocarboxy Hydroxythiocarbo-nyl	as **97** (carbo)thioic *O*-acid (C)[11]
99	$H-O-O-C(=O)-$	15	Hydroperoxy-carbonyl-	-per . . . acid (C)[11] -peroxy . . . acid (C)[11] -peroxycarboxylic acid
100	$HO-C(=O)-$	15	Carboxy-	acid (C)[11] -carboxylic acid
	stem-forms		-onium ions (cf. 9.2.1.1. p. 119)	
101	$HI^{\oplus}-$	16	Iodonio-	-iodonium
102	$HBr^{\oplus}-$	16	Bromonio-	-bromonium
103	$HCl^{\oplus}-$	16	Chloronio-	-chloronium
104	$H-Se^{\oplus}(-H)-$	16	Selenonio-	-selenonium
105	$H-S^{\oplus}(-H)-$	16	Sulfonio-	-sulfonium
106	$H-O^{\oplus}(-H)-$	16	Oxonio	-oxonium
107	$H-As^{\oplus}(H)(H)-$	16	Arsonio-	-arsonium

	Formula	Compound class group after 1	Prefix	Suffix or functional class
108		16	Phosphonio-	-phosphonium
109		16	Ammonio	-ammonium

To be interpolated between the suffixes '. . .phosphonium' and '. . .ammonium' are those of the sequence from, for example, 'diazonium', 'hydrazinium' and 'uronium'. The highest rank in group 16 includes the carbo-cations (cf. 9.3.1, p. 123).

An anion follows each onium suffix. For several anionic centres in the same structure, see 9.3.2, p. 123.

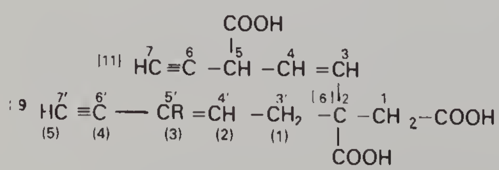
2.3 Seniority of structure elements

2.3.1 Seniority of chains

In a branched chain structure, the 'principal chain' serves as the basis of the name. This is chosen in accordance with the following criteria:

1. greatest number of principal (suffix) groups in the principal chain;
2. greatest number of multiple bonds;
3. greatest length;
4. greatest number of double bonds;
5. lowest locants for the suffixes;
6. lowest locants for multiple bonds;
7. lowest locants for double bonds;
8. greatest number of prefix substituents;
9. lowest locants for all prefix substituents;
10. the earliest letter of the alphabet for the first substituent;
11. lowest locant for the first prefix substituents in alphabetical order.

1–3



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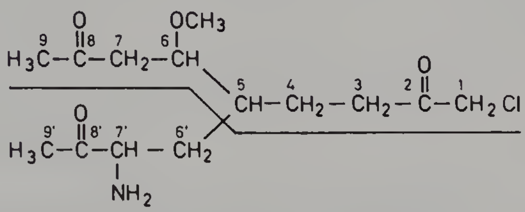
1. Greatest number of suffixes, R = H; locants in the formula 1–7: 3; 1–7′: 2; 7–7′ or 7′–7:2 2-(2-Penten-4-ynyl)-3-hepten-6-yne-1,2,5-tricarboxylic acid
2. Greatest number of multiple bonds (Mb); in all chains 3 suffixes; R = COOH; 7–7′ or 7′–7: 4; 1–7: 2; 1–7′:2.
   6-Carboxymethyl-3,7-undecadiene-1,10-diyne-3,6,9 tricarboxylic acid
   Locants in 7′–7 direction, because the double bonds take lower numbers (3, 4/7,8) against (4,5/8,9) in the opposite direction. Locants [1]–[11].
3. No Mb.s, saturated chain; R = COOH; suffixes as in 2; longest chain 7–7′ or 7′–7, 11 C. Locants as in 2.

   6-Carboxymethylundecane-3,6,9-tricarboxylic acid

   Counting direction not significant, since the saturated chain is symmetrical.

9.



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Name: 5-(2-Amino-3-oxobutyl)-1-chloro-6-methoxy-2,8-nonanedione
(Alphabetically A-c-m principal chain, A-o side-chain)

Principal chain (1–9) prefixes at 1,5,6; other, though unacceptable, possibilities would be:

chain 1,5, 9′ with prefixes in 1,5,7′ (as principal chain 1,5,7)
chain 9–1 with prefixes in 6,5,1 (4,5,9)
chain 9′–1 with prefixes in 7′,5,1 (3,5,9)
chain 9–9′ with prefixes in 6,5,7′ (4,5,7)
chain 9′–9 with prefixes in 7′,5,6 (3,5,6)

It should be noted in both formulae that the labelling of the side-chains is valid only for clarifying the choice of the principal chain. In the name, the side-chains take their own set of locants with the 'yl' position as 1.

2.3.2 Seniority of ring-systems (cf. I 5.2, p.44)

1. Heterocycles, whatever the sizes of the individual rings or ring-systems, are senior to carbocycles as parent compound.

   4-(2-Naphthyl)pyridine; not 2-(4-pyridyl)naphthalene;

2. The seniority between heterocycles is according to the sequence given in II. 2.2. b) – i) (p. 74).
3. The system with the greatest number of rings has seniority:

   Naphthylanthracene

4. The greater individual ring at the first point of difference gives seniority:

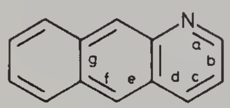
   Indanylnaphthalene

5. The greater number of atoms in common (a.i.c.) among the rings gives seniority:

	Bicyclo[3.3.3]undecane	senior to	Bicyclo[3.3.1]nonane	senior to
a.i.c.	5		3	

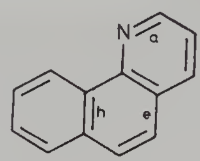
	Naphthalene	senior to	Spirobicyclohexane	senior to	Biphenyl
a.i.c.	2		1		0

6. Seniority is given by the earliest letters of the alphabet for ring junctions:



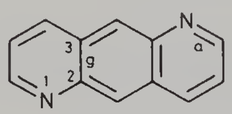
112
Benzo[*g*]quinoline

senior to



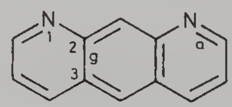
112
Benzo[*h*]quinoline

7. Seniority is given to the system with the lower numbers for ring-junctions, other bonds (for example bridges) or ring-linkages (spiro atoms, linking bonds):

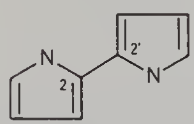


114
Pyrido[2,3-*g*]quinoline

senior to

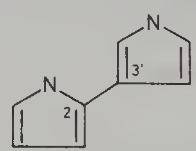


115
Pyrido[3,2-*g*]quinoline



116
2,2′-Bipyrrole

senior to



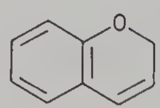
117
2,3′-Bipyrrole

8. Seniority goes to the ring with the lowest state of hydrogenation

   Pyridine senior to piperidine

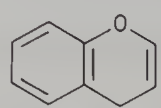
   Benzene senior to cyclohexane

9. Seniority is given to the system with the lower locants for indicated hydrogen



118
2*H*-Chromene

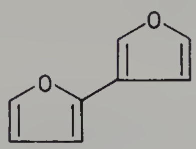
senior to



119
4*H*-Chromene

10. Seniority is given to radicals with the lower numbered 'yl' position.

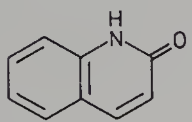
2-Furyl senior to 3-furyl



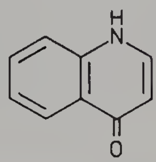
120
[2-(3-Furyl)furan]

(analogous to 2,3′-bifuran or bifuryl)
[and not 3,2′-bifuran]

11. Seniority is given to the system with the lower number for the suffix group



senior to



121
2-Quinolone
(see formula **180** p. 174)

122
4-Quinolone
(see formula **182** p. 174)

12. Seniority is given to the system with the lower set of locants, arranged in ascending order, numbering prefixes, hydro-prefixes, double bonds and triple bonds.

6-Amino-4-chloro-1,2-dihydroquinoline: 1,2,4,6 senior to

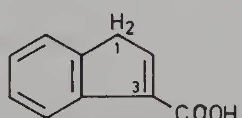
2-Amino-4-chloro-5,6-dihydroquinoline: 2,4,5,6

13. Seniority is given to the system with the lower locant for the prefix which is cited first in the name.

2.4 Numbering of compounds

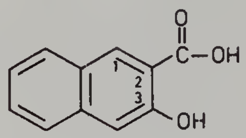
If characteristic groups are introduced as prefixes or suffixes into parent compounds (hydrocarbons Chapter I, heterocyclics Chapter II), the numbering instructions given in I and II are appropriately amplified. The lowest possible locants are given, in order, to:

1. Indicated *H*, even if it is not expressly cited in the name

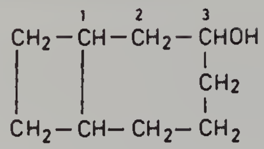


123
3-Indenecarboxylic acid

2. Substitution positions of the suffix

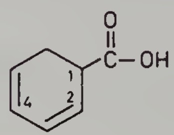


124
3-Hydroxy-2-naphthoic acid
(not the other way round)



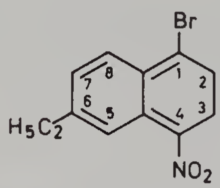
125
Bicyclo[5.2.0]nonan-3-ol
(not . . .5-ol)

3. Double bonds and then triple bonds in open-chain compounds and in cycloalkanes and poly-cycloalkanes



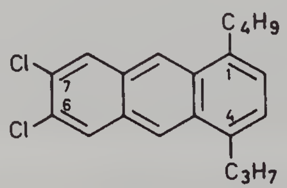
126
2,4-Cyclohexadiene carboxylic acid

4. The substitution positions of all prefixes, hydro-prefixes, double and triple bonds, ranged in ascending order in one list



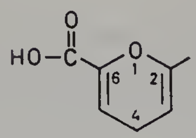
127
1-Bromo-6-ethyl-2,3-dihydro-4-nitronaphthalene
(sequence: 1,2,3,4,6)
(not 1,2,3,4,7 with nitro at 1)

5. The substitution position for the first prefix substituent occurring in the name



128
1-Butyl-6,7-dichloro-4-propylanthracene

In cyclic radicals indicated *H* has the lowest possible number as in formula **123**. After that however, deviating from 2, the position of the free valency. The above criteria are followed again if there is still a choice to be made.



129
6-Carboxy-4*H*-pyran-2yl

A locant is 'lower' than another if its number is lower or a letter is nearer the beginning of the alphabet. With locant-sets, the lowest value is given correspondingly by the first point of difference.

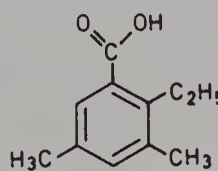
2.5 Order of prefixes (Cf. page 88 ff.)
In contrast to the suffix – the principal group which comes after the parent compound in the name the other characteristic groups – prefixes appear before the parent compound name and in alphabetical order among themselves. They are 'detachable' from the parent name. Similarly, other non-characteristic group prefixes are 'detachable', for example methyl, phenyl, cyclohexyl, pyridyl, furyl. They are placed in alphabetical order. order.

*H*ydro-prefixes (although they are additive and not substitutive units) can be arranged in alphabetical order among prefixes, but can also be treated as 'non-detachable' and cited immediately before the complete parent name (No. 8 of the following specification). The same applies to subtractive prefixes such as *a*nhydro, *d*ehydro, *d*eoxy. Heterobridges are also applied as detachable. These prefixes are arranged in order 8–1 or 9–1 before the stem of the parent names (9. hydro).

As part of the parent name and 'non-detachable' from it, are the prefixes denoting

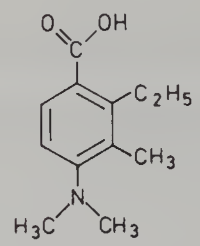
1. ring-forming (cyclo, spiro)
2. ring-breaking (seco)
3. ring-size alteration (homo, nor)
4. ring-fusion (benzo, naphtho, pyrido, furo etc.)
5. exchange of atoms in rings or chains (e.g. thia, azonia)
6. positional isomers (iso, *sec*-, *tert*-)
7. indicated *H*.
8. bridges (methano etc.)

The alphabetical order of prefixes is arranged, in the case of 'simple' prefixes, on the basis of the first letter, for example *m*ethyl, *p*henyl, *c*hloro, *a*mino, etc. If such 'simple' prefixes are combined with multiplying affixes (for example for 2 CH_3-groups, the independent unit dimethyl) this does not alter the alphabetical order. The multiplying affix is disregarded for the purposes of alphabetical order.



130
2-*E*thyl-3,5-di*m*ethyl-benzoic acid

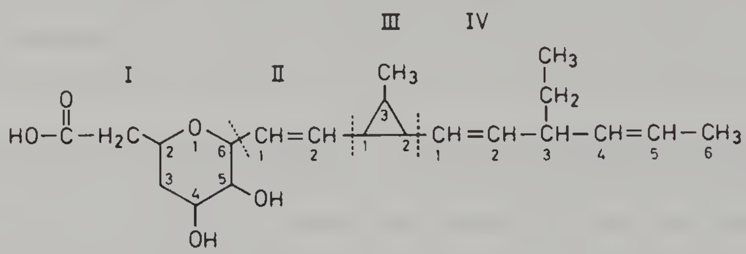
If, however, such combined 'simple' prefixes lose their independence and become part of a greater unit (composite prefix), then alphabetical order follows on the basis of the first letter of the whole name of this prefix, even if this is from the multiplying affix.



131

4-*D*imethylamino-2-*e*thyl-3-*m*ethyl benzoic acid

This principle applies also to complex names:



132

The molecule shows, in part I two kinds of characteristic (functional) groups, namely 2 alcohol OH– groups and 1 carboxylic acid group. The latter is the principal group, and the molecule is a substituted acetic acid. The substituent on the acetic acid is a tetrahydropyran ring, itself substituted. The lowest possible number for the indicated *H* and for the principal group together appear here at locant 2, so that part I is first named as tetrahydro-4,5-dihydroxy-2*H*-pyran-2-ylacetic acid. I is substituted in position 6, the substituent consisting of parts II–IV. Part II is a vinyl group with parts III–IV as substituent. Part III is a methyl-substituted cyclopropane with the further addition of substituent IV. IV is ethyl-substituted 1,4-hexadiene. The alphabetical order of substituents for part I is determined from the three substituents at 4-, 5-, and 6- positions. As the substituent at the 6- position breaks down into parts II–IV, none of which are independent with regard to part I, the alphabetical order is influenced from I to IV. The name for the combined substituent at the 6- position of I is:

II IV III II
2-[2-(3-Ethyl-1,4-hexadienyl)-3-methylcyclopropyl] vinyl-

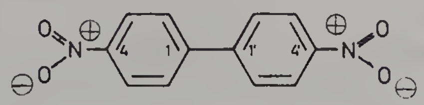
The three yl- positions of sub-substituents II, III, and IV each take the un-cited locant 1 in the context of their own group. As the combined name begins with 'e', it takes the first cited of the substituents of the base component I, including dihydroxy and also the hydro prefix tetrahydro. The name of the compound is:

6-{2-[2-(3-Ethyl-1,4-hexadienyl)-3-methylcyclopropyl]-vinyl}-tetrahydro-4,5-dihydroxy-2*H*-pyran-2-ylacetic acid

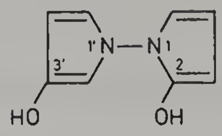
2.6 Identical units

2.6.1 Units with linking bond(s)

Ring-series with linking bonds were described at I.5.1. and II.6. Substituents on such 'identical units' are denoted by the normal prefixes or suffixes.

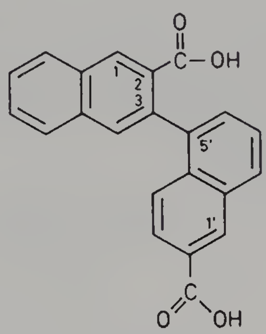


133
4,4′-Dinitrobiphenyl, as a radical (e.g.)
4,4′-Dinitro-2,2′-biphenylylene or
4,4′-Dinitro-2,2′-biphenyldiyl



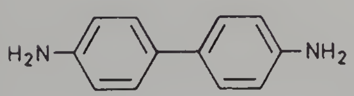
134
1,1′-Bipyrrol-2,3′-diol

Trivial names can also be combined by using a multiplying affix for such 'identical units'.

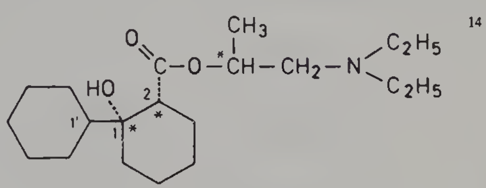


135
3,5′-Bi-2-naphthoic acid

For biphenyl derivatives, however, 'multiplied' trivial names are not applicable.



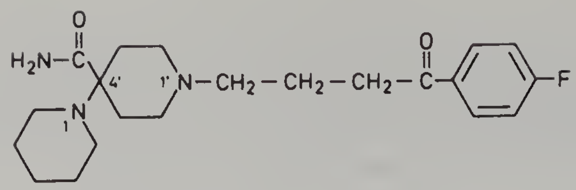
136
trivial Benzidine
syst. 4,4′-Biphenyldiamine
not 4,4′-Bianiline



137
Rociverine (INN)
2-Diethylamino-1-methylethyl *cis*-1-hydroxy-bicyclohexyl-2-carboxylate
(no hyphen in front of *cis*, English WHO)

It emerges from the last example that the lowest locant in the 'identical unit' goes to the directly connected atoms of both rings, and that the main group is considered first thereafter.

14 In this formula, * indicates an asymmetric C-atom (cf. section 10, formula 288.



138
Pipamperone (INN)
1′-[3-(*p*-Fluorobenzoyl)propyl]-1,4′-bipiperidine-4′-carboxamide

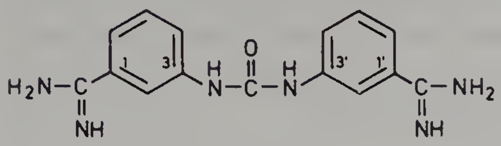
In the ‘identical unit’ (Bipiperidine), primed locants go to the partner which participates with the higher inter-connection locants. Carboxamide has seniority over ketone as a suffix.

2.6.2 Units with linking groups

The name of a compound consisting of ‘identical units’ whose only substituents are the principal groups (suffixes), and which are linked not directly to one another but to a symmetrical linking group of one or more members, begins with the bivalent (ylene) and combined linking group (central group) which is substituted at both ‘identical units’. Such polyvalent radicals are, for example,

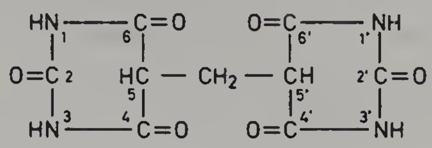
	1. Simple			2. Combined	
139	$-\overset{\overset{O}{\|}}{C}-$	carbonyldi	149	$-O-\overset{\overset{O}{\|}}{C}-O-$	carbonyldioxydi
140	$-CH_2-CH_2-$	ethylenedi	150	$-O-CH_2-O-$	methylenedioxydi
141	$-\overset{H}{N}-$	iminodi	151	$-\overset{\overset{O}{\|}}{C}-O-\overset{\overset{O}{\|}}{C}-$	‘oxydicarbonyldi’
142	$-CH_2-$	methylenedi	152	$-H_2C-O-CH_2-$	oxydimethylenedi
143	$-O-$	oxydi	153	$-O-C_6H_4-O-$	*o*-, *m*-, *p*- phenylenedioxydi
144	$-\underset{\underset{O}{\|}}{\overset{\overset{O}{\|}}{S}}-$	sulfonyldi			
145	$-S-$	thiodi			
146	$-S-S-$	dithiodi			
147	$-\overset{H}{N}-\overset{\overset{O}{\|}}{C}-\overset{H}{N}-$	ureylenedi			
148	$\underset{\|}{\overset{\diagdown\ \diagup}{N}}$	nitrilotri			

Such types of diradical names can also be combined in each case, for example **151**.



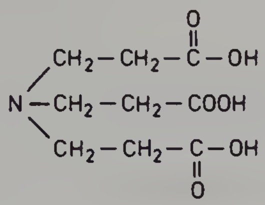
154

Amicarbalide (INN)
3,3′-Diamidinocarbanilide (WHO)
3,3′-Ureylenedibenzamidine (IUPAC) (numbering)



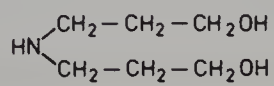
155

5,5′-Methylenedibarbituric acid



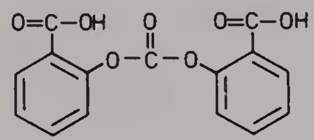
156

3,3′3″-Nitrilotripropionic acid



157

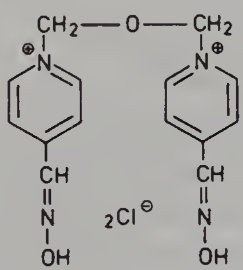
3,3′-Iminodi(1-propanol)
(cf. Improsulfan INN)



158

2,2′-Carbonyldioxydibenzoic acid

If there are other substituents on such units apart from the principal groups, these appear as prefixes and are arranged in alphabetical order before the name of the bivalent linking group.

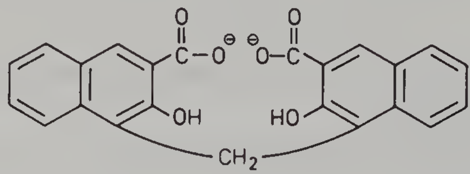


159

Obidoximechloride (INN)
(a) 1,1′-(Oxydimethylene)bis(4-formylpyridinium chloride) dioxime (WHO)
(b) 4,4′-Bis(hydroxyiminomethyl)-1,1′-oxydimethylenedipyridinium dichloride (IUPAC).

The additional prefix substituents need not be symmetrically arranged, and such a substituent can occur in just one half of the molecule.

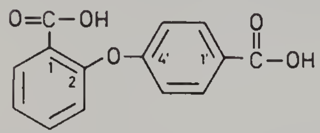
Instead of ‘di’ as the end multiplier for the base component including suffix preceded by any prefix and the linking central group (IUPAC), the prefix is not detached in WHO (CA) usage, and the doubling multiplier ‘bis’ covers the substituted base component including suffix, linked to the preceding central group. Thus the dioxime is given additive status, while in the IUPAC system, it is contained within the prefix.



160

. . . . . . embonate (INN) (Anion)
4,4′-Methylenebis(3-hydroxy-2-naphthoate) (WHO, CA)
3,3′-Dihydroxy-4,4′-methylenedi(2-naphthoate) (IUPAC)

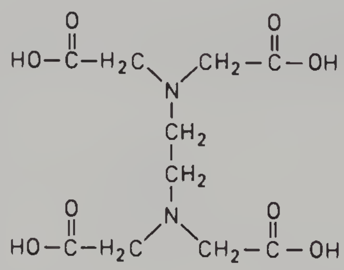
IUPAC puts the additional ‘3-hydroxy’ substituent in front (alphabet).



161

2,4′-Oxydibenzoic acid

A linking group need not join identical units at identical positions.



162

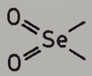
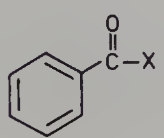
Exception (IUPAC)
Ethylenediaminetetraacetic acid

The normal ‘identical unit’ name would have been Ethylenedinitrilotetraacetic acid.

3. RADICOFUNCTIONAL NOMENCLATURE

This nomenclature procedure is not so widely applicable as is substitutive nomenclature. Suffixes are not used. In their place, functional class names, partly in anionic form, are used. The following lists give a sample of the most important functional classes, arranged in ascending order of priority. The functional class name follows the radical name as a separate word, in English.

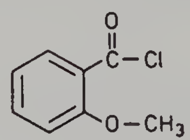
	Formula	Example	Functional class
163	$C_6H_5-\bar{N}=\overset{\oplus}{N}=\overset{\ominus}{\underline{N}}|$	Phenyl azide	Alkyl / Aryl } azide
164	$Br-CH_2-CH_2-Br$	Ethylene dibromide	

	Formula	Example	Functional class
165	H_3C-CH_2-Cl	Ethyl chloride	Alkyl halide
166			Selenone
167	$H_5C_2-\overset{O}{\underset{O}{\overset{\parallel}{\underset{\parallel}{S}}}}-C_2H_5$	Diethyl sulfone	Sulfone
168	$C_6H_5-\overset{O}{\overset{\parallel}{S}}-C_6H_5$	Diphenyl sulfoxide	Sulfoxide
169	$C_6H_5-(S)_{1-n}-C_6H_5$	Diphenyl sulfide/ polysulfide	Sulfide Polysulfide (Polysulfan)
170	$H_3C-CH_2-O-CH_2-CH_3$	Diethyl ether, Diethyl oxide	Ether, Oxide
171	$H_3C-CH_2-O-O-H$	Ethyl hydroperoxide	Hydroperoxide
172	$H_3C-\overset{SH}{\overset{\mid}{C}}H-CH_3$	Isopropyl hydrosulfide	Hydrosulfide
173	$H_3C-\overset{OH}{\overset{\mid}{C}}H-CH_3$	Isopropyl alcohol	Alcohol
174	$H_7C_{10}-\overset{S}{\overset{\parallel}{C}}-C_{10}H_7$	Dinaphthyl thioketone	Thioketone
175	$H_5C_2-\overset{O}{\overset{\parallel}{C}}-CH_3$	Ethyl methyl ketone	Ketone
176	$H_2C=CH-CH_2-N=C=S$	Allyl isothiocyanate	Isothiocyanate
177	$H_3C-CH_2-S-C\equiv N$	Ethyl thiocyanate	Thiocyanate
178	$H_3C-CH_2-\overset{\oplus}{N}\equiv\overset{\ominus}{C}$	Ethyl isocyanide	Isocyanide (see p. 90)
179	$H_3C-CH_2-CH_2-C\equiv N$	Propyl cyanide	Cyanide
180	$C_6H_5-SO_2-Cl$	Benzenesulfonyl chloride	Sulfonic acid chloride
181	$H_3C-CH_2-CH_2-CH_2-C\overset{\displaystyle\nearrow S}{\searrow Cl}$	Pentanethioyl chloride	Thiocarboxylic acid chloride
182		Benzoyl x-ide	Carboxylic acid azide/cyanide/iodide bromide/chloride/ fluoride

If a compound contains different functional class groups, the radical class name nearest the end of the list is formed. The other groups are expressed as prefixes.

$$\mathrm{HO-\overset{1}{C}H_2-\overset{2}{C}H_2-O-CH_2-CH_3}$$

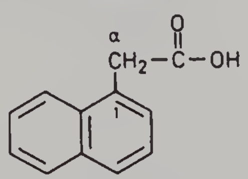
183
2-Ethoxyethyl alcohol
(Substitutive name 2-Ethoxyethanol)
[not: Ethyl (2-hydroxyethyl) ether]



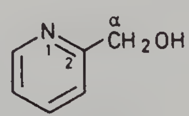
184
o-Methoxybenzoyl chloride
[not: *o*-Chloroformylphenyl methyl ether]

4 CONJUNCTIVE NOMENCLATURE
(composite names; conjunction names; composite nomenclature)

This procedure was especially used in *Chemical Abstracts* and spread from there into the literature; for example into the scientific nomenclature of the INN names of the WHO. The principle of the procedure is that a cyclic component[15] and one acyclic component (this having one principal group[16]) are linked by C-C bonding[17] that is, each is a substituent on the other. The name of the compound is formed by citing the name of the cyclic component, followed by that of the acyclic component, each being named as the molecule (not the radical).



185
1-Naphthaleneacetic acid

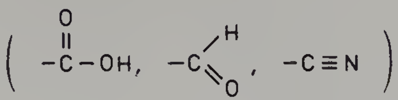


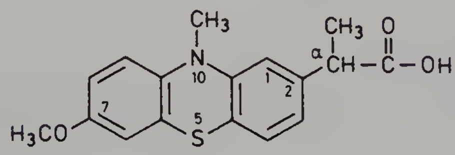
186
2-Pyridinemethanol
(cf. Pibuterol INN)

The preceding locant refers to the bonding position of the cyclic component. The C-atoms of the acyclic component are indicated with Greek letters (the α being the

15 IUPAC applies conjunctive nomenclature to benzene derivatives only if they have two or more identical side-chains.
16 Exceptions are malonic acid and succinic acid, and also compounds with several identical acyclic components (for example 2,3-Anthracenedipropionic acid).
17 Note, however, formulae 189, 191–193.

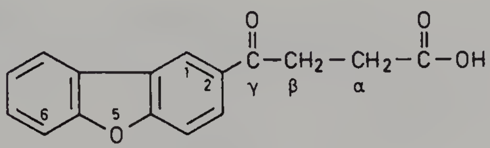
C-atom to which the principal group is attached) and proceeds to the C-atom joined to the cyclic component. Thus, C-atoms of the principal groups are not given locants.





187

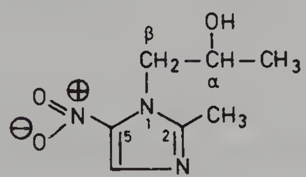
Protizinic acid (INN)
7-Methoxy-α,10-dimethyl-2-phenothiazineacetic acid
(Substitutive name: 2-(7-Methoxy-10-methyl-2-phenothiazinyl)propionic acid



188

Furobufen (INN)
γ-Oxo-2-dibenzofuranbutyric acid

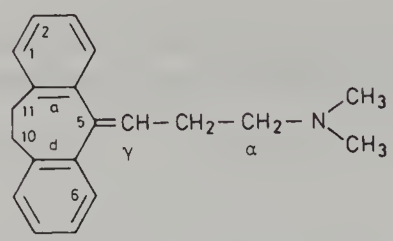
If the principal group is not at the end of the chain, the acyclic component is named as if it were so, the parts of the side-chain beyond it being cited as substituents (for N-C bonding see the Duometacin formula **193**).



189

α,2-Dimethyl-5-nitro-1-imidazole-ethanol

If cyclic and acyclic components are joined by a double bond, an upper-case Greek letter delta (Δ) is put between the two names, with the relevant locants following it as superscripts:

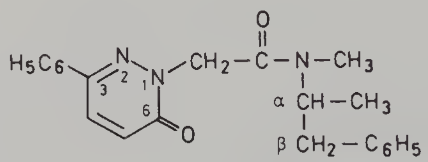


190

Amitriptylin (INN)
10,11-Di*h*ydro-*N*,*N*-di*m*ethyl-
-5*H*-dibenzo [*a*,*d*] cycloheptene-$\Delta^{5,\gamma}$-propylamine

The substituents are cited in alphabetical order (*h*, *m*).

If the insertion of the side-chain in the cyclic component causes an addition of a hydrogen atom in another ring-position, this is expressed in the name by *H* (indicated hydrogen).

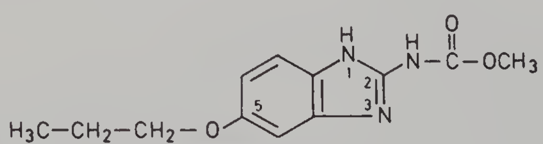


191

Isamfazone (INN)
(–)-*N*-Methyl-*N*-(*a*-methylphenethyl)-6-oxo-
3-phenyl-1(6*H*)-pyridazinacetamide

The requirement for a C-C bond in the insertion of an acyclic into a cyclic component can be disregarded for two possibilities, the application of conjunctive nomenclature to C-N- or N-C- bonding.

(a) *N* in the acyclic component with carbamic acid side-chains.[18]

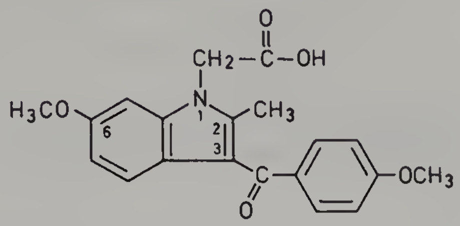


192

Oxibendazol (INN)
Methyl 5-propoxy-2-benzimidazolecarbamate

18 The IUPAC German naming of carbamic acid is not yet clarified (Carbamidsaeure, Carbaminsaeure) (cf. EP Urethane: . . . .carbamic acid . . .).

(b) *N* in the cyclic component (cf. **189, 191**)

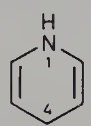


193

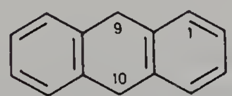
Duometacin (INN)
3-(*p*-Anisoyl)-6-methoxy-2-methyl-1-indoleacetic acid
3-(*p*-Anisoyl)-6-methoxy-2-methylindole-1-acetic acid (WHO)

5 ADDITIVE NOMENCLATURE (addition names)

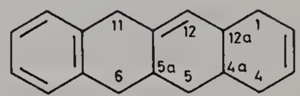
5.1 Hydro-prefixes



194
1,4-Dihydropyridine



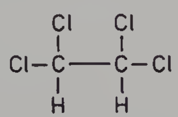
195
9,10-Dihydroanthracene



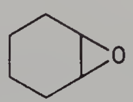
196
detachable from the parent name:
. . . .1,4,4a,5,5a,6,11,12a-octahydro. . . naphthacene. . .
(cf. Tetracycline hydrochloride EP)

Hydro-prefixes are listed among the substituents alphabetically under 'h' (detachable from the parent compound name), or may be considered as non-detachable from the parent compound name. In **196** the 'octahydro' would come then directly before 'naphthacene'. Basically in Carotenoid nomenclature hydro-prefixes are taken to be non-detachable.

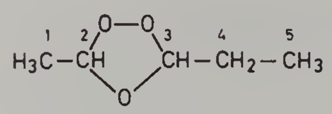
5.2 Post-positioned additions in anion-form



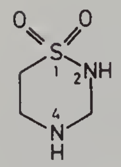
197
Acetylene tetrachloride
[the substitutive name
1,1,2,2-Tetrachloroethane
is preferred]



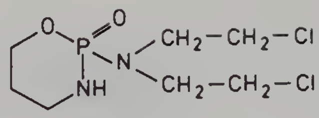
198
Cyclohexene oxide
(or 1,2-Epoxycyclohexane
or 7-Oxabicyclo[4.1.0] heptane)



199
2-Pentene ozonide (locants)
[or 3-Ethyl-5-methyl-1,2,4-trioxolane]



200
Taurultam (INN)
1,2,4-Thiadiazinane-1,1-dioxide



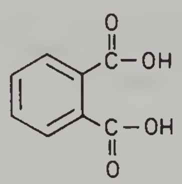
201
Cyclophosphamide (INN)
2-[Bis(2-chlorethyl)amino]-
1,3,2-oxazaphosphinane-2-oxide

In English (in contrast to German) additive nomenclature, the last part of the name (addition member) follows without hyphen after the parent name as a separate unit. (The method for the German IUPAC nomenclature is not yet fixed.)

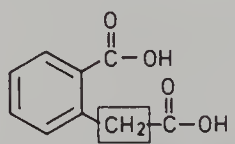
5.3 The prefix 'homo'

Ring-expansion (steroid hydrocarbons, see I.8.)

The use of 'homo' to denote a CH_2-group introduced into a parent compound should be avoided where possible. The systematic name for the compound produced by the addition is preferable.



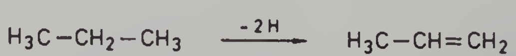
Phthalic acid



202
[⟶ Homophthalic acid]
o-Carboxyphenylacetic acid
(Priority as parent compound as at 2.3.1 number 3 p. 96)

6. SUBTRACTIVE NOMENCLATURE (subtraction names)

6.1 Endings -ene, -yne

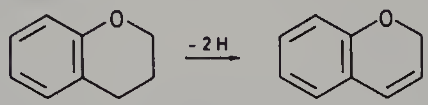


203
Propane ⟶ Propene

$$H_3C-(CH_2)_4-CH_3 \xrightarrow{-4\,H} H_3C-(CH_2)_3-C\equiv CH$$

204

Hexane ⟶ Hexyne



205

Chroman ⟶ Chromene

Codeine (see formula **206**)

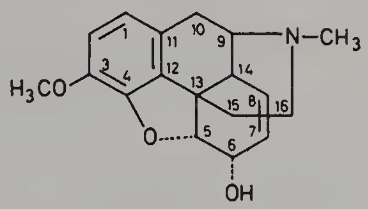
syst. 4,5-Epoxy-3-methoxy-17-methyl-7-morphinene-6-ol
cf. Ethylmorphine hydrochloride EP;
locant 17 not IUPAC)

6.2 Subtractive prefix ‘de’

Note: the subtractive prefix ‘des’ is allowable in French or German, but not in English IUPAC usage.

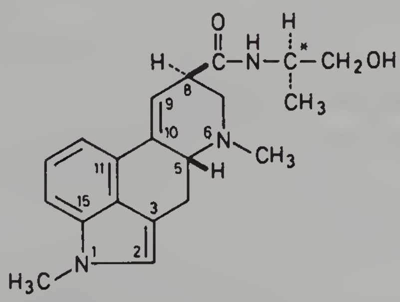
1. Removal of hydrogen: x-dehydro; trivial parent name (substituent alphabetically cited under ‘d’).

(a) *Creation of a double bond*



206

trivial: Codeine
syst.: 7,8-Didehydro-4,5 α-epoxy-3-methoxy-
N-methylmorphinan-6α-ol (cf. 6.1)



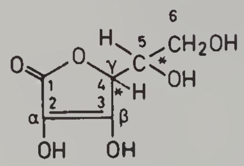
207

Propisergide (INN)
9,10-Didehydro-*N*-[(*S*)-2-hydroxy-1-methylethyl]-1,6-dimethylergoline-8β-carboxamide (WHO)

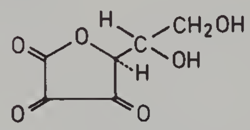
(b) *Change from –OH to =O*

Ascorbic acid[19]
L-Ascorbic acid
(OH: Enediol)

Dehydroascorbic acid[20]
Dehydro-L-ascorbic acid
Didehydro-L-ascorbic acid



$\xrightarrow{-2H}$

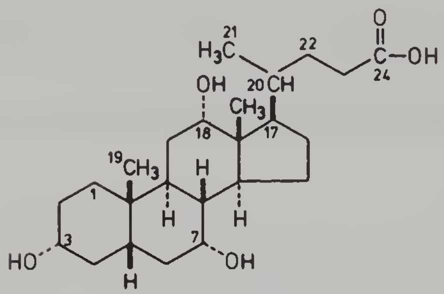


108
3-Oxo-L-gulonic acid
γ-lactone, enol form (EP)

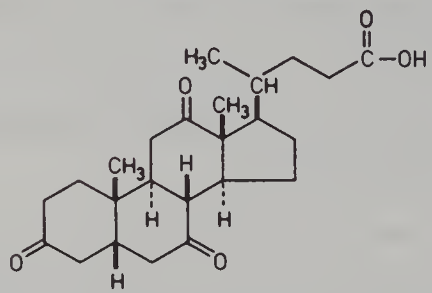
209
L-*threo*-2,3-Hexodiulosonic
acid γ-lactone

Cholic acid
(–OH: *sec.* alcohol)

Dehydrocholic acid[20] (INN)
=O



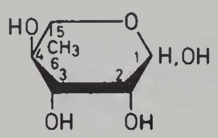
$\xrightarrow{-3H_2}$



210
3*a*,7*a*,12*a*-Trihydroxy-
5β-cholan-24-oic acid

211
3,7,12-Trioxo-5β-cholan-24-oic
acid

2. Exchange of –OH with –H, prefix 'deoxy' (German 'desoxy')



212
L-Rhamnose
6-Deoxy-L-mannopyranose
(compare (eg) Meproscillarin INN)

$C_6H_5-CH(OH)-\overset{\overset{\displaystyle O}{\|}}{C}-C_6H_5$ Benzoin

↓ OH+H

$C_6H_5-CH_2-\overset{\overset{\displaystyle O}{\|}}{C}-C_6H_5$ Desoxybenzoin

213

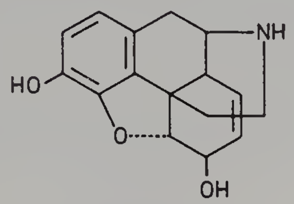
19 The example is current in pharmaceutical chemistry. It is noteworthy that the trivial name is also the INN one; these are not mutually exclusive.

20 These are commonly used, but are effectively trivial names; in the first example, correct scientific naming requires that the multiplicative prefix 'di' be added; in the second example, the 'dehydrogenation' (= oxidation) would require the correct prefix 'hexadehydro'.

3. Exchange of $-OCH_3$ with $-H$, prefix: 'demethoxy' Deserpidine (INN)
 11-Demethoxyreserpine (WHO) (not IUPAC)
 cf. also for example Vindesine (INN)

4. Exchange of $-\overset{\overset{\displaystyle O}{\|}}{C}-CH_3$ with $-H$, prefix: 'deacetyl'
 Demecolcin (INN) (not in IUPAC rules)
 Deacetyl-*N*-methylcolchicine (WHO)
 cf. also for example Vindesine (INN)

5. Exchange of $-CH_3$ with $-H$, prefix: 'demethyl'



214

De-*N*-methylmorphine (IUPAC)
Normorphine (INN)[21]
cf. also for example Vinformide (INN): *N*-Demethyl . . . . . .

6. Elimination of a ring in a steroid structure: for example Des-A . . . (see I,8.5.2.2).

6.3 Subtractive prefix 'nor'[22] ($-CH_2$, replacement of $-CH_3$ with $-H$)

1. In terpenes, see I.9 (p. 59).
2. In steroids, see I.8.2 ff. (p. 52).

Epinephrine (INN)

syst.:
(a) (-)-α-3,4-Dihydroxyphenyl-β-methylaminoethanol[24] (WHO)

(b) L-1-(3′,4′-Dihydroxyphenyl)-2-methylaminoethan-1-ol (EP) (Adrenalin tartrate)

$\xrightarrow[+H]{-CH_3}$

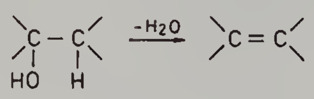
trivial:
Norepinephrine (INN) or
Noradrenalin[23]
(DAB 8) (hydrochloride)

syst.
(*R*)-2-Amino-1-(3,4-dihydroxyphenyl)-ethanol[25] (but see IV formula **140** p. 167)

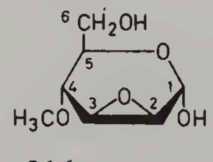
21 An INN designation is essentially not a scientific name.
22 Alternatively, 'nor' as in (for example) Norvaline, for the change of a branched chain compound (Valine) to a straight chain compound (but see footnote p. 220)
23 Nor. . is trivial here, and not to be considered systematic.
24 (−): Direction of rotation. (cf. III 10 p. 127)
25 (*R*) following Cahn-Ingold–Prelog sequence rules (cf. III 10 p. 129).

6.4 $-H_2O$, prefix: 'anhydro'[26]

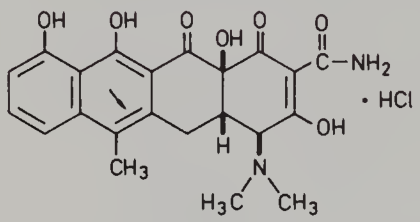
'Anhydro' signifies the intramolecular elimination of water between alcoholic OH-groups (forming an ether) (IUPAC). It is also used for the elimination of water with the production of a double bond (the example is not IUPAC). It is cited alphabetically among substituents under 'a' or as non-detachable after the substituents.



215



216
2,3-Anhydro-4-*O*-methyl-
a-D-mannopyranose



217
Anhydrotetracycline hydrochloride
(Reference material EP)
(↘ Double bond through elimination of water)

7 REPLACEMENT NOMENCLATURE (see also II.7.2 (p. 82))

7.1 Acyclic

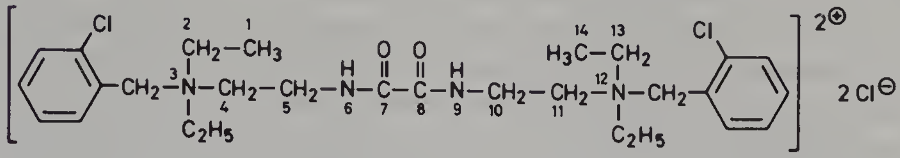
The procedure, which was discussed at II.3, for naming heterocyclic compounds, is extended to acyclic compounds. The basis of the name is an open-chain saturated compound in which CH_2-groups are replaced by hetero-atoms. Unsaturated bonds are then denoted in the normal manner (the syllable 'ene') in the name. If a number of different hetero-atoms are introduced, the 'a' terms are cited in the name in the order of precedence of the list at II.2. Cationic hetero-atoms are arranged directly following the corresponding neutral heteroatoms.

$-O-$	oxa	$-\overset{\oplus}{O}=$	oxonia
$-S-$	thia	$-\overset{\oplus}{S}=$	thionia
$-\overset{H}{N}-$	aza	$-\overset{\oplus\,|}{\underset{|}{N}}-$	azonia

Terminal hetero-atoms appear in the name as substituents (prefix or suffix), but not as 'a' terms. The same goes for other groups which may serve as suffixes, such as $-\overset{O}{\overset{\|}{C}}-NH_2$ or

26 Not for lactones.

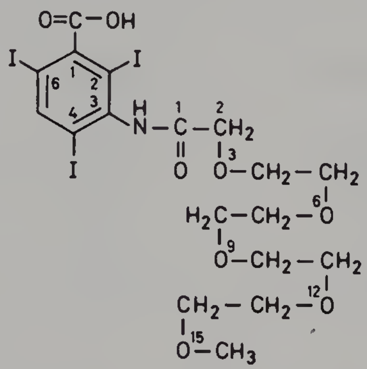
$-\overset{\overset{O}{\|}}{C}-OR$. Groups of this kind in the chains being named can be denoted by using 'a' terms.



218

Ambenonium chloride (INN)
Oxalylbis[(iminoethylene)] bis[(*o*-chlorobenzyl)-diethylammonium chloride] (WHO)
(see 2.6.) or (locants)
3,12-Bis(*o*-chlorobenzyl)-3,12-diethyl-7,8-dioxo-6,9-diaza-3,12-diazoniatetradecane dichloride

The 'a' terms are considered not detachable from the parent name, and are not cited alphabetically among the substituents (c-e-o).



219

Iotrizoic acid[27]
2,4,6-Triiodo-3-[2-[2-[2-[-(2-methoxyethoxy)ethoxy[ethoxy] ethoxy] -acetamido] benzoic acid (WHO)
or
2,4,6-Triiodo-3-[3,6,9,12,15-pentaoxahexadecanoyl)amino] benzoic acid[28]

8 PHANES, CYCLOPHANES
(IUPAC rules for this class of compound are not yet available {1984})

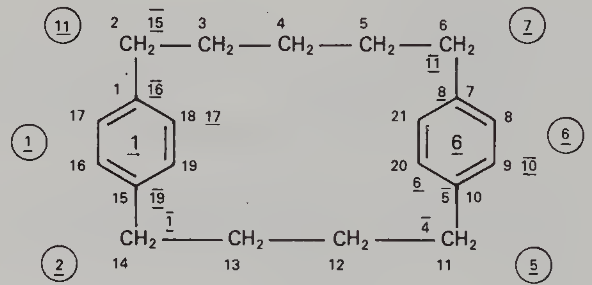
'Protophanes' are open chains consisting of units of rings joined by aliphatic groups. 'Phanes' correspond to the macro-ring closed units. 'Polyarenes' are directly joined open chains of arenes. 'Cyclopolyarenes' are corresponding groups closed to form macro-rings. 'Arene' here signifies not only aromatic hydrocarbons (benzene, naphthalene, etc.) but also much more generally, all MNC-rings and includes heterocyclics). ('Cyclophane'

27 An unofficial germanicized form of the English name: 'Iotrizoesaeure' was used in the German text.
28 The terminal 'a' of the numeric prefix is not elided before the vowel.

is the designation for ring compounds in which MNC individual rings or fused systems are bonded directly or by linking groups to macro-rings.)

Phane nomenclature belongs to replacement nomenclature. Nomenclatures of this type (matrix names) have long been concerned with the replacement of atoms by other atoms (C-atom by hetero-atom while retaining as parent name the C-compound, 'a' nomenclature, so called; hetero by C-atom, with the hetero compound as parent name; hetero by hetero, especially O by S with the retention of the O-compound name with a thio prefix). Here, however, C-atoms in aliphatic or saturated cyclic compounds are exchanged by 'arene rings'. The units entering take the ending 'a' after their parent name, analogously to the 'a'-nomenclature.

The essence of the system is the use of two sets of locants. The one set refers to the saturated hydrocarbon as base unit; the other, here called the 'exponent locants', to the entering arenes, and it conforms to the normal locants of the ring or ring-system. The 'exponent locants' are in many cases expressed as 'exponents', that is, they are put in superscript after the basis locants. In other cases, however, they are on the line and are then put in brackets. They obviously have no mathematical 'exponent' function.



220

(a) Tricyclo [$13.2.2.2^{7,10}$]henicosa-1^{17},7,9,15,18,20-hexaene. Bridged hydrocarbon. Bridgeheads 1,15. bicyclic 1–19, secondary bridge 20/21. The double bonds in the molecule, with the exception of the 1(17) double bond, are given only the lower of their two locants in each case.

(b) 1,6-Di(1,4)benzena-cycloundecaphane ('arena' name), Following the introduction of the name 'benzeno' for a normal benzene bridge, in the IUPAC rules 1979, the replacement by benzene as here, is denoted by 'benzena' instead of 'phena'.

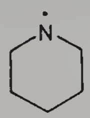
1,6 are base-component locants, (1,4) exponent locants. Two CH_2-groups of the cycloundecane base-structure are replaced with benzene in the 1,4-position. The numbering of the base-component is such as to give the lowest possible locants to the benzene rings.

(c) [4.5]-Paracyclophane.

[4.5] does not indicate locants, but the number of CH_2– groups of the base-structure standing between the two 'replacement benzenes'. For this reason the separation of the [4.5] in square brackets is by a full stop and not by a comma. Numbering runs through from 1–21 counterclockwise.

9 RADICALS AND IONS

9.1 Radicals

	As substituent		As free radical
221	Methyl	$H_3C\cdot$	Methyl
222	Hydroxymethyl	$HOH_2C\cdot$	Hydroxymethyl
223	Trimethylene	$\cdot CH_2-CH_2-CH_2\cdot$	1,3-Propanediyl
224	Methylene	$\cdot CH_2\cdot$	Methylene, Carbene
225	Propionyl	$H_3C-CH_2-\overset{\overset{O}{\Vert}}{C}\cdot$	Propionyl
226	Propionyloxy	$H_3C-CH_2-\overset{\overset{O}{\Vert}}{C}-O\cdot$	Propionyloxyl
227	Ethoxy	$H_3C-CH_2-O\cdot$	Ethoxyl
228	Anilino	$C_6H_5-\overset{H}{N}\cdot$	Phenylaminyl
229	Piperidino		1-Piperidyl
230	Hydrazino	$H_2N-\overset{H}{N}\cdot$	Hydrazyl
231	Ethylimino	$H_5C_2-N:$	Ethylaminylene

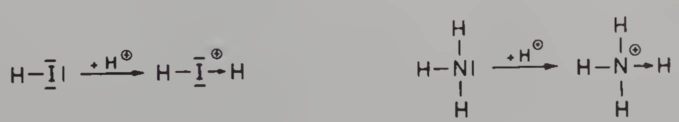
In formulae, radicals are often represented as substituents with a hyphen instead of a decimal point for the unpaired electron. (cf. p. 24 formula **23**; (p. 166/167 formulae **129--135**)

9.2 Ions

9.2.1 Cations

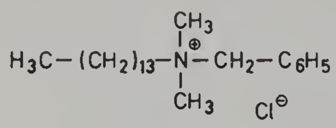
9.2.1.1 Onium ions

The parent forms of the 'onium ions' are given under formulae **101–109**; they are derived by fixation of a proton to a hetero-atom (p. 95–96).



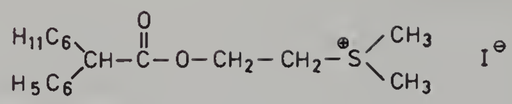
232

Examples derived by substitution (salts):



233

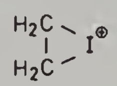
Miristalkonium chloride (INN)
Benzyldimethyltetradecylammonium-chloride (WHO) (IUPAC)
(alphabetical order of substituents)



234

Hexasonium iodide (INN)
(2-Hydroxyethyl)dimethylsulfonium iodide α-phenylcyclohexane acetate (WHO)
[2-(2-Cyclohexyl-2-phenylacetoxy)ethyl] dimethylsulfonium iodide (IUPAC)

In the WHO designation of formula **234**, the onium function (as a salt) is put as suffix to the unesterified alcohol, and the acid of the ester follows in anion form. This procedure differs from the IUPAC ruling. According to that, in choosing between the competing functions onium and ester, the senior appears as a suffix, the junior as prefix, the substituents being cited in alphabetical order (c/m in this case). The salt-forming anion follows the cation. (cf. commentary after formula **109**).



235

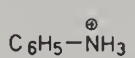
(a) Ethyleniodonium cation
or
(b) Iodiranium (cationic iodine as 'a'-term, see II.2.1, p. 71)

If the halogen cation is incorporated in a C-ring, the C-part of the name is treated as a cation-substituted alkylene radical for (a).

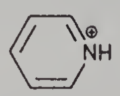
See Part 7 for 'onium ion' replacement names, p. 116.

9.2.1.2 Cations with the 'ium' ending

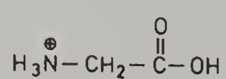
Cations can be named, using a trivial name as parent compound and adding (after elision of any terminal 'e' present) the 'ium' ending to indicate the positive charge, as in onium ions.



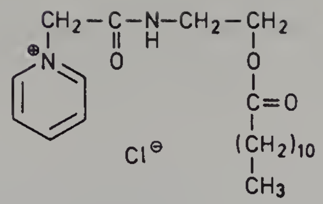
236
Anilinium



237
Pyridinium

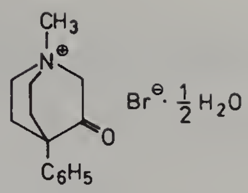


238
Glycine cation
Glycinium



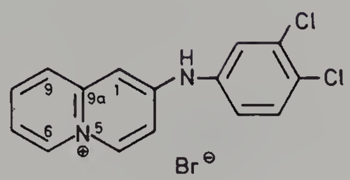
239

Lapirium chloride (INN)
1- {[(2-Hydroxyethyl)carbamoyl] methyl}pyridinium chloride laurate (ester) (WHO)
1-(2-Lauroyloxyethylcarbamoyl-methyl)pyridinium chloride (IUPAC)



240

Quinuclium bromide (INN)
1-Methyl-3-oxo-4-phenyl-quinuclidinium bromide-hemihydrate (WHO) (IUPAC)



241

Nolinium bromide (INN)
(a) 2-(3,4-Dichloroanilino)quinolizinium bromide

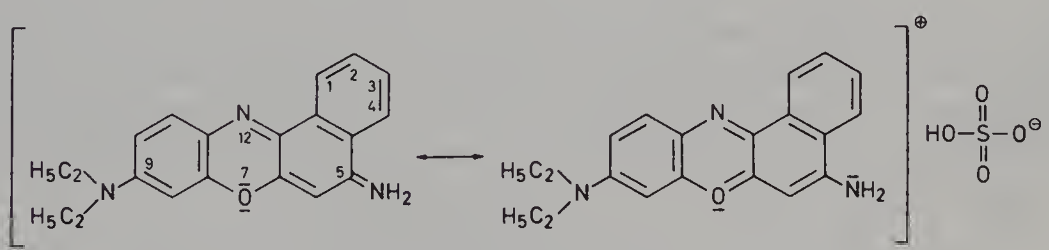
The cation here does not result from proton addition. The normal neutral MNK form for 9a*H*-quinolizine has double bonds at the 1,3,6,8 positions. Applying the MNK principle to the cation leads to the generation of 'quinolizinium' from 'quinolizine'. The name (b)

(b) 2-(3,4-Dichloroanilino)quinolizinylium bromide

is also permissible. This can be based on the concept of the loss of an electron from the 9a-quinolizinyl radical, with the mesomerism of the cation.

9.2.1.3 Cations with the 'ylium' ending

The second name of formula **241** leads to this sub-section.

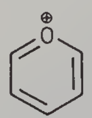


242

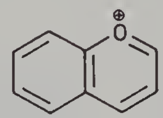
Nile blue A
5-Amino-9-diethylamino-benzo[*a*] phenoxazinylium-hydrogensulphate (EP)

The resonance form on the left exhibits an iminium group in the 5-position, which again arises through proton addition (from H_2SO_4) to a hetero-atom. The 5-amino-5-carbenium ion could have led to the mesomeric resonance form on the right. This concept is the basis for the formation of names with the 'ylium' ending.

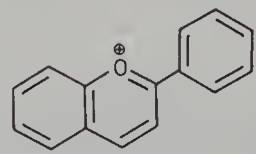
9.2.1.4 Trivial names for cations



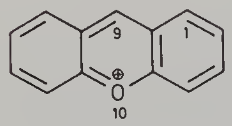
243
Pyrylium



244
Chromenylium



245
Flavylium



246
Xanthylium

$$H_3C-\overset{\oplus}{N}(CH_3)_2-CH_2-CH_2OH$$

247
Choline
(2-Hydroxyethyltrimethylammonium)

9.2.2 Anions

9.2.2.1 Ending in 'ate'

Anions take the ending 'ate' if they are derived from carbonic acids, sulfonic acids, sulfinic acids, etc. (cf. 1, Group 15). The ending is added to the stem of the names of acids whether or not trivial.

. . . acetate, . . . propionate, . . . heptanoate, . . . benzoate, . . . nicotinate,
. . . cyclohexanecarboxylate, . . . l-naphthalenesulfonate, . . . phenylarsonate.

$$H_2N-\overset{\overset{O}{\|}}{C}-O^{\ominus}$$ Glycine anion, . . . glycinate

248

9.2.2.2 Ending in 'olate'

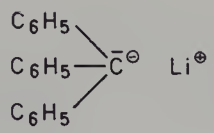
Anions take the 'olate' (or 'thiolate') ending, when they are from alcohols or phenols (or their S-analogues). 'Olates' are also designated as '. .yl oxides', and 'thiolates' as '. .yl sulfides'.

Radicofunctional names ending in 'ylate' can also be formed, but not in English.

249	$NaOCH_2-CH_2-CH_3$	Sodium propanolate Sodium propoxide
250	$NaOCH_3$	Sodium methanolate
251	$NaOC_6H_5$	Sodium phenolate Sodium phenoxide
252	$NaSCH_3$	Sodium methanethiolate Sodium methyl sulfide

9.2.2.3 Carbanions ending in 'ide'

253 $Ca^{2\oplus}$ $\bar{C}\equiv\bar{C}^{2\ominus}$ Calcium acetylide (Calcium carbide)

254 

Triphenylmethyl-lithium
(Triphenylmethanide anion)

9.2.2.4 Transcriptions

In special cases, anions are transcribed:

Sodium tryptophanate	also Tryptophan, sodium salt	
Monosodium glutamate Sodium hydrogen glutamate	also Glutamic acid, monosodium salt	
Merbromin (INN)	Disodium salt of . . .	(WHO)
Sulfamerazine-sodium (INN)	Sodium derivative of . . .	(WHO)
Thiopental-sodium (INN)	Sodium derivative of . . .	(WHO)

9.3 Two or more ions of the same type of charge in one structure

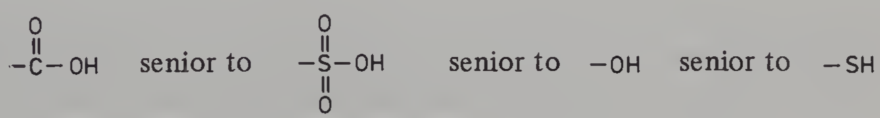
9.3.1 Cations

The highest priority cation is expressed as a suffix, and forms the parent name; the others act as substituents (prefixes). Priority is decided from the following.

1. C⊕ before heteroatom⊕ in the seniority-order of formulae **109–101** (pp. 95–96)
2. Cyclic structure ⊕ before acyclic structure ⊕
3. Priority of cyclic structures according to 2.3.2. (p. 97)

9.3.2 Anions

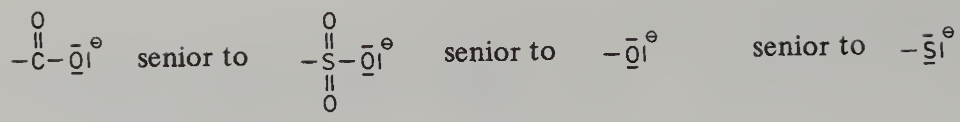
Where there is more than one anion present, the highest priority anion takes precedence in forming the parent compound, the others becoming substituents. Seniority of the acids etc. as main groups:



255

(cf. 1, groups 15 and 7) (pp. 84, 85)

Seniority of anions:

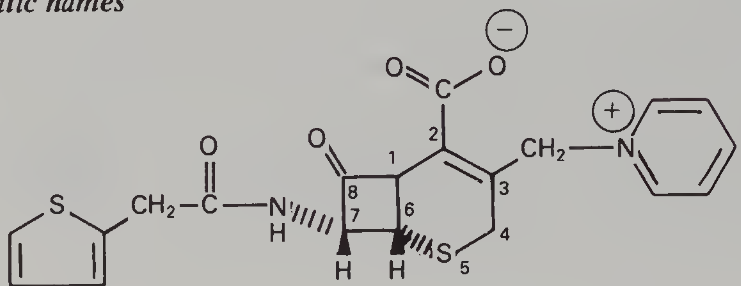


256

Suffixes:	{ carboxylate { . . . . . . oate	sulfonate	olate[29] (oxide)	thiolate (sulfide)
prefixes:	carboxylato	sulfonato	oxido	sulfido

9.4 Ions of different types of charge in the one structure (Zwitterions, 'betaine', 'inner salts', mesoionic compounds) (cf. IV. 17)

9.4.1 Systematic names



257
Cefaloridine (INN)

Naming Cefaloridin
systematic

(a) (6*R*,7*R*)-1-{[2-Carboxy-8-oxo-7-(2-(thienyl)acetamido)-5-thia-1-azabicyclo[4.2.0]oct-2-en-3-yl]methyl}pyridinium hydroxide, inner salt (WHO, without steric information)

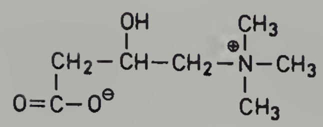
(b) (6′*R*,7′*R*)-1-[[8′-oxo-{7′β-[2-(2-thienyl)acetamido]-5′-thia-1′-azabicylo[4.2.0]oct-2′-ene-3′yl}methyl]]pyridium-2′-carboxylate

(c) (6*R*,7*R*)-8-oxo-3-(1-pyridiniomethyl)-7-[2-(2-thienyl)acetamido]-5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylate

semi-trivial:
(d) 3-(1-Pyridiniomethyl)-7-[2-(2-thienyl)acetamido]-3-cephem-4-carboxylate (EP. III) (. . .cephem. . . see II. 3.1 formula **107**)

(a) Avoids the need for information on ions by the periphrase 'inner salt', (b) following IUPAC, an anionic substituent (expressed in [[ ]] + suffix anion substituted into the cation. (c) Following IUPAC, a cationic substituent is substituted into the anion. (d) Procedure as (c), except that the anion is simplified by using the trivial stem.

29 Note the other ending 'olide' with lactones, see formula **85**.



258

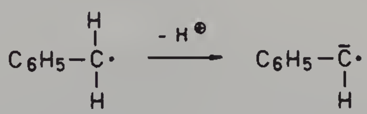
Carnitine (INN)
(a) (3-Carboxy-2-hydroxypropyl)trimethyl-ammonium hydroxide, inner salt (WHO)
(b) 3-Hydroxy-4-trimethylammoniobutyrate (IUPAC)

The cation is substituted into the anion.

259

Triphenylphosphonium benzylide

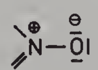
The ending 'ylide' arises where the radical ion is considered as formed by the loss of a proton from the radical.



260

Benzyl Benzylide

Finally, that type of bonding must be mentioned which is expressed by the so-called 'semi-polar' bonding (amine oxides, nitro groups).

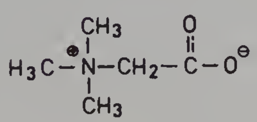


261

cf. Oxonazine (INN)
Chlordiazepoxide (INN)

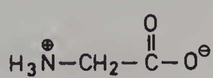
Important zwitterions, in particular those in the field of biochemistry, are not discussed here as there is a special nomenclature covering them (e.g. lecithin, cocarboxylase, cyanocobalamin) (see p. 227).

9.4.2 Trivial names



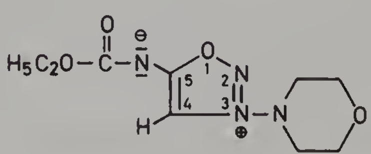
262

trivial: Betaine (IUP)
syst.: Trimethylammonioacetate



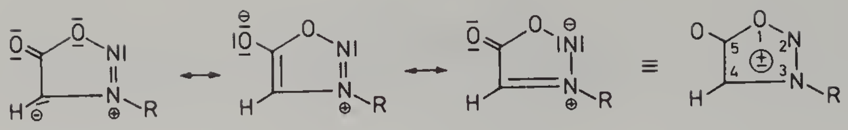
263

Glycinamphion
Ammonioacetate



264

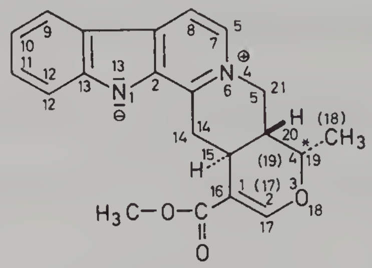
Molsidomine (INN)
N-Carboxy-3-morphinolinosydnone-imine, ethyl ester (WHO)



265 266 267 268

R-syndrone (R: e.g. phenyl, morpholino)

The arrangement of the hetero-atoms in the ring corresponds to that in 1,2,3-oxadiazole. The illustration shows three mesomeric resonance forms with the generalized formula which dispenses with the information on localized charges.

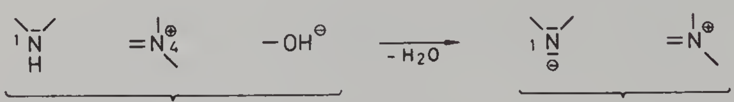


269

Serpentine[30]

a) (outer locants for oxayohimbanium)
b) (inner locants (17), (19), with (18) for Corynan)
c) (inner locants 1–14 IUPAC, systematic)

Serpentine is a so-called 'anhydronium base'. It can be derived by the loss of water from the hydroxide of the quaternary base.



270

Systematic names can be envisaged in various ways.

(a) 3,4,5,6,16,17-Hexadehydro-16-methoxycarbonyl-19*a*-methyloxayohimbanium (Merck-Index).

The name, even together with consideration of the Yohimbane formula established by IUPAC, gives no definitive structure for the compound. Information on the position of the ring-oxygen is lacking, and there is no indication of the zwitterion.[30]

(b) (*S*)-17,19-Epoxy-16-methoxycarbonyl-coryna-3,5,16-trieniumbetaine.

30 Name (a) does not conform to the IUPAC replacement nomenclature principle, by which 'a' terms of hydrocarbons can be combined (II.3.1). This exercise effects the combination of an 'a' term with a trivial name of a heterocyclic natural product. (New IUPAC Rule F? not yet in the 1979 Rules.)

Through the trivial name Corynan (Beilstein, CA) the name is simplified. The methyl substituent no longer need be specifically cited, the oxygen can be fitted in as an epoxy bridge, and, in the Corynan base-component framework, does not have its own locants; apart from which, the introduction of the unsaturated bond by means of the 'ene' ending is preferable to the 'dehydro' procedure. Finally, a zwitterion is specified by the use of 'betaine'. Here, 'betaine' is a general name, a class of compound. (cf. however, the substance 'Betaine' has the formula **262**.)

(c) (*S*)-4,4a,5,13,14,14a-Hexahydro-1-methoxycarbonyl-4α-methyl-indolo[2,3-*a*]pyrano[3,4-*g*]quinolizin-6-ium-13-ide

Here, the ring-system is systematically named and numbered according to IUPAC, starting with hydrogenation of the MNC position. All substituents are indicated as in (a). The zwitterion appears in the form ium/ide with locants.

The IUPAC Rules on zwitterions (9.4) do not give exhaustive information on naming them in this case. According to IUPAC (see 9.2.2.3), 'ide' is the ending for a carbanion. Here, however, a ring nitrogen atom is being considered, and there is a view that 'ide' can be recommended in this case too (see, 87, *5).

10 STEREOCHEMICAL NAMING METHODS

10.1 Chiral centres (asymmetric C-atoms)
(The asymmetric C-atom is bonded to four different atoms or groups.)

10.1.1 Direction of rotation

The information on the direction of rotation of polarized light (the D-line of the sodium lamp) by a liquid substance or of a material in solution, conveys no evidence as to the configuration of the substance or the material in question. One differentiates as follows:

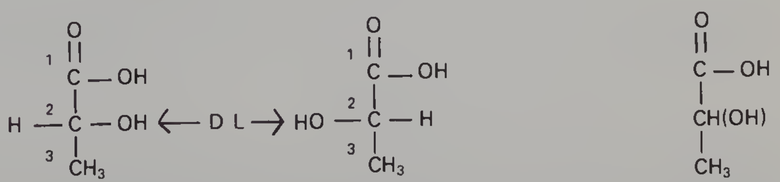
(a) 'dextrorotatory': (+). The earlier indicator '*d*' is outdated. For a complete description of the relation between direction of rotation and configuration, c.f. Tartaric acid (**441**), but also Griseofulvin IV.9.2.2 (p. 173), named according to EP II.

(b) 'laevorotatory': (-). The earlier indicator '*l*' is outdated. cf. Fosfomycin (INN) IV.15 formula **341**, here combined with information on the configuration according to the *RS*-system. cf. Epinephrine (INN) III 6.3 p. 115 name (a).

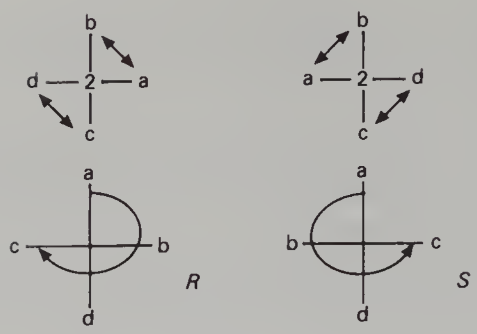
(c) 'optically inactive': (±). The earlier designation (*dl*) is outdated. cf. 15.4.7.6 p. 225. The optically active ingredients of such a mixture are designated 'optical antipodes'; the optically inactive mixture as a 'racemate'.

Example: Lactic acid (cf. IV.15.4.6.3) formula **437**.

Fischer projections:



(−)−;D−;(*R*)− Lactic acid **271a** | (+)−;L−;(*S*)− Lactic acid **271b** | (±)−;DL−;(*RS*)− Lactic acid **271c**



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Configurations according to the C.I.P. –Rule (*see* 1.2.2)

10.1.2 Configuration. (D- from Dextrose, L- from Laevulose)
The information on the configuration does not indicate the direction of rotation.

10.1.2.1 Fischer projection
A molecule with one or more asymmetric C-atoms is considered as a projection from the level of the paper, according to the position of the substituents to the right (D-) or left (L-) of the chain in which is the asymmetric C-atom, the C(1) of which chain has at the same time the highest degree of oxidation, and is depicted at the top of the chain drawn vertically. The C-atoms of the chain are in the plane of the drawing or below it, the substituents on the chain are above the plane of the drawing, so that the Fischer projection with a plane formula shows the ordered position of the substituents with regard to the chain.

Examples
1. asymmetric C-atom

Trivial: Serine (cf. IV.15.4.7.1 formula **464**)

Aminoacids take the L-configuration when no configuration is specified. A D-configuration must be specified.

systematic:
L-2-Amino-3-hydroxypropionic acid
L-2-Amino-3-hydroxypropanoic acid
(*S*)-2-Amino-3-hydroxypropanoic acid

2. asymmetric C-atoms cf. Tartaric acid IV.7.2.2 formula **138**.

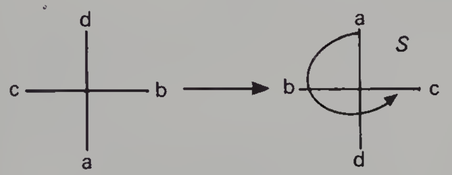
IV.15.4.6.3 (formula **437**).
V.3.4.2 formulae **59/60**.

More than 2 asymmetic C-atoms, see under Carbohydrates V.1 p. 231 and following (abbreviation[2]) see under Cyclitols V 8 p. 254 ff.

10.1.2.2 Implementing the sequence rules (CIP)

The four ligands at the asymmetric C-atom are given an order of preference (a) to (d), such that (a) is the ligand of the highest preference, with decreasing preference through (b), (c), (d), giving ligand (d) lowest preference. The steric arrangement is drawn with (d) at the bottom of the projection and below the plane of the paper. Viewed from the front and from above, the sequence (a) to (c) is then either clockwise (= R, rectus, right) or anticlockwise (= S, sinister, left). The absolute and correct molecular model structure can then be read. One can, however, start from the Fischer projection, but frequently this must first be changed to a proper CIP structure. Racemates get the characteristics (RS). (cf. formula 271c).

Conversion of Fischer projection to CIP structure (substituent exchange):



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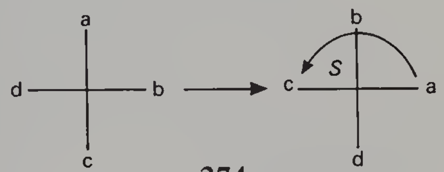

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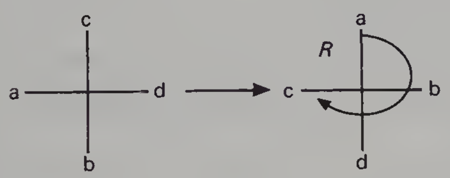
Fischer-Projection



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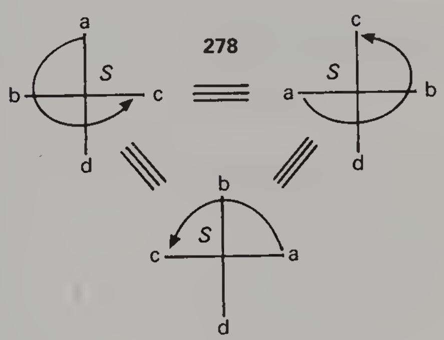
Fischer-Projection



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CIP[31] Order of Preference: Important rules.

1. Preference decreases with decreasing atomic number of the elements directly bound to the asymmetric C-atom (for example, Cl > S > C > B)

2. Where the elements directly bonded to the asymmetric C-atom have the same atomic number, the elements of the 'second sphere' are considered in the same way; that is, those directly bound to the elements considered above. (for example, $-PCl_2 > -PO > PNH_2$). If no distinction is possible at this level, then one is sought on the basis of the atoms in the 'third sphere', and so on.

3. Between like atoms, precedence goes with the greater number, (for example, $-SO_3H > -SO_2H > -SOH$).

31 CIP: from the initial letters of the names of its three authors:
Robert Sidney *C*ahn, 1899–1981, London University and Industrialist. Editor of the *Journal* of the Chemical Society. Member of the IUPAC Nomenclature Commission for Organic Chemistry.
Sir Christopher Kelk *I*ngold, 1893 (Ilford, England) –1970, University College London.
Vladimir *P*relog, 1906 (Sarajewo) ETH Zurich. Nobel prize for Chemistry 1975.

4. Multiply bound atoms count as multiple simple atoms (cf. Table and illustrations).
5. A branch increases in order of preference as the number of its sub-branches increases (each with fewer H), and as these are nearer to the asymmetric C-atom.

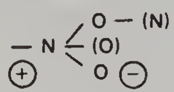
Linked Elements in the (R, S)-system (Sequence Rules CIP[31])

Element	Atomic number	Oxidation states Valency Radicals
I	53	$-IO_2$(V) iodyl; $-IO$ (III) iodosyl; $-I$ (I) iodo
Br	35	$-BrO_3$ (VII) perbromyl, otherwise analogous to Iodine;
As	33	$-AsO(OH)_2$ (V) arsono/arsonic acid; $-As(O)H_2$ (V) arsinoyl $-AsH_4$ (V) arsoranyl; $-AsH_2$ (III) arsino;
Cl	17	ClO_3 (VII) perchloyl, otherwise analogous to iodine;
S	16	$-SO_3H$ (VI) sulfo/sulfonic acid; $-SO_2NH_2$ (VI) sulfamoyl, sulfamide $-S(O)CH_3$ (IV) methylsulfinyl; $-SH_2+$ (cation) sulfonio; $-SCH_3$ (II) methylthio; $-SH$ (II) mercapto;
P	15	$-PCl_2$ (III) dichlorophosphino; $-P(S)H_2$ (V) thiophosphinoyl; $-PO(OH)_2$ (V) phosphono; $-P(O)H_2$ (V) phosphinoyl; $-P(OH)_2$ (III) dihydroxyphosphino; $-PH_2$ (III) phosphino;
F	9	$-F$ (I) fluoro;
O	8	$-OR$ (II) acyloxy; glucosyloxy; phenoxy; benzyloxy; methoxy; $-OH$ (II) hydroxy/ol

Element	Atomic number	Oxidation states Valency Radicals	
N	7	$-NO_2$ (IV) nitro;[a]	
		$-N{=}N-CH_3$ (III) methylazo;[b]	
		$-NH-NH_2$ (III) hydrazino;	
		$-NR_3+$ (cation) e.g. trimethylammonio/ . . . ammonium	
		$-NR_2$ (III) e.g. dimethylamino;	
		$-NHC(O)R$ (III) e.g. acetylamino	
		$-NHR$ (III) e.g. methylamino;	
		$-NH_3^+$ (cation) ammonio/ammonium;	
		$-NH_2$ (III) amino/amine;	
C	6	$-CCl_3$ (IV)	trichloromethyl
		$-C(O)Cl$	chloroformyl/carbonyl chloride
		$-CH_2Cl$	chloromethyl
		$-COOR$	alkoxycarbonyl/carboxylic acid ester
		$-\overset{\overset{O}{\|}}{C}-OH$ c)	carboxy/carboxylic acid
		$-CO(NH_2)$	carbamoyl/carboxamide
		$-CHO$	formyl/carbaldehyde
		$-C{\equiv}N$ d)	cyano/carbonitrile
		$-CH{=}NH$ e)	iminomethyl
		$-C_6H_4OH$ (2)	*o*-hydroxyphenyl
		$-C{\equiv}C-CH_3$ (f)	1-propynyl
		$-C_6H_4OH$ (4)	*p*-hydroxyphenyl
		$-C_6H_5$ g)	phenyl
		$-C{\equiv}CH$	ethynyl
		$-C({=}CH_2)-CH_3$	isopropenyl
		$-C(CH_3)_3$	*tert*-butyl
		$-CH{=}CH-CH_3$ h)	1-propenyl
		$-C_6H_{11}$	cyclohexyl
		$CH(CH_3)CH_2-CH_3$	*sec*-butyl
		$-CH{=}CH_2$	ethenyl, vinyl
		$-CH(CH_3)_2$	isopropyl, 2-propanyl 1-methylethyl
		$-CH_2-C_6H_5$	benzyl
		$-CH_2-C{\equiv}CH$	2-propynyl
		$-CH_2-C(CH_3)_3$	neopentyl
		$-CH_2-CH{=}CH_2$ i)	2-propenyl, allyl

Element	Atomic number	Oxidation states Valency Radicals	
C	6	$-CH_2-CH(CH_3)_2$	isobutyl
		$-CH_2-CH_2-CH(CH_3)_2$	isopentyl
		$-CH_2-(CH_2)_3-CH_3$	pentyl
		$-CH_2-CH_2-CH_3$	propyl
		$-CH_3$	methyl
B	5	$-BCl_2$ (III)	dichloroboryl
		$-BH_2$	boryl
D ^2H	1		
H ^1H	1		
Z	0	(Phantom atom of atomic number 0 for saturation of duplicate or triplicate atoms)	
–	0	(free electron-pair instead of substituent)	

Inserted in the above sequence with duplicate atoms (double bonds), or triplicate atoms (triple bonds):

(a) 

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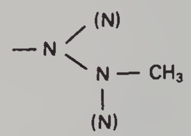
(b) 

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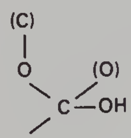
(c) 

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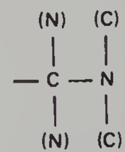
(d) 

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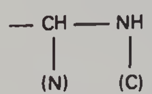
e) 

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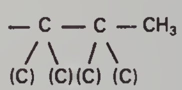
(f) 

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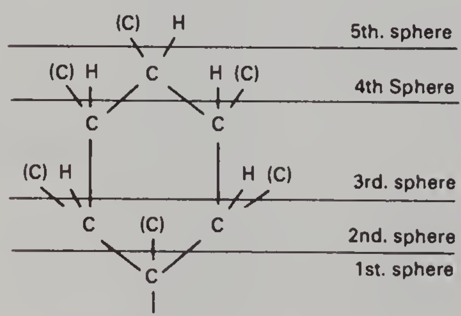
(g) 

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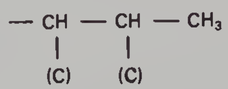
(h) 

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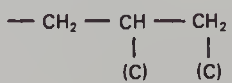
(i) 

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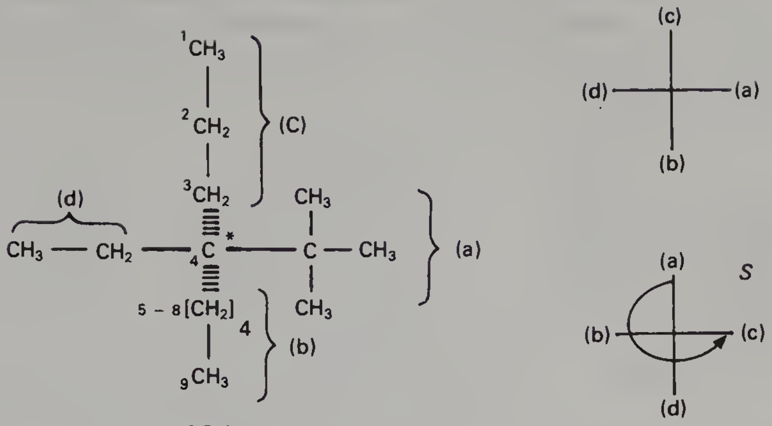
Examples



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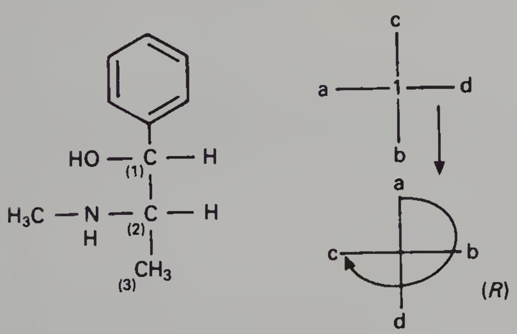
*1 asymm. C atom CIP sequence: a/b/c/d

Longest chain 9 C (1–9), other chains 8,8,6,6,5 C

(a) The highest CIP preference is given to the *tert*-butyl group, on the C-atom *4 of the principal chain. The preference is based on the doubled branching of the 'yl' position compared to the other three groups directly linked to the C-atom 4, unbranched methylene groups.

(b/c/d) The decreasing chain-length is the single criterion for selecting preference.

Name: (*S*)-4-*tert*-Butyl-4-ethylnonane



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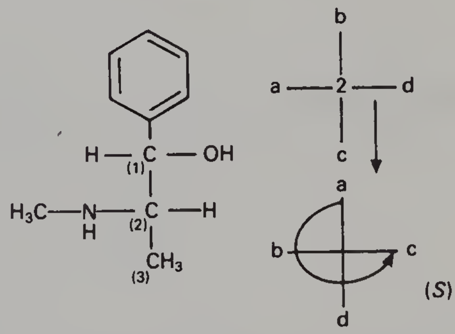
L-(-)-Ephedrine
(an *erythro*-form Fischer projection)
L-*erythro*-2-Methylamino-1-phenyl-1-propanol
(1*R*,2*S*)-2-Methylamino-1-phenyl-1-propanol



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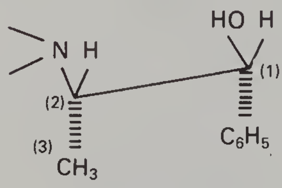
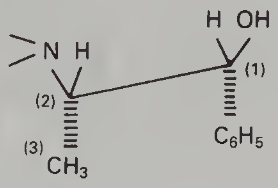
L-(+)-Pseudoephedrine
(a *threo*-form Fischer projection)
L-*threo*-2-methylamino-1-phenyl-1-propanol
Lg-*threo*-2-Methylamino-1-phenyl-1-propanol
(1*S*,2*S*)-2-Methylamino-1-phenyl-1-propanol

Ephedrin and Pseudoephedrin are a diastereoisomeric pair. There is no pseudo-asymmetric C-atom. In the threo-form, in order to eliminate any doubt as to interpretation at the L-*threo*, the position on the left side of the Fischer projection at the higher numbered chiral centre, is cited as 'Lg' (g = Glyceraldehyde), whereby the 2-methylamino group is unambiguously established as being in the L-position. The presentation of the formulae as so-called 'saw-horse' formulae (perspective) and as 'Newman' projection (staggered, with 180 degree rotation of the atoms towards the front) shows the steric behaviour particularly well.

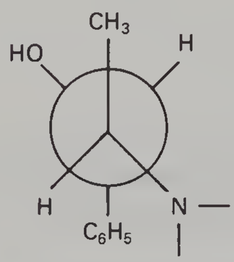
"Saw-horse"



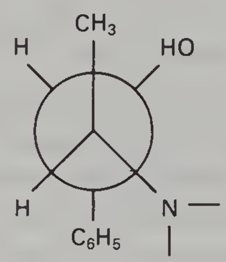
289a



290a

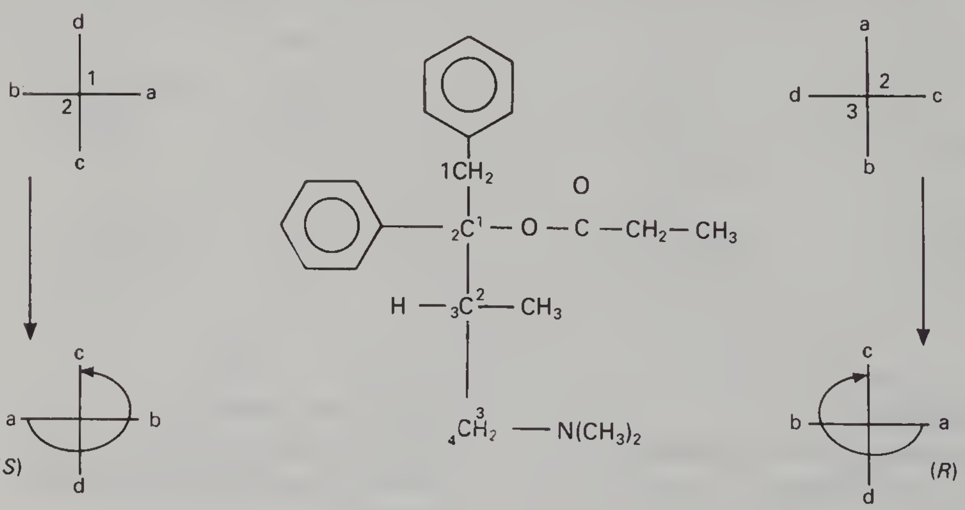


"Newman"



289b
L-(-)-Ephedrine

290b
L-(+)-Pseudoephedrine



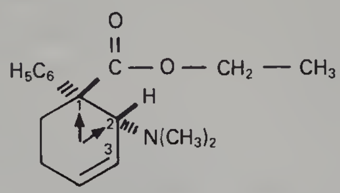
291
Dextropropoxyphen (INN)

systematic:

(a) longest chain, locants left 1–4, 'yl' position as 2 (2*S*,3*R*)-4-Dimethylamino-3-methyl-1,2-diphenyl-2-butanyl propionate

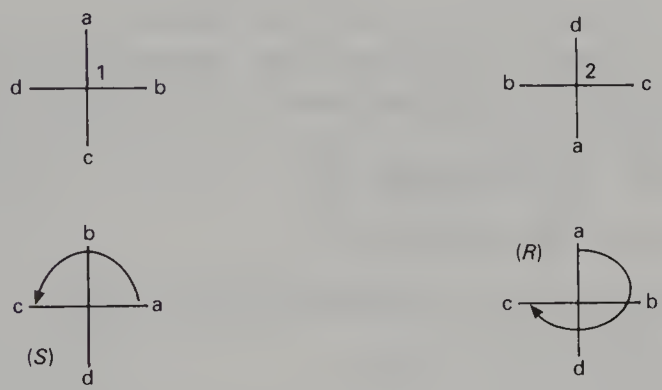
(b) yl position as 1, locants right 1–3.
(1*S*,2*R*)-1-Benzyl-3-dimethylamino-2-methyl-1-phenylpropyl propionate (IUPAC)

(c) α-(+)-4-Dimethylamino-1,2-diphenyl-3-methyl-2-butanol propionate (ester) WHO[32]



292
Dextilidine (INN)

(a) (+)-(1*S*,2*R*)-Ethyl 2-dimethylamino-1-phenyl-3-cyclohexene-1-carboxylate (IUPAC)



(b) (+)-Ethyl *trans*-2-(dimethylamino)-1-phenyl-3-cyclohexene-1-carboxylate (WHO)

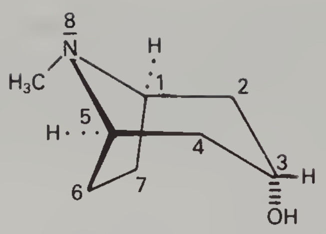
10.2 Pseudoasymmetric atoms

In this case, one of the four ligands to a C-atom is the mirror image of one of the other three. That is, these two (enantiomers) have the same structure except that the configurations are diametric opposites.

(a) See, for example, formulae **43** and **44** on p. 236. In both Adonitol and Xylitol, the C-atom 3 is pseudoasymmetric and the C-atoms 2 and 4 are in each case enantiomeric. The C-atom 2 has (*S*)- and the C-atom 4 (*R*)- configuration. Both formulae are congruent with their mirror images; the compounds are not divisible into enantiomers; they are meso-forms.

32 This name appeared as a valid name in the WHO Cumulative List (1982). It is interesting, since as a forerunner of those indicators of configuration used in IUPAC names to distinguish between two diastereomers, it employs the indicator α (in contrast to β) for the less soluble of two diastereomers (β the more soluble).

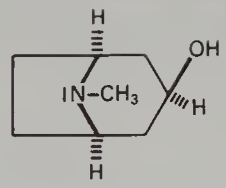
(b)



293A

trivial: Tropine (293A)
semitrivial: 1α*H*,5α*H*-3α-Tropanol
syst.: (1*R*,3*r*,5*S*,8*s*)-8-Methyl-8-azabicyclo[3.2.1]octan-3-ol
(endo: cf. p. 141)

(3*r*)



293B

trivial: ψ(=psi, for β) Tropine, Pseudotropine (293B)
semitrivial: 1α*H*,5α*H*-3β-Tropanol
syst.: (1*R*,3*s*,5*S*,8*s*)-8-Methyl-8-azabicyclo[3.2.1]octan-3-ol
(exo: cf. p. 142)

(3*s*)

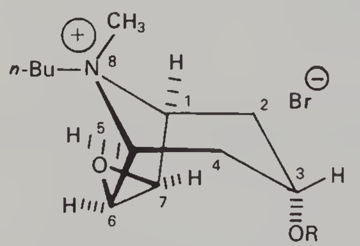
The methyl group is equatorial, as X-ray structure studies have confirmed. The configurations are (1*R*,5*S*,8*s*) (N is pseudo-asymmetric as is 3), (3*r* in Tropine; 3*s* in Pseudotropine).
The order of precedence a) – d) is for Tropine at 3:

(a) OH; (b) 1*R*; (c) 5*S*; (d) H; giving 3*r*

For Tropine and Pseudotropine we find at position 8, according to CIP:

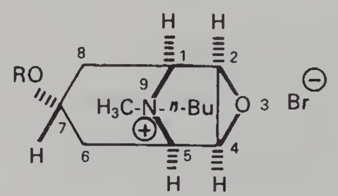
(a) 1*R*; (b) 5*S*; (c) CH_3; (d) –: giving 8*s*

(c) In Butylscopolaminium bromide (formula **294**) because of the epoxide ring, an alteration of the priorities for ligands at the 1 and the 5 positions arises. The *n*-butyl radical (= *n*-Bu) here takes up an equatorial position. The spatial arrangement is (1*S*,3*s*,5*R*,6*R*,7*S*,8*r*). [R = (2*S*)-Tropate].



a

294



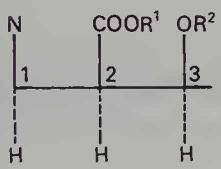
b

semitrivial:
(1) 8-Butyl-6β,7β-epoxy-3α-(*S*)-tropoyloxy-1α*H*,5α*H*-tropanium-bromide
systematic
(2) (1*S*,3*s*,5*R*,6*R*,7*S*,8*r*)-8-Butyl-6,7-epoxy-8-methyl-3-[(*S*)-(3-hydroxy-2-phenyl-propionyl)oxy]-8-azoniabicyclo[3.2.1]octane bromide

(3) (1*R*,2*R*,4*S*,5*S*,7*s*,9*r*)-9-Butyl-9-methyl-7-[(*S*)-tropoyloxy]-3-oxa-9-azoniatricyclo[3.3.1.$0^{2,4}$]nonane bromide

10.3 No pseudoasymmetric C-atoms

The prefix 'pseudo' does not always signify pseudoasymmetric C-atoms; for example, α-, β-Ionone: Pseudoionone (see p. 171); Cumene (see p. 45); Pseudocumene (=1,2,4-Trimethylbenzene). Ecgonine (→ Cocaine) (E/C) and Pseudoecgonine (→ Pseudococaine) (Ps/ps) have no pseudoasymmetric C-atoms in them, they are divisible diastereomers. While the hydroxyl or benzoyloxy groups respectively in both cases occupy the 3β-position like the OH- group in Pseudotropine, the distinction between E/C and Ps/ps is based on an inversion of the carboxyl and methoxycarbonyl groups respectively in the 2-position. These groups are β- in E/C, but α- in Ps/ps. The compounds contain 4 asymmetric C-atoms (1,2,3,5), which normally would correspond to $4^2 = 16$ optical isomers. However, as C-atoms 1 and 5 are here ring members and the 6–7 bridge is sterically fixed, only 8 optically active forms arise.



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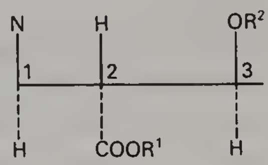
Ecgonine $R^1 = R^2 = H$

Cocaine $R^1 = CH_3-$
$R^2 = C_6H_5CO-$

Possible configurations according to CIP

C-atoms	1	2	3	5	
forms	(R)	(R)	(S)	(S)	E/C
	(R)	(S)	(S)	(S)	Ps/ps
	(R)	(S)	(R)	(S)	
	(R)	(R)	(R)	(S)	

and mirror images



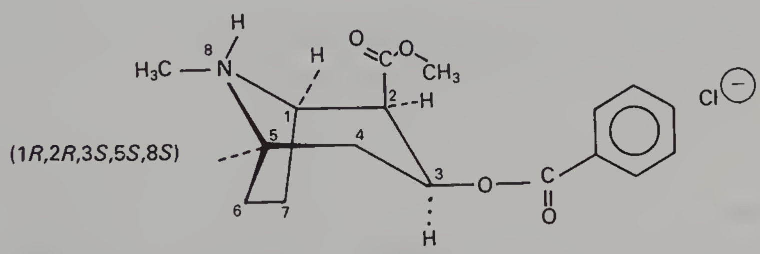
296

$R^1 = R^2 = H$ Pseudoecgonine

$R^1 = CH_3-$
$R^2 = C_6H_5CO-$ Pseudococaine

10.4 Chiral nitrogen

Cocaine hydrochloride is another example showing chiral nitrogen:



297

syst.: (-)-Methyl[3β-benzoyloxy-2β(1α*H*,5α*H*)-tropancarboxylat] hydrochloride (DAB 9)

10.5 Spatial isomerism about double bonds or ring systems

10.5.1 cis/trans *isomerism*

10.5.1.1

This deals with positional isomerism at the double bonds in a chain (no optical activity) (= geometrical isomerism). Following long-standing usage, the isomers are differentiated by use of the prefixes '*cis*' and '*trans*' (*see* IV.15.4). Note that in formula **401** the *cis*-isomer of the 3-phenylpropenoic acid is generally designated 'allocinnamic acid', the other two polymorphic forms appearing as 'isocinnamic acid'.

See also IV.11.2.1 and 2 (Citral formula **222**, Cinnamaldehyde formula **226**) p. 183/84.

10.5.1.2

In Carotenoid Hydrocarbons (I.7), *cis*- and *trans*-prefixes are also used to differentiate the arrangement at the double bonds combined in groups (for example, 'all-*trans*'), in cases where there is an unbroken series of conjugated double bonds in a carbon chain (cf. Retinoids p. 166, 213).

10.5.1.3

Polymers, cf. VI.2.5. p. 272.

10.5.1.4

Cyclitols (V. 8. p. 254 *et seq*.)

In this type of representation, comparable with the Haworth formulae in V, '*c*' (*cis*) corresponds to the β-position in the steroids (see I p. 51, 52) or the β-anomers in position 1 of the Haworth formulae (p. 231 and following). The '*t*' (*trans*) corresponds to the α-position or to the α-anomers.

10.5.1.5

Triterpene Hydrocarbons I. p. 62,

Here the indicators *c*/*t* are applied in systematic names for a relative steric description, whereby an absolute configuration is cited only for a position serving as a reference (reference '*r*').

10.5.1.6

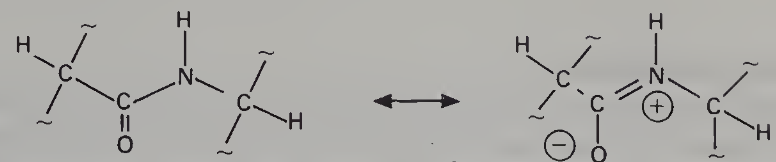
See also the stereo prefixes in carbohydrates and cyclitols. (V p. 230–255).

10.5.2 **Z/E** *isomerism*

As the *cis*/*trans* concept was not without dispute with regard to double bonds at the end of chains or between rings and chains, prefixes, connected to the (CIP) sequence rule, were defined by IUPAC. These are '*Z*' (generally = *cis*, from the German 'zusammen', together) and '*E*' (generally = *trans*, from the German 'entgegen', opposite), and they ensure uniform interpretation. In formula **385** p. 208 with 'all-Z' for example, all 4 double bonds have an H-atom attached to each of the 2 C-atoms linked by the double bond, and these H-atoms are on the same side of the bond in each case. The C-chains are thus also both on the same side of the double bond. The two units of lower precedence according to the sequence rules are thus both on the same side, and the two of higher precedence are similarly both on the same side. In Retinol (p. 166 formula **124**) ('all-*E*') they are in each case on opposite sides.

cis/trans or *Z/E*:
Compounds with partially double bond (=) character:

(a) *Acid amides*: the peptide bond



–*cis or Z*

298

(b) *N-Nitrosoamines*

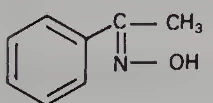
trans or *E*

299

This stereochemical differentiation is used in characterizing the rotamers of nitroso-amines.

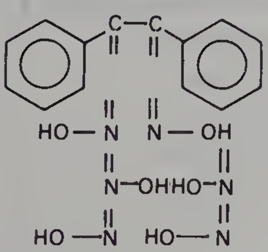
10.5.3 **syn/anti**

The designations '*syn*' and '*anti*' for distinguishing the steric arrangements of double-bonded nitrogen are outdated and are replaced with '*Z*' and '*E*' prefixes (cf. 10.5.2).



300

(*E*)-Acetophenone oxime
The hydroxyl group is (*E*) to the C_6H_5 group which has (CIP) preference to CH_3.



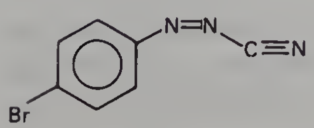
301

Benzil dioxime

[*anti*] = (*Z*, *Z*)

[*syn*] = (*E*,*E*)

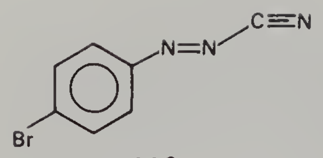
[*amphi*] = (*Z*, *E*)



302

4-Bromobenzenediazocyanide

[(*syn*), (*cis*)] = (*Z*)

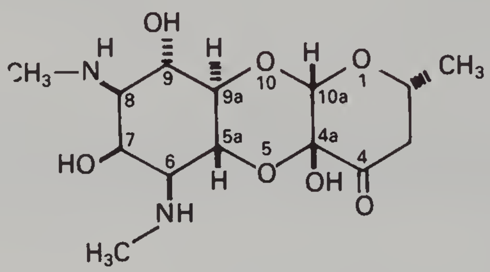


303

[(*anti*), (*trans*)] = (*E*)

10.5.4 cis/cisoid/trans/transoid

The 'IUPAC Rules E' dealing with the steric relationships in polycyclic systems with more than 1 pair of saturated bridgeheads, allow prefixes '*cisoid*' or '*transoid*' to denote the steric arrangement at the nearest atoms to the '*cis*' and '*trans*' bridgheads respectively. They are placed between the designations of the steric arrangement at the individual bridgeheads of the pairs concerned, from which they are separated by the smallest number of atoms (or none). The lowest locant only of a bridgehead pair is cited after the stereo-prefix.



304

Spectinomycin (INN)

Decahydro-4aβ,7β,9α-trihydroxy-2α-methyl-6β,8β-bis(methylamino)-*cis*-4a-*cisoid*-4a,5a-*trans*,5a-4*H*-pyrano[2,3-*b*] [1,4] benzodioxin-4-one

The steric information is read as follows:

cis-4a. . Bridgehead pair 4a/10a carry an OH– substituent (*see* . .4aβ-hydroxy. .) and an H-atom, which are *cis* to one another.

. . .*cisoid*-4a,5a. . The OH-substituent at 4aβ and the H-atom at 5a (separated by an O-atom) are *cis* to one another.

. . .*trans*-5a. . Both H-atoms of the bridgehead-pair 5a/9a bear a *trans* relationship to each other.

10.5.5 α, β-systems

10.5.5.1

See Steroid Hydrocarbons I. 8, p. 51 *et seq.*
Triterpene Hydrocarbons I. 9 p. 62 *et seq.*
Cholic acid IV 15.4.4.1 formula **419** p. 213.

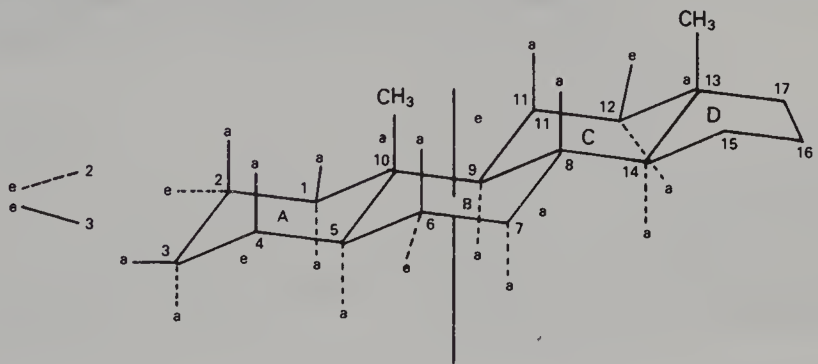
α and β are used here to express definite relative steric arrangements within projection formulae (convention). Starting at ring C-atoms in the plane of reference, α (. . .)-bonds lie below, and β-bonds above the plane. α and β have no direct information as to optical activity and chirality.

cf. II 4 formula **112** p. 79
II 3.2 formula **108** p. 78.
III 9.4.2 formula **271** with names (a) and (c).

10.5.5.2
See anomers in Carbohydrates V.1.1.3 and 1.1.4 p. 231 *et seq*.

10.5.6 a(axial)/e(equatorial)

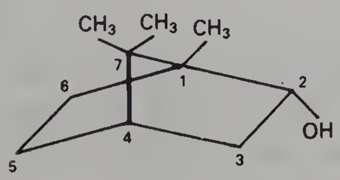
If hydrogenated rings (here Cyclohexane, analogue Piperidine, Morpholine, Tetrahydropyran) are depicted, not as projection-formulae, but as **configuration**-formulae (see V formulae **15, 27, 31–32**; formulae **79, 81a, 85, 91**; the substituents or H-atoms in the Haworth formulae (for example, formula **14**), above or below the projection level are changed in consideration of their positions referred to the now multiple ring planes due to ring folding and the tetrahedral structure of each ring C-atom is visible. The bonding direction denoted as 'e' (= equatorial) forms an angle of 109.5° (= middle point angle in a regular tetrahedron) with the vertically running axis through the ring centre. The bonding direction of 'a'-bonds (= axial) runs parallel to the axis.



305
Axis of symmetry of one six-ring

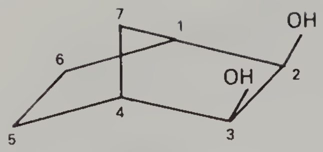
Locants for the sterol framework 1–17
here: linkages AB, BC, CD *trans*
rings A, B, C in chair-form
dotted bonds in the projection α-bonds
drawn out bonds in the projection β-bonds
axial bonds: parallel to axis of symmetry
equatorial bonds: 109.5° angle to axial bond lying approximately in the equatorial plane

10.5.7 endo/exo



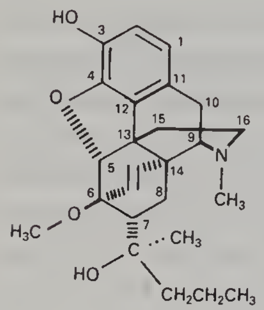
306

Borneol; 2-*endo*-Bornanol
The bridgeheads are 1,4; the 3 bridges are 2,3/5,6 and 7. '*endo*' signifies that the OH-substituent in 2 refers to the lower numbered of the nearby two bridges (5,6/7) and thus to bridge 5,6. (Bn).



307

2-*exo*,3-*exo*-Trinorbornanediol
Here the substituents at 2 and 3 are directed towards the higher numbered nearby bridge 7 and away from the lower numbered bridge 5,6 (cf. diagram).



308

Etorphine (INN)
6,7,8,14-Tetrahydro-7α-(1-hydroxy-1-methylbutyl)-6,14-*endo*-ethenooripavine (WHO)

4,5α-Epoxy-7α-(1-hydroxy-1-methylbutyl)-6-methoxy-*N*-methyl-6α,14α-ethenomorphinan-3-ol (IUPAC *et al.*) *al.*)

'*endo*' is used in the WHO name in a different sense from that in the first case. Here it signifies simply the position as a bridge inside a ring. Nonetheless a parallel can be drawn with the first case, which is clearly shown from (7α,6α/14α) in the IUPAC name, namely the spatial approach of the 7α-substituent at the etheno-bridge.

11 SILICON COMPOUNDS

Silicon (atomic number 14) is the next higher homologue to carbon (atomic number 6) in group IV of the Periodic Table.

11.1 Silicon hydrides

11.1.1 Silicon chains, saturated

The simplest silicon hydride of formula SiH_4 (**309**) is named silane. Silane forms the silyl radical $SiH_3\cdot$ (**310**) (the term disilyl is used for 2 $SiH_3\cdot$) and the silanediyl radical SiH_2: (**311**). The next in the homologous silicon hydride series is disilane $SiH_3{-}SiH_3$ (**312**) with the radicals

disilanyl	$SiH_3{-}SiH_2\cdot$ (**313**),
1,2-disilanediyl	$\cdot SiH_2SiH_2\cdot$ (**314**) and
1,1,1-disilanetriyl	$SiH_3Si{\equiv}$ (**315**).

The third member is trisilane $SiH_3{-}SiH_2{-}SiH_3$ (**316**).

11.1.2 Silicon chains, unsaturated

Monomeric compounds of the 'silicoethylene' or 'silicoacetylene' type are unknown, but polymers are known, poly-silicon dihydrides of the formula (SiH_2) (**317**). In these, instead of the usual polymerisation factor '*n*', the mathematical sign for infinity (∞) is used to indicate a very high factor.

11.2 Substituted silanes

Names are formed on the prefix/suffix system, with silane as either the base compound or, as a radical, the prefix.

318	$SiHCl_3$	trichlorosilane, 'silicochloroform'
319	$(CH_3)_2SiCl_2$	dichlorodimethylsilane
320	$(C_2H_5)_4Si$	tetraethylsilane
321	$(CH_3)_3Si{-}O{-}CH_3$	methoxytrimethylsilane
322	$(C_6H_5)_3Si{-}COOH$	triphenylsilylcarboxylic acid or carboxytriphenylsilane
323	SiH_3NH_2	aminosilane or silylamine
324	$C_2H_5{-}(SiH_2)_4{-}N(C_2H_5)_2$	4,*N*,*N*-triethyltetrasilanylamine
325	SiH_3OH	silanol (anion: . . . .olate)
326	$(H_3Si{-}O{-}H$	radical: $H_3Si{-}O\cdot$ (**326**) siloxy (contracted)
327	SiH_3SH	silanethiol, radical: $H_3Si{-}S\cdot$ (**328**) silylthio (not contracted here)
329	$Si(OH)_4$	Tetrahydroxysilane or silanetetrol are not commonly used. The commonly used name is orthosilicic acid, esters of which are known. In this respect it is similar to orthocarbonic acid.
330	$H_6Si_2O_7$	Orthodisilicic acid is known, as are other polysilicic acids.

The higher polymer metasilicic acids $(H_2SiO_3)_\infty$ (**331**) are also known.

332	$Si(OC_2H_5)_4$	Tetraethyl orthosilicate (tetra-ester with ethanol).
333	$(CH_3CH_2COO)_4Si$	In a compound of this type, there is a tetra-anhydride of the orthosilicic acid, with a carboxylic acid. For this example the official names are: – Tetrapropionyl orthosilicate (acylated orthosilicic acid) – Tetra(propionato)silicon (complex with central atom) – Tetrapropionyloxysilane. In this name reference is made to the tetrahydroxysilane or silanetetrol, not generally used as the basis for names.

11.3 Mixed hetero-chains

11.3.1 Silicon/oxygen: Siloxanes; analogue Silicon/sulphur: Silathianes

Chain compounds with end-position Si and alternating Si and O atoms in the chain, are named siloxanes (trivial). In the name the citation order of hetero-atoms, sil. . .ox. . ., is entirely different from the systematic nomenclature of the Hantzsch–Widman system or replacement nomenclature (II 2.1, II 3) where oxygen is cited before silicon.

334 $H_3Si-O-SiH_3$

335 $(H_3Si \leftrightarrows \bar{O}-SiH_3)$ Disiloxane

336 $H_3Si-O-SiH_2\cdot$ Disiloxanyl

337 $H_3Si-O-SiH(OH)-O-SiH_2-O-SiH_2OH$ 1,5-Tetrasiloxanediol

7 6 5 4 3 2 1

The numerical prefix of the name refers to the number of silicon atoms in the chain, while the number of oxygen atoms is self-evident, given the alternation of Si and O. (Generalized formula, unsubstituted $Si_nH_{2n+2}O_{n-1}$)

11.3.2 Polymers

338 $(CH_3)_3Si-[O-Si(CH_3)_2]_n-O-Si(CH_3)_3$ Dimeticon (INN) (n = 20–400)
Polydimethylsiloxane (WHO)

syst.: α-Trimethylsilyl-ω-trimethylsiloxypoly(dimethylsiloxane)

The complicated ω-substituent is necessary in order to comply with the definition of siloxanes, by which the end atoms of the hetero-chain must be silicon atoms. The structural formula is based on the precedence of oxygen over silicon in the polymer chain (cf. 11.5).

Under the general name 'silicones' are collected together organic substituted (C–Si compounds) polymeric siloxanes of various structural forms (linear, branched, sheet structures, and three-dimensional structures).

11.3.3 Silicon/Nitrogen: Silazanes

Chain-form compounds with end-position silicon atoms and nitrogen atoms alternating with silicon atoms in the chain, are named 'silazanes'. This name also represents trivial nomenclature, since the citation order sil. . .az. . ., is the reverse of that of the systematic names of the Hantzsch–Widman and replacement nomenclatures. The multiplying prefix refers to the number of silicon atoms, the nitrogen atoms being self-evident, as above. Hydrogen atoms, on either nitrogen or silicon atoms of the chain, may be replaced by other substituents.

339 $H_3Si-(NH\text{-}SiH_2)_2-NH\text{-}SiH_3$ Tetrasilazane

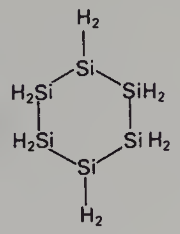
4 3
7 2 1
6 5

11.4 Cyclic compounds

11.4.1 Cyclic silanes

These take the prefix 'cyclo' before the name of the open-chain compound with the same number of silicon atoms.

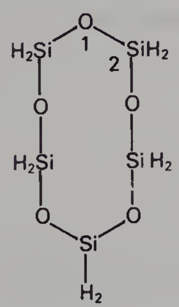
340



Cyclohexasilane is the silicon analogue of cyclohexane.

11.4.2 Cyclic siloxanes

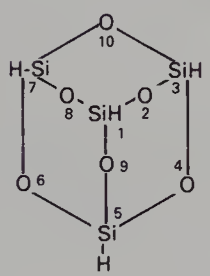
341



Cyclopentasiloxane (10-member ring).
Like the open-chain siloxanes, cyclic siloxanes have like numbers of oxygen and silicon atoms, and the general formula $Si_nH_{2n}O_n$.

The distribution of locants here does not follow the order of precedence of hetero-atoms in the trivial name. With 1 at an oxygen atom it corresponds to the order of precedence found in the Hantzsch–Widman nomenclature.

342



Tricyclo[3.3.1.1.]tetrasiloxane
or
Tetrasilasesquioxane ($Si_{2n}H_{2n}O_{3n}$, here $n = 2$)
The special feature of the structure is that each silicon atom is bound to 3 oxygen atoms. The resulting general formula shows that there are equal numbers of silicon and hydrogen atoms but that the number of oxygen is one and a half times (sesqui) the number of silicon atoms.

11.5 Replacement names with silicon

11.5.1 Chains

Silicon atoms can, as 'sila', be inserted into carbon chains, and also with other hetero-atoms. With the seniority O/S/Si, the sequence of the hetero-atoms follows the normal pattern in this type of nomenclature system.

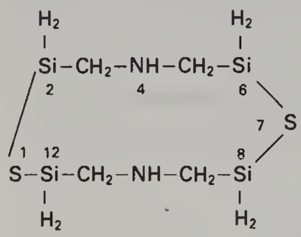
343 $\underset{11}{CH_3}-CH_2-\underset{9}{S}-CH_2CH_2-\underset{6}{SiH_2}-CH_2-CH_2-\underset{3}{O}-CH_2-\underset{1}{CH_2}-NH_2$

3-Oxa-9-thia-6-silaundecylamine

11.5.2 Rings (see also Hantzsch–Widman nomenclature)

11.5.2.1 More than 10 ring-members

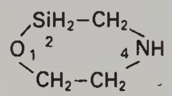
344



1,7-Dithia-4,10-diaza-2,6,8,12-tetrasilacyclododecane

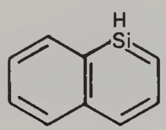
11.5.2.2 Others

345



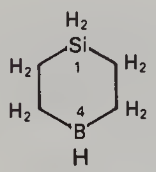
1-Oxa-4-aza-2-silacyclohexane
(NOT 2-Silamorpholine)

346



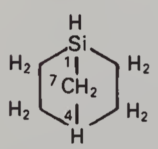
1-Silanaphthalene (cf. II.3.1 formula **103** p. 77)

347



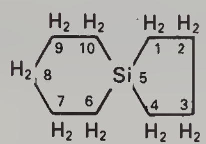
1-Sila-4-boracyclohexane

348



1-Silabicyclo[2.2.1]heptane

349



5-Silaspiro[4.5]decane

IV

Characteristic groups; functional compounds

0.[†] SUBSTITUTIVE NAMES WITH NO SUFFIX DESIGNATION, PREFIX ONLY; RADICOFUNCTIONAL NAMES

0.1 Halogenated hydrocarbons

H_3C-CH_2-Cl

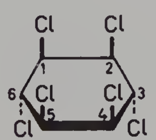
1

Chloroethane (subst.)
Ethyl chloride (radicofunctional = rf.)

$Br-CH_2-CH_2-Br$

2

1,2-Dibromoethane (subst.)
Ethylene dibromide (rf. and also additive name)



3

Lindane (INN)
γ-1,2,3,4,5,6-Hexachlorocyclohexane (WHO) (see also appendix V.8)

$CHCl_3$, $CHBr_3$, CHI_3

4

trivial: Chloroform, bromoform iodoform[1]. Trichloro-,tribromo-, triiodomethane (subst.)[1]

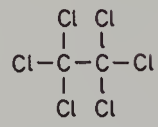
1. The syllable ‘form’ reflects the relationship to formic acid (1 C-atom).

† The second German edition (of which this English edition is a translation) maintained, for ease of cross-reference from edition to edition, the section-numbering system of the first edition; hence the use of ‘0’ for this added section.

CCl_4

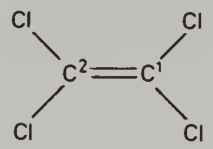
5

Carbon tetrachloride
Tetrachloromethane (subst.)



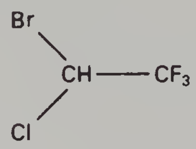
6

Perchloroethane (subst.)



6A

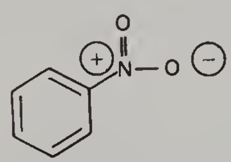
Tetrachloroethylene



6B

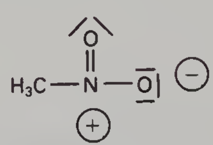
Halothane (INN)
syst.: (RS)-2-Bromo-2-chloro-1,1,1-trifluorethane

0.2 Nitro compounds



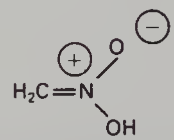
7

Nitrobenzene



8

Nitromethane
(detailed presentation of the nitro group)

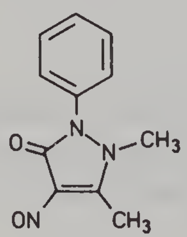


9

aci-Nitromethane
('Nitronic acid')

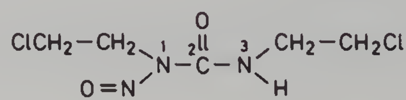
'Nitroglycerine', (syst. 1,2,3-propanetriyl trinitrate; glycerol trinitrate) is not a nitro compound, but a triester of glycerol with nitric acid (cf. **6** p. 161).

0.3 Nitroso compounds



10

trivial: 'Nitroso-antipyrine' (Antipyrine)
syst.: 1,2-Dihydro-1,5-dimethyl-4-nitroso-2-phenyl-3*H*-pyrazol-3-one. Nitroso in the alphabetical order among the prefixes

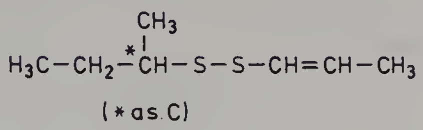


11

Carmustine (INN) 1,3-Bis(2-chlorethyl)-1-nitrosourea

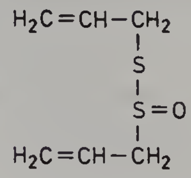
1. POLYSULFIDES, PEROXIDES

1.1 Disulfides (S- analogues of peroxides), S-chains, (polysulfides, sulfanes[2])



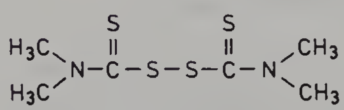
12

syst.: *sec*-Butyl 1-propenyl disulfide (rf.)



13

trivial: Allicin
syst.: Diallyl disulfide *S*-oxide or
2-Propenethiosulfinic acid *S*-allyl ester,
S-Allyl-2-propenethiosulfinate

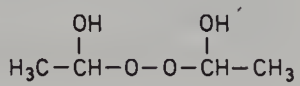


14

Thiram (INN)
syst. a) Bis(dimethylthiocarbamoyl) disulfide (WHO)
b) Tetramethylthiuram disulfide (IUPAC)

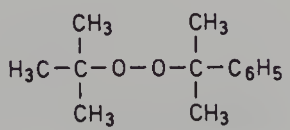
1.2 Peroxides

(Radicofunctional names (Ozonide see III 5) p. 112 formula **199**
(Bridge prefix: epidioxy), (Prefix:dioxy)



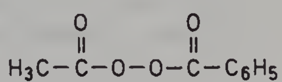
15

Bis(1-hydroxyethyl) peroxide



16

tert-Butyl α-cumyl peroxide (CA)
syst.: a) *tert*-Butyl (1-methyl-1-phenylethyl) peroxide;
b) *tert*-Butyl (α,α-dimethylbenzyl) peroxide

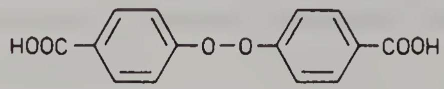


17

Acetyl benzoyl peroxide

2 Analogous to 'disulfides' R-S-S-R', are trisulfides R-S-S-S-R', tetrasulfides R-S-S-S-S-R', and so on e.g. methyl pentyl tetra-sulfide or 1-(methyltetrathio)pentane. The S-chain can be particularly emphasized by the terminal designation 'sulfane'. The main groups directly attached to the S-chain, like other substituents, appear as prefixes: $H_3C{-}CH_2{-}CH_2{-}S{-}S{-}S{-}S{-}OH$ 1-hydroxy-4-propyltetrasulfane (inorganic parent compound).

Subordinate function

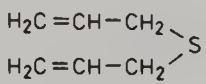


18
4,4′-Dioxydibenzoic acid (identical unit)

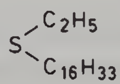
2 SULFIDES, ETHERS

2.1 Sulfides

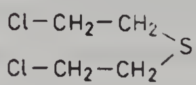
(no suffix, prefix . . .thio, rf. . . . sulfide)
(S-analogues of ethers)
(cf. Chapter II. Heterocycles and III.7. replacement names)
The function is expressed in radicofunctional names, not as . . . ‘thioether’, but as . . . ‘sulfide’:



19
Diallyl sulfide

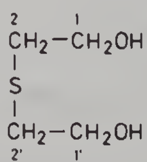


20
a) Ethyl hexadecyl sulfide (rf.)
Alkyl radicals in alphabetical order
In the form ‘ethyl hexadecyl sulfide’, the spaces indicate that the ‘ethyl’ is not a substituent on the ‘hexadecyl’
b) 1-(Ethylthio)hexadecane (subst.)



21
trivial: Mustard gas
syst.: a) Bis(2-chloroethyl) sulfide (rf.) (IUPAC)
b) 1,1′-Thiobis(2-chloroethane) (subst.) (CA).

Subordinate function



22
Thiodiglycol (INN)
syst.: 2,2′-Thiodiethanol
(identical units) (WHO, IUPAC)

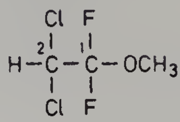
2.2 Ethers

(Prefix . . .oxy; no suffix; rf.: ether, oxide[3])
(see also Chapter II heterocycles, III, 7 replacement names, Chapter IV acetals and Chapter V polyhydric alcohols)

$H_5C_2-O-C_2H_5$

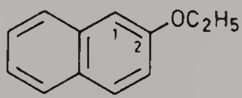
23

'Anaesthetic ether' (E.P. III)
syst.: Diethyl ether (rf.)



24

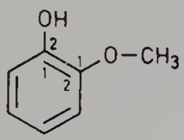
Methoxyflurane (INN)
syst.: (2,2-Dichloro-1,1-difluorethyl) methyl ether (rf.) (WHO, IUPAC)
The composite radical with d as initial letter precedes methyl, (alphabetical order of radicals)



25

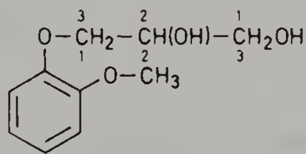
2-Ethoxynaphthalene (subst.) The senior hydrocarbon becomes the parent compound

Subordinate function



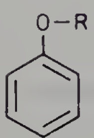
26

trivial: Guaiacol
syst.: a) *o*-Methoxyphenol (inner locants) (ether is subordinated to . . . .phenol)
b) Pyrocatechol methyl ether } outer
c) 1-*O*-methylpyrocatechol } locants



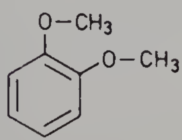
27

Guaifenesin (INN)
syst.: a) 3-(*o*-Methoxyphenoxy)-1,2-propanediol (locants above) (WHO, IUPAC)
The ether groups are subordinated to the OH-groups the former are therefore given as prefixes, the latter as the suffix.
b) Glycerol (1-*o*-methoxyphenyl) ether (locants below)
c) 1-*O*-(*o*-Methoxyphenyl)glycerol



$R=CH_3$ **28** Anisole
$R=C_2H_5$ **29** Phenetole

Trivial names

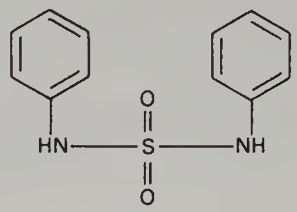


30

Veratrole

3 Hardly ever used in English for such compounds.

3 DERIVATIVES OF INORGANIC ACID NOT COMING UNDER SECTIONS 6 AND 14 (p. 84, 85)



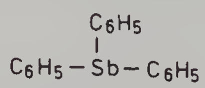
30A

a) *N,N′*-Diphenylsulfuryldiamide
b) *N,N′*-Diphenylsulfonyldiamide
c) *N,N′*-Diphenylsulfuric acid diamide

4 STIBINES – AMINES

4.1 Stibines

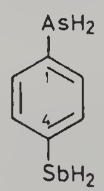
(Suffix: stibine, prefix: stibino)



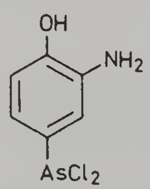
31
Triphenylstibine

4.2 Arsines

(Suffix: arsine, prefix: . . .arsino. . .)



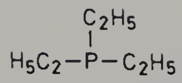
32
4-Stibinophenylarsine



33
Dichlorphenarsine (INN)
syst.: a) 2-Amino-4-dichlorarsinophenol (WHO)
. . .arsine as subordinate function (prefix) in an organic compound.
b) (3-Amino-4-hydroxyphenyl)dichloroarsine as inorganic coordination compound.
c) 3-Amino-4-hydroxyphenylarsonous dichloride as acid chloride.

4.3 Phosphines

(Suffix: . . .phosphine, prefix: . .phosphino. .)



34
Triethylphosphine
(vgl. Auranofin (INN))

4.4 Nitrogen chains

4.4.1 More than 2 N

$-\overset{1}{N}=N-\overset{3}{N}H-$

35
Diazoamino,
1-Triazene-1,3-diyl

$H_2N-N=\overset{1}{N}-$

36
1-Triazeno

$\underset{3}{HN}=\underset{2}{N}-\underset{1}{\overset{H}{N}}-$

37
2-Triazeno

$H_2N-\overset{H}{N}-\overset{H}{N}-\overset{H}{N}-$

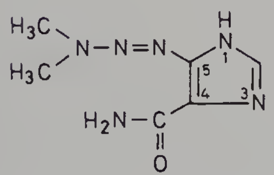
38
Tetrazano

$\overset{1}{H}\overset{}{N}=\overset{2}{N}-\overset{3}{N}=\overset{4}{N}H$

39
1,3-Tetrazadiene

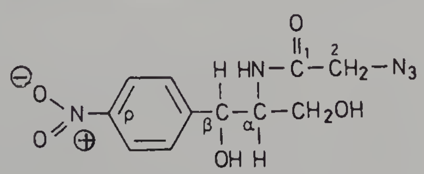
$H_2N-N=N-NH_2$

40
2-Tetrazene
(not to be confused with
tetracene = naphthacene,
see I.2.2.1.1. No. 20) p. 30, 31



41
Dacarbazine (INN)
5-(3,3-Dimethyl-1-triazeno)imidazole-4-carboxamide
(Triazeno as prefix, subordinate substituent)

42
Azido (prefix; functional: . . . azide)

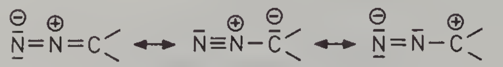


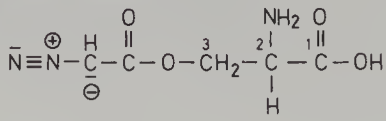
42a
a) Azidamfenicol (INN)
D-(–)-(*threo*)-2-Azido-*N*-[β-hydroxy-α-(hydroxymethyl)-*p*-nitrophenethyl] acetamide
The acid amide is the highest seniority compound class, giving the suffix in the substitutive name.

$C_6H_5-N_3$

43
Phenylazide

4.4.2 Diazo groups

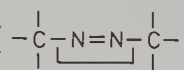
(prefix only; )



44
Azaserine (INN)

a) L-Serine diazoacetate ester (WHO)
The diazo group is a substituent of the acetic acid. The (esterified) OH-group is implicit in the name of the amino-acid. The ester is stated explicitly, to avoid confusion between this compound and the salt formed between the diazoacetic and the amino-acid, in view of the similarity of the nomenclature in both cases.
b) 3-*O*-(diazoacetyl)serine (locants) (IUPAC/IUB)
This name gives useful clarification of particular biochemical relevance.
c) 3-(Diazoacetoxy)alanine (IUPAC)
In this systematic name, the esterified OH-group is treated as a substituent of the OH-free amino-acid, of which the unesterified carboxyl group is the principal group of the compound.

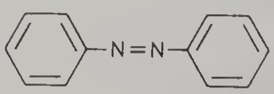
4.4.3 Azo compounds

( azo-prefix, and also bridge; no suffix)

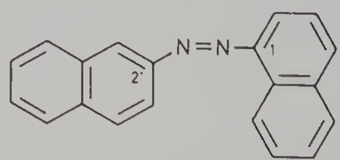
Cis/trans isomerism of the double bond, (*E*) or (*Z*) form.

In the general formula R–N=N–R_1, if R and R_1 are identical, the prefix as . .azodi. . after the prefixes for other substituents.

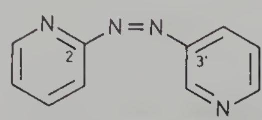
If R = R_1 and they are aromatic hydrocarbons, then the following trivial names are valid:



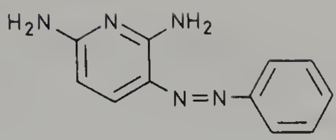
45
Azobenzene



46
1,2′-Azonaphthalene
The corresponding names for heterocycles apply

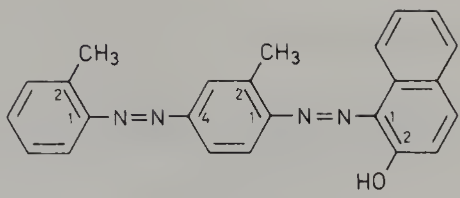


47
2,3′-Azopyridine
The higher locant is primed



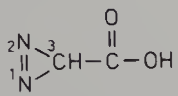
48

Phenazopyridine (INN)
2,6-Diamino-3-(phenylazo)pyridine (WHO)
If R ≠ R_1, the azo group is treated as a substituent of the parent compound formed by the ring of higher seniority.



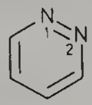
49

trivial: Cochineal; scarlet red
syst.: 1-[2-Methyl-4-(2-methylphenylazo)-phenylazo]-2-naphthol
The stem is that part of the molecule which bears the suffix, it also has an azo group substituent, which has itself, as substituent, an identical group.



50

Diazirine-3-carboxylic acid

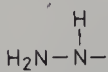


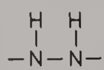
51

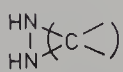
Pyridazine
The compound is named as a heterocycle, if the azo group forms part of a ring.

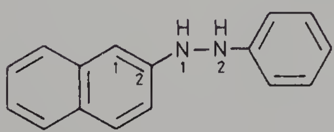
4.4.4 Hydrazines

(Suffix: . .hydrazine; prefixes

hydrazino 

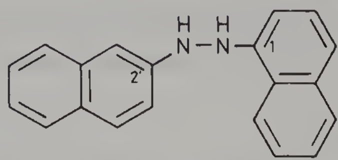
hydrazo  as a bridge, biimino

hydrazi 



52

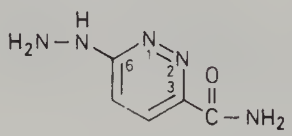
1-(2-Naphthyl)-2-phenylhydrazine
Alphabetical order of the substituents



53

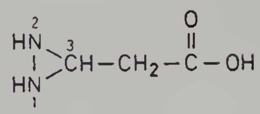
1,2′-Hydrazonaphthalene
Short name as hydrogenated azonaphthalene.
Like substituents, different substitution positions.

Subordinate function



54

Hydracarbazine (INN)
6-Hydrazino-3-pyridazinecarboxamide (WHO, IUPAC)



55

3-Hydrazipropionic acid
Hydrazi prefix, subordinate function as heterocycle
3-Diaziridineacetic acid (conjunctive) (locants)

4.5 One nitrogen atom

4.5.1 Hydroxylamine

(Oximes, see aldehyde and ketone derivatives)

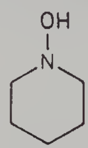
Prefix H_2N-O- aminooxy

$R-O-\overset{H}{\overset{|}{N}}-$ R-yloxyamino

H_2NOH

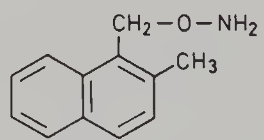
56

Hydroxylamine
The name is outside the scope of the organic chemistry nomenclature rules (no C!). The OH-group is a substituent of ammonia



57

a) 1-Hydroxypiperidine
The name is analogous to hydroxylamine
b) 1-Piperidinol
The name with the OH-suffix follows the organic chemistry rules.



58

Nafomine (INN)
O-[(2-Methyl-1-naphthyl)methyl] hydroxylamine (WHO, IUPAC)
Hydroxylamine as substituted parent compound

4.5.2 Imines

(Suffix: . . .imine (or . . .amine); prefix: imino)
(cf. Amfecloral INN)

$H_3C-(CH_2)_3-CH=NH$

59

a) 1-Pentanimine
Single function as suffix

b) Pentylidenamine
Substituted ammonia

4.5.3 *Amines*

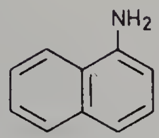
4.5.3.1 *Primary amines*

(Suffix: . .amine; . . .ylamine (subst. NH_3 or rf.); prefix: . .amino. .) 'amine' is the designation for substituted ammonia.

$H_5C_2-NH_2$; $\cdots\overset{H}{N}-$

60

Ethylamine, radical: ethylamino
Ethanamine (substitutive name with suffix)



61

1-Naphthylamine
α-Naphthylamine

$H_2N-CH_2-CH_2-NH_2$

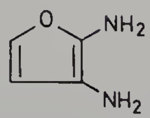
62

Ethylenediamine (rf.)
The substituent of 2 NH_3 is named as a radical.
1,2-Ethanediamine

$H_2N-(CH_2)_6-NH_2$

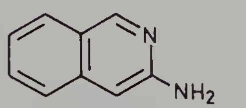
63

Hexamethylenediamine
1,6-Hexanediamine (subst.)



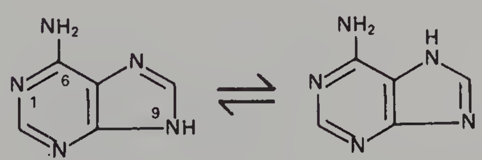
64

2,3-Furandiamine
Primary amines can also be named substitutively with 'amine' after the parent compound (as a suffix). Here the NH_2-group is substituted into the parent compound.



65

3-Isoquinolylamine
3-Isoquinolineamine
3-Aminoisoquinoline
N-heterocycles with substituted NH_2-groups can be named as amines or as aminoheterocycles.



66

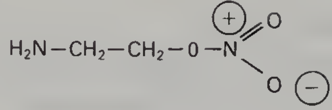
trivial: Adenine (three letter symbol Ade)
syst.: 6-Amino-7*H*-purine; 6-Purinamine
(see also nucleosides p. 250, formula **92** Adenosine
Tautomeric forms of Purine (cf. p. 68 No. 47)

Amines as subordinate function

$H_2N-CH_2-CH_2OH$

67

['Ethanolamine']
This commonly used designation is not IUPAC-compatible, as both functions are cited as suffixes.
syst.: 2-Aminoethanol (IUPAC)
The amine function, subordinate to the alcohol function, appears as a prefix.



68

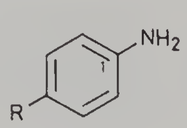
Aminoethyl nitrate (INN)
syst.: 2-Aminoethyl nitrate (WHO, IUPAC)
The amino function, subordinate to the ester function, appears as a prefix.

$H_2N-(CH_2)_5-C(=O)-OH$

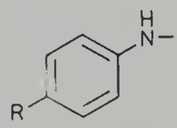
69

Aminocaproic acid (INN)
syst.: 6-Aminohexanoic acid (WHO, IUPAC)
The amino function, subordinate to the acid function, appears as a prefix.

Trivial names

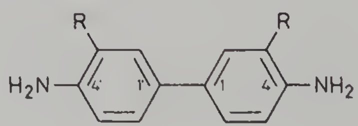


bzw.



	70	71
$R=H-$	Aniline	Anilino
$R=H_3C-$	*p*-Toluidine	*p*-Toluidino
$R=H_3CO-$	*p*-Anisidine	*p*-Anisidino
$R=H_5C_2O-$	*p*-Phenetidine	*p*-Phenetidino

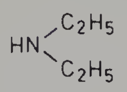
Analogous *o*-position stereoisomers.



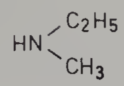
72

$R=H-$	Benzidine
$R=H_3C-$	*o*-Tolidine
	syst.: 3,3′-Dimethylbenzidine (IUPAC)
	3,3′-Dimethylbiphenyl-4,4′-diamine (C.A.)
	3,3′-Dimethyl-4,4′-biphenyldiamine (IUPAC)

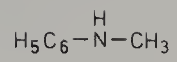
4.5.3.2 Secondary amines
(Suffix: . . .amine, . . .imine, prefix . .amino, . . .imino)



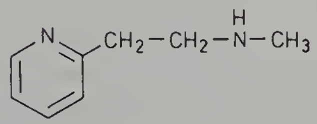
73
Diethylamine
Two like radicals as substituents of an NH_3 molecule



74
Ethylmethylamine
Two different radicals in alphabetical order

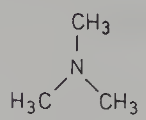


75
N-Methylaniline
One radical attached to the N of the base, using its trivial name

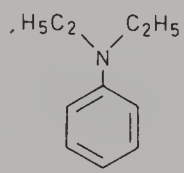


76
Betahistine (INN)
2-[2-(Methylamino)ethyl] pyridine (WHO, IUPAC)
Secondary amine as prefix in the substituted side-chain of the heterocycle

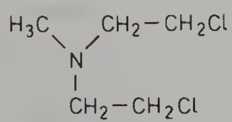
4.5.3.3 Tertiary amines
(Suffix: . . .amine, prefix: amino, nitrilo)



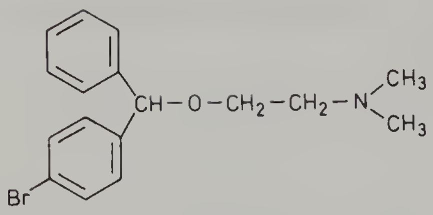
77
syst.: Trimethylamine
substituted ammonia



78
semi-trivial: *N,N*-Diethylaniline
Primary amine doubly substituted at the N

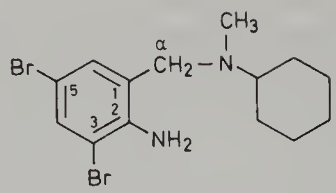


79
Chlormethine (INN)
2,2′-Dichloro-*N*-methyldiethylamine (WHO, IUPAC)
The two like radicals, having seniority before substitution, give rise to the name of the parent amine. The substituents (Cl) are dealt with separately from those radicals, chloro and methyl then being cited in alphabetical order



80

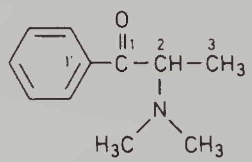
Bromazine (INN)
2-(*p*-Bromo-α-phenylbenzyloxyethyl-*N*,*N*-dimethylamine (WHO)
The senior radical gives the parent amine. The substituents at C and N are cited alphabetically (B/m). In expressing the group in brackets, either of the two synonyms. (*p*-bromobenzhydryloxy) and (*p*-bromodiphenylmethoxy) could be used.



81

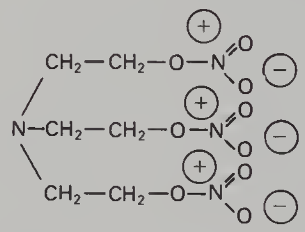
Bromhexin (INN)
syst.: a) 3,5-Dibromo-N^{α}-cyclohexyl-N^{α}-methyltoluene-α,2-diamine (WHO, IUPAC)
The parent amine is substitutively named (with a suffix) as a double primary amine. The substituents are cited alphabetically.
b) 2-Amino-3,5-dibromo-*N*-cyclohexyl-*N*-methylbenzylamine
All substituents are cited alphabetically. The parent amine derives from the radicals with seniority before substitution (IUPAC, DAC).

subordinate function



82

Metamfepramone (INN)
2-Dimethylaminopropiophenone (WHO, IUPAC)
Prefix, substituted secondary amino group, the principal group is a ketone.



83

Trolnitrate (INN)
syst.: a) Nitrilotriethanol trinitrate (WHO)
Tertiary amino group as substituent, prefix nitrilo. Identical unit alcohol ester additive.
b) 2,2′,2″-Nitrilotris(ethyl nitrate) (IUPAC)†
Identical unit is an ester
c) Nitrilotriethylene trinitrate
Polyvalent radical + inorganic anion (IUPAC)

† The rules are not ideally clear on ester-assemblies but, in my opinion, a correct interpretation gives instead: Nitrilotriethylene trinitrate, i.e. name the polyvalent radical.

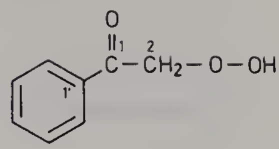
5. HYDRODI(POLY)SULFIDES, HYDROPEROXIDES

$H_3C-CH_2-CH_2-S-SH$

84
Propyl hydrodisulfide
Propyldisulfane

H_3C-CH_2-O-OH

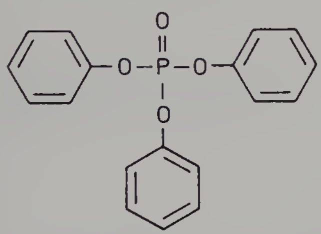
85
Ethyl hydroperoxide



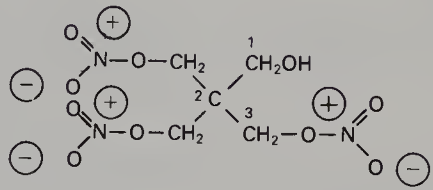
86
2-Hydroperoxyacetophenone
The ketone is the senior class of compound and occurs as suffix, the hydroperoxy group as prefix.

6. INORGANIC, NEUTRAL ESTERS OF PHENOLS AND ALCOHOLS, UNIFIED CLASS OF COMPOUNDS

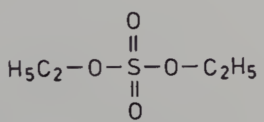
(not with halogen hydride acids)



87
syst.: Triphenyl phosphate



88
semi-trivial: Pentaerythritol trinitrate (WHO) (INN: Pentrinitrol)
syst.: 3-Nitrooxy-2,2 -bis(nitrooxymethyl)-propan-1-ol
The 3 inorganic, neutral ester groups are subordinate to the OH-group (suffix) and appear as prefixes.

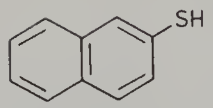


89
syst.: Diethyl sulfate
Competing compound classes are not applicable to esters. Therefore designation is as with esters of carboxylic acids (see 13.14.)

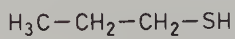
7. PHENOLS, ALCOHOLS

7.1. S-Analogues of phenols and alcohols (SH-) (unified class of compounds)

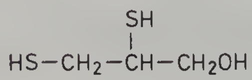
(Suffix: . .thiol, prefix: mercapto. ., rf. . . .hydrosulfide)



90
2-Naphthalenethiol

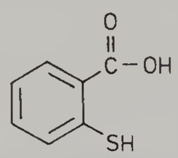


91
1-Propanethiol
rf. Propyl hydrosulfide

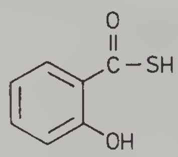


92
Dimercaprol (INN)
syst.: (*RS*)-2,3-Dimercaptopropanol (E.P. I)
-OH has seniority as suffix over -SH which therefore appears as prefix. Locant 1 for the OH is omitted as self-evident.

Subordinate function



93
trivial: Thiosalicyclic acid
syst.: 2-Mercaptobenzoic acid
-COOH has seniority as suffix over –SH which therefore appears as a prefix.

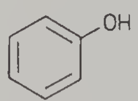


94
[NB. Unlike 'Thiosalicyclic acid' (93) this compound is not given a trivial name:
syst.: 2-Hydroxy(thiobenzoic) *S*-acid]

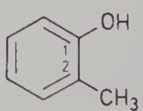
7.2 Phenols and alcohols (OH) (unified compound class)

7.2.1 Phenols
(Suffix: . . .ol, prefix: hydroxy)

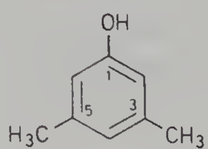
7.2.1.1 Carbocyclic phenols



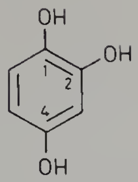
95
semi-trivial: Phenol
radical C_6H_5—O—
Phenoxy



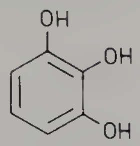
96
semi-trivial: *o*-Cresol
syst.: 2-Methylphenol



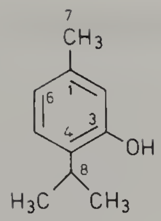
97
semi-trivial: 3,5-Xylenol
syst.: 3,5-Dimethylphenol



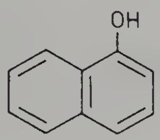
98
semi-trivial: Hydroxyhydroquinone
syst.: 1,2,4-Benzenetriol
As all 3 OH-groups are equal, they are grouped together as suffixes.



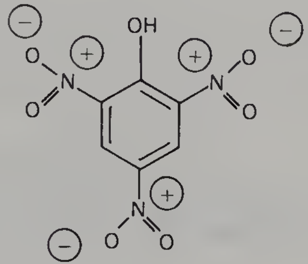
99
semi-trivial: Pyrogallol
syst.: 1,2,3-Benzenetriol



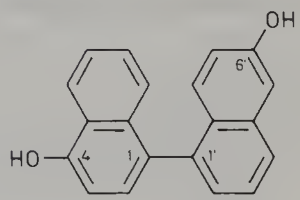
100
semi-trivial Thymol (locants)
syst.: 2-Isopropyl-5-methylphenol



101
semi-trivial: 1-Naphthol
syn. α-Naphthol

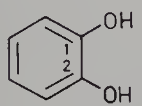


102
trivial: Picric acid
syst.: 2,4,6-Trinitrophenol
radical: Picryl
2,4,6-Trinitrophenyl

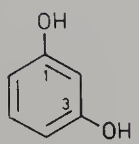


103
syst.: 1,1′-binaphthyl-4,6′-diol

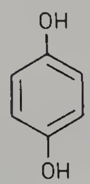
Trivial names



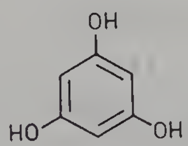
104
Pyrocatechol
syst.: 1,2-Benzenediol



105
Resorcinol
syst.: 1,3-Benzenediol



106
Hydroquinione
syst.: 1,4-Benzenediol



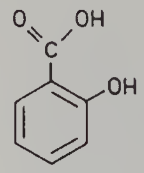
107
Phloroglucinol
syst.: 1,3,5-Benzenetriol

Salts

$H_5C_6O^{\ominus}\ Na^{\oplus}$

108
Sodium phenolate
Sodium phenoxide

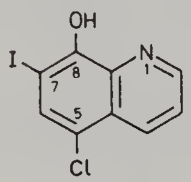
Subordinate function



109

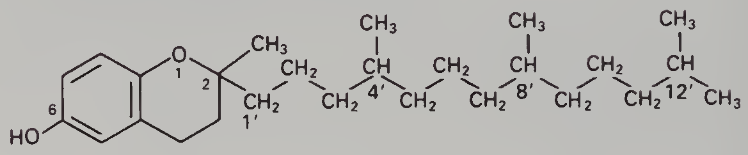
trivial: salicyclic acid
syst.: 2-Hydroxybenzoic acid
–COOH has seniority as suffix
–OH is therefore a prefix

7.2.1.2 Heterocyclic phenols



110

Clioquinol (INN)
5-Chloro-7-iodo-8-quinolinol



111

trivial: tocol
syst.: 2-Methyl-2-(4,8,12-trimethyltridecyl)-6-chromanol
Primed locants of the formula are not necessary in names where they appear in brackets.

7.2.2. Alcohols

(Substitutive names: prefix: hydroxy, suffix: ol, radicofunctional names . . .yl alcohol)
(subst. derived from hydrocarbon name with suffix, after elision of terminal e)

H_3COH

112

subst.: Methanol;
Methyl alcohol (rf.)

H_3C-CH_2OH

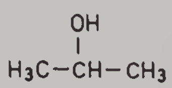
113

subst.: Ethanol;
Ethyl alcohol (rf.)

$H_3C-CH_2-CH_2OH$

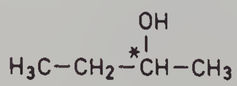
114

subst.: 1-Propanol;
Propyl alcohol (rf.)



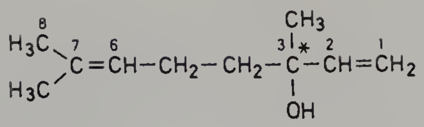
115

subst.: 2-Propanol; Isopropyl alcohol (rf.)
(Not: Isopropanol as no hydrocarbon named 'isopropane' exists.)



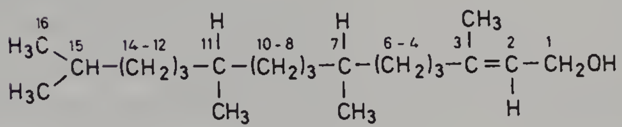
116

subst.: 2-Butanol; *sec*-Butyl alcohol (rf.)
1-Methyl-1-propanol



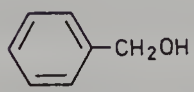
117

trivial: (±)-Linalool; (+)-coriandrol
syst.: 3,7-Dimethyl-1,6-octadien-3-ol
(DAB 8, IUPAC)
The hydrogen is named according to its longest C-chain, the substitution position of the OH-group takes its locants in the context of the established numbering of the C-chain.



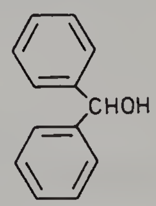
118

trivial: Phytol
syst.: (2*E*)-(7*R*,11*R*)-3,7,11,15-Tetramethyl-2-hexadecen-1-ol



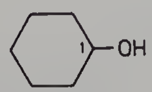
119

subst.: Phenylmethanol;
Benzyl alcohol (rf.)



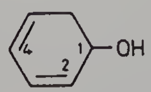
120

Benzhydryl alcohol (rf.)
(IUPAC)
subst.: Diphenylmethanol



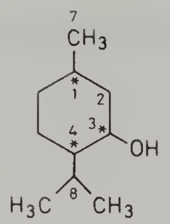
121

subst.: Cyclohexanol



122

subst.: 2,4-Cyclohexadienol
The substitution position of the OH-group and not the double bond, takes the lowest locant.



123

semi-trivial: Menthol
syst.: (1*R*,3*R*,4*S*)-3-p-Menthanol
(Formula without steric details,[3]
asymm. C)

HOH_2C-CH_2OH

125

semi-trivial: Ethylene glycol
syst.: 1,2-Ethanediol

$H_3C-CH(OH)-CH_2OH$

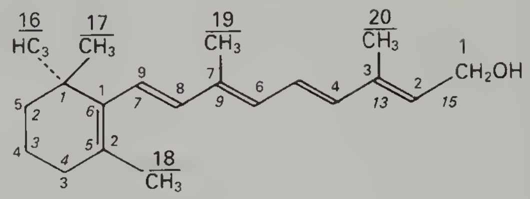
126

semi-trivial: Propylene glycol
syst.: (RS)-1,2-Propanediol

$HOH_2C-CH(OH)-CH_2OH$

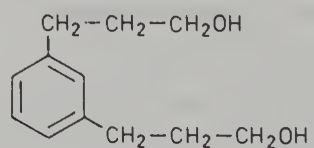
127

semi-trivial: Glycerol (cf. Lecithin 17.2) (see also V.2)
syst.: 1,2,3-Propanetriol
triradical: . .glyceryl[3] (IUPAC–IUB) lipid nomenclature)
= 1,2,3-Propanetriyl)



124

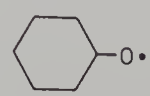
trivial: Axerophthol; Retinol (INN) (all-*trans* or all-*E*) (locants IUPAC-IUB, cf. Carotenoids p. 47) Vitamin A
syst.: a) (2*E*,4*E*,6*E*,8*E*)-3,7-Di*m*ethyl-9-(2,6,6-*t*rimethyl-1-cyclohexen-1-yl)-2,4,6,8-nonatetraen-1-ol (IUPAC–IUB; WHO without stereo-designators)
b) *15*-Apo-β-caroten-*15*ol (cf. retinoic acid p. 213)
In a) the substituents of the fourfold unsaturated chain are cited in alphabetical order (*m*,*t*). OH- is the suffix. IUPAC–IUB excludes Retinol expressly from the Carotenes because it does not have both central 20/20′ methyl substituents. Despite this, the designation as apocarotene can be used with the group 20′ replaced (with 1′–19′). In this designation the all-*trans* configuration is not indicated, as it is implicit in the . . .carotene basis of the name)
lit.: (see Europ. J. Biochem 129 (1982) 1. Nomenclature of Retinoids)



128

subst.: 3,3′-*m*-Phenylenedipropan-1-ol (identical units IUPAC)
1,3-Benzenedipropanol (IUPAC) (conjunctive)

Radicals

$H_3C-O\bullet$	$H_5C_2-O\bullet$	$H_7C_3-O\bullet$	$H_9C_4-O\bullet$	$H_{11}C_5-O\bullet$	
129	**130**	**131**	**132**	**133**	**134**
Methoxy	Ethoxy	Propoxy	Butoxy	Pentyloxy	Cyclohexyloxy

3 The use of this designation for the 2,3-Dihydroxypropyl radical is also found in the literature, however.

$$\bullet O-CH_2-CH_2-O\bullet$$

135

Ethylenedioxy (cf. III.9.1)

Salts $Na^{\oplus}\ H_5C_2O^{\ominus}$

136

Sodium ethanolate

The anion has the 'olate' ending from the hydrocarbon name.

Sodium ethoxide (derived from the 'ethoxy' radical)

Sodium ethyl alcoholate (rf.)

Sodium ethylate (rf.)

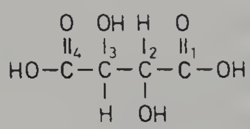
$Na^{\oplus}\ H_{11}C_5O^{\ominus}$

137

Sodium pentyl oxide

(from the 'pentyloxy' radical)

Subordinate function



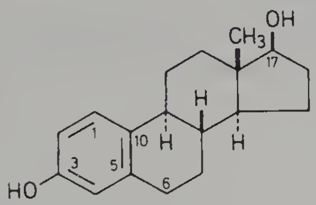
138

trivial: Tartaric acid

syst.: (2*R*,3*R*)-2,3-Dihydroxysuccinic acid (E.P. III, IUPAC)

In the presence of a senior suffix group, here '. . acid' (trivial for a carboxylic acid) the alcoholic OH-groups are denoted by the 'hydroxy' prefix.

7.2.3 Phenolic and alcoholic OH-groups in the same compound

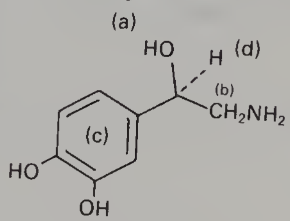


139

trivial: Estradiol-17β

syst.: 1,3,5(10)-Estratriene-3,17β-diol (IUPAC)

Here there is no distinctive order for the OH-groups, indeed phenolic and alcoholic groups are grouped together as suffixes.



140

Norepinephrine (INN)

a) (−)-α-(Aminomethyl–protocatechuyl alcohol (WHO)

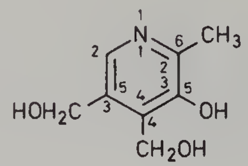
b) (*R*)-4-(2-Amino-1-hydroxyethyl) -1,2-benzenediol (IUPAC)

c) pyrocatechol (like b) but suffix trivial)

d) (*R*)-2-Amino-1-(3,4-dihydroxyphenyl)-ethanol (DAB 8)

In b) the greater number of phenolic OH-groups appear in the suffix, while the 1 alcoholic group is denoted as a prefix.[4]

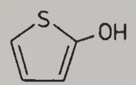
4 I am indebted to Dr Powell, IUPAC Secretariat, for clarification of this problem.



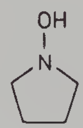
141
Pyridoxine (INN)

syst.: 3-Hydroxy-4,5-di(hydroxymethyl)-2-methylpyridine (WHO) (inner locants)
This name does not conform to IUPAC as it lacks a suffix. Correct IUPAC is (5-Hydroxy-6-methyl-3,4-pyridinediyl)dimethanol (outer locants)
This is numbered such that the two methanol groups are at the ring atoms with the lowest possible locants. Alcohols and phenols are treated equally and are also arranged so that the suffix is given by the class representing the major number of them. The corresponding conjunctive name is:
5-Hydroxy-6-methyl-3,4-pyridinedimethanol.
In biochemistry the following are also used:
4,5-Bis(hydroxymethyl)-2-methyl-3-pyridinol
3-Hydroxy-4,5-bis(hydroxymethyl)-2-methylpyridine

7.2.4 Prefix as exception



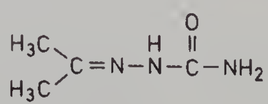
142
(syst.: 2-Thiophen/ol due to confusion with Thiophenol C_6H_5-SH)
Therefore here
Thiphen-2-ol or
2-Hydroxythiophene



143
syst.: 1-Pyrrolidinol but also:
1-Hydroxypyrrolidine
The latter name should be considered as analogous to 'Hydroxylamine' (cf. 4.5.1 p. 156)

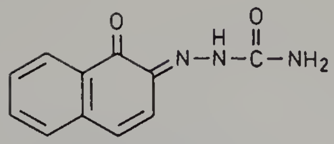
8. KETONE DERIVATIVES

8.1 Semicarbazone



144
Acetone semicarbazone
The designation of the functional derivative is added to the name of the ketone.

Subordinate function

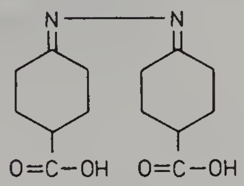


145

Naftazone (INN)
a) 1,2-Naphthoquinone-2-semicarbazone (WHO)
The procedure here is that of the first example.
b) 2-Semicarbazono-1(2*H*)naphthalenone (IUPAC)
The functional derivative is junior to the ketone as compound class and therefore is given as a prefix.

8.2 Azine

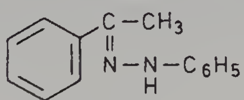
Subordinate function



146

4,4′-Azinodi(cyclohexanecarboxylic acid)
(Identical unit)
The derivative designation is a prefix, while the senior, carboxylic acid forms the suffix.
'Azine' designates the doubled hydrazone formed from one molecule of hydrazine with 2 molecules of a ketone.

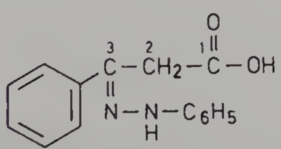
8.3 Hydrazones



147

Acetophenone phenylhydrazone
The function name is added to the name of the ketone.

Subordinate function

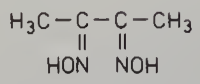


148

3-Phenyl-3-(phenylhydrazono)propionic acid
The subordinate function is a prefix cited alphabetically with other substituents.

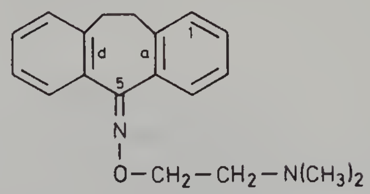
8.4 Oximes

Single function



149

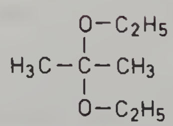
'Dimethylglyoxime' (DAB 8)
syst.: 2,3-Butanedione dioxime (IUPAC, DAB 8)
Biacetyl dioxime (IUPAC)
The first name is derived on the basis of the dialdehyde glyoxal. It is classified as trivial.
The function name systematically follows the name of the ketone.



150

trivial: Noxiptiline (INN)
a) 10,11-Dihydro-5*H*-dibenzo[*a,d*] cyclo-hepten-5-one *O*-[2-(dimethylamino)-ethyl] oxime (WHO, IUPAC)
b) 10,11-Dihydro-5*H*-dibenzo[*a,d*] cyclo-hepten-5-one oxime (2-dimethylaminoethyl) ether (IUPAC)

8.5 Ketone acetals



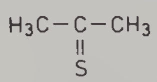
151

a) Acetone diethyl acetal
b) 2,2′-Diethoxypropane
The designation is derived either from combination of names, ketone radical acetal or substitutively as with ethers (see 2.2. p. 151)

9. THIONES, KETONES

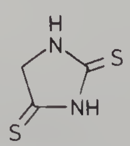
9.1. S-analogues of ketones

(Suffix: . . .thione, prefix: . . .thioxo. .)



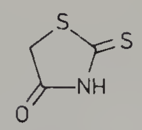
152

trivial: Thioacetone
syst.: 2-Propanethione



153

trivial: Dithiohydantoin
syst.: 2,4-Imidazolidinedithione
In the trivial name the oxygen of the parent compound is replaced by S.

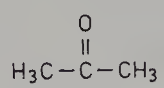


154
trivial: Rhodanine
syst.: 2-Thioxo-4-thiazolidinone
The =S function (prefix) is subordinate to the =O function (suffix).

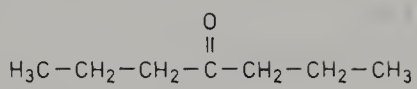
9.2 Ketones

(rf. -ketone, suffixes; . . .one; -quinone; prefix: . .oxo-)

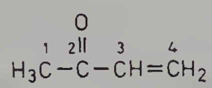
9.2.1 Aliphatic and carboxyclic ketones



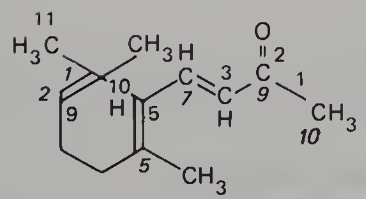
155
trivial: Acetone
syst. (rf.): Dimethyl ketone
syst. (subst.): 2-Propanone



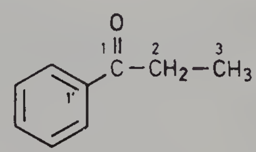
156
trivial: Butyrone
syst. (rf.): Dipropyl ketone
syst. (subst.): 4-Heptanone



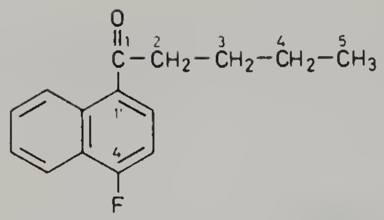
157
syst. (rf.): Methyl vinyl ketone
syst. (subst.): 3-Buten-2-one
The radicals are cited alphabetically.
The '-one' suffix, in preference to an unsaturated bond, takes the lowest possible numbered locant.



158
trivial: ψ-Ionone
syst.: (3*E*,5*E*)-10-Methyl-3,5,9-undecatrien-2-one
semi-syst.: 9-Apo-ψ-caroten-9-one

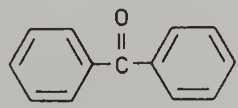


159
trivial: Propiophenone (exception)
The name is trivial and commonly used.
The systematic, uncommon name is propionophenone
(The derivation is from the acyl group designation in carboxylic acids . . .ic acid → . .ophenone with the phenyl radical or . .onaphthone from the . .naphthyl radical).



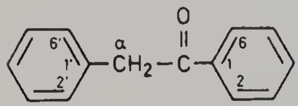
160

syst.: 4′-Fluoro-1′-valeronaphthone
The substituted acyl radical has unprimed locants, the locants of phenyl or naphthyl radicals are primed.



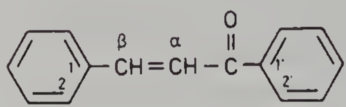
161

syst.: Benzophenone



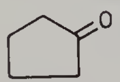
162

semi-trivial: Deoxybenzoin



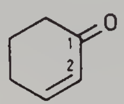
163

trivial: Chalcone



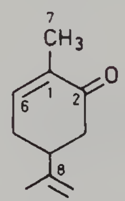
164

Cyclopentanone



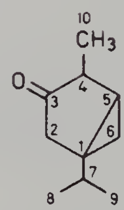
165

2-Cyclohexenone
The suffix, in preference to the double bond, has claim to the lowest locants.
(1 not denoted)



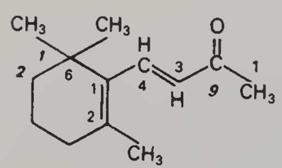
166

trivial: Carvone
syst.: 6,8-*p*-Mentha-dien-2-one
(cf. Limonene, p. 60)



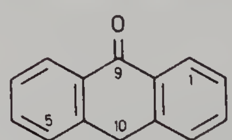
167

trivial: Thujone
syst.: 3-Thujanone
(cf. Thujane, p. 60)



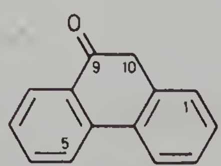
168

trivial: β-Ionone
syst.: *trans*-4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-3-buten-2-one
semi syst.: $\underline{9}$-Apo-β-caroten-$\underline{9}$-one



169

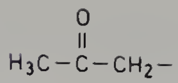
syst.: (contraction) Anthrone
(9(10*H*)-Anthracenone)



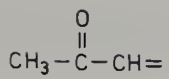
170

syst.: (contraction) Phenanthrone
(9(10*H*)-Phenanthrenone)

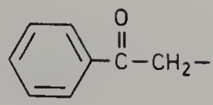
Radicals



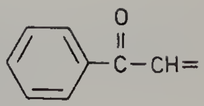
171
Acetonyl



172
Acetonylidene

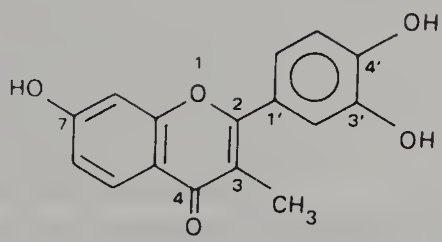


173
Phenacyl



174
Phenacylidene

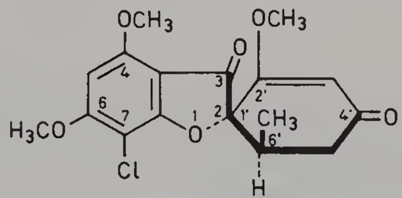
9.2.2. Heterocyclic ketones



175

semi-trivial: 3,3′,4′,7-Tetrahydroxyflavone
syst.: 2-(3,4-Dihydroxyphenyl)-3,7-dihydroxy-4*H*-chromen-4-one
4*H*-[1] benzopyran-4-one

In the semi-trivial name the locants, both primed and unprimed, are put into ascending order and where there are both primed and unprimed locants of the same numerical value, the primed locants follow their unprimed equivalent (but see Carotenes I 7.3, page 50 example (c)).



176
Griseofulvin (INN)

syst.: 7-Chloro-2′,4,6-trimethoxy-6′-methylspiro[benzofuran-2(3*H*),1′-[2] cyclohexene]-3,4′-dione (WHO); with the configuration (1′*S*,6′*R*) DAB9.

Sequence Rules would denote the configuration of the two asymmetric C-atoms (1′,6′) by the indicators 1′(*S*),6′(*R*), in place of the rotation direction in front of the E.P. II name.

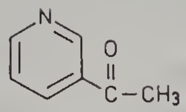
semi-trivial: 7-Chloro-2′,4,6-trimethoxy-6′-methylgris-2′-ene-3,4′-dione

Only the substituents are systematically designated, the spirane base compound is trivial.

IUPAC does not allow for the designation . . .2(3*H*). . for spirans, which gives rise to the following nomenclature:

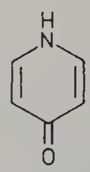
. . .spiro[2,3-dihydrobenzofuran-2,1′-2′-cyclohexene]. . .

This gives rise to the difficulties in ketone name, as the dihydro component requires an 'oxo-' prefix for it, but the cyclohexene requires an 'one.' suffix. The difficulty does not arise with the 2(3*H*)- formula for the spiran.



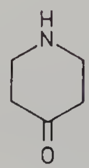
177

systematic (subst.): 1-(3-Pyridyl)ethanone
(rf.): Methyl 3-pyridyl ketone
(subst.): 3-Acetylpyridine
The first name is, starting from 3-ethylpyridine, easily understood. The third name is an acceptable alternative.



178

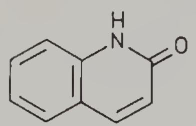
4-Pyridone
(acceptable contraction of 4(1*H*)-pyridinone)



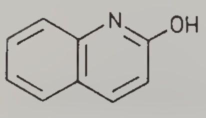
179

4-Piperidone (contraction of 4-piperidinone)

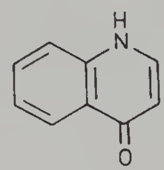
Systematic names of ketones derived from carbocyclic or heterocyclic aromatic ring systems are so constructed that first a —CH= group is replaced by $\underset{\underset{\displaystyle \mathrm{O}}{\|}}{-\mathrm{C}-}$ and the MNK system set up thereafter (cf. 5,8-Quinolinedione 9.2.3.3) or individual H-atoms established as 'indicated H' as the case may be. Thereby the carbonyl group takes precedence for the lower locant number (cf. 9(10*H*)-phenanthrenone 9.2.2) insofar as the established numbering system of a heterocycle gives something else (cf. 4(1*H*)-pyridinone for the former, and 2- and 4(1*H*)-quinolinone for the latter).



180 trivial: Carbostyril (C.A.)
syst.: 2(1*H*)-Quinolinone



181 2-Quinolinol
(see III formula 121 p. 99)

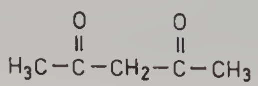


182

4-Quinolone (contraction of 4(1*H*)-Quinolinone)
(see III formula 122 p. 99)

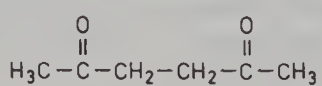
9.2.3 Polyketones

9.2.3.1 Aliphatic



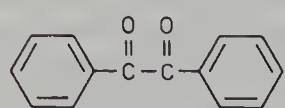
183

Acetylacetone
2,4-Pentanedione
(suffix)



184

semi-trivial: Acetonylacetone
syst.: 2,5-Hexanedione

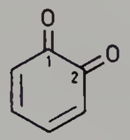


185

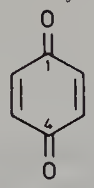
trivial: Benzil
syst.: Diphenylethanedione
Bibenzoyl

9.2.3.2. Quinones

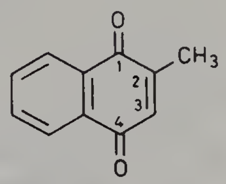
(Cyclic diketones with the maximum number of non-cumulative double bonds, derived from aromatic compounds; *o*- or *p*-quinonoid bond-systems.



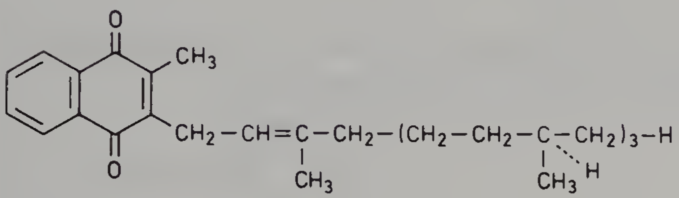
186
o-Quinone
o-Benzoquinone



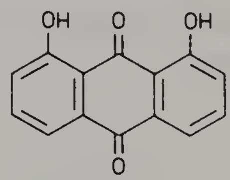
187
p-Benzoquinone
'Quinone'
['Hydroquinone' with aromatic bonding, is produced by hydrogenation of 'quinone' (addition of 2 H-atoms) cf. phenols]



188
Menadione (E.P. I)
syst.: 2-Methyl-1,4-naphthoquinone

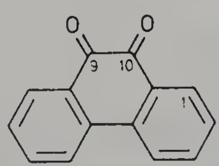


189
Phytomenadione (INN) trivial: Vitamin K
Phylloquinone
syst.: 2-Methyl-3-phytyl-1,4-naphthoquinone



190
Dantrone (INN)
1,8-Dihydroxyanthraquinone
(. . .anthraquinone:
. . ,9,10-anthracenedione)

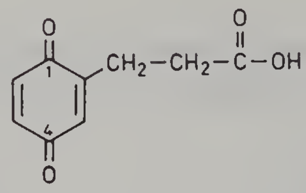
While in the named examples a quinone suffix was combined with a contraction of an aromatic hydrocarbon name, this contraction is not applicable in other examples.



191
Phenanthrenequinone
9,10-Phenanthrenedione

Radicals

From . . .quinone names, C-'radical' names of the form . .quinonyl. . are derived, when naming compounds with a group having seniority over oxo-acid, as suffix (exception! two suffix groups; between them . . .yl):

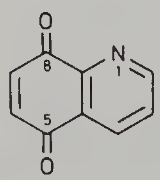


192

3-(1,4-Benzoquinon-2-yl)propionic acid
The locant 2 need not be cited in this simple case. The carbonyl C-atoms point of attachment is cited first, the quinone locants take precedence over the 'yl' position for lowest locants.

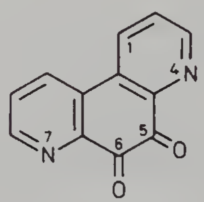
9.2.3.3. Heterocyclic diketones

Heterocyclic diketones with quinonoid bond systems are designated not as quinones but as diketones.



193

5,8-Quinolinedione
5,8-Dioxo-5,8-dihydroquinoline

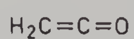


194

Phanquinone (INN)
syst.: 4,7-Phenanthroline-5,6-dione (WHO, IUPAC)

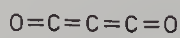
9.2.4 Ketenes

These are characterized by the terminal double bond carbonyl group (see formula 195). The nomenclature of this compound-class is formed using substitutive names. In cyclic ketenes the carbonyl group appears as a prefix 'carbonyl' before the name of the ring system.



195

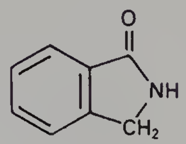
Ketene (parent compound of the class)



196

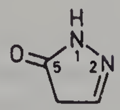
inorganic: Carbon suboxide
Tricarbon dioxide
(Propadienedione ?)

9.2.5 *Lactams as heterocyclic ketones*[6]



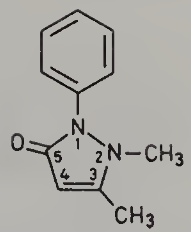
197

trivial: Phthalimidine
syst.: 1-Isoindolinone



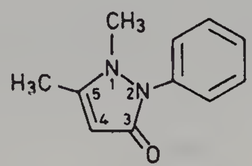
198

a) 2,3-Didehydropyrazolidin-5-one
b) 4,5-Dihydro-1*H*-pyrazol-5-one (IUPAC)
c) contraction: 5-Pyrazolone
d) acceptable: 5-Oxopyrazole



199

Phenazone (INN)
(2,3-Dimethyl-1-phenyl-3-pyrazolin-5-one)
(WHO)

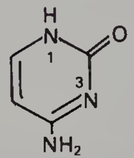


200

1,5-Dimethyl-2-phenyl-3(2*H*)-pyrazolone
(IUPAC, E.P. III, C.A.)

199 $\equiv$ 200

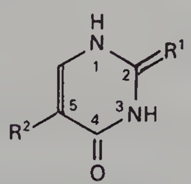
9.2.6 *Cyclic ureas as ketones*



201

trivial: Cytosine (three-letter symbol Cyt)
syst.: 4-Amino-2(1*H*)-pyrimidinone

9.2.6a) *Pyrimidine bases*



202

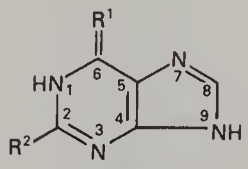
	Trivial	R^1	R^2	TLS*
α)	Thiouracil	=S	—H	Sur
β)	Uracil	=O	—H	Ura
γ)	Thymine	=O	CH_3	Thy
	Unspecified Pyrimidine base	–	–	Pyr

* Three-letter symbol

syst.: α) 2,3-Dihydro-2-thioxo-4(1*H*)-pyrimidinone
β) 2,4(1*H*,3*H*)-Pyrimidinedione
γ) 5-Methyl-2,4(1*H*,3*H*)-Pyrimidinedione

6 cf. lactams, p. 193.

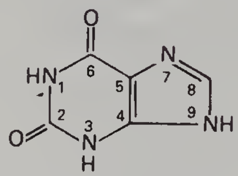
9.2.6b) Purine bases



203

syst.: α) 9*H*-Purine-6(1*H*)-thione
β) 2-Amino-9*H*-purine-6(1*H*)-one
γ) 9*H*-Purine-6(1*H*)-one

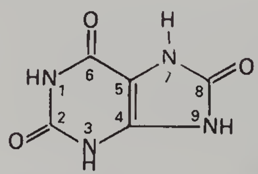
	Trivial	R^1	R^2	TLS
α)	9*H*-Thiohypoxanthine	=S	—H	Shy
β)	9*H*-Guanine	=O	NH_2	Gua
γ)	9*H*-Hypoxanthine	=O	—H	Hyp
	Unspecified purine base	—	—	Pur



204

trivial: 9*H*-Xanthine (TLS:Xan)
syst.: 9*H*-Purine-2,6(1*H*,3*H*)-dione

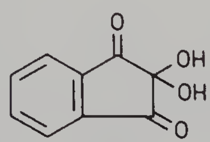
9.2.6c) Uric acid



205

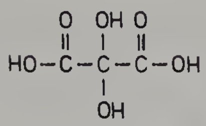
7*H*-Purine-2,6,8(1*H*,3*H*,9*H*)-trione

9.2.7. Ketone hydrates



202

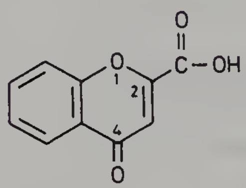
trivial: Ninhydrin (E.P. II)
1,2,3-Indantrione monohydrate (E.P. II)
syst.: 2,2-Dihydroxy-1,3-indandione
The 'ketone hydrate' appears under the designation as the prefix 'dihydroxy' (subordinate function before the '-one' suffix).



203

trivial: Mesoxalic acid hydrate or monohydrate
syst.: Dihydroxymalonic acid
The hydrate names do not form their own class of ketone derivatives; they simply express the addition of water to the ketone or the oxo-group. In the other (syst.) names by contrast, the seniority of the functional groups comes to the fore (O= or –COOH) rank senior to the –OH); the –OH groups therefore are cited as prefixes. This is not given as indicating equality with alcoholic –OH groups, merely an analogy in the nomenclature.

9.3 Subordinate function

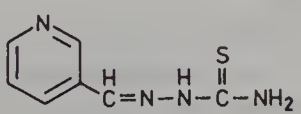


204

Chromocarb (INN)
4-Oxo-4*H*-1-benzopyran-2-carboxylic acid (WHO)
4-Oxo-4*H*-2-chromenecarboxylic acid (IUPAC)
Instead of using a senior suffix, a ketone acid is designated by means of the 'oxo' prefix.

10. ALDEHYDE DERIVATIVES

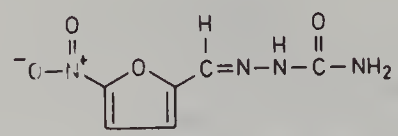
10.1 Thiosemicarbazones



205

Nicothiazone (INN)
Nicotinaldehyde thiosemicarbazone (WHO)
The word 'thiosemicarbazone' follows the aldehyde name.

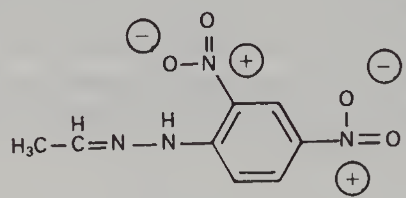
10.2 Semicarbazones



206

Nitrofural (INN)
5-Nitro-2-furaldehyde semicarbazone (WHO, IUPAC)
NB. As 'furaldehyde' is trivial, this name uses two nomenclature styles.

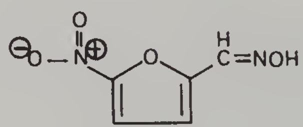
10.3 Hydrazones



207

Acetaldehyde 2,4-dinitrophenylhydrazone (IUPAC)

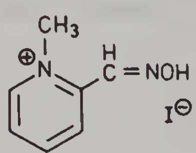
10.4 Oximes



208

Nifuroxime (INN)
5-Nitro-2-furaldehyde oxime (IUPAC)
The word 'oxime' follows the name of the aldehyde; 'furaldehyde' is trivial.

Subordinate function



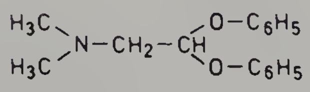
209

Pralidoxime iodide (INN)
a) 2-Formyl-1-methylpyridinium iodide oxime (WHO)
The oxime function is denoted additively after the salt of the quarternary base. The aldehyde is denoted as a prefix.
b) 2-Hydroxyiminomethyl-1-methylpyridinium iodide
The aldehyde oxime is denoted as a unified prefix in alphabetical order of prefixes. The primary group is the quaternary base (as a salt) which forms the suffix.

10.5 Acetals[8]

(Etherified aldehyde hydrates) (aldehyde hydrates see 11.3)

10.5.1. Open (acyclic) acetals



210

Medifoxamine (INN)

a) Dimethylaminoacetaldehyde diphenyl acetal (WHO, IUPAC)

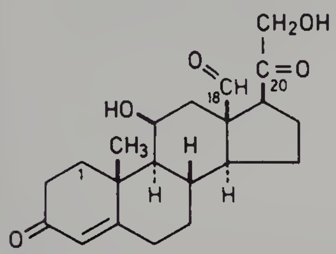
The name of the aldehyde (forming the hydrate) is cited first and then the names (in alphabetical order) of the substituents of both O-atoms (or where two identical radicals are involved, the substituent name following the number indicator) and then the word 'acetal'. The aldehyde derivative has seniority over the amine as principal group.

b) *N,N*-Dimethyl-2,2-bis(phenoxy)ethylamine (IUPAC)

The amine has seniority over the ether in this type of designation.

10.5.2. Closed acetals

Cyclic acetals



211

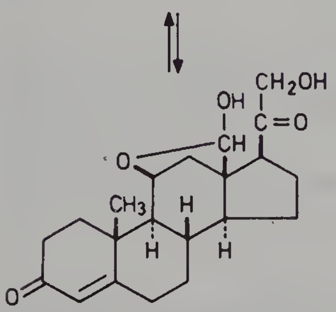
Aldosterone (INN)

a) 11β,21-Dihydroxypregn-4-ene-3,18,20-trione (WHO)

In this designation, there is no distinction between aldehyde and ketone structures; no acetal.

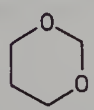
b) 11β,21-Dihydroxy-3,20-dioxopregn-4-en-18-al (IUPAC)

Here aldehyde and ketone structures are separated, aldehyde has seniority as suffix; no acetal.



212

In this isomer structure there is a hemiacetal, only one of the two hydroxy groups of the aldehyde hydrate is intramolecularly etherified. This structure is denoted, using the previous IUPAC name with the addition '18,11-hemiacetal' (instead of . .18-al).



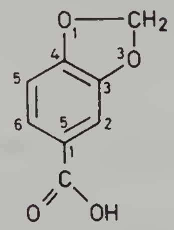
213

1,3-Dioxan (IUPAC)

This type of cyclic acetal (of formaldehyde in this case) is named according to the rules for heterocycles.

8 Acetals belonging to the carbohydrates are dealt with in Chapter V.

Subordinate function

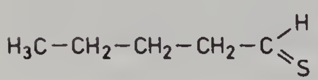


214

trivial: Piperonylic acid
1,3-Benzodioxole-5-carboxylic acid
(inner locants)
3,4-Methylenedioxybenzoic acid
(outer locants)
(Substitutive name, the carboxylic acid has seniority over the ether as suffix or the acetal of formaldehyde).

11. THIOALDEHYDES, ALDEHYDES

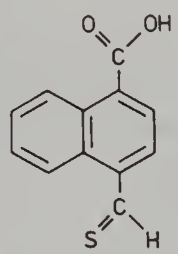
11.1 Thioaldehydes



215

Pentanethial (IUPAC)
All C-atoms are attached to the the hydrocarbon, on which the S-atom is terminally attached, this appears together with the 1 H of the hydrocarbon as the suffix . . .thial.

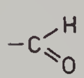
Subordinate function



216

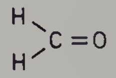
1-(4-Thioformyl)naphthoic acid
The carboxylic acid is the preferred function (suffix). The carbothialdehyde group becomes the prefix.

11.2 Aldehydes



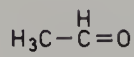
(Suffixes: . . .(C.A.); prefixes . . .) . .aldehyde, -al, carbaldehyde (IUPAC) carboxaldehyde (C.A.), oxo, formyl

11.2.1. Aliphatic aldehydes



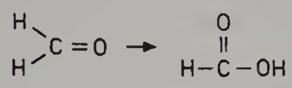
217

trivial: Formaldehyde
The (uncommon) syst. name would be methanal: base hydrocarbon: Methane CH_4, function as aldehyde –H, =O. The syllable 'form' of the trivial name originates in the fact that oxidation produces formic acid.

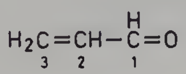


218

trivial: Acetaldehyde
syst.: Ethanal

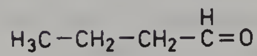


219



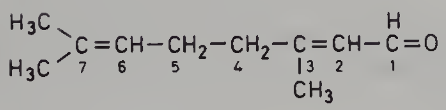
220

trivial: Acrylaldehyde (acrolein)
syst.: 2-Propenal



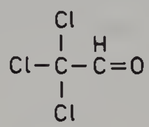
221

trivial: Butyraldehyde
syst.: Butanal
The suffix 'al' refers to the structure $(\text{-C})^{-H}_{=O}$ being attached to one of the end C-atoms of the parent compound



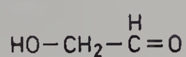
222

trivial: Citral (DAB 8)
(mixture of geranial (*trans*) and neral (*cis*))
syst.: 3,7-Dimethyl-2,6-octadienal



223

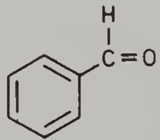
trivial: Chloral
syst.: Trichloracetaldehyde
Hydrate cf. formula **237**



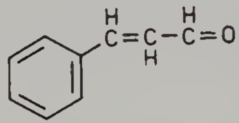
224

trivial: Glycolaldehyde
syst.: 2-Hydroxyethanal
2-Hydroxyacetaldehyde

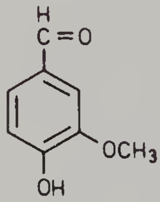
11.2.2 Cyclic aldehydes



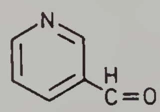
225
trivial: Benzaldehyde



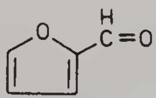
226
trivial: Cinnamaldehyde (formula trans)
syst.: (*E*)-3-Phenyl-2-propenal



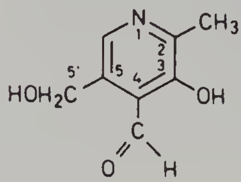
227
trivial: Vanillin (DAB 8)
syst.: 4-Hydroxy-3-methoxybenzaldehyde
(Alphabetical order of substituent prefixes)



228
trivial: Nicotinaldehyde
syst.: 3-Pyridinecarbaldehyde
(IUPAC)

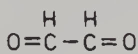


229
trivial: 2-Furaldehyde
Furfural (E.P.II)
syst.: 2-Furancarbaldehyde (IUPAC)
2-Furancarboxaldehyde (C.A.)

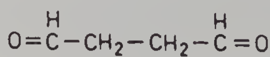


230
trivial: Pyridoxal (with 5′)
symbol: PL
syst.: 3-Hydroxy-5-hydroxymethyl-2-methyl-4-pyridinecarbaldehyde

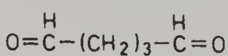
11.2.3 Dialdehydes



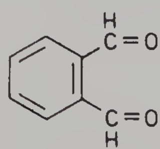
231
trivial: Glyoxal
syst.: Ethanedial



232
trivial: Succinaldehyde
syst.: Butanedial

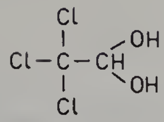


233
trivial: Glutaraldehyde
syst.: Pentanedial
Locants are not needed for the systematic name, as the 'al' suffix can only apply to terminal groups.



234
trivial: Phthalaldehyde

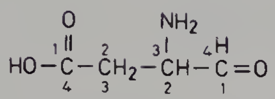
11.2.4



235

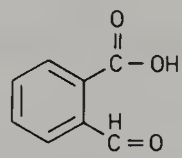
trivial: Chloral hydrate
(Trichloroacetaldehyde hydrate)
syst.: 2,2,2-Trichloroethane-1,1-diol (E.P. II)
The hydrate nomenclature does not establish a class of compounds for aldehyde derivatives, but simply expresses the addition of water to the aldehyde. The substitutive name does not constitute any relationship of the compound to the alcohols.

11.3



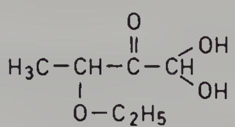
236

trivial: Aspart-1-al
The stem of the trivial name of the parent compound is attached to the 'al' suffix, when there is a further senior carboxyl group also available. (Lower locants) (cf. 15.4.7.2.)
syst.: 3-Amino-4-oxobutanoic acid (upper locants).



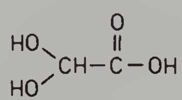
237

Phthalaldehydic acid
syst.: 2-Formylbenzoic acid
Trivially named dicarboxylic acids of which one of the carboxyl groups is changed to an aldehyde group can form the combined name . .aldehydic acid
(NB. this is exceptional; 2 suffixes).



238

Ketoxal (INN)
3-Ethoxy-1,1-dihydroxy-2-butanone (WHO, IUPAC)



239

Glyoxylic acid monohydrate
2,2-Dihydroxyacetic acid

The aldehydrate loses the senior rank of aldehyde and the ketone becomes senior.

12. ISOCYAN-(ATE, IDE)

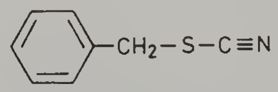
12.1 Isothiocyanates

$H_2C{=}CH{-}CH_2{-}N{=}C{=}S$

240

trivial: 'Mustard oil'
syst.: Allyl isothiocyanate (rf.)

12.2 Thiocyanates



241

trivial: Benzyl rhodanide
syst.: Benzyl thiocyanate

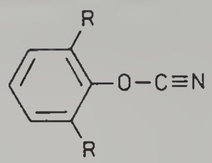
12.3. Isocyanates

$H_5C_2-N=C=O$

242

Ethyl isocyanate

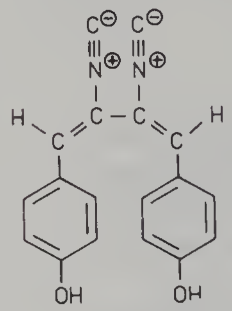
12.4 Cyanates



243

2,6-Di-R-phenyl cyanate

12.5. Isocyanides



244

Component of Xanthocillin (INN)
trivial: Xanthocillin X
syst.: Bis(*p*-hydroxybenzylidene)ethylene diisocyanide
(Zwitterions see III 9.4.)

12.6. Cyanides (nitriles)

(Suffixes: nitrile, carbonitrile; prefix[9] : cyano. . ; anion; cyanide)

9 The prefix 'nitrilo' denotes a tertiary amino group $\bar{N}$ as substituent, see p. 160 formula 83.

$H_3C-CH_2-CH_2-CH_2-C\equiv N$

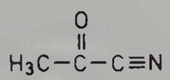
245

a) Pentanenitrile (subst. - -N). All the C-atoms included in the named parent hydrocarbon.
b) Valeronitrile
The trivially named carboxylic acids include all the C-atoms and form the nitrile name by changing the '. .ic acid' (just as the '. .oic acid'), to '. .onitrile'.

$H_3C-C\equiv N$

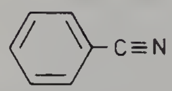
246

Ethanenitrile, acetonitrile, methyl cyanide (rf.)



247

a) Pyruvonitrile, b) acetyl cyanide



248

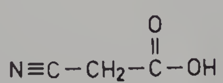
a) Benzonitrile, b) phenyl cyanide

$N\equiv C-CH_2-C\equiv N$

249

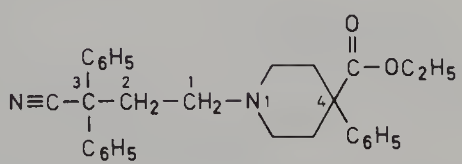
a) Propanedinitrile (all C-atoms belong to an hydrocarbon)
b) Malononitrile (name derived from dicarboxylic acid, cf. formula 245)
Carboxylic acid has priority over cyano as principal group.
In the case of an acid ending with 'carboxylic acid', nitrile ending is 'carbonitrile'.

Subordinate function
(Prefix: . . .cyano)



250

Cyanoacetic acid
Carboxylic acid has priority over cyano as principal group.
In the case of an acid ending with 'carboxylic acid', nitrile ending is 'carbonitrile'

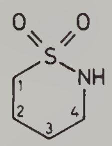


251

a) Diphenoxylate (INN)
b) syst.: a) 1-(3-Cyano-3,3-diphenylpropyl-4-phenylpiperidine-4-carboxylic acid ethyl ester (WHO)
The substituent alphabetical order (c/d/p) is chosen. Cyano is a prefix while the ester group, which has priority, forms the suffix.
c) Ethyl 1-(3-cyano-3,3-diphenylpropyl)-4-phenyl-4-piperidinecarboxylate (IUPAC)

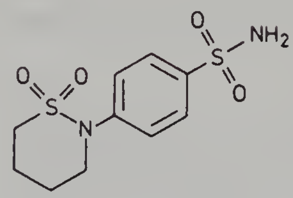
13. ACID DERIVATIVES

13.1. Sultams
(cyclic sulfonic acid amides)



252

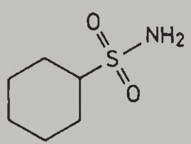
a) Butanesultam (inner locants)
The SO_2 group is on the C-atom bearing the lowest possible locant.
b) 1,2-Thiazinane 1,1-dioxide (locants
Oxidation of the S gives rise to addition names.
c) 1,1-Dioxo-1λ^6-1,2-thiazinane
(λ-convention)
[S with bonding number 6 (standard 2)]



253

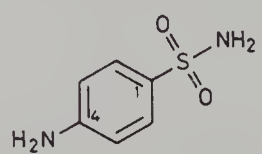
Sultiame (INN)
a) *p*-(Tetrahydro-2*H*-1,2-thiazin-2-yl)-benzenesulfonamide *S,S*-dioxide (WHO)
b) *p*-(1,2-Thiazinan-2-yl)benzenesulfonamide 1,1-dioxide
The sultam is subordinate to the sulfonamide and is cited as prefix in the systematic name, oxidation is cited thereafter.
4(1,1-Dioxo-1λ^6-1,2-thiazinane-2-yl)-benzolsulfonamide

13.2 Sulfonamides



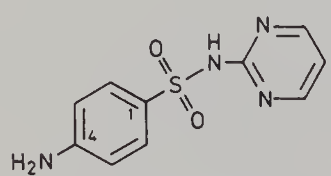
254

Cyclohexansulfonamide



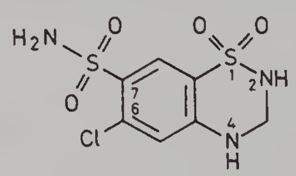
255

trivial: Sulfanilamide
syst.: *p*-Aminobenzolsulfonamide



256

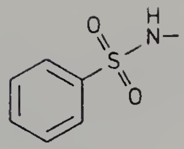
Sulfadiazine (INN) (E.P. III)
a) N^1-2-Pyrimidinylsulfanilamide (WHO)
b) 4-Amino-*N*-(2-pyrimidinyl)benzenesulfonamide (E.P. III)
Both names can be regarded as acceptable IUPAC, even though the distinction between N (from N as in sulfanilamide) is not expressly provided for.



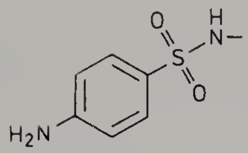
257

Hydrochlorothiazide (INN)
a) 6-Chloro-3,4-dihydro-2*H*-1,2,4-benzothiadiazine-7-sulfonamide 1,1-dioxide (WHO)
b) 6-Chloro 1,1-dioxo-2*H*-1λ^6-1,2,4-benzothiadiazine-7-sulfonamide

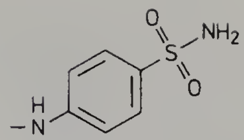
Radicals



258
Benzenesulfonamido



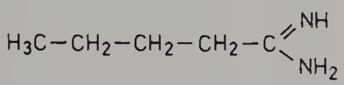
259
Sulfanilamido



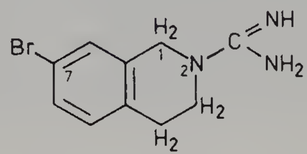
260
4-Sulfamoylanilino

13.3. Amidines

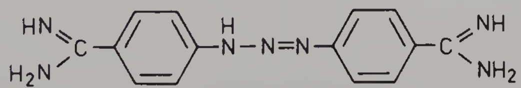
Suffixes: . . .amidine, carboxamidine; prefix: amidino (not guanyl)



261
Pentanamidine, Valeramidine
Derivation from the (carbonic) acid name 'amidine' includes no C!)

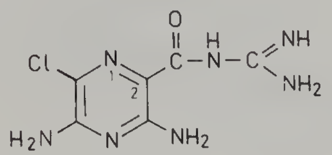


262
Guanisoquine (INN)
a) 7-Bromo-3,4-dihydro-2(1*H*)-isoquinoline-carboxamidine (WHO)
b) 7-Bromo-1,2,3,4-tetrahydro-2-isoquinolinecarboxamidine (IUPAC)
Here 'carboxamidine' is a suffix, there being no priority groups. It is to be noted that the $-C(NH)NH_2$ group is denoted 'carboxamidine' while the prefix -inclusive of the C-atom-, is simply denoted 'amidino' and not 'amidino-methyl'. The systematic 'carbamimidoyl' is optional.



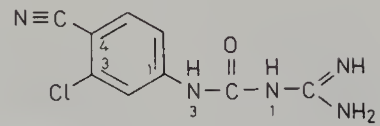
263
Diminazene (INN)
4,4′-(Diazoamino)benzamidine
'Diazoamino' is a biradical which, linking with two identical groups, does not take any multiplying prefix.

Subordinate function



264

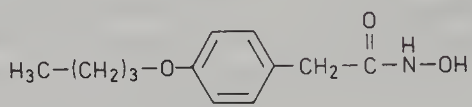
Amiloride (INN)
N-Amidino-3,5-diamino-6-chloro-pyrazinecarboxamide (WHO) (IUPAC)
'Amidino' is cited as substituent (prefix), the carboxamide group having priority, forming the suffix. There is no IUPAC provision for naming it as an acylated guanidine. The locant 2 for the suffix is not cited, there being no possible alternative.



265

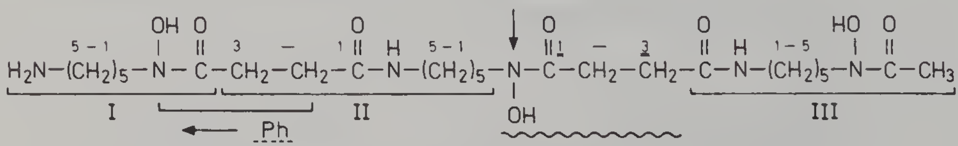
Cloguanamil (INN)
1-Amidino-3-(3-chloro-4-cyanophenyl)urea (WHO) ('amidino' includes 1 C)

13.4. Hydroxamic acids (N-hydroxamides)



266

Bufexamac (INN)
a) *p*-Butoxyphenylacetohydroxamic acid
b) *p*-Butoxy-*N*-hydroxy-phenylacetamide
A hydroxamic acid is thus not an N-hydroxy derivative of an '. . .amic acid' (half-amide of a dicarboxylic acid), but is derived from a monocarboxylic acid.

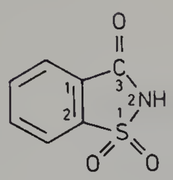


267

Deferoxamine (INN)

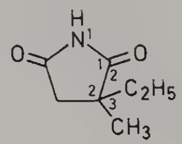
a) *N*-(5- {3-[(5-Aminopentyl)hydroxycarbamoyl] propionamido}pentyl)-3- {[5-(*N*-hydroxyacetamidopentyl] carbamoyl}propionohydroxamic acid (WHO)
3 hydroxamic acid structures are contained within the name. The middle (N,3) forms the stem for the principal (suffix) group; the other two in the substituent groups are cited as prefixes. These lose their own propionohydroxamic acid (ph) order of numbering, because the direction for the substituent is opposite to that for the parent compound and it is shared between substituents I and II.
A permissible replacement nomenclature designation would be
b) 30-Amino-3,14,25-trihydroxy-3,9,14, 20, 25-pentaazatriacontan-2,10,13,21,24-pentone (Order of number).

13.5 Imides



268

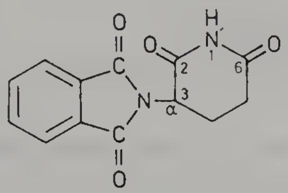
a) 2-Sulfobenzoic acid imide
(cf. DAB 7 saccharin-sodium)
(locants in the benzene ring)
b) 1,2-Benzisothiazol-3(2*H*)-one 1,1-dioxide (IUPAC)
(locants in the 5-member ring)
The ring-system is named as a heterocycle. Thereby the 'imide' designation is dropped, and the oxo-function at the 3 position takes priority and appears as the suffix '-one'. The 1 position dioxide is an additive nomenclature component, which does not affect the status of the '-one' suffix of the preceding independent part of the name.



269

Ethosuximide (INN)
a) 2-Ethyl-2-methylsuccinimide (IUPAC)
(inner locants)
b) (*RS*)-3-Ethyl-3-methyl-2,5-pyrrolidine-dione
(DAC 1979, IUPAC)
(outer locants)

c) 1,1-Dioxo-2*H*-1λ^6-1,2-benzisothiazol-3-one (locants in the five ring) (according to λ-convention).



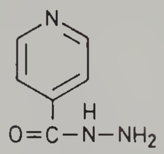
270

Thalidomide (INN)

a) *N*-(2,6-Dioxo-3-piperidyl)phthalimide (WHO, IUPAC) (inner locants)
The compound consists of two mutually substituted imides. Naming depends on deciding which imide is considered the more important. In the above name this is taken to be phthalimide, which becomes the principal component of the name. The glutarimide substituted on it is not designated as such, but as a heterocycle, because it is not joined by means of its N, but by a C-atom.
b) α-(*N*-Phthalimido)glutarimide (WHO) (outer locants)
In this name the glutarimide serves as base-component. The phthalimide is a substituent on it. Citing the N in brackets is superfluous, as the radical ending '. .imido' already establishes this.

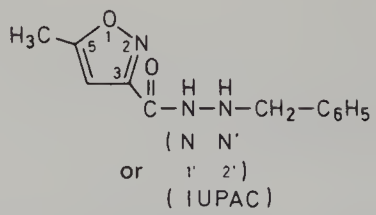
If considered as a substitution product of two heterocycles, then on the basis of III 2.3., isoindoline has preference as the base component over piperidine. The following name thereby results (p. 97):
c) 2-(2,6-Dioxo-3-piperidyl)-1,3-isoindolinedione (IUPAC).

13.6 Hydrazides



271

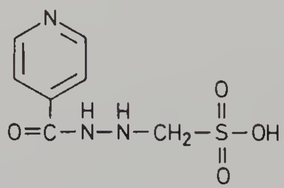
Isoniazide (INN)
a) Isonicotinic acid hydrazide (WHO)
b) Isonicotinohydrazide (IUPAC)
If the carboxylic acid has a trivial name with the '. .ic acid' ending, the hydrazide is named by adding '. .ohydrazide' to the stem of the carboxylic acid name.



272

Isocarboxazide (INN)
a) 5-Methyl-3-isoxazolecarboxylic acid 2-benzylhydrazide (WHO)
b) N'-Benzyl-5-methyl-3-isoxazolecarbohydrazide (IUPAC) (locants)
Here the substituents of the hydrazide considered as a unit are positioned before it, the unit following. The acetylated N-atom is unprimed, the alkylated N- is primed.

Subordinate function

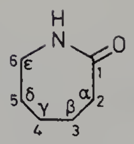


273

Methaniazide (INN)
a) Isonicotinic acid 2-(sulfomethyl)hydrazine (WHO)
This, from List 6 of INN recommended scientific names is not an acceptable IUPAC name (hydrazine instead of hydrazide).
b) N'-(Isonicotinoylhydrazino)methanesulfonic acid (IUPAC)
The base component of the name is the senior sulfonic acid. The junior carboxylic acid hydrazide is cited as prefix.

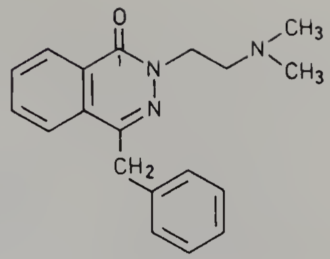
13.7 Lactams

(intramolecular amides) (cf. ketones 9.2.5.)
Many compounds considered elsewhere fall into this group because of their structures, e.g. penicillin, cephalosporin, pyrazolone. Since lactams by their nature are always N-heterocycles, most are so named.



274

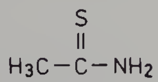
a) 6-Hexanelactam (IUPAC) (outer locants)
b) ϵ-Caprolactam (IUPAC)
This name is derived from the outdated name 'caproic acid' for hexanoic acid. (inner locants)
c) Hexahydro-2*H*-azepin-2-one (IUPAC)
d) Hexahydro-2-azepinone (IUPAC)



275

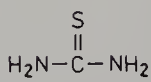
Talastine (INN)
2-[2-(Dimethylamino)ethyl]-4-benzyl-1(2*H*)phthalazinone
Lactam named as a heterocyclic ketone.

13.8. Thiocarboxylic acid amides



276

Thioacetamide (E.P. I)
The amide of thioacetic *O*-acid $H_3C-\overset{\overset{S}{\|}}{C}-OH$, which can be thought of as acetamide with an O replaced by S.

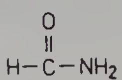


277

Thiourea
Replacement of O by S in urea

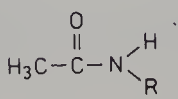
13.9 Carboxylic acid amides

13.9.1 Amides of monocarboxylic acids



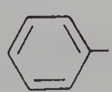
278

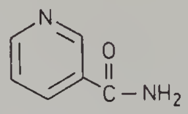
Formamide (E.P. I)



279

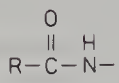
R=H Acetamide

R=  Acetanilide; IUPAC gives substituents on the phenyl group primes.

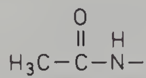


280
trivial: Nicotinamide
syst.: 3-Pyridinecarboxamide (E.P. II)

Radicals

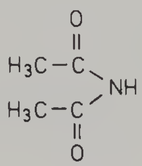


281
. . .Carboxamido

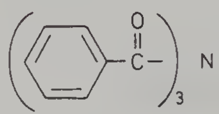


282
Acetamido, Acetylamino

13.9.2. [Bis(tris)carboxylic acid] amides

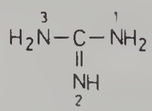


283
Diacetamide

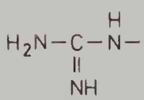


284
Tribenzamide

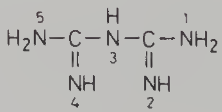
13.9.3. Amides of carbon acids and substitution products (and radicals)



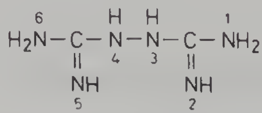
285
Guanidine



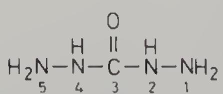
286
Guanidino



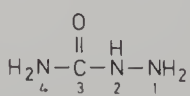
287
Biguanide



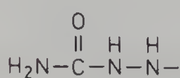
288
Biguanidine



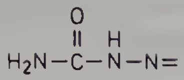
289
Carbonohydrazide
(also carbohydrazide,
carbazide)



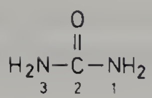
290
Semicarbazide



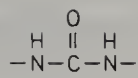
291
Semicarbazido



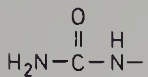
292
Semicarbazono



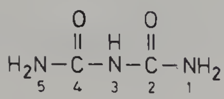
293
Urea



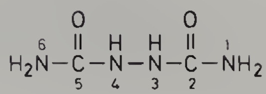
294
Ureylene



295
Ureido



296
Biuret

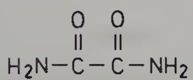


297
Biurea

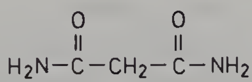
Replacement of =O by =S in urea and semicarbazide gives rise to thiourea and thiosemicarbazide.

'Carbamic acid' and its derivatives, also carboxylic acids of urea follow 1·5.4.6.2 on p. 217.

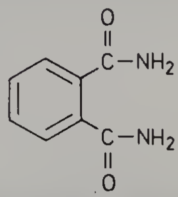
13.9.4. Dicarboxylic acid amides



298
Oxamide
(cf. also formula 422a)



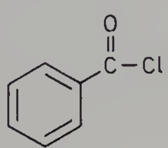
299
Malondiamide
(also malonamide)
(cf. also formula 422b)



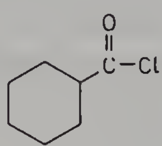
300
Phthaldiamide
(also phthalamide)

13.10 Carboxylic acid halogenides

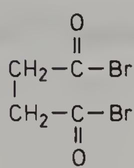
Acid halogenides are named using radicofunctional nomenclature:



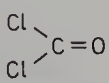
301
Benzoyl chloride (E.P. I)



302
Cyclohexanecarbonyl chloride

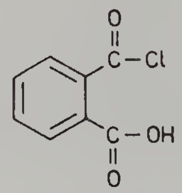


303
Succinyl dibromide



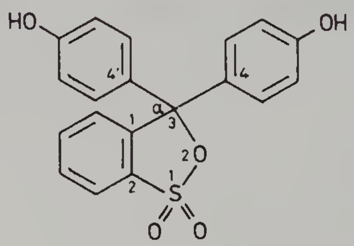
304
trivial: Phosgene
syst.: Carbonyl dichloride
(derived from carbonic acid H_2CO_3)

When groups having priority for citation as principal group are present, the -C-halogen group is given the prefix haloformyl, thus as the acyl of halogenated formic acid:



305
o-Chloroformylbenzoic acid

13.11 Sultones



306
trivial: Phenol red
Phenolsulfonephthalein

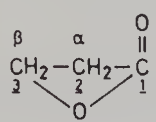
syst.: a) 4,4′-(3*H*-2,1-Benzoxathiol-3-ylidene)bisphenol *S,S*-dioxide (C.A.) (outer locants) In this name, the sultone group is denoted as a heterocyclic dioxide. Thereby 'phenol' is both parent compound and suffix.
b) There is a strong possibility that the substance has the structure of a zwitterion corresponding to the name

2-[Bis(4-hydroxyphenyl)methylio] benzenesulfonate

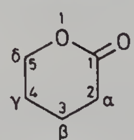
rather than that shown with a closed sultone ring.

13.12 Lactones/lactides

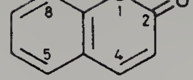
13.12.1. Intramolecular carboxylic acid esters (lactones) (heterocycles)



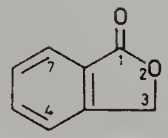
307
Propiolactone (INN)
syst.: a) *β*-Propiolactone (WHO, not IUPAC)
b) 3-Propanolide (IUPAC) (The basis is a non-hydroxylated carboxylic acid)
c) Hydracrylolactone (IUPAC) (The basis is a hydroxylated carboxylic acid).



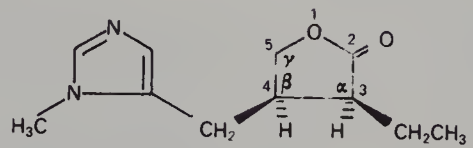
308
a) 5-Pentanolide
b) δ-Valerolactone (not a method of naming, generally applicable; IUPAC)
c) Tetrahydro-2-pyrone



309
trivial: Coumarin
radical: 2-Oxo-2*H*-chromen-x-yl



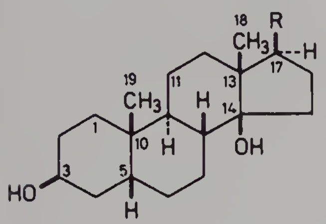
310
trivial: Phthalide
radical: (Phthalidyl)



310A
Pilocarpine

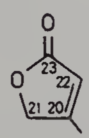
a) α-Ethyl-β-(1-methyl-5-imidazolylmethyl)-γ-butyrolactone (IUPAC)
b) (3*S*,4*R*)-3-Ethyl-4,5-dihydro-4-(1-methyl-5-imidazolylmethyl)-2(3*H*)-furanone (IUPAC) (outer locants).
In naming this as a heterocyclic ketone, the carboxylic acid derivative (lactone) group (which would have been the group of highest priority) is not cited.
c) 2-Ethyl-3-(1-methyl-5-imidazolylmethyl)-4-butanolide (IUPAC)

13.12.2. Steroid lactones

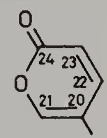


311

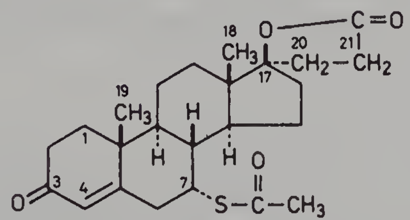
R:



311a
a) trivial: Digitoxigenin
syst.: 3β,14-Dihydroxy-5β, 14β-card-20(22)-enolide



311b
b) trivial: Bufalin
syst.: 3β,14-Dihydroxy-5β, 14β-bufa-20,22-dienolide

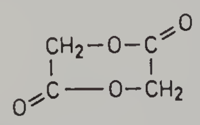


312
Spironolactone (INN)

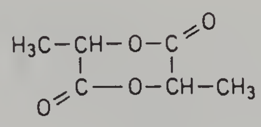
a) 17-Hydroxy-7-mercapto-3-oxo-17α-pregn-4-ene-21-carboxylic acid lactone 7-acetate (WHO) (locants)
This WHO name departs from IUPAC rules for steroid lactones, in a number of aspects. According to them, '17-hydroxy' is not denoted as lactonised OH-group, and the thio-

ester is cited as a prefix. The result is the IUPAC:
b) 7α-Acetylthio-3-oxo-17α-pregn-4-ene-21,17-carbolactone
Designation as a spiran is equally possible: the lactone group disappears and the thioester becomes a function (rf. see III p. 91 however):
c) *S*(3,5′-Dioxo-4-androstene-17-spiro-2′-tetrahydrofuran-7α-yl)

13.12.3. Intermolecular esters of hydroxy acids, producing ring-closure by double esterification (lactides)



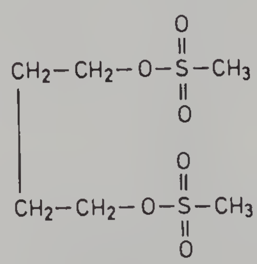
313
Glycolide (from glycolic acid)
1,4-Dioxan-2,5-dione



314
Dilactide (from lactic acid)

Where there is a trivial name for the acid, the name can be formed by adding '-ide' to the stem of the acid name prefixed by 'di' or 'tri' as the case may be. If there is no trivial name, the compound is named as an heterocycle.

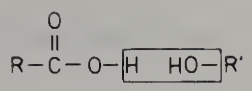
13.13 Sulfonic acid esters



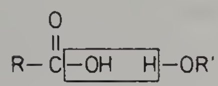
315
Busulfan (INN)
a) Tetramethylene ester of methanesulfonic acid (WHO)
b) Tetramethylene bis(methanesulfonate) (IUPAC)

13.14 Carboxylic acid esters

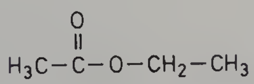
The esters are named by the 'yl/ate' method (cf. Chapter III). First, the alcohol in the form of the hydrocarbon radical remaining after elimination of the OH-group is named, followed by the acid in its anion form. The procedure gives rise to a name of the form: radical + anion, implying that a neutral molecule is not produced. Further, it is not the acid anion but the anion form of the name of the acid which is cited. Apart from this, the 'yl/ate' method of naming is in contrast to the actual reaction sequence of an esterification, which is not



but



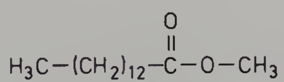
which produces:



316

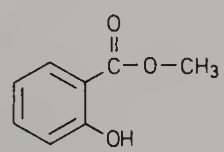
a) Ethyl acetate
b) Acetic acid ethyl ester

In English, ester names are written with the anion following the radical as a separate word and without a hyphen. Esters may also be named on the model 'acetic acid methyl ester', in which case the words again are all separate and not joined by hyphens.



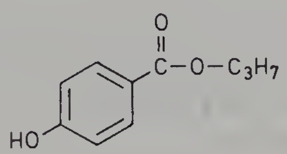
317

trivial: Methyl myristate
syst.: Methyl tetradecanoate



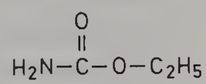
318

Methyl salicylate (E.P. II),
Methyl 2-hydroxybenzoate
Salicyclic acid methyl ester



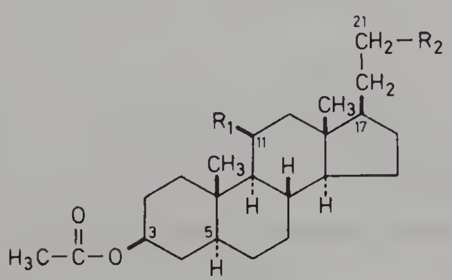
319

a) Propyl 4-hydroxybenzoate (E.P. II)
b) Propyl *p*-hydroxybenzoate
c) *p*-hydroxybenzoic acid propyl ester



320

trivial: Urethane
syst.: a) Carbamic acid ethyl ester (E.P. I)
b) Ethyl carbamate (IUPAC)

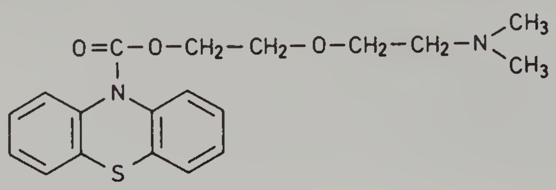


321a/b

321 a) $R_1 = R_2 = H$
Alcohol: 5α-Pregnan-3β-ol
Ester: 5α-Pregnan-3β-yl acetate
$\left.\right\}$ 17β must not be cited
Naming esters of steroid alcohols follows the usual yl/ate method

321 b) $R_1 = OH$, $R_2 = -O-\overset{\overset{\displaystyle O}{\|}}{C}-CH_2-CH_3$
Ester: 5α-Pregnan-3β,11β,21-triol 3-acetate 21-propionate
Esters of steroid polyalcohols (poly >1) are denoted by means of the suffix 'ol' (with multiplying prefix), the acids (in anion form) follow, cited in alphabetical order.

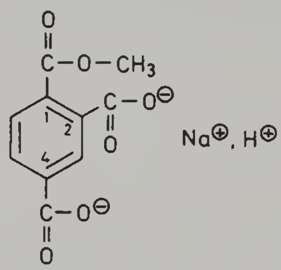
If the name of an acid ends in 'carboxylic acid', then the anion form in esters is expressed as 'carboxylate'.



322

Dimethoxanate (INN)
syst.: a) 2-(2-Dimethylaminoethoxy)ethyl 10-phenothiazine-carboxylate (IUPAC)
b) . .phenothiazin-10-carboxylate (WHO)

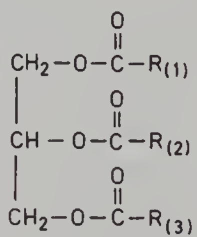
If a polycarboxylate is partially esterified and the free carboxyl groups are partly as salts, so that Na+, H+, and ester are all present, their citation in the name follows in sequence; cation, alkyl or aryl, hydrogen, anion:



323

Sodium 1-methyl hydrogen 1,2,4-benzenetricarboxylate
The locants of the unesterified free acid are retained
(but see esters as subordinate compound class)
(cf. formula 325)

In *Biochemical Names* (IUB), appropriate, trivial names of alcohols are combined with the names of acid anions in naming esters.



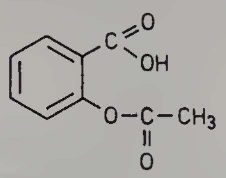
324

a) Glycerol 1,2-dipalmitate 3-stearate (IUB)
b) but: 1,2,3-Propanetriyl 1,2-dipalmitate 3-stearate (IUPAC)

Glycerol tristearate or tristearoylglycerol or tri-*O*-stearoylglycerol, but: 1,2,3-Propanetriyl tristearate ($R_1 = R_2 = R_3$).

Ester as subordinate compound class

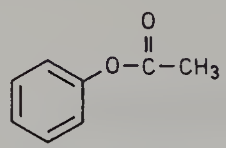
In the presence of senior compound class groups, the ester group is cited as a prefix:



325

trivial: Acetylsalicyclic acid

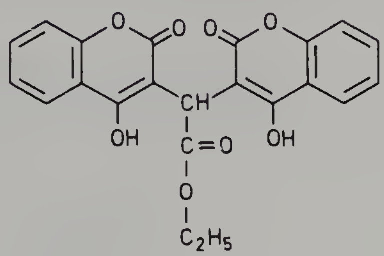
syst.: 2-Acetoxybenzoic acid



326

Phenyl acetate

Ester and lactone



327

Ethylbiscoumacetate (INN)

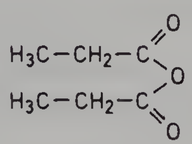
a) Ethyl ester of bis(4-hydroxy-2-oxo-2*H*-1-benzopyran-3-yl)acetic acid (WHO)

b) Ethyl bis(4-hydroxy-2-oxo-2*H*-chromen-3-yl) acetate (IUPAC)

As compound class, lactone is below ester and is therefore cited as a prefix in the name. (Steroid lactones are treated differently, cf. Spirolactones §13.12.2.)

13.15 Acid anhydrides

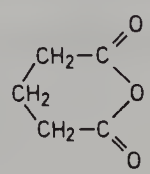
These arise from the elimination of water between two carboxyl groups of the same or of different carboxylic acids or between other similar or different acid groups of other classes of acid.



328

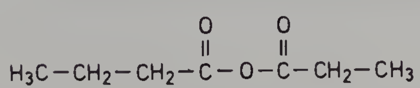
Propionic anhydride or

Propionic acid anhydride (E.P. I)



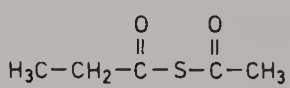
329

Glutaric (acid) anhydride



330

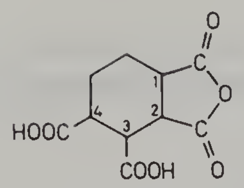
Butyric propionic anhydride



331

Acetic propionic thioanhydride

(carboxylic acids are cited alphabetically)

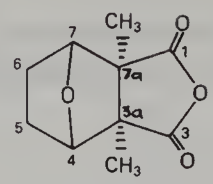


332

1,2,3,4-Cyclohexanetetracarboxylic acid 1,2-anhydride

This example from IUPAC shows clearly the additive nature of 'anhydrides'.

The principal group (suffix) is '. . .carboxylic [acid]' (cf. Chapter III 1e) As a substitutive name, the insertion of the anhydride as '3,4-oxydicarbonyl' into a 1,2-cyclohexanedicarboxylic acid would be conceivable. IUPAC does not recommend this method.



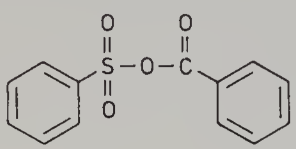
332A

Cantharidin

a) 2α,3α-Dimethyl-7-oxabicyclo[2.2.1] heptane-2,3-dicarboxylic acid anhydride

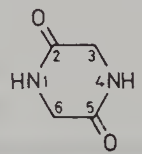
b) 4,5,6,7-Tetrahydro-3aα,7aα-dimethyl-4,7-epoxy-1,3[3a*H*,7a*H*]isobenzofurandione

(locants)



333

Benzoic benzenesulfonic anhydride



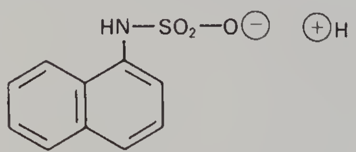
334

2,5-Piperazinedione

(also Glycinic anhydride (exception))

The numbering of piperazine is in that direction which gives the lowest possible locants to the oxo groups. The compound belongs to the heterocyclic ketones §9.2.5.

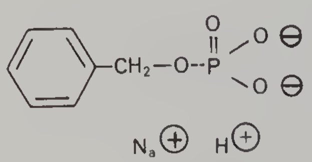
14. ORGANIC DERIVATIVES (STILL REMAINING ACIDIC) OF INORGANIC ACIDS



334A

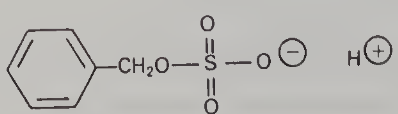
a) *N*-(1-naphthyl)sulfamidic acid

b) 1-naphthylamidosulfuric acid



334B

Sodium benzyl hydrogenphosphate

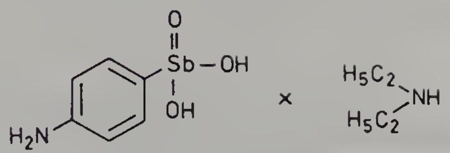


334C

Benzyl hydrogensulfate

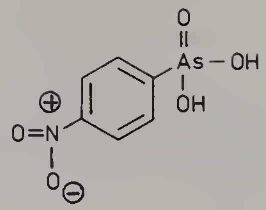
15. ACIDS

15.1. Heteroacids



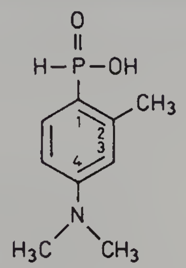
335

Stibosamine (INN)
Diethylamine *p*-aminobenzenestibonate (WHO)
(*p*-Aminobenzenestibonic acid, salt with diethylamine)
p-Aminophenylantimony dihydroxide oxide, salt with diethylamine (IUPAC)



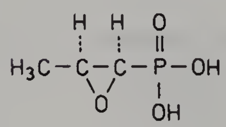
336

Nitarsone (INN)
p-Nitrobenzenearsonic acid (WHO) (subst. benzene with suffix)
p-Nitrophenylarsonic acid (IUPAC) (substituted arsonic acid)



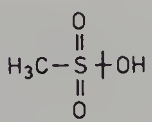
337

Toldimfos (INN)
[4-(Dimethylamino)-*o*-tolyl] phosphinic acid (WHO)



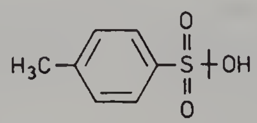
338

Fosfomycin (INN)
(-)-(1*R*,2*S*)-(1,2-Epoxypropyl) phosphonic acid



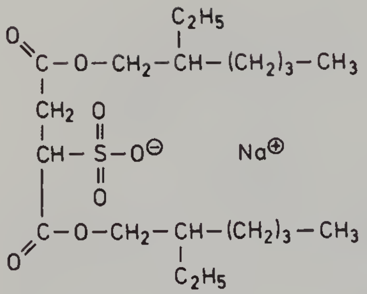
339

Methanesulfonic acid (subst. methane suffix) Radical: mesyl
Anion: methanesulfonate (not mesylate)



340

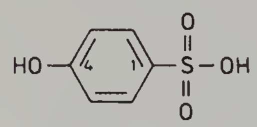
p-Toluenesulfonic acid
Radical |: tosyl
Anion: *p*-toluenesulfonate (not tosylate)



341

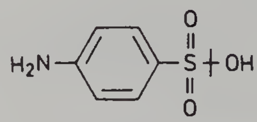
a) Sulfosuccinic acid bis(2-ethylhexyl) ester sodium salt (WHO not IUPAC)
b) Sodium 1,2-bis(2-ethylhexyloxycarbonyl)ethanesulfonate (IUPAC DAC 1979)

In IUPAC, sulfonic acid has preference as suffix over carboxylic acid ester.



342

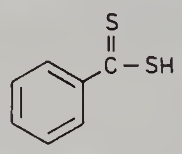
4-Hydroxybenzenesulfonic acid (IUPAC)
(also permitted: 4-phenolsulfonic acid)



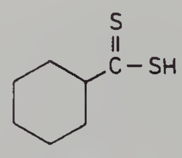
343

trivial: Sulfanilic acid
syst.: 4-Aminobenzenesulfonic acid
Radical: sulfanilyl

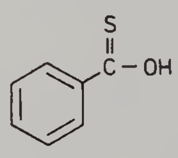
15.2. Thiocarboxylic acids



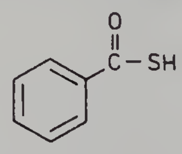
344
Dithiobenzoic acid



345
Cyclohexanecarbodithioic acid

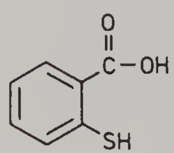


346
Thiobenzoic *O*-acid

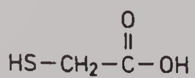


347
Thiobenzoic *S*-acid

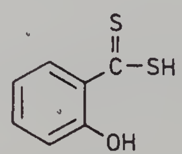
If the base component of a thioacid is the trivial name of a hydroxycarboxylic acid, the prefix thio denotes the hydroxyl group and not the carboxyl group.



348
Thiosalicylic acid
o-Mercaptobenzoic acid

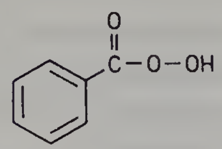


349
Thioglycolic acid
Mercaptoacetic acid

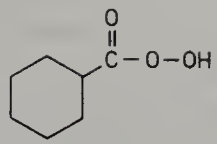


350
o-Hydroxydithiobenzoic acid
not dithiosalicylic acid

15.3 Peroxy acids (peroxycarboxylic acids)



351
semi-trivial: Perbenzoic acid
syst.: Peroxybenzoic acid



352
syst,: Cyclohexaneperoxycarboxylic acid

Names based on trivial names, or on the -oic name of the corresponding acid are formed by prefixing the name with 'peroxy-'. Systematic names of the form '. . .carboxylic acid' are changed to '. . .peroxycarboxylic acid'.

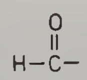
15.4 Carboxylic acids

15.4.1. Aliphatic monocarboxylic acids (examples) a) syst., b) trivial

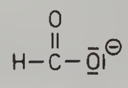
15.4.1.1. Saturated ($C_nH_{2n}O_2$)

Acid	Acyl	Anion
1) a) Methanoic acid	Methanoyl (**353**)	methanoate (**354**)
b) Formic acid	Formyl	formate
2) a) Ethanoic acid	Ethanoyl (**355**)	ethanoate
b) Acetic acid	Acetyl	acetate
3) a) Propanoic acid	Propanoyl (**356**)	propanoate
b) Propionic acid	Propionyl	propionate
4) a) Butanoic acid	Butanoyl (**357**)	butanoate
b) Butyric acid	Butyryl	butyrate
5) a) 2-Methylpropanoic acid	2-Methylpropanoyl	2-methylpropanoate
b) Isobutyric acid (**358**)	Isobutyryl (**359**)	isobutyrate
6) a) Pentanoic acid	Pentanoyl	pentanoate
b) Valeric acid	Valeryl	valerate
7) a) 3-Methylbutanoic acid	3-Methylbutanoyl	3-methylbutanoate
b) Isovaleric acid (**360**)	Isovaleryl (**361**)	isovalerate
8) a) 2,2-Dimethylpropanoic acid	2,2-Dimethylpropanoyl	2,2-dimethylpropanoate
b) Pivalic acid (**362**)	Pivaloyl (**363**)	pivalate
9) a) Dodecanoic acid	Dodecanoyl	dodecanoate
b) Lauric acid	Lauroyl	laurate
10) a) Tetradecanoic acid	Tetradecanoyl	tetradecanoate
b) Myristic acid	Myristoyl	myristate
11) a) Hexadecanoic acid	Hexadecanoyl	hexadecanoate
b) Palmitic acid	Palmitoyl	palmitate
12) a) Octadecanoic acid	Octadecanoyl	octadecanoate
b) Stearic acid	Stearoyl	stearate

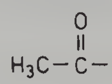
Acid	Acyl	Anion
13) a) Icosanoic acid	Icosanoyl	icosanoate
b) Arachidic acid	Arachidoyl	arachidate[9]
14) a) Docosanoic acid (**364**)	Docosanoyl	docanosoate
b) Behenic acid	Behenoyl	behenate[9]



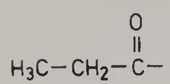
353



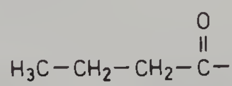
354



355



356



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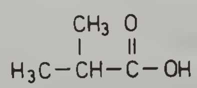

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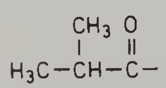

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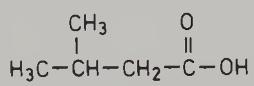

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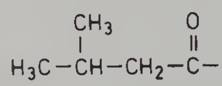

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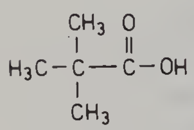

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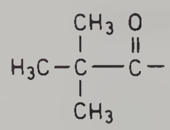

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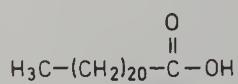


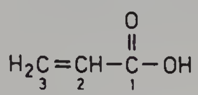
364

9 These trivial names are not permissible IUPAC names.

15.4.1.2. Unsaturated

Acid	Acyl	Anion
15) a) Propenoic acid (**365**)		propenoate
b) Acrylic acid	Acryloyl (**366**)	acrylate (**367**)
16) a) Propynoic acid (**368**)		propynoate
b) Propiolic acid	Propiolyl (**369**)	propiolate (**370**)
17) a) 2-Methyl-2-propenoic acid (**371**)		
b) Methacrylic acid	Methacryloyl (**372**)	methacrylate (**373**)
18) a) *trans*-2-Butenoic acid (**374**)		
b) Crotonic acid	Crotonoyl (**375**)	crotonate (**376**)

Acid	Acyl	Anion
19) a) *cis*-2-Butenoic acid		
b) Isocrotonic acid (**377**)	Isocrotonoyl (**378**)	isocrotonate (**379**)
20) a) *cis*-9-Octadecenoic acid		
b) Oleic acid (**380**)	Oleyl	oleate
21) a) *trans*-9-Octadecenoic acid		
b) Elaidic acid (**381**)	Elaidoyl	elaidate
22) a) *trans,trans*-2,4-Hexadienoic acid (*E,E*)-2,4-Hexadienoic acid		
b) Sorbic acid (**382**)	Sorboyl	sorbate
23) a) *cis, cis*-9,12-Octadecadienoic acid (*Z,Z*)-9,12-Octadecadienoic acid		
b) Linoleic acid (**383**)	Linoleoyl	linoleate
24) a) (*cis,cis,cis*)-9,12,15-Octadecatrienoic acid (*Z,Z,Z*)-9,12,15,-Octadecatrienoic acid		
b) Linolenic acid (**384**)	Linolenoyl	linolenate
25) a) all *Z*-5,8,11,14-Icosatetraenoic acid		
b) Arachidonic acid (**385**)[10]		



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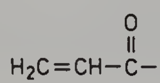

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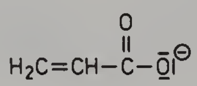

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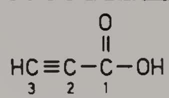

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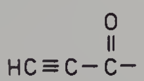

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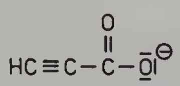

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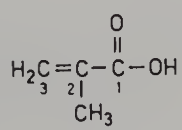

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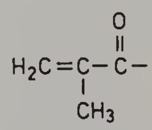


372

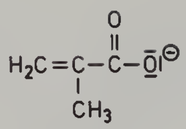
10 A special, simplified kind of numbering, chiefly used for natural fatty acids in connection with biochemical problems and dietetics, begins with the locant 1 at the highest numbered C(20) of the systematic numbered chain. Beginning with 1 at the 'wrong' end of the chain is marked by prefixing the whole name with an 'omega' (ω). The first locant in the name after the 'omega' is that for the first unsaturation reached in the new direction of numbering in the group of several isolated double-bonds. In this way the name 'ω-6-Icosatetraenoic acid' is developed. It is improved by inclusion of the number 4, signifying the sum of isolated double-bonds '4ω-6-Icosatetraenoic acid'. For the discussion in the field of fatty acids of natural origin a further simplification is introduced, which at the same time signifies another improvement. The last name gets the form (20:4ω6) and appears first as a provisorium. 'Linolenic acid' (384) is reproduced in this way by (18:3ω3).

The impression of a provisorium disappcars, if the severely reduced instructions are upvalued by two preconditions:

1. the configurations on all double-bonds are Z;
2. each group of C-atoms beginning with a double-bond, holds 3 C-atoms so, between two double-bonds only 1 CH_2-group stands.

With these preconditions, all natural scientists may handle the shortest 'names' as sure as if they were systematic names.

My thanks are due to Dr. U. Hörcher, Luwigshafen for his most kind communications.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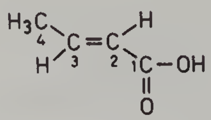
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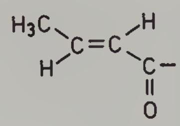
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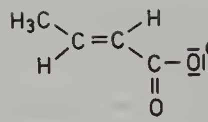
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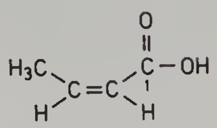
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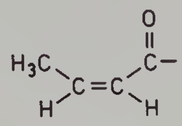
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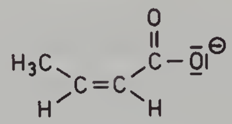
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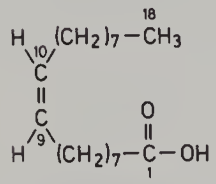
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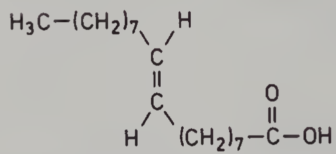
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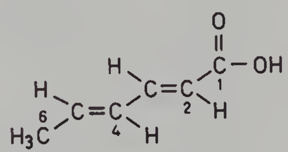
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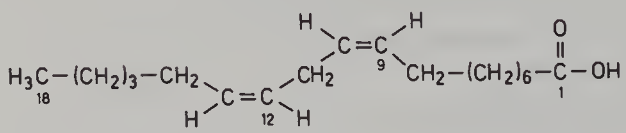
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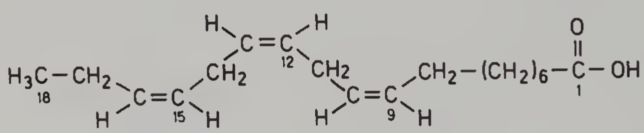
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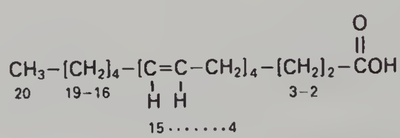

385 (20:4ω6)[10]

15.4.2. Aliphatic dicarboxylic acids (examples) a) syst., b) trivial

15.4.2.1 Saturated (general list of IUPAC permitted trivial names)

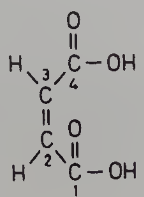
$HOOC{-}(CH_2)_n{-}COOH$ 386

Acid	Diacyl and (monoacyl)	Anions
26) a) Ethanedioic acid $n = 0$ b) Oxalic acid	Ethanedioyl Oxalyl (Oxalo)	ethanedioate oxalate (hydrogenoxalate)
27) a) Propanedioic acid $n = 1$ b) Malonic acid	Propanedioyl Malonyl (Carboxyacetyl)	propanedioate malonate (hydrogenmalonate)

Acid	Diacyl and (monoacyl)	Anions
28) a) Butanedioic acid $n = 2$ b) Succinic acid	Butanedioyl Succinyl (Carboxypropionyl)	butanedioate succinate
29) a) Pentanedioic acid $n = 3$ b) Glutaric acid	Pentanedioyl Glutaryl (4-Carboxybutyryl)	pentanedioate glutarate
30) a) Hexanedioic acid $n = 4$ b) Adipic acid	Hexanedioyl Adipoyl (5-Carboxyvaleryl)	hexanedioate adipate
31) a) Heptanedioic acid $n = 5$ b) Pimelic acid	Heptanedioyl Pimeloyl (6-Carboxyhexanoyl)	heptanedioate pimelate
32) a) Octanedioic acid $n = 6$ b) Suberic acid	Octanedioyl Suberoyl (7-Carboxyheptanoyl)	octanedioate suberate
33) a) Nonanedioic acid $n = 7$ b) Azelaic acid	Nonanedioyl Azelaoyl (8-Carboxyoctanoyl)	nonanedioate azelate (azelainate)
34) a) Decanedioic acid $n = 8$ b) Sebacic acid	Decanedioyl Sebacoyl (9-Carboxynonanoyl)	decanedioate sebacate (sebacinate)

15.4.2.2. *Unsaturated*

Acid	Diacyl and (monoacyl)	Anions
35) a) *cis*-Butenedioic acid (*Z*) b) Maleic acid (387)	 Maleoyl (388)	 maleate (hydrogenmaleate) (389)
36) a) *trans*-Butenedioic acid (*E*) b) Fumaric acid (390)	 Fumaroyl	 fumarate
37) a) *cis*-Methylbutenedioic acid (*Z*) b) Citraconic acid (391)	 Citraconoyl	 citraconate
38) a) *trans*-Methylbutenedioic acid (*E*) b) Mesaconic acid (392)	 Mesaconoyl	 mesaconate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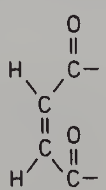
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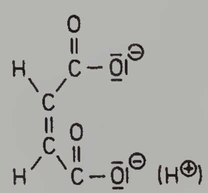
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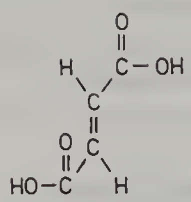

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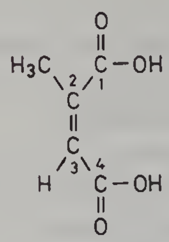

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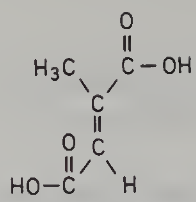
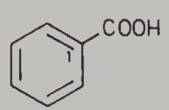


392

15.4.3. Carbocyclic carboxylic acids (examples) a) syst. b) trivial

Acid	Diacyl (and monoacyl)	Anions
39) a) Benzenecarboxylic acid		
b) Benzoic acid (**393**)	(Benzoyl)	benzoate
40) a) 1,2-Benzenedicarboxylic acid		
b) Phthalic acid (**394**)	Phthaloyl (*O*-Carboxybenzoyl)	phthalate hydrogen phthalate
41) a) 1,3-Benzenedicarboxylic acid		
b) Isophthalic acid (**395**)	Isophthaloyl	isophthalate hydrogen isophthalate
42) a) 1,4-Benzenedicarboxylic acid		
b) Terephthalic acid (**396**)	Terephthaloyl	terephthalate
43) a) 2-Napthalenecarboxylic acid		
b) 2-Naphthoic acid (**397**)	2-Napthoyl	2-naphthoate
44) a) x-Methylbenzenecarboxylic acid		
b) 2-Tcluic acid (**398**)	2-Toluoyl	σ-toluate
45) a) 2-Phenylpropanoic acid		
b) Hydratropic acid (**399**)	Hydratropoyl	hydratropate
46) a) 2-Phenylpropenoic acid		
b) Atropic acid (**400**)	Atropoyl	Atropate
47) a) *trans*-3-Phenylpropenoic acid		
b) Cinnamic acid (**401**)	Cinnamoyl	Cinnamate



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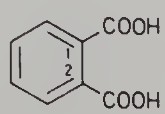

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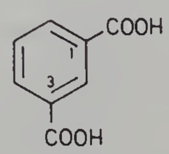

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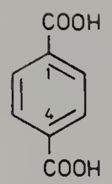

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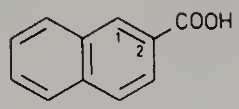

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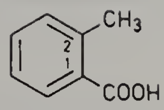

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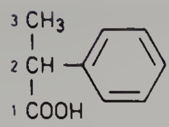

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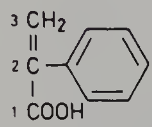

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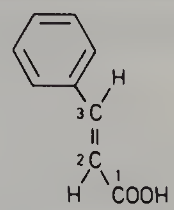
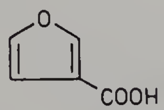


401

15.4.4. Heterocyclic carboxylic acids (examples)

48) Pyromucic acid
3-Furancarboxylic acid (**402**)
acyl: 3-Furoyl (**403**)
anion: 3-furoate (3-furancarboxylate) (**404**)



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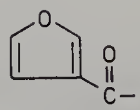

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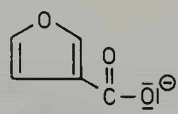
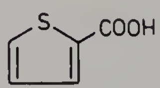


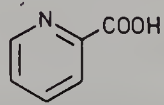
404

49) 2-Thiophenecarboxylic acid (**405**)
acyl: 2-Thenoyl (2-Thiophenecarbonyl)
anion: 2-thenoate
(2-Thiophenecarboxylate)



405

50) 2-Pyridinecarboxylic acid
Picolinic acid (**406**)



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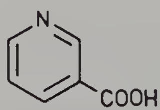
51) 3-Pyridinecarboxylic acid
Nicotinic acid (**407**)



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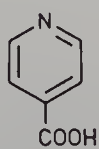
52) 4-Pyridinecarboxylic acid
Isonicotinic acid (**408**)



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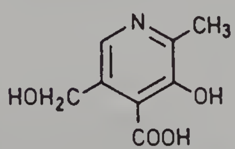
53) 3-Hydroxy-5-hydroxymethyl-2-methyl-4-pyridinecarboxylic acid
(4)-Pyridoxic acid (**409**)



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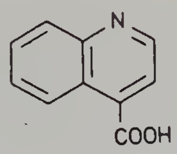
54) 4-Quinolinecarboxylic acid
cinchonic acid (**410**)



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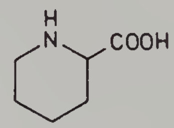
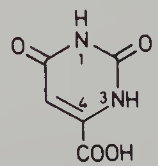
55) 2-Piperidinecarboxylic acid
Pipecolinic acid (**411**)



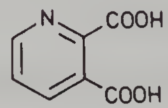
411

56) 1,2,3,6-Tetrahydro-2,6-dioxo-4-pyrimidinecarboxylic acid[13]
Orotic acid (**412**)



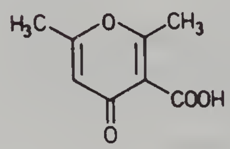
412

57) 2,3-Pyridinedicarboxylic acid
Quinolinic acid (**413**)



413

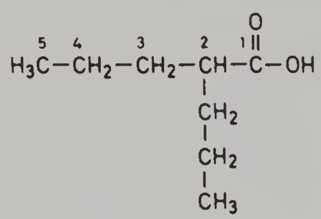
58) 2,6-Dimethyl-4-oxo-4*H*-pyrancarboxylic acid (**414**)



414

15.4.5. Special examples

15.4.5.1. Individual cases involving various chemical groups



415

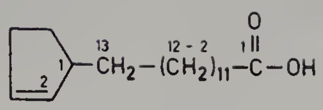
Valproic acid
2-Propylvaleric acid (WHO, IUPAC)
syst.: 2-Propylpentanoic acid (IUPAC)
A 5-C-chain acid has a 3-C-chain as a substituent.

$$\overset{11}{H_2C}=\overset{10}{CH}-\overset{9-2}{(CH_2)_8}-\overset{1}{\underset{}{C}}(=O)-OH$$

416

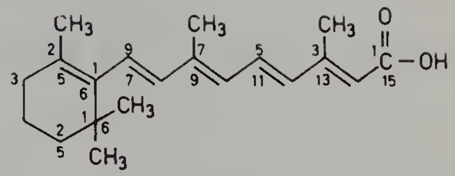
trivial: Undecylenic acid
syst.: 10-Undecenoic acid
The acid C-atom is included in the 11 C-atoms total.

13 This locant distribution, corresponding to the general IUPAC rule, is of particular importance for nucleosides, as the glycosidic N here takes the locant 1. As 'uracil-6-carboxylic acid' or as '1,2,3,4-tetrahydro-2,4-dioxo-6-pyrimidinecarboxylic acid', this N takes the locant 3. (cf. uracil §9.2.6β).



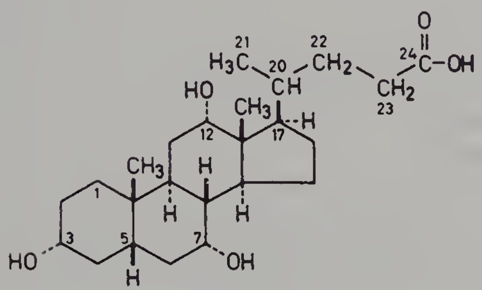
417

Chaulmoogric acid
syst.: 13-(2-Cyclopentenyl)tridecanoic acid (subst.)
2-Cyclopentenetridecanoic acid (conjunctive) (IUPAC)



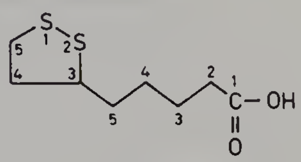
418

trivial: all-*trans* / all-(E) } -Retinoic acid (trivial locants inside/lower (cf. formula **124**, p. 166)
'Vitamin A acid', Tretinoin (INN)
syst.: 3,7-Dimethyl-9-(2,6,6-trimethyl-1-cyclohexenyl)-2,4,6,8-nonatetraenoic acid (locants outer/above)
15-Apo-β-caroten-15-oic acid



419

trivial: Cholic acid
syst.: 3α,7α,12α-Trihydroxy-5β-cholan-24-oic acid



420

trivial: α-Lipoic acid
Thioct acid
syst.: 5-(1,2-Dithiolan-3-yl)valeric acid (subst.)
1,2-Dithiolan-3-valeric acid (conjunctive)

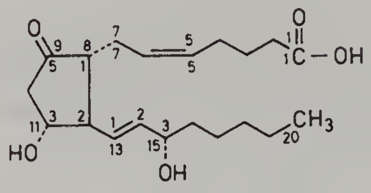
15.4.5.2. Prostaglandins

Literature: Norman A. Nelson (*J. Med. Chem.* **17**, 9[1974] 911)
Ph. Fresenius (*Ph.Ztg.* **120**, 32[1975] 1173)

The scientific nomenclature is based on the hydrocarbon prostane (see I 6, formula **201**).

From this, are derived 'prostanoic acid' and '*ent*'-prostanoic acid (inverse position of the side-chains) semi-systematic names). Other purely systematic methods dispense with the use of the trivial Prostanoic acid as an intermediate step.

One other trivial nomenclature system comprises 'prostaglandin families' (each based on different substituents on the pentane ring, and each designated by a set of roman capital letters, indicating the substituents on the pentane ring). Further subdivision is by numerals (and Greek letters where applicable) according to the steric disposition in the side-chains (a).



421

Dinoprostone (INN)
a) PGE_2 (WHO)
b) 7-[3-Hydroxy-2-(3-hydroxy-1-octenyl)-5-oxocyclopentyl]-5-heptenoic acid (inner locants) (WHO, IUPAC)
c) (5*Z*,11α,13*E*,15*S*)-11,15-Dihydroxy-9-oxoprosta-5,13-dienoic acid (outer locants) (C.A.)

Summary of prostaglandin (PG) families

A. Main divisions

Abbreviation	Substituents and unsaturated bonds in the positions of the 5 member ring					
Family	8	9	10	11	12	15
PG A		=O	10=11			OH
PG B	=12	=O			=8	OH
PG C		=O		11=12		OH
PG D		. .OH		=O		OH
PG E		=O		. .OH		OH
PG F α		. .OH		. .OH		OH
PG F β		—OH		. .OH		OH
PG G or PG H PG R		O. . . | O. . .(11)		O. . . | O. . .(9)		O—OH OH

All substituents in the table are included in the 'PG' family name (name **421a**). In systematic or semi-systematic (prostanoic acid) names, they are cited separately (names b and c). PGH and PGR are identical. PGH(PGR) is the same as PGG only in respect of the ring portion of the molecule. Additional Greek letters are used with family F, to distinguish between 9α/9β-isomers.

B Subdivision

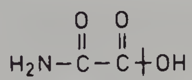
This is concerned with the two chain components of the molecule, bonded to the 5-member ring.

Subdivision number of double bonds	Double bonds in positions		
1		t 13 = 14	
2	c 5 = 6	t 13 = 14	
3	c 5 = 6	t 13 = 14	c 17 = 18

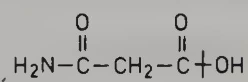
c = *cis* at the double bond, whilst t = *trans*

15.4.6. Further carboxylic acids

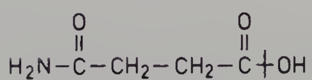
15.4.6.1. (. .amic acids and subst.) (: *radicals*)



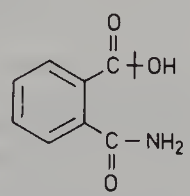
422a
Oxamic acid
: Oxamoyl



422b
Malonamic acid
: Malonamoyl



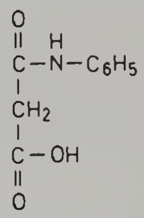
423
Succinamic acid
: Succinamoyl



424
Phthalamic acid
: Phthalamoyl

Dicarboxylic acids having a trivial name change the name to . .amic acid when one of the carboxyl groups is replaced by a carboxyamide (IUPAC)
Deviating from this rule are the . .amidic acids e.g. malonamidic acid. (Not IUPAC, two suffixes) (cf. amino acids, asparagine. glutamine (15.4.7.2.)

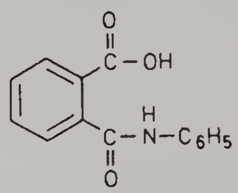
N-Phenyl substituted . .amic acids can be named as such:



425

N-Phenylmalonamic acid

Systematic designation as . . .anilic acid is however also permitted.

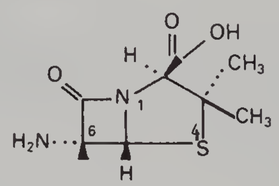


426

Phthalanilic acid

Note that this procedure is also applied in forming trivial names of quite different structures (anthranilic acid = *o*-aminobenzoic acid; carbanilic acid (see formula **428**), sulfanilic acid = *p*-aminobenzenesulfonic acid (formula **343**).

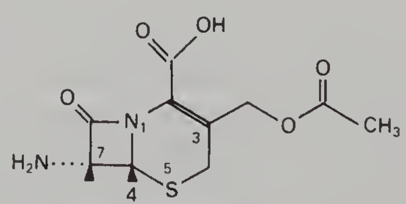
15.4.6.2. β-Lactam–Antibiotic



426A

a) trivial: 6-Aminopenicillanic acid

b) syst.: (2*S*,5*R*,6*R*)-6-Amino-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo-[3.2.0] heptane-2-carboxylic acid

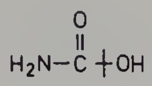


426B

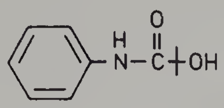
a) trivial: 7-Aminocephalosporanic acid

b) syst.: (6*R*,7*R*)-3-Acetoxymethyl-7-amino-5-thia-1-azabicyclo[4.2.0] oct-2-ene-2-carboxylic acid

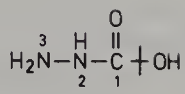
15.4.6.3. 'Carbamic acid' and derivatives; urea – carboxylic acids



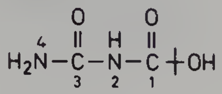
427
trivial: Carbamic acid
: Carbamoyl



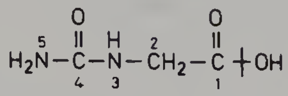
428
trivial: Carbanilic acid
: Phenylcarbamoyl



429
trivial: Carbazic acid
: Carbazoyl



430
trivial: Allophanic acid
: Allophanoyl



431
trivial: Hydantoic acid
: Hydantoyl

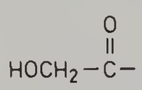
15.4.6.4 Hydroxycarboxylic acids

a) syst. b) trivial c) acyl d) anion

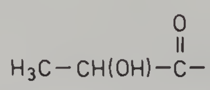
			c	d
1	a)	Hydroxyethanoic acid		
	b)	Glycolic acid	glycoloyl (**432**)	glycolate
2	a)	2-Hydroxypropanoic acid		
	b)	Lactic acid	lactoyl (**433**)	lactate
3	a)	2,3-Dihydroxypropanoic acid		
	b)	Glyceric acid	glyceroyl (**434**)	glycerate
4	a)	Hydroxypropanedioic acid		
	b)	Tartronic acid	tartronoyl (**435**) (hydroxymalonoyl)	tartronate hydrogen tartronate
5	a)	Hydroxybutanedioic acid		
	b)	Malic acid	maloyl (**436**)	malate hydrogen malate
6	a)	2,3-Dihydroxybutanedioic acid		
	b)	Tartaric acid (. . . D- or L- or meso) Tartaric acid (DL)	tartaroyl (**437**)	tartrate hydrogen tartrate
7	a)	3-Hydroxy-2-phenylpropanoic acid		
	b)	Tropic acid	tropoyl (**438**)	tropate
8	a)	2-Hydroxy-2,2-diphenylethanoic acid		
	b)	Benzilic acid	benziloyl (**439**)	benzilate

		c	d
9	a) *o*-Hydroxybenzoic acid		
	b) Salicylic acid	salicyloyl (**440**)	salicylate
10	a) 2-Hydroxy-1,2,3-propanetricarboxylic acid		
	b) Citric acid	2-Hydroxy-1,2,3-propanetricarbonyl (**441**)	citrate hydrogen citrate dihydrogen citrate
11	a) 2-Phenylglycolic acid	2-Phenylglycoloyl	mandelate
	b) Mandelic acid (D, L, DL) (**442**)		

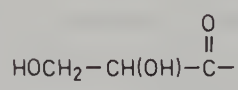
Carbamic acid, the monoamide of carbonic acid, is cited on p. 217 with the other trivial names.



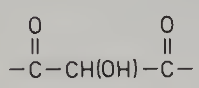
432



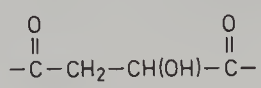
433



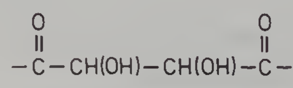
434



435



436



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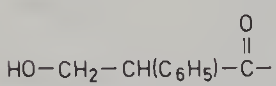

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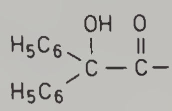

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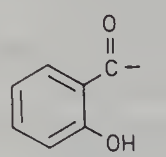

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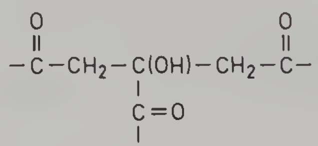

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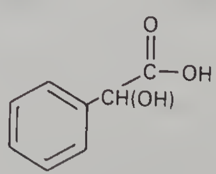
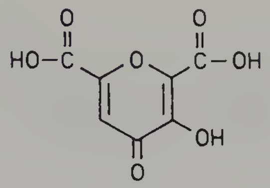


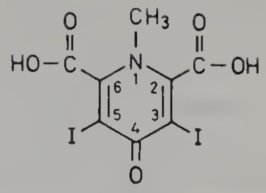
442

15.4.6.4. Oxocarboxylic acids



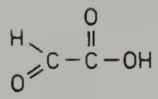
442a

Meconic acid
3-Hydroxy-4-oxo-4*H*-pyran-2,6-dicarboxylic acid



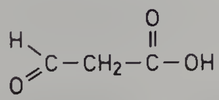
443

1,4-Dihydro-3,5-diiodo-1-methyl-4-oxo-2,6-pyridinecarboxylic acid
(di-Na salt: sodium iodomethamate)



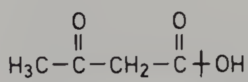
444

trivial: Glyoxylic acid
syst.: 2-Oxoacetic acid



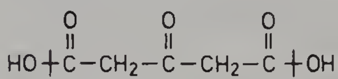
445

3-Oxopropionic acid
The oxo substituent can be in a terminal or mid-position (e.g. formula 449)
also: Malonaldehydic acid (exception)
The name is permissible even though it conflicts with the principle that, of two functional groups, only the principal group can appear as the suffix.



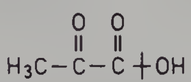
446

Acetoacetic acid
: Acetoacetyl



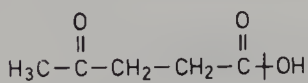
447

Acetonedicarboxylic acid
3-Oxoglutaric acid
: 3-Oxopentanedioyl



448

Pyrotartaric acid (obsolete)
Pyruvic acid (S. IUPAC C416.3)
2-Oxopropanoic acid



449

Laevulinic acid
4-Oxovaleric acid
4-Oxopentanoic acid
: Laevulinoyl

15.4.7. α- and β-Amino acids

15.4.7.1. Aminocarboxylic acids a) semi-trivial b) trivial

Names: a) syst. b) trivial			Symbol	Biochem	Acyl (R. .CO–)	Formula of the acid
1	a)	2-Aminopropionic acid				
	b)	Alanine	Ala		alanyl	(450)
2	a)	2-Amino-5-guanidino-valeric acid				
	b)	Arginine	Arg		arginyl	(451)
3	a)	2-Amino-3-mercapto-propionic acid				
	b)	Cysteine	Cys		cysteinyl	(452)
					hemi cystyl(-S. . .CO-)	
4	a)	2-Amino-3-(3,4-dihydroxy-phenyl)propionic acid		3,4-Dihydroxy-phenylalanine		
	b)	Dopa				(453)
5	a)	Aminoacetic acid				
	b)	Glycine	Gly		glycyl	(454)
6	a)	α-Amino-1*H*-imidazole-4-propionic acid		1*H*-Imidazole-4-alanine		
	b)	Histidine	His		histidyl	(455)
7	a)	2-Amino-3-methyl-valeric acid				
	b)	Isoleucine	Ile		isoleucyl	(456)
8	a)	2-Amino-4-methyl-valeric acid				
	b)	Leucine	Leu		leucyl	(457)
9	a)	2,6-Diaminohexanoic acid				
	b)	Lysine	Lys		lysyl	(458)
10	a)	2-Amino-4-(methylthio) butyric acid				
	b)	Methionine	Met		methionyl	(459)
11	a)	2,5-Diaminovaleric acid		5-Aminonorvaline[14]		
	b)	Ornithine	Orn		ornithyl	(460)
12	a)	2-Amino-3-phenylprop-ionic acid				
	b)	Phenylalanin	Phe		phenyl-alanyl	(461)

14 Norvaline as a trivial name for 2-aminopentanoic acid (and likewise norleucine for 2-amino-hexanoic acid) is no longer recommended by IUPAC–IUB (*Pure and App. Chem.* 56, 5,595 [1984]), as this does not accord with the established sense in which the prefix 'nor' is used, (= demethyl; $-CH_2$). (cf. Chapter III 6.3).

Names:	a) syst.	b) trivial	Symbol	Biochem.	Acyl (R. .CO–)	Formula of the acid
13	a)	5-Oxo-2-pyrrolidine-carboxylic acid (Pidolinic acid INN)		5-Oxoproline (also WHO) 5-Pyrrolidone carboxylic acid		
	b)	Pyroglutamic acid	Glp		pyroglutamyl	(462)
14	a)	2-Pyrrolidinecarboxylic acid				
	b)	Proline	Pro		prolyl	(463)
15	a)	2-Amino-3-hydroxy-propionic acid				
	b)	Serine	Ser		seryl	(464)
16	a)	2-Amino-3-hydroxybutyric acid				
	b)	Threonine	Thr		threonyl	(465)
17	a)	*O*[4]-(4-Hydroxyphenyl)-tyrosine		4-(4-hydroxy-phenoxy) phenylalanine		
	b)	Thyronine			thyronyl	(466)
18	a)	2-Amino-3-(3-indolyl)-propionic acid		α-Amino-1*H*-indole-3-propionic acid		
	b)	Tryptophan	Trp		tryptophyl	(467)
19	a)	2-Amino-3-(4-hydroxy-phenyl)-propionic acid		3-(4-Hydroxy-phenyl)alanine		
	b)	Tyrosine	Tyr		tyrosyl	(468)
20	a)	2-Amino-3-methylbutyric acid				
	b)	Valine	Val		valyl	(469)

$$H_3C-CH(NH_2)-COOH$$

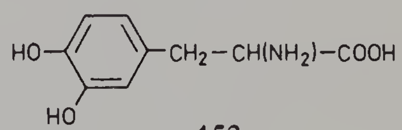
450

$$H_2N-\underset{\underset{NH}{\|}}{C}-\overset{H}{N}-CH_2-CH_2-CH_2-CH(NH_2)-COOH$$

451

$$HS-CH_2-CH(NH_2)-COOH$$

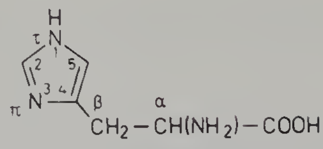
452



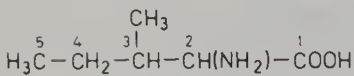
453

H_2N-CH_2-COOH

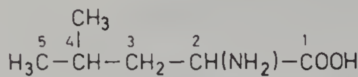
454



455[15]



456



457

$H_2N-\underset{\varepsilon}{\overset{6}{CH_2}}-\underset{\delta}{\overset{5}{CH_2}}-\underset{\gamma}{\overset{4}{CH_2}}-\underset{\beta}{\overset{3}{CH_2}}-\underset{\alpha}{\overset{2}{CH(NH_2)}}-\overset{1}{COOH}$

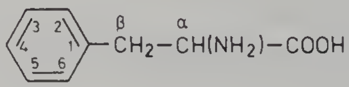
458

$\overset{6}{H_3C}-\overset{5}{S}-\overset{4}{CH_2}-\overset{3}{CH_2}-\overset{2}{CH(NH_2)}-\overset{1}{COOH}$

459

$H_2N-\overset{5}{CH_2}-\overset{4}{CH_2}-\overset{3}{CH_2}-\overset{2}{CH(NH_2)}-\overset{1}{COOH}$

460



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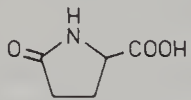

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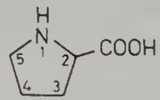


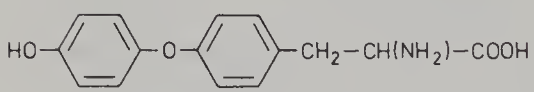
463

$HO-CH_2-CH(NH_2)-COOH$

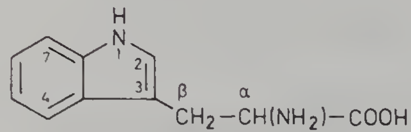
464

$H_3C-CH(OH)-CH(NH_2)-COOH$

465



466



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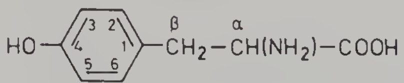
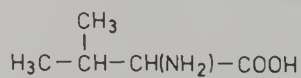


468



469

15 π (pi) for 'pros' (near) / τ (tau) for 'tele' (distant) } with respect to the position of the side chain.

15.4.7.2. Aminodicarboxylic acids and derivatives a) semi-trivial, b) trivial

			Symbol		Acyl
21	a)	2-Aminosuccinic acid	Asp	(470)	Aspartoyl
	b)	Aspartic acid		(470α/β)	α-/β-Aspartyl
22	a)	2-Aminosuccinamic acid	Asn	(471)	Asparaginyl
	b)	Asparagine	Asp $\vert$ NH_2		
23	a)	2-Aminoglutaric acid	Glu	(472)	Glutamoyl
	b)	Glutamic acid		(472α/β)	α-/γ-Glutamyl
24	a)	2-Aminoglutaramic acid	Gln	(473)	Glutaminyl
	b)	Glutamine	Glu $\vert$ NH_2		

$$HO+\overset{O}{\overset{\|}{C}}-CH_2-CH(NH_2)-\overset{O}{\overset{\|}{C}}+OH$$

470

$$HOOC-\overset{\beta}{CH_2}-\overset{\alpha}{CH}(NH_2)-\overset{O}{\overset{\|}{C}}-$$

470α

$$-\overset{O}{\overset{\|}{C}}-\overset{\beta}{CH_2}-\overset{\alpha}{CH}(NH_2)-COOH$$

470β

$$H_2N-\overset{O}{\overset{\|}{C}}-CH_2-CH(NH_2)-\overset{O}{\overset{\|}{C}}+OH$$

471

$$HO+\overset{O}{\overset{\|}{C}}-CH_2-CH_2-CH(NH_2)-\overset{O}{\overset{\|}{C}}+OH$$

472

$$HOOC-\overset{\gamma}{CH_2}-CH_2-\overset{\alpha}{CH}(NH_2)-\overset{O}{\overset{\|}{C}}-$$

472α

$$-\overset{O}{\overset{\|}{C}}-\overset{\gamma}{CH_2}-CH_2-\overset{\alpha}{CH}(NH_2)-COOH$$

472β

$$H_2N-\overset{O}{\overset{\|}{C}}-CH_2-CH_2-CH(NH_2)-\overset{O}{\overset{\|}{C}}+OH$$

473

15.4.7.3. α-Amino acid ions

e.g.

$$R-CH(NH_2)-\overset{O}{\overset{\|}{C}}-O^{\ominus} \quad \text{a) anion}$$

($R = CH_3$) Alanine

$$R-CH(NH_3)^{\oplus}-\overset{O}{\overset{\|}{C}}-OH \quad \text{b) cation}$$

($R = H$) Glycine

$$R-CH(NH_3)^{\oplus}-\overset{O}{\overset{\|}{C}}-O^{\ominus} \quad \text{c) amphion}$$

474

SALTS

a) with bases

$$H_3C-CH(NH_2)-\overset{\overset{\displaystyle O}{\|}}{C}-O^{\ominus}\ \ Na^{\oplus}$$

475
Sodium alaninate

b) with acids

$$H_3\overset{\oplus}{N}-CH_2-\overset{\overset{\displaystyle O}{\|}}{C}-OH\ \ Cl^{\ominus}$$

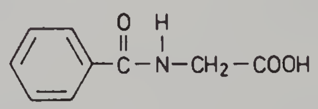
476
Glycine hydrochloride
Glycinium chloride

ESTERS

$$H_5C_2-O-\overset{\overset{\displaystyle O}{\|}}{C}-(CH_2)_2-CH(NH_2)-\overset{\overset{\displaystyle O}{\|}}{C}-O-C_2H_5$$

477
Diethyl glutamate

15.4.7.4. Acylated amino acids



478
trivial: Hippuric acid
syst.: *N*-Benzoylglycine
the acid radical is called Hippuroyl

15.4.7.5. Peptides

In defining a peptide formula with the help of the three-letter symbols, its α-NH_2-group is situated on the left of the symbol or its structural formula, the carbonyl or carboxyl group being on the right side:

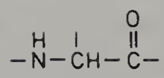
$$-\mathrm{Ala}-:\quad -\overset{\displaystyle H}{N}-\overset{\overset{\displaystyle CH_3}{|}}{CH}-\overset{\overset{\displaystyle O}{\|}}{C}-$$

If arrows are used in place of hyphens, the amino group is at the point of the inward pointing arrow, the carboxyl group at the tail of the outward pointing arrow:

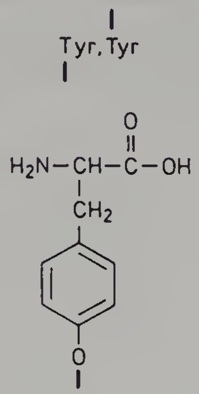
$$\rightarrow\mathrm{Ala}\rightarrow:\quad -\overset{\displaystyle H}{N}-\overset{\overset{\displaystyle CH_3}{|}}{CH}-\overset{\overset{\displaystyle O}{\|}}{C}-$$

This is specially significant with cyclic peptides, where, if the direction in which arrow 1 is drawn changes from left to right, then arrow 2 must change from right to left.

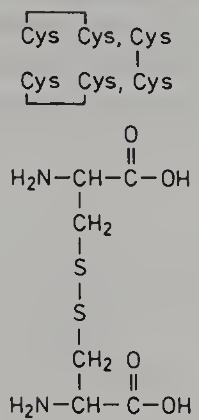
The three-letter symbol therefore is always in the horizontal plane of the atomic symbol



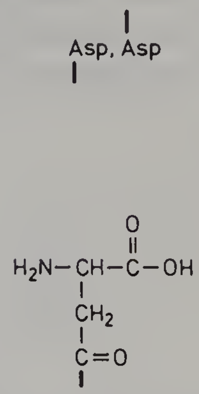
the other parts of an α-amino acid lie in the vertical plane. That means, for example:



479

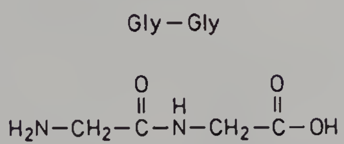


480

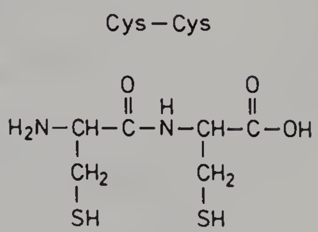


481

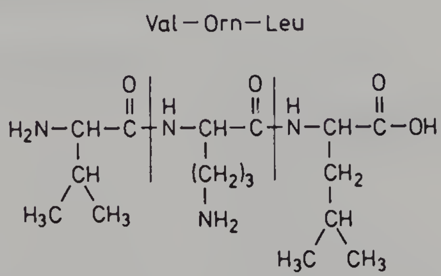
(The thickly drawn lines merely serve to improve clarity on this aspect.) In contrast the following signify as shown:



482



483



484

15.4.7.6. Configuration at the α-C

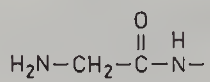
The names given in the table give no consideration to this configuration, the formulae are given as racemates.

In a racemate formula expressly citing the α-C as inactive, the name should have the prefixes [DL] or (±).

In dealing with the amino acid as an enantiomer from a protein, the L-configuration is assumed and the L-prefix is not required. A D-configuration must always be cited.

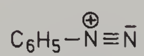
To avoid mixing up configuration indications, the index relevant to the amino acid can be given 's' (Serine), for example $\mathrm{L_s}$. The relevant prefix to the highest numbered as-C of the carbohydrate takes the index 'g' (glyceraldehyde), e.g. $\mathrm{D_s}$. (Instead of indexes g and s, G and S can be used.) An α-L configuration in an amino corresponds, for the most part, to the *S*-configuration of the sequence rules. (Exceptions e.g. L-Cystine and L-Cysteine.)

Radicals

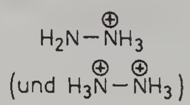


485
Glycylamino

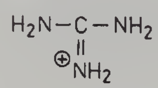
16. CATIONS
(cf. Chapter III formulae 101–109, 2.2.2. and §§8.2.1., 8.3.1.)



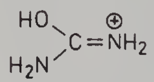
486
Diazonium



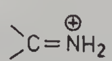
487
Hydrazinium



488
Guanidinium



489
Uronium

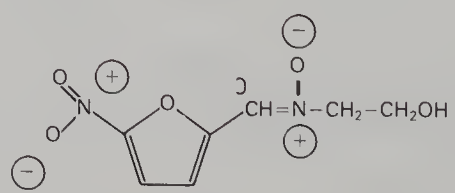


490
Iminium

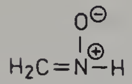
17. APPENDIX: ZWITTERIONS

1. Nitrones

a) Compound class



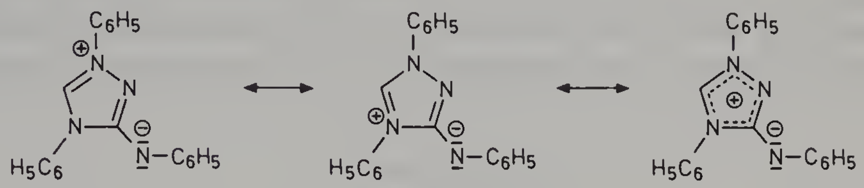
491
Nifuratrone (INN)
N-(2-Hydroxyethyl)-α-(5-nitro-2-furyl)nitrone
(WHO, not IUPAC)
The basic nitrone structure is



491A

Names are formed as substituted nitrone
or as N-oxide of an azomethine (Schiffs base)
2-[(5-Nitrofurfurylidene)amino] ethanol *N*-oxide
(IUPAC)
Schiffs base as prefix, OH as principal group

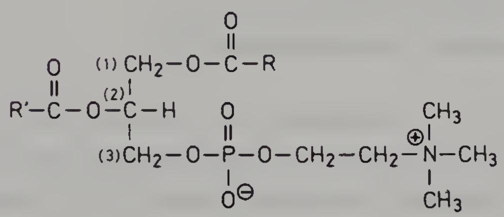
b) Trivial name (reagent with HNO)



492

N-[1,4-Diphenyl-3-(1,2,4-triazolio)] anilide (IUPAC)

2. Lecithins

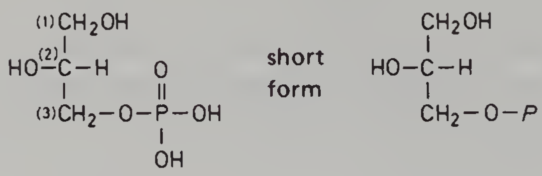


493

pharm.: Lecithin (formula shows α-)
R ≢ R' (In natural products, the alkyl- etc.
radicals are most important)

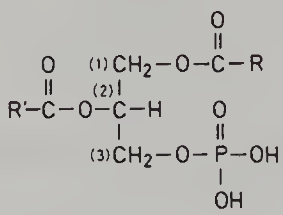
Radical	corresponding	carboxylic acid
$C_{15}H_{31}$		Palmitic acid
$C_{17}H_{35}$		Stearic acid
$C_{17}H_{33}$		Oleic acid
$C_{17}H_{31}$		Linolic acid
$C_{17}H_{29}$		Linolenic acid
$C_{19}H_{31}$		Icosatetraenoic acid (Arachidonic acid)

For lecithin nomenclature, the so-called stereospecific numbering '*sn*' of the glycerol part of the molecule is essential. In contrast to free 1,2,3-propanetriol, which has no asymmetric centre, the C-2 of the lecithins becomes a chiral centre through non-identical esterification of C-3 and C-1. An agreed form of numbering is here prescribed in order for unambiguous descriptions to be made. If in the Fischer projection, (vertical arrangement) the OH group on the C-2 is on the left side of the chain, then the formula demonstrates the L-3-glycerol phosphoric acid (1-3-glycerol phosphate[17]) (ident: D-glycerol-1 phosphate).



494a **494b**

This numbering starts from the '*sn*' in the lecithin nomenclature. In this, the trivial name 'phosphatidic acid' is used for the ester of 1 glycerol, 2 fatty acids and 1 phosphoric acid, which therefore contains 2 acid equivalents (from the phosphoric acid) left unesterified:

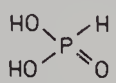


495
Phosphatidic acid
(Formula: 3-Phosphatidic acid
obsolete: α-Phosphatidic acid)

If the substituents of C-2 and C-3 are exchanged, 2- (formerly β-)phosphatidic acid is produced (from which: β-lecithin). 1 phosphatidic acid esterified with 1 choline gives rise to the pharmaceutical product commonly known as 'lecithin' but for which, as the group name, is recommended 3-sn-phosphatidylcholine. The systematic name for the general form is:

1,2-Diacyl-*sn*-glycero-3-phosphocholine

The multiplicity of naming procedures for glycerolphosphoric acid merits some clarification. 'Phosphono' is the name for the $H_2O_3P\cdot$ radical



496

17 Lit.: Hoppe-Seyler's *Z. Physiol. Chem.* 350, 279 (1969); 358, 599 (1977); 358, 617 (1977) (IUPAC–IUB).
syn. *sn*-Glycerol 3-dihydrogenphosphate
sn-Glycerol-3-phosphate
sn-Glycero-3-phosphate
biochem;
3-*O*-phosphono-*sn*-glycerol
3-Phospho-*sn*-glycerol
sn-Glycerol-3-*P*

as substituent in organic compounds. 'Phospho' is an abbreviation of 'phosphono' as substituent at O. *P* is a common (in biochemistry) abbreviation for the $H_2O_3P\cdot$ radical, for use in formulae. The ester formation with glycerol is applied as with carbohydrates and the acyl radical appears in the names as an O-substituent on the glycerol, whereby the express reference to the O may also be omitted.

V

Polyols, carbohydrates, cyclitols

1. OPEN-CHAIN POLYOLS WITH SIMPLE OXO-FUNCTIONS OR O-HETEROCYCLES (HEMIACETALS), $C_nH_{2n}O_n$

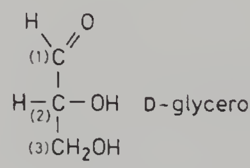
(Lit.: *Eur. J. Biochem.* 21 (1971) 455 (IUPAC–IUB)

1.1. Aldoses (aldehyde sugars)

Function end-positioned

Systematic and trivial names of aldehyde sugars (monsaccharides) have the ending . . .ose, (NB not: glycerose)

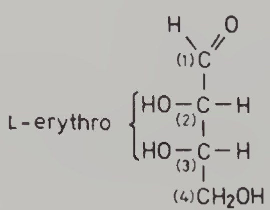
1.1.1. Trioses (3 C-atoms)

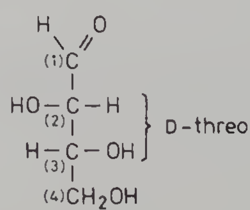


1

D-Glyceraldehyde

1.1.2. Tetroses (4 C-atoms)





2

L-Erythrose

L-*erythro*-Tetrose

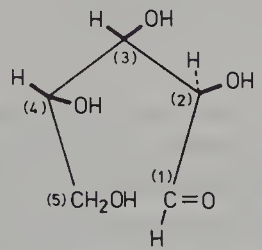
3

D-Threose

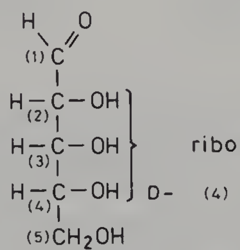
D-*threo*-Tetrose

Configuration designations D- and L- are according to the position of the OH-group on the asymmetric C-atom furthest from C-atom 1 of the chain (i.e. the asymmetric C atom bearing the highest locant = the reference C-atom). The D-configuration prefix is used if, in the Fischer projection, the OH-group is on the right side; if it is on the left, then L- is used. The relative positions of all the OH-groups together is expressed in systematic names, by means of special stereoprefixes which (in italics) come after the configuration-prefix (in small capital letters).

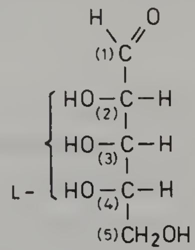
1.1.3. Pentoses (5 C-atoms)



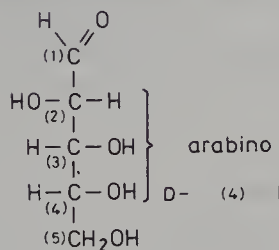
4
D-Ribose



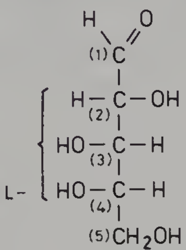
5
D-Ribose (Rib)[1]



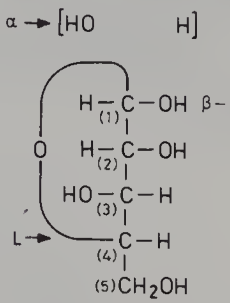
6
L-Ribose
L-*ribo*-Pentose



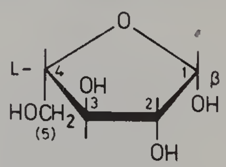
7
D-Arabinose (Ara)[1]



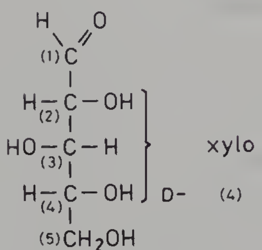
8
L-Arabinose
L-*arabino*-Pentose



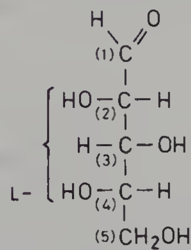
9
β-L-Arabinofuranose



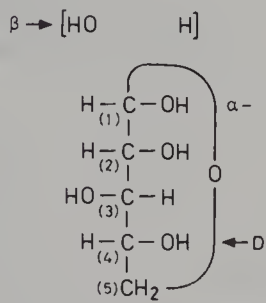
10
Haworth-formula
(cf. 15)



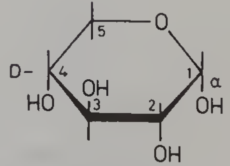
11
D-Xylose (Xyl)[1]
D-*xylo*-Pentose



12
L-Xylose

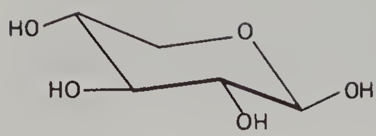


13
α-D-Xylopyranose

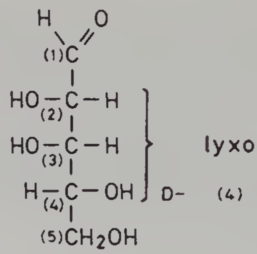


14
Haworth-formula
(cf. 13) (α–D)

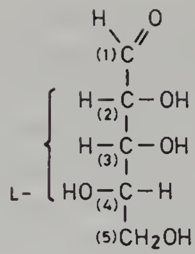
1 Three-letter symbols for monosaccharides are used only in indicating the monomers in macromolecules, and not for the monosaccharide itself.



15
β-Xylopyranose
(formal conformation)



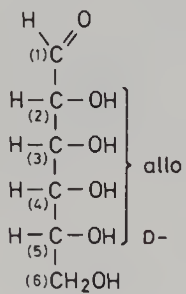
16
D-Lyxose
D-*lyxo*-Pentose



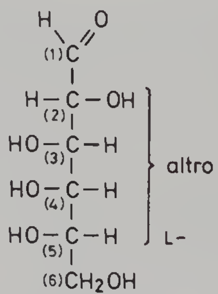
16a
L-Lyxose

In the hemiacetal formula **13** (. . .pyranose) and **15** (. .furanose) the C-atom 1 additionally is asymmetric. For steric designation of the two isomeric forms (anomers) the Greek letters α and β are used. The anomeric OH-group is in α-position, if (in the Fischer projection) it is on the same side as the D-OH-group. It is in the β position if on the opposite side. In the Haworth formula **14** on the other hand, the OH-groups 1 and 4 are on the same side of the ring-plane, in formula **16** the OH-group 1 is below the ring-plane, the furan oxygen atom is in the ring-plane. In names of the hemiacetal form, based on the size of the heterocycle, the 'stereoprefix' is written not as a separate prefix in italics, but joined to the stem-name as one word.

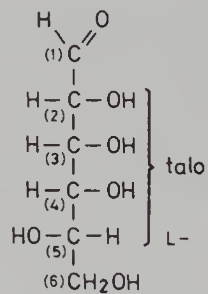
1.1.4. Hexoses (6 C-atoms)



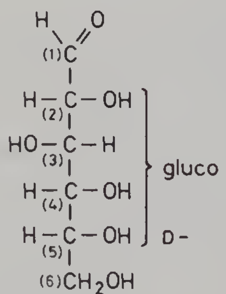
17
D-Allose



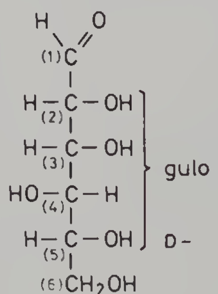
18
L-Altrose



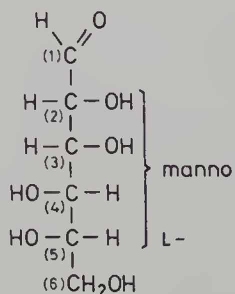
19
L-Talose



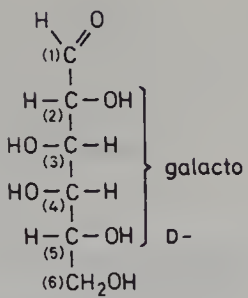
20
D-Glucose, D-*gluco*-Hexose (Glc)[1]



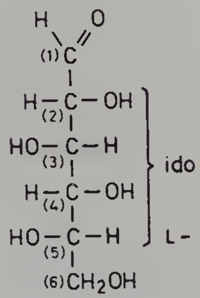
21
D-Gulose



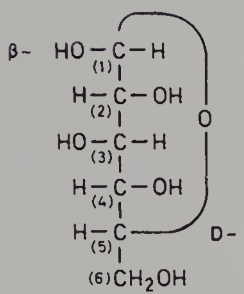
22
L-Mannose (Man)[1]
L-*manno*-Hexose



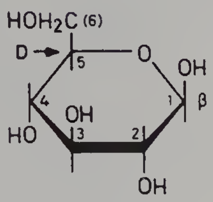
23
D-Galactose, D-*galacto*-Hexose (Gal)[1]



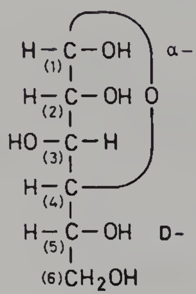
24
L-Idose



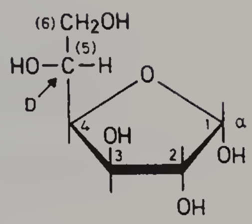
25a
β-D-Glucopyranose
Fischer[2]-Projection



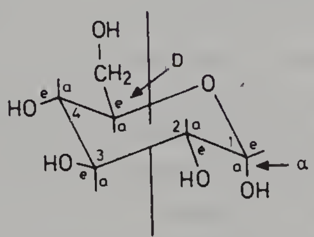
25b
β-D-Glucopyranose
Haworth-Formula



26a
α-D-Glucofuranose
Fischer-Projection



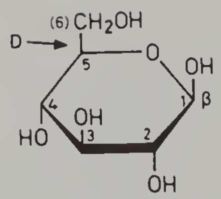
26b
α-D-Glucofuranose
Haworth-Formula



27
a conformation formula (chain)
(cf. Dextrose, α-D-Glucopyranose E.P.)
syn. Dextrose

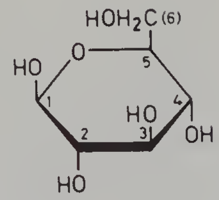
2 Fischer-Tollens.

mirror



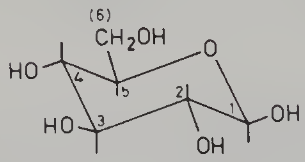
28

Haworth-Formula
β-D-Glucose
conformation-formula

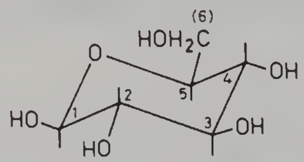


29

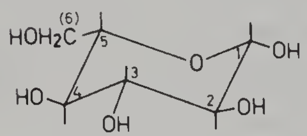
Haworth-Formula
β-L-Glucose
conformation-formula



Mirror



31



32

β-L-Glucose

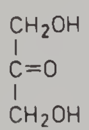
1.1.5. Naming sugars with a greater number of C-atoms

> 6 C-atoms in the chain, > 4 asymmetric C-atoms

The C-chain is numbered in the normal way with the aldehyde group as (1). The C-atoms from (2) onwards are divided into groups of 4 C-atoms finishing with a grouping [which may be] less than 4. Each grouping takes its own stereoprefix. In the complete name, these are cited one after another beginning with the highest numbered grouping, then the numerical prefix for the number of C-atoms in the chain, with the ending . .ose. In Anglo-American literature the stereoprefixes named in 1.1.2. and 1.1.4. are used also in cases where there is a row of asymmetric C-atoms interrupted by non-asymmetric groups (see formula 71 p. 242).

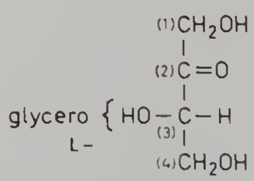
1.2. Ketoses (monosaccharides)

Mid-positioned function.



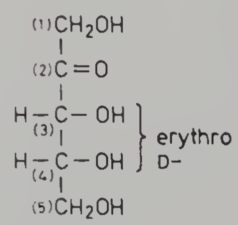
33

a) 1,3-Dihydroxy-2-propanone
b) Dihydroxyacetone
c) Glycerone (biochem.)



34

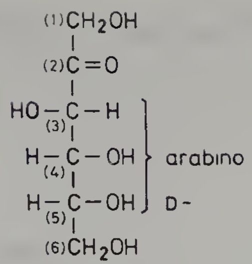
L-*glycero*-2-Tetrulose



35

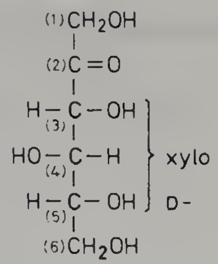
D-Ribulose
D-*erythro*-2-Pentulose

The smallest ketose is named systematically by the usual rules of organic nomenclature.



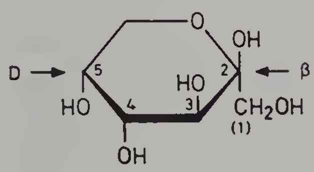
36

D-Fructose (Fru)[1]
D-*arabino*-2-Hexulose
(see also laevulose (cf. p. 128)
β-D-Fructopyranose E.P.)



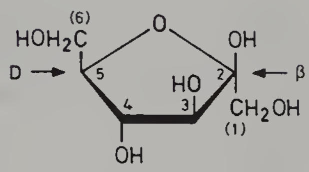
37

D-Sorbose
D-*xylo*-2-Hexulose



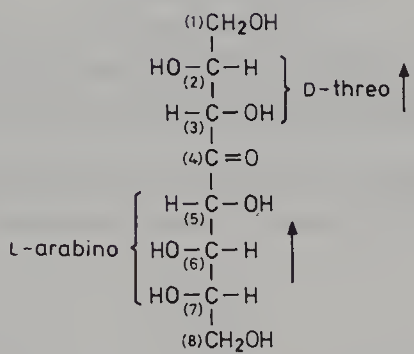
38

β-D-Fructopyranose



39

β-D-Fructofuranose



40

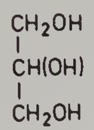
L-*arabino*-D-*threo*-4-Octulose

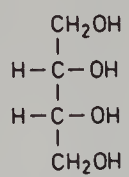
The stereoprefixes are established from the highest numbered chain-member in the direction towards the C-atom (1) and cited in the name. If there is an odd number of C-atoms in the chain and the oxo group is on the middle C-atom of the chain, the stereoprefixes are cited in alphabetical order. In the case of identical stereoprefixes, D- takes precedence over L-.

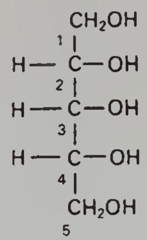
1.3. Derivatives of monosaccharides

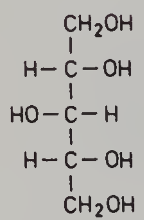
Derivatives of monosaccharides which could have been derived from configuratively different parent compounds the designation with the earliest name in alphabetical order takes preference (e.g. gluco before gulo). In the case of identical parent names, D- comes before L-. In other cases (e.g. alphabetical order of substituents) the solution is preferred which involves the lowest alteration of locants.

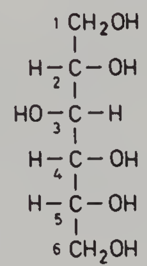
2.[3] REDUCTION, POLYOLS WITHOUT AN OXO GROUP $C_nH_{2n}O_2$, ALDITOLS

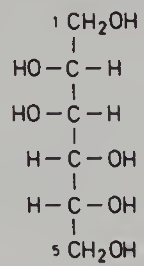

41
Glycerol
(see also IV. 7.2.2.)


42
Erythritol
(cf. Eritrityl tetranitrate INN)


43
trivial: Adonitol
meso-Ribitol

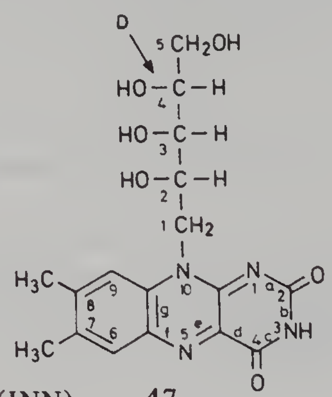

44
Xylitol
meso-Xylitol


45
D-Glucitol
trivial: Sorbitol


46
D-Mannitol (Mannite)
(cf. Mannitol hexanitrate INN)

With the exception of glycerol, polyalcohols take the ending . .itol instead of . .ose of the aldoses or ketoses. The ending follows after the stem of the stereoprefix forming one word with it.

The polyols allitol and galactitol also require the meso-prefix. Threitol and arabinitol for example still have the D- or L- prefix, ('lyxitol' is not used, cf. §1.3. p. 235).



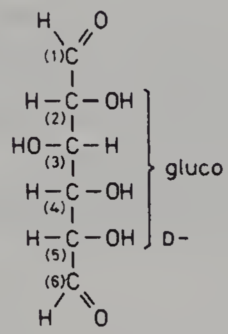
trivial: Riboflavin (INN) **47**
Vitamin B_2, Lactoflavin
syst.: a) 7,8-Dimethyl-10-(D-ribit-1-yl)-iso-alloxazine (WHO)
Ring-system: Benzo[*g*] pteridine
b) 7,8-Dimethyl-10-(D-ribo-2,3,4,5-tetrahydroxypentyl)isoalloxazine
c) 7,8-Dimethyl-10-(D-ribo-2,3,4,5-tetrahydroxypentyl)-3*H*,10*H*-benzo[*g*] pteridine-2,4-dione (IUPAC)
d) 7,8-Dimethyl-10-(1-D-ribityl)-2,4(3*H*,10*H*)benzo[*g*] pteridinedione

3 See Appendix §8.

In the context of carbohydrate nomenclature, there is no IUPAC rule allowing for the derivation of the 'ribityl' group (formula **47**). There is, however, authorization for established trivial names for materials of biochemical significance.

3. OXIDATION

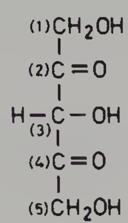
3.1. Dialdoses



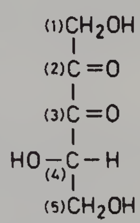
48
D-*gluco*-Hexodialdose

If the primary alcohol group of an aldose is oxidized to an aldehyde, a dialdose is produced. The name is formed by . .dialdose being added after the stem designation for the number of C-atoms in the chain. The stereoprefix is put in front of the name, and it is preceded by a configuration-prefix insofar as this is required. 'Gluco' is preferred to 'gulo' (alphabetical order).

3.2. Diketoses



49
meso-2,4-Pentodiulose

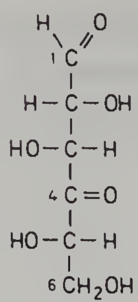


50
L-*glycero*-2,3-Pentodiulose

Diketoses have the systematic ending '. .diulose'. The oxo group locants are given in the context of the C-chain numbering.

3.3. Aldoketoses

The compounds corresponding to this group designation take the ending . . .osulose. Aldehyde is senior to ketone, and in names based on compound classes the construction . . .oxo. . .al is used (e.g. 4-oxohexanal).



51

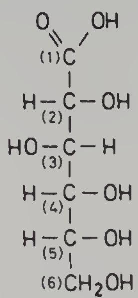
(α) L-*glycero*-L-*threo*-4-Hexosulose (IUPAC)
C.A. require only one stereoprefix by virtue of bringing together all chiral centres without consideration of any intermediate achiral C-atoms. This gives rise to
(β) L-*arabino*-4-Hexosulose
2-Hexosuloses were formerly designated as 'osones'.

3.4. Carboxylic acids

3.4.1. Monocarboxylic acids

3.4.1.1. The C-atom (1) being oxidized

a) Aldoses form aldonic acids.

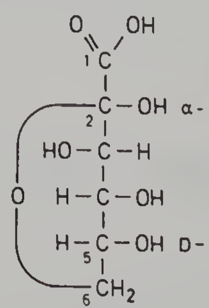


D-Glucose
↓
D-Gluconic acid

52

D-Gluconic acid

b) Ketoses (here fructose) form ketoaldonic acids:

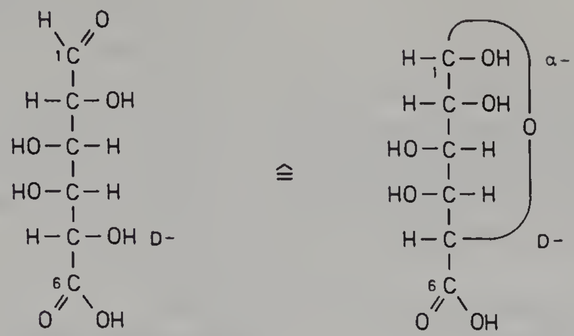


53

2-Keto-D-gluconic acid (biochem)
syst.: α-D-*arabino*-2-Hexulopyranosonic acid (IUPAC)

3.4.1.2. The C-atom (6) being oxidized

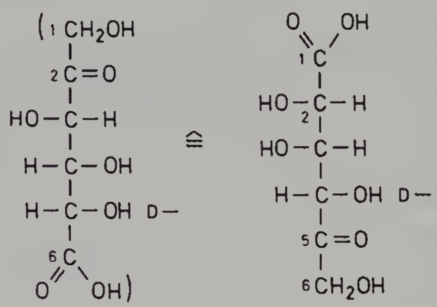
a)



54 D-*Galacturonic* acid — **55** α-D-Galactopyranuronic acid

The . . .ose ending of the aldose (galactose) is replaced by the ending '. . .uronic acid'. Carbon atom keeps locant 1; the carboxyl carbon atom takes locant 6.

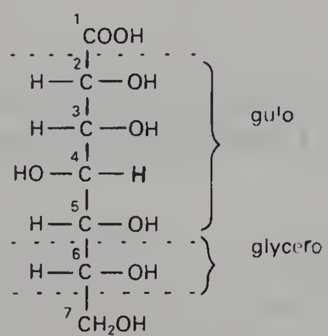
b)



56 **57**
(6 oxidized Fructose) D-*lyxo*-5-Hexulosonic acid)

The compound is considered as 5-oxidized gulonic acid, and not as 6-oxidized fructose. It is accordingly numbered as gulonic acid and not as fructose. The carboxyl group takes locant 1 (cf. formula **52**). Again it is a question of a ketoaldonic acid (cf. formula **53**).

3.4.1.3. Carboxylic acids with 7 C-atoms, by cyanhydrin synthesis from glucose

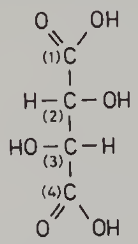


58

a) trivial: D-Glucoheptonic acid
b) syst.: D-Gluco-D-gulo-heptonic acid (locants) (cf. 1.1.5 p. 234). Here the chain is named in the direction 6–2, in 2 groups each of 4 atoms of carbon (6–3: D-gluco and 5–2: D-gulo).
c) syst.: D-*Glycero*-D-*gulo*-heptonic acid

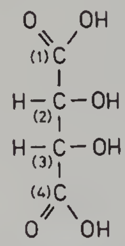
The 2-epimer form is named D-Glycero-D-ido-heptonic acid (the configuration is reversed at 2)

3.4.2. Dicarboxylic acids (aldaric acids) (. . .aric acids)



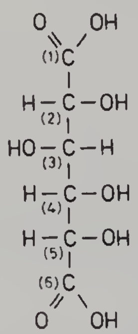
59

trivial: L(+)-Tartaric acid
(see also IV 15.4.6.3.)
with stereoprefix: L-Threaric acid
with configuration prefix:
(2*R*,3*R*)-2,3-Dihydroxysuccinic acid



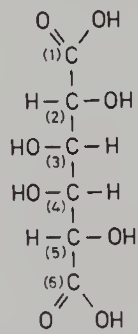
60

meso-Tartaric acid
Erythraric acid
(2*R*,3*S*)-2,3-Dihydroxysuccinic acid



61

trivial: Saccharic acid
D-*gluco*-Saccharic acid
D-Glucaric acid
(2*R*,3*S*,4*S*,5*S*)-2,3,4,5-Tetrahydroxyadipic acid



62

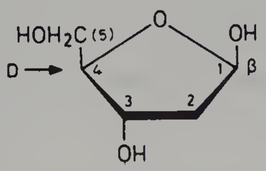
trivial: Mucic acid
meso-Galactaric acid
(2*R*,3*S*,4*R*,5*S*)-2,3,4,5-Tetrahydroxyadipic acid
Salts: Mucates
meso-Galactarates

4. DE(S)OXY. . .OSES

Because of their special significance these are not dealt with in association with group 2 (reduction), but are given their own separate section. An H- is (automatically) introduced in place of the lost OH-group.

4.1. De(s)oxypentoses

4.1.1. Without additional substituents



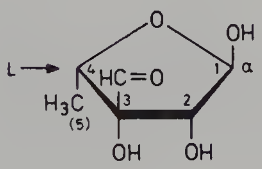
63

a) biochem. trivial: Deoxy-(β-D)ribose
b) syst.: 2-Deoxy-β-D-erythro-pentose
2-Deoxy-β-D-erythro-pentofuranose

The stereoprefix '-erythro' in (b) takes up the position of the –OR substituent or the –OH in 4,3 of the C-chain 1–5.

Radical 1β:2-Desoxy-β-D-ribosyl

4.1.2. With additional substituents

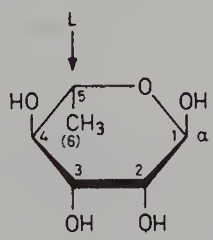


64

5-Deoxy-3-*C*-formyl-α-L-lyxose
trivial: Streptose
from streptomycin

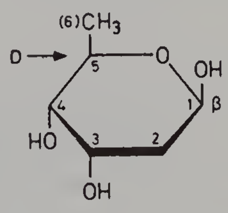
4.2. De(s)oxyhexoses (6 C)

4.2.1. Without additional substituents



65

trivial: (+)-α-L-Rhamnose
syst.: 6-Deoxy-L-mannose (here α-)

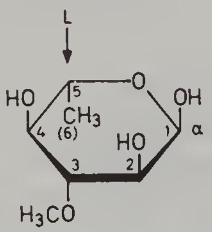


66

trivial: Digitoxose
syst.: 2,6-Dideoxy-β-D-*ribo*-hexose
2,6-Dideoxy-β-D-*ribo*-hexopyranose

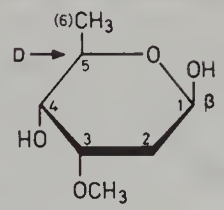
The configuration and stereoprefix 'D-*ribo*' refers to the arrangement at the C-atoms 5,4,3 of chain 1–6. A designation with the parent sugar 'allose' or 'altrose' (e.g. 2,6-dideoxyallose) is not permitted, because (e.g.) in allose the C(3) is (*R*)-configured, whereas it is in an (*S*)-configuration in digitoxose, under the influence of the 2-deoxy grouping (–CH_2–). The configuration in the parent sugar and the deoxy-sugar derived from it must however have their corresponding asymmetry centres the same.

4.2.2. With additional substituents



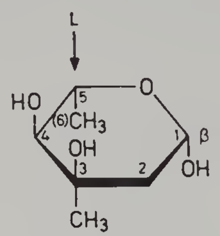
67

6-Deoxy-3-*O*-methyl-L-glucose
(here: α-)
trivial: L-Thevetose (from peruvoside)



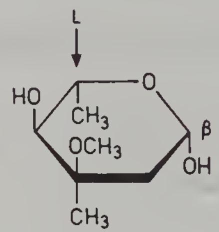
68

2,6-Dideoxy-3-*O*-methyl-D-*ribo*-hexose
(here: β-)
[3-*O*-Methyl-digitoxose]
trivial: Cymarose (from strophanthine-K)



69

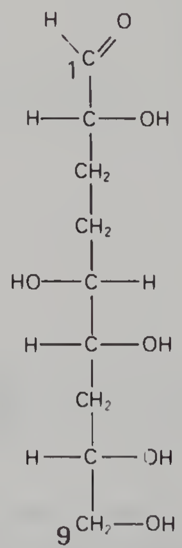
2-6-Dideoxy-3-*C*-methyl-L-*ribo*-hexose
(here: β)
trivial: L-Mycarose (from Carbomycin, Spiramycin)



70

2,6-Dideoxy-3-*C*-methyl-3-*O*-methyl-L-*ribo*-hexose
3-*O*-Methylmycarose (here: β)
trivial: Cladinose (from Erythromycin)

4.3. Deoxy-sugars, >6 C



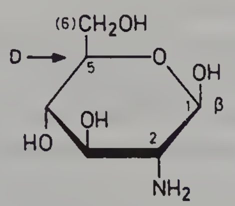
71

3,4,7-Trideoxy-D-gluco-nonose
Here the configurations at the non-directly-bonded asymmetric C-atoms 8-(6/5)-2 are joined together as D-gluco (Anglo/American). (see rule 1.15)

5. AMINO COMPOUNDS

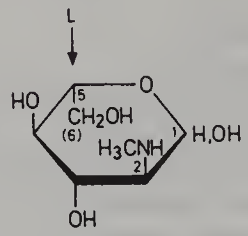
5.1. Amino. . .oses

Amino-acids are named with the alphabetical sequence of the prefixes (amino/deoxy) on the basis of the substituent sequence $OH/H/NH_2$, i.e. the introduction of an amino-group in place of an H in a methyl group. As parent names, for trivial names the carbohydrate of the same Fischer projection, or for systematic names the corresponding stereoprefixes, are used.



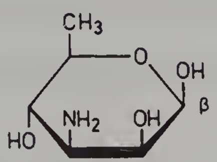
72

trivial: Chitosamine
biochem. trivial: (β)-D-Glucosamine
syst.: 2-Amino-2-deoxy-β-D-glucopyranose
The trivial name is also valid for the anomeric form



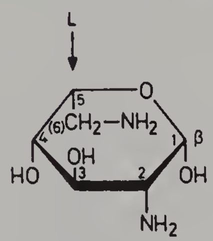
73

N-Methyl-L-glucosamine
(from streptomycin)



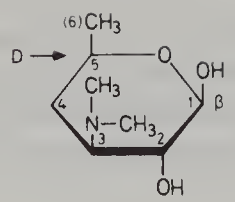
74

trivial: Mycosamine
(from Nystatin, Amphotericin)
syst.: 3-Amino-3,6-dideoxy-β-D-manno-pyranose



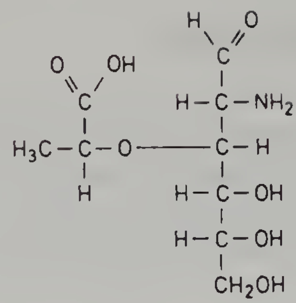
75

trivial: Neosamine B
(from Neomycin B)
syst.: 2,6-Diamino-2,6-dideoxy-β-L-ido-pyranose



76

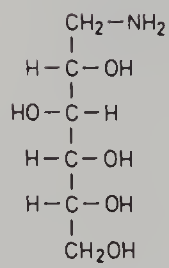
trivial: Desosamine
(from erythromycin)
semi-trivial: 3,4,6-Trideoxy-3-dimethylamino-β-D-glucose
The configurations in 2,3 and 5 are the same as in D-glucose (2*R*,3*S*,5*R*). Thus glucose can be used as the parent name.
syst.: 3,4,6-Trideoxy-3-dimethylamino-β-D-*xylohexopyranose*
D-xylo refers to the interrupted row 5,3,2 of the C-parent atoms 1–6.



77

trivial: Muraminic acid
syst.: 2-Amino-3-*O*-[1-(*S*)-carboxyethyl]-2-deoxy-*aldehydo*-D-glucose
The substituent prefixes, including subtractive prefixes are cited in alphabetical order. The 'aldehydo' prefix indicates the presence of the non-cyclic form of glucose.

5.2. Amino. .ols



78

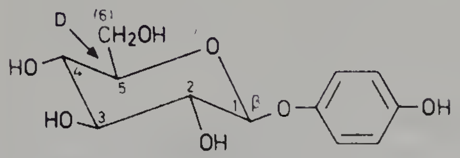
trivial: Glucamine
syst.: 1-Amino-1-deoxy-D-glucitol
The N-methyl derivative is meglumine (INN)

6. GLYCOSIDES

(cf. §7.4 so-called N-glycosides)

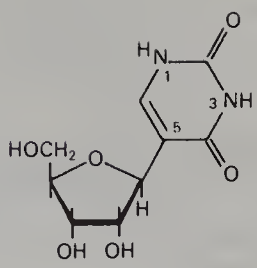
Glycosides are ether-type compounds formed by the reaction of an anomeric hydroxyl group of a sugar molecule with a phenolic or alcoholic hydroxyl group, which may also belong to a sugar molecule, and which may also be anomeric. 'Glycoside' is a class designation which may in individual cases provide the name by adding its ending to the sugar stem, e.g. glucoside, galactoside, riboside, fructoside.

6.1 Monosaccharide glucosides



79

syst.: a) *p*-Hydroxyphenyl β-D-glucoside
b) *p*-Hydroxyphenyl β-D-gluco-pyranoside-(1,5)
trivial: Arbutin



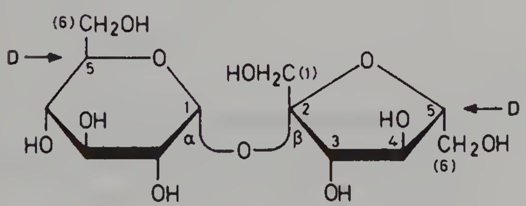
80

Pseudouridine (cf. 'pyrimidine bases', IV 9.2.6. a, p. 177 and nucleosides V 7.4) (C-glycoside! exception). Ψrd
syst.: 5-(β-D-Ribofuranosyl)uracil.

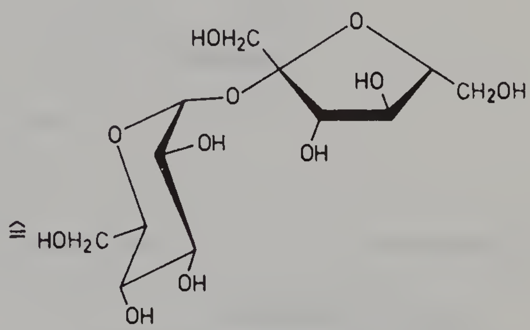
The aldehyde group which is established as a hemiacetal in the pyranose form of the glucose has become a full acetal in the glycoside. The phenol group appears in the name as a substituent of the anomeric hydroxyl group.

6.2. Disaccharides, trisaccharides

6.2.1. Non-reducing disaccharides



81



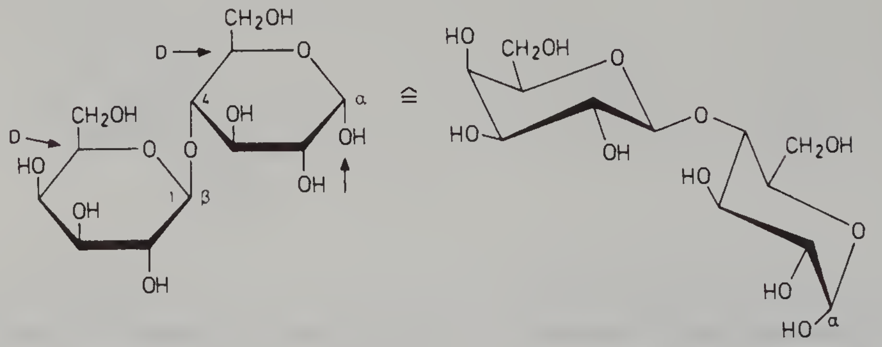
81(a)

trivial: Sucrose, Saccharose E.P. (cane-sugar) (beet-sugar)
β-D-Fructofuranosyl-α-D-glucopyranoside

D-Glucose and D-fructose have reacted at their anomeric hydroxyl groups. Both reducing groups are no longer reactive as such. In the systematic name, alphabetical order is followed (f/g). The fructose radical (. . .osyl: here . .furanose minus anomeric OH-group) is a substituent in place of the H- of the anomeric OH-group of the glucose in the glycoside (ether) formation. The reaction is classed as elimination of water.

6.2.2. *Reducing disaccharides, trisaccharides*

6.2.2.1. *Free anomeric hydroxyl group (↑) reducing*

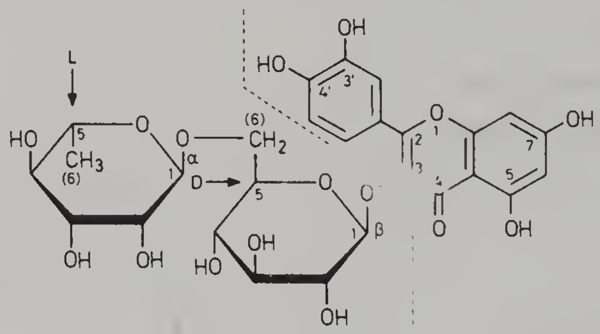


82 82a

trivial: Lactose (as monohydrate in E.P.) milk sugar
syst.: 1) 4-*O*-β-D-Galactopyranosyl-α-D-glucopyranose
2) *O*-β-D-Galactopyranosyl-(1→4)-α-D-glucopyranose

The anomeric hydroxyl group of the galactose reacted with the alcoholic hydroxyl group in the 4-position of the glucose. The anomeric (↑)hydroxyl group is still free. The component with the 'free aldehyde group' is the base component in the name. (Seniority of –CHO or OH– over OR.)

6.2.2.2. *Glycosidic anomeric hydroxyl groups, non-reducing*



83

α-L-Rhamnose β-D-Glucose

Rutinose (reducing)
6-*O*-(6-Deoxy-α-L-mannopyranosyl)-
β-D-glucopyranose (cf. 84)

1) 2-(3,4-Dihydroxyphenyl)-5,7-dihydroxy-4*H*-1-benzopyran-4-one
2) 3′,4′5,7-Tetrahydroxyflavone

trivial: Rutin, Rutoside
syst.: 3-[6-*O*-(6-Deoxy-α-L-mannopyranosyl)-β-D-glucopyranosyl]oxy-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-4*H*-1-benzopyran-4-one

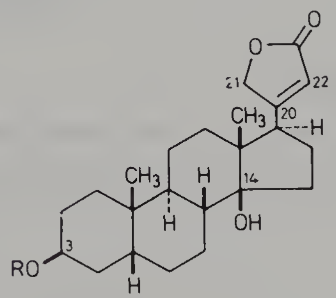
-4-chromenone
Alphabetical order: De/di/h

The disaccharide appears (in the systematic name) as prefix, as the carbonyl group has seniority as compound class and forms the suffix.

In E.P.III, rutin was named on the same principle, but with the use of 'rhamnose' for 'desoxymannose'. Thereby the alphabetical sequence is altered, and, taking account of the water of crystallization, the result is:

2-(3,4-Dihydroxyphenyl)-5,7-dihydroxy-3-(O^6-α-L-rhamnopyranosyl-β-D-gluco-pyranosyloxy)-4-chromenone, trihydrate (see Rutoside DAB 8).

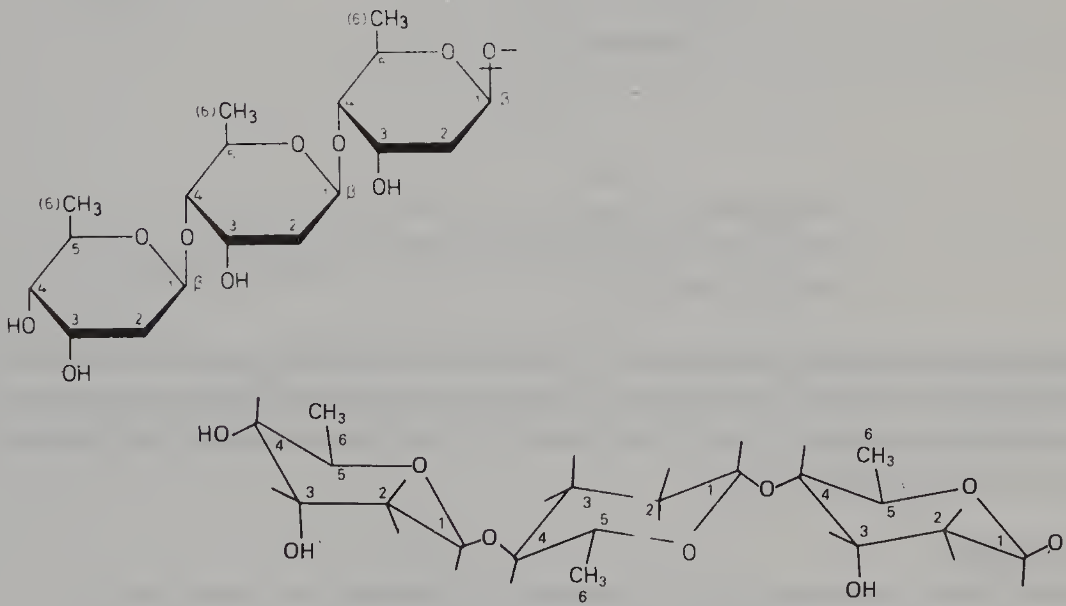
The reducing power of rutinose is lost after glycoside formation with the flavone.



84

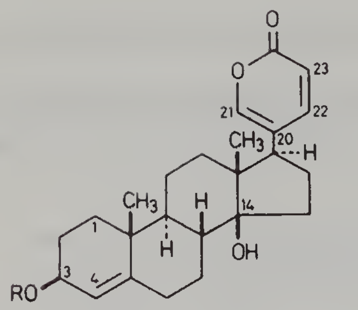
Digitoxin (R see 85)

3β-[2,6-Dideoxy-*O*-β-D-ribohexopyranosyl-(1→4)-2,6-dideoxy-*O*-β-D-ribohexopyranosyl-(1→4)-2,6-dideoxy-β-D-ribohexopyranosyloxy]-14-hydroxy-5β,14β-card-20(22)-enolide



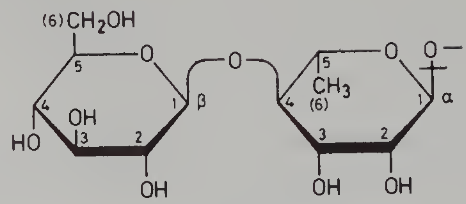
85

R-O- (*see* formula 84)
3α-Digitoxose (trisaccharide)
(Tridigitoxoside)
syst.: [O^4-(O^4-β-D-Digitoxopyranosyl-β-D-digitoxopyranosyl)-β-D-digitoxopyranosyloxy]



86

Scillaren A (R see 87)
3β-[4-*O*-β-D-Glucopyranosyl-α-L-rhamnopyranosyloxy]-14-hydroxy-bufa-4,20,22-trienolide



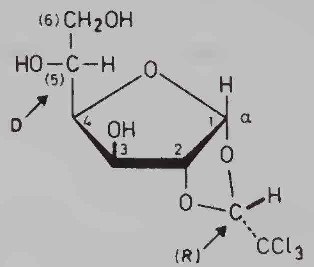
87 (to 86)

R = Scillabiose
(disaccharide, free reducing)

The lactone groupings take first place as a compound class. '. .cardenolide' or '. . .bufa-trienolide' respectively are therefore the base components of the names. (cf. formula 79)

7. SPECIAL DERIVATIVES

7.1. Acetals (cf. §6.1.)



88

Chloralose (INN) α-Chloralose (WHO)
(*R*)-1,2-*O*-(2,2,2-Trichlorethylidene-α-D-glucofuranose (WHO)

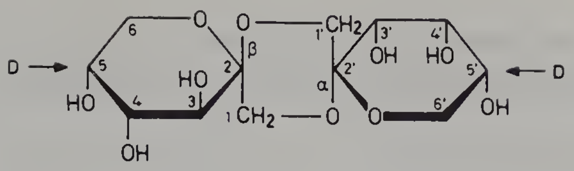
The polyhydroxy-compound serves as the parent name; the acetal appears in the name as *O*-alkylidene substitution product. Chloral (trichloroacetaldehyde) is the acetal-source. The substitution locations of the oxygen atoms are cited by two locants and therefore introduced once only in the name.

7.2. Anhydrides

The naming follows the general organic nomenclature procedure for the grouping

$$R-\overset{\overset{\displaystyle O}{\|}}{C}-O-\overset{\overset{\displaystyle O}{\|}}{C}-R$$

e.g. Acetic (acid) anhydride, ...carboxylic acid anhydride (acid derivative). In the field of carbohydrates however, it is applied to double glycoside formation between two sugar molecules:



89

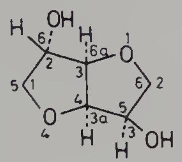
Fructose Psicose

β-D-Fructopyranose-α-D-psicopyranose-1,2′;2,1′-dianhydride

The names of the carbohydrates are cited in alphabetical order (f/p). The locants for the anhydride grouping are given likewise.

7.3. Ethers

The nomenclature possibilities of glycosides (see §6) and as *O*-substituted . . .oses (see 4.2.2.) etc. are already mentioned. For example, instead of 4-*O*-methyl-D-mannose, the name D-mannose 4-methyl ether can also be used. For intramolecular ethers, subtractive names can be used with the prefix 'anhydro'.



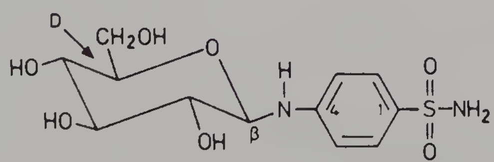
90

trivial: Isosorbide
(cf. Isosorbide dinitrate INN)
as polyol syst.: 1,4,3,6-Dianhydro-D-glucitol (inner locants)
as fused ring system syst.: (3*R*,3a*R*,6*S*,6a*R*)-Furo[3,2-*b*]-furan-3,6-diol (outer locants)

7.4. So-called N-Glycosides

7.4.1. General

This is not a matter of glycosides as defined in 6. It is more a question of the elimination of water between anomeric hydroxyl groups and primary or cyclic amino groups. There is a direct (⋛C-N<) bond.



91

N_4-(β-D-Glucopyranosyl)sulfanilamide

To this group belong also the:

7.4.2. *Nucleosides (sugar: ribose and 2′-Deoxyribose)*

Literature: Hoppe-Seyler's *Z. Physiol. Chem.* **351**, 1055, 1970

(a) *With pyrimidine bases* (cf. IV 9.2.6)

Cyt*idine* 1-(β-D-Ribofuranosyl)cytosine; Cyt-Rib; Cyd; rCyd; (C).

Oro*tidine* 3-(β-D-Ribofuranosyl)orotic acid; Ord; (O).

Ur*idine* 1-(β-D-Ribofuranosyl)uracil; Urd; (U). (Pseudouridine see glycosides) (p. 245, formula **80**) . . .1-Ribosylthymine; Thd; rThd; (T).

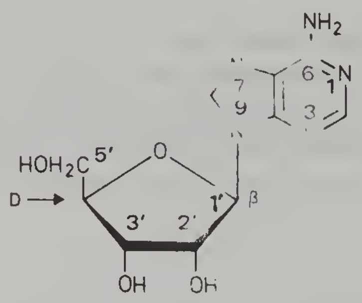
Thym*idine* 1-(2′-Deoxy-ribosyl)thymine; dThd; (dT).

Thiour*idine* 1-(β-D-Ribofuranosyl)thiouracil; Srd; s^2 U*; (S).

Pyrimidine nucleoside (non specific) Pyd; (Y)

The trivial ending 'idine' indicates that the nucleosides are based on pyrimidine bases.

(b) *With purine bases*



92

trivial: Adenosine
semitrivial: 9-(β-D-Ribofuranosyl)adenine
syst.: 6-Amino-9-(β-D-ribofuranosyl)-9*H*-purine
(Adenine see formula **66** p.157)
The trivial ending 'osine' indicates that this nucleoside is formed from a purine base.

Symbols Ade-Rib[1]; Ado[2]; rAdo[3]; (A)[4].

1) Adenine-ribose;
2) Adenosine; (1 & 2 three letter symbols)
3) r: for ribo with special significance;
4) Single letter symbol only for oligo- and poly-nucleotides, not for mononucleotides and nucleosides.

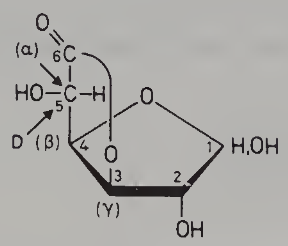
* s^2 U: for Thiouracil-nucleosid (cf. p. 177 formula **202** structure α).

Further examples: (without formulae) on the adenosine structure principle.
Deoxyaden*osine*: 9-(2′-Deoxy-β-D-ribofuranosyl)adenine; dAdo(d: deoxy)
Guan*osine*: 9-(β-D-ribofuranosyl)guanine; Gua-Rib; Guo; rGuo; (G)
In*osine*: 9-(β-D-ribofuranosyl)hypoxanthine; Hyp-Rib; Ino; rIno; (I)
Thioin*osine*: 6-Mercapto-9-(β-D-ribofuranosyl)purine; Shy-Rib; Sno.
Xanth*osine*: 9-(β-D-ribofuranosyl)xanthine; Xan-Rib; Xao; rXao; (X)
Purine nucleoside (ribo) (non-specific); Puo; (R)

The use of the letter symbols presupposes that the 'N-glycoside' is formed on the 1-position of the pyrimidine or the 9-position of the purine respectively, and that in the absence of indication otherwise, the β-D-ribosyl radical is the sugar component, and that in the case of 'deoxyriboses' it is a matter of a 2′-deoxy compound, and that (from left to right) only 3′–5′ bonds occur.

(c) (ribo) Nucleosides (unspecified, unknown) Nuc; (N).

7.5. Lactones



93

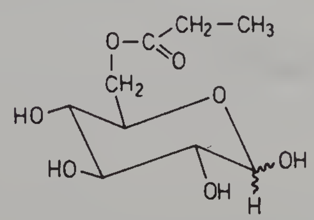
Glucurolactone (INN)
syst.: D-Glucofuranuronic acid γ-lactone (WHO)
D-Glucofuranurono-6,3-lactone (IUPAC)

In general (IUPAC) names are of the form . .o. .lactone, and not . . .acid. . .lactone. The lactone ring-size is indicated by the locants, that for the carboxyl group being cited first. In uronic acid it takes the highest locant. The steric disposition at the C-atom 1 is not established.

7.6 Esters

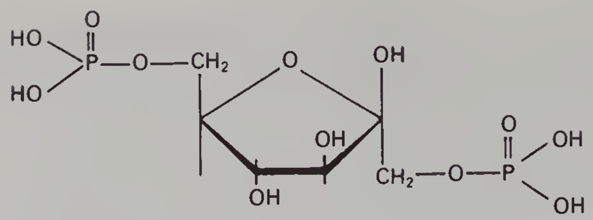
7.6.1. General

Naming is possible: 1) as an O-substitution product and
2) as an ester



94

1. 6-*O*-Propionyl-D-glucopyranose
2. D-Glucopyranose 6-propionate



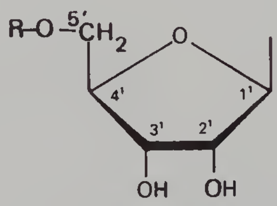
95

1. D-Fructose 1,6-bis(phosphate) (biochem.)
2. D-Fructofuranose 1,6-bis(dihydrogen phosphate) (syst.)
3. Fructose 1,6-P_2
4. Fru(1,6)P_2
5. 1,6-Di-*O*-phosphono-D-fructose (biochem.)
6. 1,6-Bis(phospho)-D-fructose (biochem)
7. Harden-Young-ester

7.6.2. Nucleotides
(cf. nucleosides § 7.4.2) (P cf. lecithin IV 17.2)
By nucleotides is understood esters of nucleosides with phosphoric acid. 'Mono' nucleotides are the building blocks for 'oligo-' and 'poly-' nucleotides.

1) Purine base adenine (Ade)
Nucleoside adenosine (Ado)
Nucleotides

a) Adenosine 5′-dihydrogenphosphate
≡ AMP (Adenosine monophosphate)
≡ Muscle adenylic acid
≡ Ado-5*P*≡*P*5′-Ado≡*P*-Ado (if the *P* is on the left without a locant, then it is 5′)



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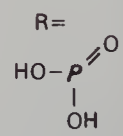
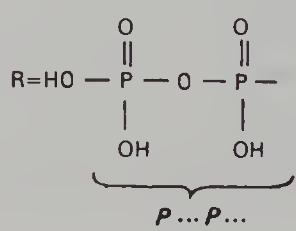


97

b) ADP (Adenosine diphosphate)
≡ 5′-Adenosine pyrophosphate
≡ Adenosine 5′-diphosphate
≡ Adenosine-5′*PP*≡Ado-5′*PP*≡*PP*-Ado



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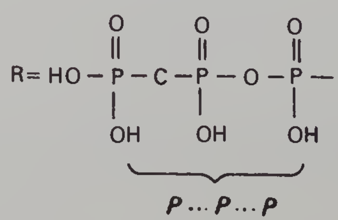
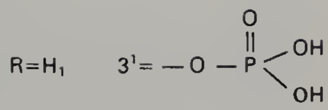
c) ATP (Adenosine triphosphate)



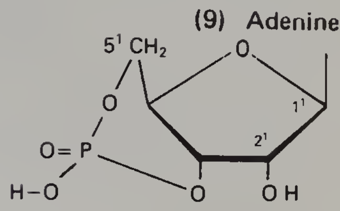
99

d) Adenosine 3′-phosphate
≡ Yeast adenylic acid
≡ Ado-3′*P*≡*P*3′-Ado≡Ado-*P* (if the *P* is on the right without a locant, then it is 3′)



100

e) Cyclic ester
Cyclo-AMP
≡ Ado-3′:5′*P*≡*P*3′:5′-Ado



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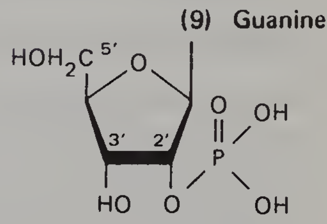
2) Purine base guanine (cf. p. 178)
Nucleoside Guanosine
Nucleotide guanosine-2′ phosphate
≡ Guo-2′*P*≡*P*2′-Guo



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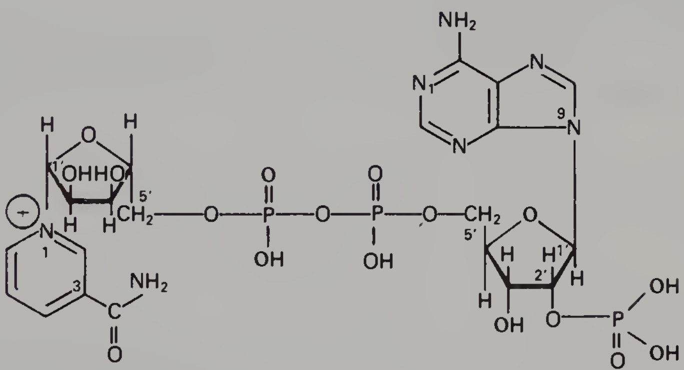

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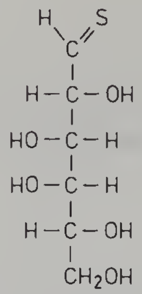
Nicotinamide-adenine-dinucleotide phosphate
NADP$^{\oplus}$
Codehydrase II

Here addition of AMP esterified at 2′ with phosphoric acid and a ‘pyridine’ nucleotide produces a dinucleotide by diphosphate formation (at 5′/5′). (cf. Nadide INN, however)

7.7. S-Analogues

If S takes the place of O in a carbohydrate or a derivative of a carbohydrate, in general by the insertion of ‘thio’ into the name, the oxygen atom replaced by S is indicated (but not expressly named), e.g.



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1-Thio-*aldehydo*-D-galactose

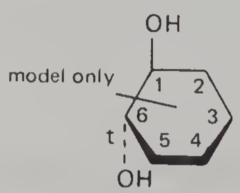
8. APPENDIX: CARBOCYCLIC POLYOLS CYCLITOLS AND DERIVATIVES

(Literature Hoppe-Seyler's *Z. Physiol. Chem.* **350**, 523, 1969 IUPAC–IUB)

These are hydroxyl-substituted cycloalkanes. Representing this group were the inositols (and analogues) which will be discussed here. Depending upon the steric arrangement of the OH-groups, there are three procedures for naming them:

by means of special steric prefixes;
by means of fraction prefixes formed from locants;
(by means of Greek letter prefixes)

loc	arrangement of OH-substituents							base component
1	c	c	c	c	c	c	c	c	
2	c	c	c	c	c	c	c	t	
3	c	c	c	c	c	t	t	c	
4	c	c	c	t	t	c	c	t	
5	c	c	t	t	c	c	t	c	
6	c	t	t	t	t	t	t	t	
stereo-prefixes	*cis*	*epi*	*allo*	*neo*	*myo* (*meso*)	*muco*	*chiro*	*scyllo*	Inositol
fraction-prefixes	1,2,3,4,5,6/0	1,2,3,4,5/6	1,2,3,4/5,6	1,2,3/4,5,6	1,2,3,5/4,6	1,2,4,5/3,6	1,2,4/3,5,6	1,3,5/2,4,6	Cyclohexanehexol
letter prefixes	ι (iota)	θ (theta)	η (eta)	ϵ (epsilon)	δ (delta)	γ (gamma)	α (alpha)	β (beta)	Inositol
optical isomerism	*meso*	*meso*	*meso*	*meso*	*meso*	*meso*	*rac*	*meso*	



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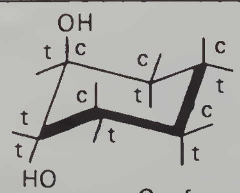
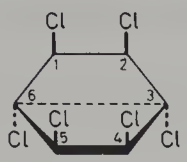


Conformation

Inositols
(Inositol, inosite) (Cyclohexanehexol)

If 6 Cl-atoms are substituted for the OH-groups, taking up the steric configuration as in the inositols, the letter prefixes as well as the fraction prefixes can be used (without a suffix) in forming substitutive names. If up to two OH-groups are replaced by other prefix-substituents, the name is formulated as a substitutive one on the inositol base-component. Substitutive naming using the break prefix is also possible.



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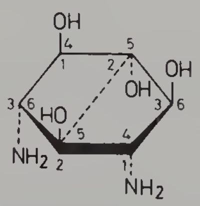
Trivial: Gammexane; Lindane
syst.: γ-1,2,3,4,5,6-Hexachlorocyclohexane
(DAB 6,3. Supplement)
1,2,4,5/3,6-Hexachlorocyclohexane: axis of symmetry
muco-1,2,3,4,5,6-Hexachlorocyclohexane

The first systematic name follows the normal rules of substitutive nomenclature. The steric specificity is achieved by the letter prefix preceding the name. In the second systematic name, locants are arranged in a fraction prefix sequence taken from inositol nomenclature. In the third systematic name, steric specificity is achieved using the corresponding inositol stereoprefix.



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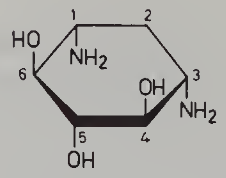
trivial: Streptamine
syst.: a) 4,6-Diamino-4,6-dideoxy-*scyllo*-inositol
b) 1,3,5/2,4N,6N-Diaminocyclohexanetetrol
(inner locants)
The fraction prefix can also be applied directly to the diamine by adding N to the corresponding locants.

By IUPAC the substitution points are assigned the lowest locants which do not interfere with the locant sequence describing an existing configuration. By CA on the other hand, the substitution points are assigned the lowest locants. This gives rise to the name:

syst.: c) 1,3-Diamino-1,3-dideoxy-*scyllo*-inositol (C.A.)
(outer locants)

From 'streptamine' (locants as syst. c), '2-deoxystreptamine' (meso-form) is derived.



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from this, by glycosidation, important antibiotics are formed, (INN: gentamicin, kanamycin, neomycin, sisomycin).

The ending . . .micin is fixed for antibiotic of the species Micromonospora, the ending . .mycin for such of Streptomyces.

VI

Polymers

A. GENERAL PRINCIPLES

The nomenclature of polymers has numerous special concepts that need not concern us here to any great extent. However, a few of them must first be explained and a few general comments can be made.

One, or rather THE, role in systematic (structure-based) polymer nomenclature is played by the 'structural repeating unit' (RU). That is the smallest repeating unit in the polymer, which can itself consist of sub-units. In the name, the RUs are preceded by the indeterminate prefix 'poly' indicating that they are linked, forming single-strand[1] chains of indeterminate length and indeterminate molecular weight. The indeterminate nature of 'poly' is expressed by the use of 'n' generally (though another lower-case letter may also be used), following the RU set in brackets. The RU generally is divalent, a ranking sequence is observed with regard to its construction from sub-units. The RU is written from left to right. Each sub-unit shall be as large as possible, i.e. the number of sub-units shall be as small as possible. Sub-units can be individual atoms, chains or rings, including heterocycles. RUs and sub-units can also have substituents.

In nomenclature one must distinguish between structure-based and production-based names. Apart from which, there are trivial or semi-systematic names. The order of naming a structure-based RU begins with the most senior ranking sub-unit and goes on to the next most senior one, by the shortest means. The ranking sequence of sub-units is:

heterocycle/chain with heteroatom(s)/carbocycle/hydrocarbon chain.

1 Single-strand: two end-position atoms in the RU.

Polymer structures are designated as endless structures, i.e. the divalent chain has no ending on either side. The so-called end-groups are missing. They may well be unknown and have practically no effect on molecule size and little influence on the properties of the polymer. They can be cited only in those cases where the polymer is a unitary one in this respect and in so far as they are known.

Citing the end-groups, if at all, must include both end groups of the divalent RU being named. They are then cited as prefixes, the end-group on the left end of the (correctly aligned) RU is in this context the α and the right end one is the ω.

A polymer with a small 'n' value is known as an oligomer. No fixed size of 'n' is laid down as the dividing line between oligomers and polymers. The decisive factor is that the removal or the addition of one RU would not significantly alter a polymer's properties, but would alter an oligomers physical properties. If the value of 'n' is precisely known, then the prefix 'poly' is replaced by the exact Greek numerical prefix.[2]

- A homopolymer consists of only one type of monomer.
- A copolymer consists of more than one type of monomer.
- A block polymer consists of linear polymers linked together to form blocks. The blocks can be linked together either directly or by means of other structural units.

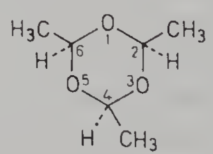
A trimer is an oligomer where n = 3 (e.g. paraldehyde from acetaldehyde[3]). One must distinguish a trimer from a 'terpolymer', which is formed from three different monomers.

The very wide range and variety which polymer chemistry covers, imposes a limit on those nomenclature possibilities we can deal with here. The limited area covered is that of 'regular single-strand organic polymers', and it is that area to which the explanations of RU etc. refer.

The details, given in this section, on oligo- and polynucleotides and nucleic acids follow on with those (see V 7.4.2 and 7.6.2) for nucleosides and nucleotides. They differ importantly from those given with regard to special polymer nomenclature, e.g. in not using the RU concept and in applying the special symbols and abbreviations, normal to biochemistry.

2 In the case of polymers with a factor 'h' it is clear that the product must be a mixture of materials without stoichiometric composition. This is not the case here with a fixed value for n. Here, particularly in the case of an oligomer, a fixed n may signify a pure substance, but only in association with the end-groups being cited and a determined molecular weight.

3 Paraldehyde has the formula



Citing this as an oligomer is misleading, as it is a defined pure substance. The systematic name

a) until 1979: 2,4,6-Trimethyl-1,3,5-trioxan

b) 1979–1982: 2,4,6-Trimethyl-1,3,5-trioxixan

c) Since 1983 the name is again 2,4,6-Trimethyl-1,3,5-trioxan (see II 2.1)

B. INDIVIDUAL POLYMERS

1. Chains with hetero-atoms

1.1. Polyethylene glycols DAB 8 (Monograph)
It can be seen from the heading that this monograph deals with a structure-based nomenclature in the sense of the IUPAC polymer rules. In one important aspect the monograph differs from that type of nomenclature. The structure given as

1 $HO-CH_2-(CH_2-O-CH_2)_n-CH_2OH$

does not conform to IUPAC, particularly with regard to the formulation of the RU as

2 $+CH_2-O-CH_2+$

which by IUPAC would be

3 $+O-CH_2-CH_2+$

The structure-based IUPAC name (without end groups) derived from this is

Poly(oxyethylene) (trivial: polyethylene oxide) (abb. PEO)

The hetero-atom has seniority over the hydrocarbon chain and stands at the left (α) end.
The end groups are known to be H- on the left and -OH on the right. Thus one arrives at the IUPAC name (with end groups)

α-Hydro-ω-hydroxy-poly(oxyethylene)

Were this a question of an oligomer with (e.g.) n = 3, the formula according to DAB 8 gives a different product or a different pure material as does the IUPAC formula

DAB 8 a) 3,6,9-Trioxa-1,11-undecanediol (MG 194)
b) α-Hydro-ω-hydroxy-tetra(oxyethylene)

IUPAC a) 3,6-Dioxa-1,8-ocatanediol (MG 150)
b) α-Hydro-ω-hydroxy-tri(oxyethylene)

The difference is not significant in the case of the polymer. The names (a) stand for the pure substances; the names (b) for the oligomers; all names correspond to IUPAC.

1.2. Polyethylene glycol esters

(a) *Polyethylene glycol-400 stearate (DAB 8) (Macrogolstearat)*
The number 400 signifies the average molecular weight of the unesterified polyethylene glycol. In the light of the comments made at [2], there is a limited need to stress that an

α-Hydro-ω-hydroxy-nona(oxyethylene) (MG 414)

is a stoichiometric defined compound not to be confused with a

Polyethylene glycol-400.

The latter, defined in terms of average i.e. mean molecular weight, is not in reality a stoichiometric compound but a mixture of compounds with $n \lesseqgtr 9$ (DAB 9 $n \approx 8$, calculated MG. 370). With regard to the end group, the stearate is unambiguously written in DAB 8 as monoester. Thus a polymer formula can be drawn. The ester group is outside the RU

$$4 \qquad H\!-\!\left[O-CH_2-CH_2\right]_n\!-\!O-\overset{\overset{\displaystyle O}{\|}}{C}-C_{17}H_{35}$$

The polymer name for this would be

α-Hydro-ω-stearoyloxypoly(oxyethylene)

(b) *Polyethylene glycol succinate [poly(ethylene glycol succinate)] (E.P. III)*
In a chemicals list, this substance would appear as the trivial

polyethylene glycol succinate,

and under this, as a scientific name,

poly(ethylene glycol succinate).

This name expresses the correct position with regard to the ester, that it is within the RU, and thus, in contrast to (a), governed by the factor 'n'. This name is not correct in the sense of the IUPAC rules, as the formula given by it,

$$5 \qquad HO\!-\!\left[\overset{\overset{\displaystyle O}{\|}}{C}-CH_2-CH_2-\overset{\overset{\displaystyle O}{\|}}{C}-O-CH_2-CH_2-O\right]_n\!-\!H$$

must first be put into the correct naming order. This gives the formula

$$6 \qquad H\!-\!\left[O-CH_2-CH_2-O-\overset{\overset{\displaystyle O}{\|}}{C}-CH_2-CH_2-\overset{\overset{\displaystyle O}{\|}}{C}\right]_n\!-\!OH$$

From this comes the IUPAC polymer name:

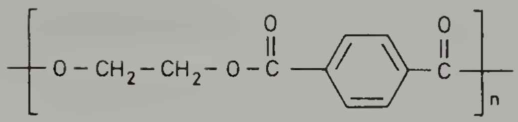
α-Hydro-ω-hydroxy-poly(oxethylenoxysuccinyl)

(c) *Polyethylene glycol adipate [(polyethylene glycol adipate)] (E.P. III), DAB 9 Macrogoladipate*
This gives, as an analogue to (b), the formula and the name

$$7 \qquad H\!-\!\left[O-CH_2-CH_2-O-\overset{\overset{\displaystyle O}{\|}}{C}-(CH_2)_4-\overset{\overset{\displaystyle O}{\|}}{C}\right]_n\!-\!OH$$

α-Hydro-ω-hydroxypoly(oxyethylenoxyadipoyl)

(d) *Sterile polyester fibres ([E.P. II] [Diolene, Trevira, Terylene according to the commentary])*
The product consists of polyethylene terephthalate. This name corresponds to the IUPAC trivial name for the following polymer:

8 

The trivial name is ambiguous, being consistent with interpretation as either

Poly(ethylene terephthalate)

or

(Polyethylene) terephthalate

Brackets as with the former should therefore be preferred. The RU contains four sub-units. From the formula, the scientific name can be read as

Poly(oxyethylenoxyterephthaloyl) (no end groups)

Taking the end-groups into account (from the Merck-Index, –H left, $-OCH_3$ right) gives

α-Hydro-ω-methyoxypoly(oxyethylenoxyterephthaloyl)

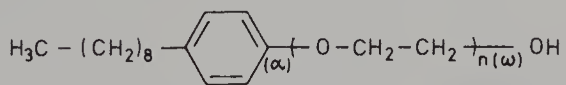
There is no indication of the polymerization factor in the documents cited above. The abbreviation for the product is PETP.

1.3. Polyethylene glycol ethers

(a) *Nonoxinol (INN)*

A number following the INN 'Nonoxinol' indicates the approximate number of oxyethylene units (RUs) in the named polymer, so that the 'n' must remain only for the general case. That is so for the formula and for the structure-based name.

WHO gives the general formula

9 

α-(p-Nonylphenyl)-ω-hydroxypoly(oxyethylene)

is the name which refers to that formula.

This name also conforms to IUPAC. If the alphabetical sequence for the substituents were followed, hydro could be α and '*p*-nonylphenoxy' ω. This does not seem to be covered by a binding rule. Individual nonoxinol type compounds take the following names:

Nonoxinol 4": α-(*p*-Nonylphenyl)-ω-hydroxy-tetra(oxyethylene)

Nonoxinol 30": α-(*p*-Nonylphenyl)-ω-hydroxy-triaconta(oxyethylene)

DAB 9 brings with the name 'Octoxinol 10R' a product of the same chemical group with the sidechain 1,1,3,3-Tetramethylbutyl (instead of nonyl), n = 10 and the scientific name; α-[4-(1,1,3,3-Tetramethylbutyl/phenyl] -ω-hydroxypoly(oxyethylene).

(b) *Polidocanol (INN)*

WHO describes this material as 'polyethylene glycol monododecyl ether (average 'n', 9; nonaethylene glycol monododecyl ether)'. From the name, following DAB 8 would lead to the construction of a formula:

10 $H_{25}C_{12}-O-CH_2 \left[CH_2-O-CH_2 \right]_9 CH_2OH$

WHO gives no structure-based formula. An IUPAC name derived from that formula above would be:

α-Dodecyl-ω-hydroxy-deca(oxyethylene): C_{32} . . .

(c) *Polyoxyethylene glycerol monostearate (DAC 1979)*
The preparation is a mixture. A major-component is defined, leaving open the question of positional isomers. Glycerol retains one free OH-group, forms an ester with stearic acid at another OH-position, and forms an ether at a third OH-group with polyethylene glycol (n ~ 20). It remains open whether these conversions of the glycerol can be considered as regular in the sense that a formula can be envisaged. The following details should therefore be considered as applying to an idealized formula.

The possible isomers can be grouped together as follows:

Substituents on the propane

11

$\underset{(\alpha)}{H}\!+\!O-CH_2-CH_2\underset{(\omega)}{+_n}O-$ (a)

$C_{17}H_{35}\overset{\overset{O}{\|}}{C}-O-$ (b)

$HO-$ (c)

With these substituents, the following isomers can be constructed:

12

I	II	III	
a	a	b	$-_1CH_2$
b	c	a	$-_2CH$
c	b	c	$-_3CH_2$

With alphabetical order of 'end groups', the polymer forms the structure-based name in all cases:

α-Hydro-ω-(R)poly(oxyethylene)

The R to be inserted into the formula is:

I: [3-hydroxy-2-(stearoyloxy)propoxy] (loc.)

II: [2-hydroxy-3-(stearoyloxy)propoxy] (loc.)

III: [(1-hydroxymethyl-2-stearoyloxy)ethoxy]

All the idealized structures are single-string, and can be subject to regular systematic naming procedures.

(d) *Poloxamer (INN)*
WHO gives the following general form:

13

$$H\!+\!\overset{RU\ (I)}{(O-CH_2-CH_2)_a}\overset{RU\ (II)}{(O-\underset{\underset{CH_3}{|}}{CH}-CH_2)_b}\overset{RU\ (I)}{(O-CH_2-CH_2}\!+_c OH$$

„MG" RU (I) 44

RU (II) 58

The WHO name for which is:

'α-Hydro-ω-hydroxypoly(oxyethylene)poly(oxypropylene)poly(oxyethylene) block-copolymer'

This is explained as follows:

'Each poloxamer name is followed by a three-digit number, such as: Poloxamer 188, 331, 407, and so on. The first two digits, multiplied by 100, correspond to the average molecular weight of the poly(oxypropylene) part. The third, multiplied by 10, gives the percentage by weight of the poly(oxyethylene) part.'

In the example named, the end-groups are given on the α,ω-basis. Two different RUs are available. In a poloxamer 188, for example, the molecular weight (MW) of the (RU $II)_b$ would be around 1800, and the percentage by weight of the sum of (RU $I)_{a+c}$ around 80%. The index 'b' calculates out at around 31, (= 1800:58). If the MW 1800 corresponds to around 20% (100–80), then the sum of the indexes, 'a+c' calculates out at about 164 (7200:44) (the MW for 'a+c' is [80%] 4×1800 = around 7200). On the basis of these amounts, an approximate picture of the product is formed. The total MW of the polymer is 7200 + 1800 = (approx.) 9000. A structure-based nomenclature is only possible by citing the nomenclature for individual blocks one after another. 'Block-copolymers' are formed from linear linked blocks of more than one type of monomer.

(e) *Poloxalene (INN) (cf. 21. rec. list)*
WHO here gives an explanation, no name but simply:

Polymers of the polyoxypropylene-polyoxyethylene type

Further, it is stated that the molecular weight is ~3000, and that 67% is allotted to polyoxypropylene.

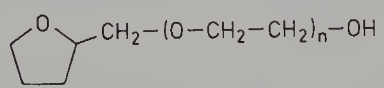
On the basis of the similar calculation as was applied above to poloxamer (INN), one arrives at a MW for the polypropylene part of approx. 2000, with a 'b' of about 34, with a MW for the polyethylene part of approx. 1000, with an 'a+c' of about 23.

Once again here, one can by this kind of calculation derive some idea of the product, if the type of polymer is correctly described. Whether the description is accurate is open to question.

(f) *Glycofurol*
The material is described unambiguously and is satisfactorily recognizable in the field of pharmaceutical law, by the official name:

α-Tetrahydrofurfuryl-ω-hydroxyoligo(oxyethylene)-1(2)

It is a monoether within the scope of the oligoethylene glycols (i.e. a polyethylene glycol according to DAB 8, with a small polymerization factor 'n'). The formula is

14 

In the name, 'n' is given as '. . .1(2)' and can be calculated as approx. 1.5.[4] Ideally the material therefore consists of a mixture of two compounds:

2-(Tetrahydrofurfuryloxy)ethanol $C_7H_{14}O_3$(146)n = 1 and

2-[2-(Tetrahydrofurfuryloxy)ethyoxy]ethanol $C_9H_{18}O_4$(190) n = 2

in proportions by weight to their molecular weights.

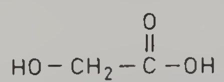
The special feature of the scientific name here lies in the information, not available in the existing polymer rules, on the size of the polymer or oligomer factor. Knowledge of this fact is of fundamental interest. With polymers (high n) an approximation of the factor, such as 50, 300, 6000 must suffice, giving accordingly limited information on the parameters of the substance. In the preceding case however, with an extremely low n, the most accurate value for the factor is important. The relationship of the factor to the scientific name would seem to be more useful, if an 'n' were included. It would be even clearer if expressed in such a form as '. .n(1–2)'. Its nature as a multiplying factor, as opposed to (e.g.) locants, would thus be more easily recognized.

1.4. Polyglycolic acid (INN)

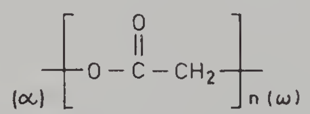
WHO gives the empirical formula $(C_2H_2O_2)_n$ and the name

Poly(oxycarbonylmethylene)

The glycolic acid monomer has the formula

15 

From this, the formula of the polymer (without end-groups) conforming to the empirical formula is given as:

16 

The WHO name has three sub-units in the RU. The name following IUPAC would have two sub-units, one of them substituted (largest possible sub-units):

Poly[oxy(1-oxoethylene)]

The RU name begins on the left with the hetero-atom. The sequence for the other atoms results from the seniority of O– substituted C over $-CH_2-$. It should be emphasized from this especially clear-cut example that 'polyglycolic acid' is properly called . . .acid, but that in many monomer molecules all the carboxyl groups but one no longer exist as . . . .acid, i.e. as carboxyl groups, but have taken other functions; here that of ester. Only one end group is still . . .acid. If the WHO also give no indication as to end-groups, it can be assumed that the α end-group is an –H, therefore belonging to a carboyxl group, but the ω end-group is an –OH.

4 My thanks to Hoffman-La Roche AG. Grenzach-Wyhlen for their kind comments.

The corresponding situation exists with other trivial polymer names, e.g. in the case of polyethylene glycol.

1.5. Paraformaldehyde, paraform

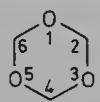
This is a question of a polymer of formaldehyde (CH_2O). With end-groups,[5] one arrives at the formula:

17 $H \left[O - CH_2 \right]_n OH.$

The RU is called 'oxymethylene' and, the polymer with end-groups, 'n' = 30 – 100, is:

α-Hydro-ω-hydroxypoly(oxymethylene), abbr. POM

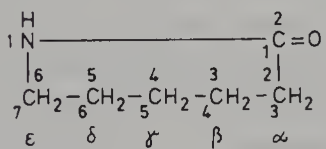
The old synonym, 'trioxymethylene' (in Suppl. Vol. B.6), is no longer acceptable, as it describes quite another type of polymeric formaldehyde, namely a cyclic trimer of the formula

18 

which can be given the exact organic chemistry name 1,3,5-Trioxan (cf. p. 258 footnote 3).

1.6. Sterile polyamide 6 fibre (E.P. II, Perlon)

(a) According to the monograph, the material is synthesized by the polymerization of ϵ-caprolactam [= hexanelactam, (inner locants) until 1982; hexahydro-2-azepinone (outer locants) since 1982: not yet decided]. The monomer has the formula:

19 

and IUPAC allows any of the above names. The first of these may be regarded as somewhat archaic, since the use of 'caproic acid' for hexanoic acid, has long been discarded.

There is no scientific name for the polymer given in E.P. II. As a trivial name, IUPAC gives consideration to:

Poly(ϵ-caprolactam)

This designation suggests a ring series with linking bonds

The correct structure is in fact depicted by a polymer chain:

20 $\left[\overset{H}{N} - \overset{O}{\overset{\|}{C}} - (CH_2)_5 \right]_n$

5 Auterhoff, *Lehrbuch der Pharmazeutischen Chemie*, 10th edn. Wissenschaftliche Verlagsgesellschaft, Stuttgart 1980.

The RU is to be read as 'imino-(1-oxohexamethylene), and the scientific polymer name (without end-groups) is therefore

Poly[imino(1-oxohexamethylene)]

According to the Merck-Index, n ~ 200. No information on this matter is given in the Commentary to E.P.

IUPAC denotes these and other polymer structures as idealized, which must give rise to a certain reservation with regard not only to the structure, but also to the name derived therefrom. This is something which must be kept in mind.

(b) *Policapram (INN)*
WHO includes under this INN, a scientific name:

Poly(iminocarbonylpentamethylene)

which unambiguously complies with the same RU met at (6a). While at (6a) there are two sub-units in the RU, (. .imino and . .hexamethylene, the latter substituted), there are three sub-units in the WHO name, (-imino, -carbonyl and -pentamethylene). IUPAC does not use 'carbonyl' if the C-atom is part of a C-chain. Different nomenclature principles are used in the two cases.

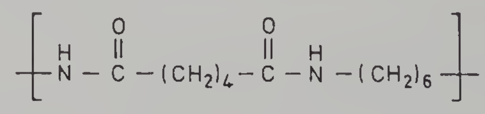
The molecular weight given by WHO as 'approximately 5668', in combination with the molecular formula $C_{300}H_{552}N_{50}O_{51}$ leads to a polymerization factor 'n' = 50. Therein lies the distinction between (6a) and (6b), having identical RUs, they differ only in the size of the polymerization factor.

1.7 Sterile polyamide 6/6 fibres ([E.P. II] [Nylon group])
From the description, the material is obtained by 'polycondensation' of hexamethylenediamine and adipic acid (syst.: hexanedioic acid). The acyl radical of adipic acid is named 'adipoyl'. The formula for hexamethylenediamine is

21 $H_2N-(CH_2)_6-NH_2$

In polyamide 6/6, the first 6 indicates the number of C-atoms separating the two nitrogen atoms, and therefore represents 'hexamethylenediamine'. The second 6 refers to the number of C-atoms in the dicarboxylic acid, and thus the 'hexanedioic acid'.

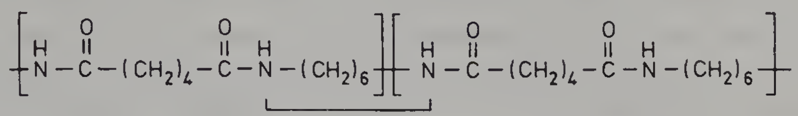
The pharmacopaeia gives no more precise information as to the nature of the polymer, nor does the commentary. One may assume from this that it is a matter of a regular linear polymer, the RU of which has the formula:

22 

There are three possible designations, following IUPAC:

a) trivial: Polyhexamethyleneadipamide
b) structure-based: Poly(iminoadipoyliminohexamethylene)
c) structure-based: Poly[imino(1,6-dioxohexamethylene)iminohexamethylene]

As the formula for the RU shows, the hexamethylenediamine component cannot be seen directly, unless two RUs are put one after another:

23 

The order of citation in the structure-based names becomes clearer if yet a further criterion is added. Both hydrocarbons have 6 C-atoms, and they are of equal length and the criterion of the shortest distance from the first to the second hetero-atom does not resolve matters. Here it is valid to use the criterion that the substituted chain has seniority over the unsubstituted one.

The reversed arrangement in the trivial name creates confusion.

1.8 Polyetadene (INN) (hetero atoms in chains and/or rings?)
The description laid down in WHO says:

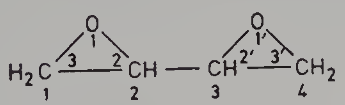
'1,2:3,4-Diepoxybutane polymer with ethyleneimine'

This conveyed by the formula:

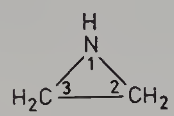
$(C_4H_6O_2)_m(C_2H_5N)_n$

These provide two facts only: knowledge that both monomers are used in producing the polymer, and that these are not in a (1:1) molar ratio in the end-product, but in some indeterminate (m:n) ratio.

The monomers are

24 

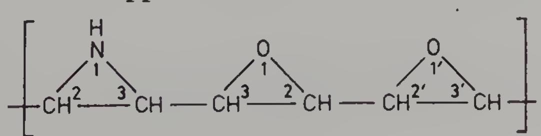
1,2:3,4-Diepoxybutane
(outer locants)
(Bioxirane) (inner locants) (1979)

25 

Ethylenimine
(Aziridine) (locants)

There is no information given on the type of bonding of the monomer in the polymer nor whether the polymer contains only cyclic, or both cyclic and acyclic groups. The empirical formula gives us only the separate empirical formulae of the monomers set next to each other, but there is no RU. Thus all that information is lacking which is the pre-requisite to the construction of a scientific name. An RU cannot be identified. The polymer is classified as an 'indeterminate copolymer'.

This case may, however, serve to illustrate the principles of heterocycles occurring in RUs. The RU might have an approximate formula

26 

This contains only heterocycles and no chains. The heterocycles have a priority for citation, by which N-rings have seniority. Other heterocycles follow in the ranking order O/S/P etc. Other citation order criteria are the number of rings in a ring-system, the size of individual rings, and the number of the same and different hetero-atoms.

The numbering is such as to give the lowest possible locants to those ring atoms which form the principal chain, retaining the original numbering of the rings. The above RU would be designated:

. . .(2,3-aziridinediyl-3,3′-bioxiranediyl)

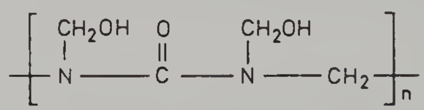
The lowest locant of the aziridine (2 not 3) is put on the left side.

1.9 Polynoxylin (INN)

The WHO designation is:

'Poly{methi[bis(hydroxymethyl)] ureylene } amer'.

It is somewhat unusual in this form and is found first from the formula in the Merck-Index pattern:

27 

According to this, it is a polymerization of urea and formaldehyde. It is a single strand substituted polymer. The naming order is determined on the basis of the seniority of the hetero atom with the shortest substituted route to other hetero atoms. This forms the sub unit 'ureylene' in the complete RU. The structure-based designation thus formed is

Poly[1,3-bis(hydroxymethyl)ureylenemethylene]

1.10 Polyhexanide (INN)

The WHO designation is:

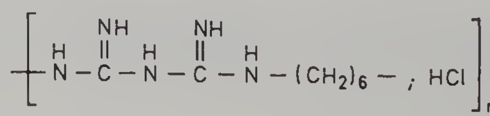
'Poly[imino(imidocarbonyl)imino(imidocarbonyl)imino(hexamethylene) monohydrochloride]' ($C_8H_{17}N_5$xHCl)

Only the outer brackets are present in the WHO name, and were inserted here to aid recognition of the sub-units. Without the salt designation, this name requires six sub-units in the RU.

'Imidocarbonyl' is a permitted C.A. diradical for the group

28 $HN{=}C<$

The structure which the name yields is

29 

'Imidocarbonyl' is not a recommended IUPAC term. If necessary 'iminomethylene' would be an acceptable IUPAC term. However, the type of name formed above, because of the imino/imido contrast, is a suitable means of making the name (without the brackets) understandable. Such a structure-based name following IUPAC principles can also be formed, making use of replacement nomenclature and thereby greatly simplifying matters. This gives rise to an RU with no sub units:

Poly(2,4-diimino-1,3,5-triazaundecamethylene hydrochloride).

From the nomenclature here it is noteworthy that the use of this poly(diradical), can give rise to a change of C to N at the beginning or end position of the chain. If it were a case not of a diradical, but a similar 'a' molecule, such a change would not be permitted. In such a case,the molecule would have to be named by replacement nomenclature as:

1,3-Diimino-2,4-diazadecan-1-amine hydrochloride.

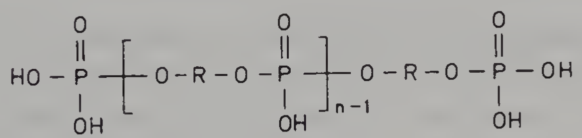
It must be noted that such recognized radical names as amidino and guanidino may not be used here, since they are monoradicals, while names for diradicals are needed here.

1.11 Polyestradiol phosphate (INN)
The WHO states only:

'Estradiol phosphate polymer; approximately $(C_{18}H_{22})_m(O_4P)_n$'

In the empirical formula, the organic part corresponds to the estradiene diradical. There is no H in the inorganic part. That can be taken as an indication that a multiple esterification occurred, and no single strand polymer remains, which could have made a structure-based designation feasible. Merck-Index (9. Ed. 1976) has the formula for a namable polymer which must, however, be considered as much idealized:

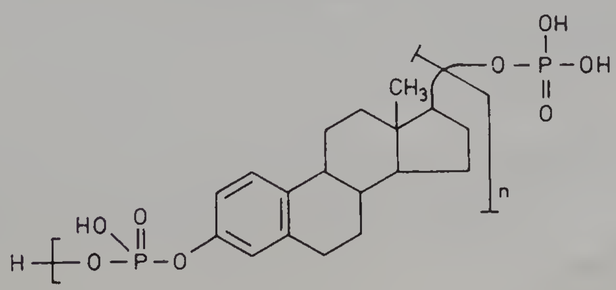
30



-O-R-O- is the diradical from estradiol; n ≈ 80.

All the same, it is interesting to discuss the possible nomenclature for this idealized formula, even though it does not fit the empirical formula in principle. Several subunits are combined to form the RU. They consist of heteroatoms and a carbocyclic compound. The oxygen has seniority and thereafter the phosphorus. This is not cited as such, but appears in the form of an oxidation stage. The repeating unit (RU) for the nomenclature shows a modification of the above formula, the structure:

31



This results in the composite RU

[oxy(phosphinico)oxy(1,3,5(10)-estratriene-3,17β-ylene)].

The end groups, from the Merck-Index, are 'hydro' and 'phosphonoxy'.

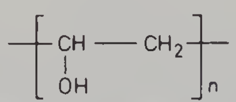
2. Substituted C-chains

2.1. Polyvinyl alcohol, polyvinyl chloride

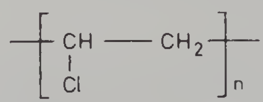
These two polymers, which merit some discussion here, are by no means insignificant in the pharmaceutical area. The two monomers have analogous structures:

32 $H_2C = CH(OH)$	**33** $H_2C = CHCl$
Vinyl alcohol (unstable)	Vinyl chloride

Likewise, the resulting polymers have analogous formulae, analogous RUs, and analogous names:

34 

trivial:
Polyvinyl alcohol
structure based:
Poly(1-hydroxyethylene)
short: PVAL

35 

trivial:
Polyvinyl chloride
structure based:
Poly(1-chloroethylene)
short: PVC

The names cite the OH-group and the Cl-atom respectively as prefixes, representing substituents on the polymer C-chain. The treatment of the OH-group in polymer nomenclature is shown here to be different from the usual organic chemistry nomenclature for 'alcohols', while the nomenclature for the halogen compound follows the usual nomenclature procedure.

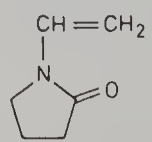
2.2 Polyvinyl pyrrolidone (trivial)

Polyvidone (INN) (DAB 9)

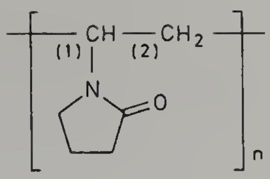
In the WHO third cumulative list, the substance is described as

'Polymer of 1-vinyl-2-pyrrolidinone'

Thus the monomer has the structure:

36 

The following resulting polymer is:

37 

syst.: DAB 9: Poly[(2-oxo-1-pyrrolidinyl)ethylene]$_n$

From the WHO description, at least the trivial name can be derived. A structure-based name should go further and show that the pyrrolidone is not in the principal chain, but is a substituent in a side chain. It must therefore appear in the name as a prefix. The IUPAC acceptable name would be:

Poly[(2-oxo-1-pyrrolidinyl)ethylene]

2.3 Polymethacryl acid esters

(Example methyl ester ‘Perspex®’)

‘Methacrylic acid’ is the IUPAC acceptable trivial name for

38 $$\underset{(3)}{H_2C} = \underset{(2)}{\overset{CH_3}{\overset{|}{C}}} - \underset{(1)}{\overset{O}{\overset{\|}{C}}} - OH$$

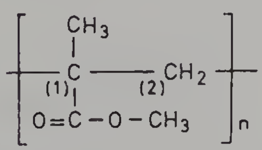
2-Methylpropenoic acid (cf. IV formula 371)

The methyl ester

39 $$H_2C = \overset{CH_3}{\overset{|}{C}} - \overset{O}{\overset{\|}{C}} - O - CH_3$$

Methyl methacrylate, methacrylic acid methyl ester
Methyl 2-methacrylate, methyl 2-methylpropenoate

polymerises easily to a polymer of the formula

40 

which shows a substituted RU.

The IUPAC name is

trivial: Polymethyl methacrylate, short: PMMA
structure based: Poly[1-(methoxycabonyl)-1-methylethylene].

The pharmaceutical preparation Eudragit®, which is used as a coating medium, belongs to this group of polymers.

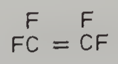
The substituents on the same C-atom of the chain are cited in alphabetical order. The substituted C-atom has seniority over the $-CH_2-$ and is put at the left end of the RU, and bears locant 1.

2.4 Polytef (INN)

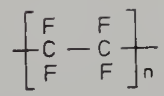
The WHO name is:

'Poly(tetrafluoroethylene)'

From this are given the structures:

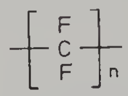
41 

Monomer

42 

Polymer; short form: PTFE

The WHO name is also the IUPAC one. There is also

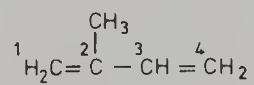
43 

Poly(difluoromethylene)

for the halved formula (halved RU).

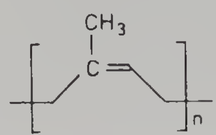
2.5 Polyisoprene

Isoprene is an unsaturated branched hydrocarbon of the formula

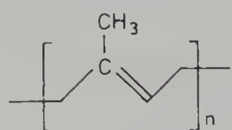
44 

systematic name: Methylbutadiene (cf. I formula **61**).

Isoprene polymers are natural rubbers and guttapercha, which differ by virtue of their steric dispositions.

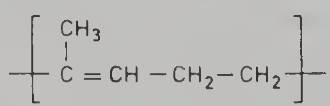
45 

Rubber
all-*cis*-Polyisoprene (all-*Z*)

46 

Guttapercha
all-*trans*-Polyisoprene (all-*E*)

The polymer nomenclature is carried out so as to give the lowest possible locant to the double bond, which is at the left, and of the structural repeating unit. While the polymer formulas above are automatically produced from the isoprene formula, the formula arrangement for nomenclature purposes leads to the following form:

47 

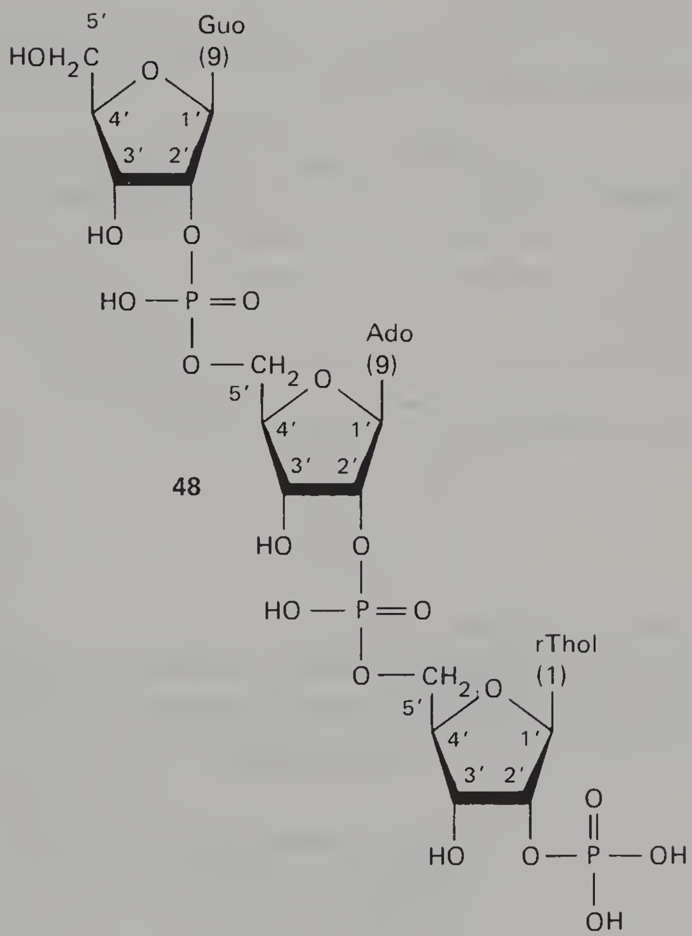
From this comes the systematic name of the polymer:

(all-*Z*)
or -Poly(1-methyl-1-butenylene).
(all-*E*)

3. Oligo-, polynucleotides
(Literature: Hoppe-Seyler's *Z. Physiol. Chem.* **351**, p. 1055 [1970])
(cf. Nucleosides V7.4; Nucleotides V. 7.6)

Designating junction points between mononucleotides which are linked 3′/5′ is unnecessary. Other linking can be designated in two ways:

(a) Single junction, e.g. Guo-2′*P*5′-rAdo
(b) Series of junctions e.g. (2′-5′)Guo-*P*-Ado-*P*-rThd-2′*P* (formula **48**)



48

In a row of nucleotides without locants, end-position *P* is taken as

end-position *P* left, a 5′-phosphate

end-position *P* right, a 3′-phosphate

Using single-letter symbols, phosphoric acid ester radicals are designated by 'p' (not italic):

(c) . .-Ap . . .Adenosine- 3′-phosphate (3′ in the symbol is not cited)
(d) . .A2′p5′I. . Adenosine- 2′-phosphate ester with 5′-Inosine
(e) . .A3′-5′I. . with 3′-5′, 'p' is replaced by '-' (known sequence)
(f)[6] . .A-I. . if no locants are cited, the esterification of phosphoric acid left in 3′ and right in 5′ is understood.
(g)[6] . .A,I. . if the sequence is not known, then the '-' in (f) is simply replaced by ','.
(h)[6] (3′-5′)A-I-A-I. . Phosphoric acid is esterified in each case left in 3′, right in 5′ (Ado-3′P5′-Ino-3′P5′-Ado-3′P5′Ino. .).
(i) A→I→A→I. . as (h); the arrow direction denotes the direction of the 3′-5′ ester bond, without citing the locants however.

In (c) 'p' signifies (end-position) -$PO(OH)_2$, and thus simple esterification. In (d)–(h) 'p' or '-' signify mid-position –PO(OH)–, and thus double esterification.

Where esterification is not in the 3′-5′ direction, or not in the arrow direction, respectively, but in the reverse direction, the locants in the reverse order can be placed before the name in brackets.

[h):(5′-3′)] or the arrow direction can be changed [i):←] .

The symbols can alternatively be simply written upside-down.

4 Nucleic acids

4.1 High-polymer nucleotide chains

For the representation of, or exchange of ideas on, this group, the simplest possible means, the conventional, established specific single-letter symbols, are used. They are combined on the pattern analogous to that of the oligo-nucleotides, with the indeterminate prefix 'poly'.

poly(N)	polynucleotide (unspecified)
poly(I-dT)	copolymer of alternating inosine/thymidine nucleotide units
$)_{80}$	chain length 80 units

6 In current literature, single-letter symbols are placed one next to the other without hyphens.

$)_{\overline{80}}$	average chain length 80 units
$)_{70-90}$	range of chain length
	A number index 'n' signifies 'unknown'. Further such indices within the same polymer are designated with other small letters.
poly(I,dT)	The subunits are statistically distributed.
poly[d(I-T)] or poly(dI-dT) or $d(I\text{-}T)_n$ (without 'poly')	The subunits 2′-deoxyinosine and thymidine alternate in the polymerized nucleotide.

Non-covalent bonds (e.g. hydrogen bonds) are not given with hyphens but with raised decimal points (not full stops) (association):

poly[d(I-T)] · poly[d(I-T)] or

poly[d(I-T)· d(I-T)

Lack of association between chains is indicated by (+):

poly[dI) + poly(dT)

4.2 Trivial name abbreviations

The following are established trivial designations:

RNA (ribonucleic acid)	
DNA	deoxyribonucleic acid
mRNA	messenger RNA
rRNA	ribosomal RNA
nRNA	nuclear RNA
tRNA	transfer RNA
cRNA	complementary RNA
mtRNA	mitochondrial RNA
mtDNA	mitochondrial DNA

Alanine tRNA	non-acylated alanine specific transfer RNA
Alanyl-tRNA or Ala-tRNA or $\text{Ala-tRNA}^{\text{Ala}}$	aminoacylated alanine specific transfer RNA

(here the hyphens represent the aminoacyl bonds).

VII

Etymological and other guidance on the derivation and explanation of scientific terms

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abeo from the Latin *abire* to go away
acetate from the Latin *acetum* vinegar (acetic acid)
acetone see preceding entry
acid from the Latin *acidus*, sour
aliphatic from the Greek *aliphar*, salve, oil; refers generally to a C-chain structure; the Greek stem-name refers to fats and fatty materials ('mineral oils').
alkaloid from the Arabic *ali-quali* salt-containing plant ash, + the Greek *eidos* appearance (. . .*oid*, of similar form).
allose from the Greek *allo* other.
altrose from the Latin *alter* other
amphion from the Greek *amphi* on both sides, all around.
amphoteric from the Greek *amphoteros* of both kinds.
androstane from the Greek *andros* a man.

anellation from the Latin *anellus* a ring.
aniline from the Portuguese *anil* indigo plant
anomer from the Greek *ano* above + *meros* part (in sugars, change in the configuration at the 1 position)
anthracene from the Greek *anthrax* coal
antimony from the Arabic *al ithmidum* grey antimonite (Sb_2S_3)
apo from the Greek *apo* from, away
arabinose from the Latin *arabia* from its occurrence in 'gum arabic'
arachidonic acid from the botanical name of the peanut, *arachis hypogaea*
asymmetry from the Greek *a* (negation): un. . ., without, and symmetry
atropine from the Greek *a*, see above, + *tropin* turn; cf. Atropos Green goddess of fate
azo from the French *azote* nitrogen (from the Greek *a* + *zoe* life)
azulene from the Spanish *azul* blue

bilin from the English *bile*
bisma from the German *Wismut* (latinized to bismutum)
bora, boron from the Arabic *bauraq* borax
bromine from the Greek *bromos* stink
bufenolide from the Latin *bufo* toad
butane from the Greek *butyron* butter

carb. . from the Latin *carbo* coal
cardenolide from the Greek *kardia* heart
catechin from the Malay *katechu* extract from the wood of *Acacia catechu*
chiral from the Greek *cheiro* hand, fist
chloro from the Greek *chloros* yellow-green
chloroform see form. .
chlorophyll see chloro plus the Greek *phyllon* leaf: leaf green
chol. . . from the Greek *chole* gall
chromo from the Greek *chroma* colour
cocaine from the Quechua (ancient Peruvian) *coca*
coumarin from *coumaru*, the indigenous name in northern South America for the seeds (tonka beans) of *dipteryx odorata*. These contain melilotoside, from which coumarin is formed.
cyano from the Greek *kyanos* blue
cyclo from the Greek *kyklos* circle, ring
cystine from the Greek *kystis* bladder
cytidine, cytosine from the Greek *kytos* hollow, cell . . .

desmotropy from the Greek *desmos* bond and Greek *trope* (see tropine)
digitoxin from the Latin *digitus* finger and Greek *toxicon* (arrow)poison

ecgonine from the Greek *ekgonos* derived from (with reference to cocaine)
enantiomer (ent) from the Greek *enantios* opposite, opposing + *meros* part
enantiomorph see above, plus Greek *morphe* shape or form

epi from the Greek *epi* at, on
epimer see above and . . . .*mer*; with sugars, change of configuration at the 2 position
erythro from the Greek *erythros* red (for the configuration of the tetrose from the red algae erythrina, = erythrose)
estro. . (oestro. .) from the Greek *oistros* frenzy, sting; in a broad sense, lust, heat
ether from the Greek *aither*, space

flavin from the Latin *flavus* yellow
flavone see above (yellow flower colouring)
fluoro from the Latin *fluere* flow (on account of the use of fluorspar CaF_2 as a flux)
form. . ., . . .form from the Latin *formica* ant (formic acid 1C; and likewise formaldehyde, the formyl group and for example chloroform)
fulven from the Latin *fulvus* reddish yellow
furan, furfuryl from the Latin *furfur* bran

galactose from the Greek *galactos* milk
gem. . from the Latin *gemini* twins
glucose from the Greek *glykys* sweet
glutamic acid from the Latin *gluten* glue
glycerol from the Greek *glykeros* sweet
glycine see glucose
gonene from the Greek *gone*, offspring
guanidine from Quechua *huano* guano (bird-dung)
gum from the Greek *kommi*
gutta-percha from the Malay *guttah* gum + *percha* a tree producing it

halogen from the Greek *halos* salt + *gennao* to produce
hemi from the Greek *hemysis* half
hemin from the Greek *haima* blood
hetero from the Greek *heteros* different, foreign
hippuric acid from the Greek *hippos* horse + Latin *urina* urine (on account of its occurrence in horse-urine.
histidine from the Greek *histos* web
homo from the Greek *homos* same, like (e.g. homogeneous)
homologous from the Greek *homologeo* corresponding (in nomenclature, a homologous series has a constant difference between successive members of the series (+ CH_2)
hydro from the Greek *hydor* water (a prefix for added hydrogen)
hyper from the Greek *hyper* above
hypo from the Greek *hypo* below

iodine from the Greek *ioeides* violet-blue (from the colour of iodine vapour)
iso from the Greek *isos* equal
isomerism see *iso* and . .*mer*

lactose from the Latin *lac* milk
leucine from the Greek *leukos* white
lyse break down, decompose from the Greek *lysis* loosening

macro from the Greek *makros* large
maleic acid from the Latin *malus* apple
malic acid from the Latin *malus* apple
malonic acid from the Latin *malus* apple
mannose from the Aramaic/biblical *manna*
mer from the Greek *meros* part
mercapto from the Latin *mercurio captum* (due to the mercury-capturing behaviour of thioalcohols, mercaptans, which form mercury salts) or mercurio aptum
mercury from the Latin *Mercurius* the messenger of the gods; Mercury
meso from the Greek *mesos* middle
methane from the Greek *meta* within, between, behind (indicating the change of the substrate, forming methane by fermentation)
morphine from the Latin *Morpheus* the god of dreaming

naphthalene from the Persian *nafta* flammable liquid
nicotine from J. *Nicot*, french diplomat 1530 to 1600, who brought tobacco to France.
nitro from the Greek *nitron* saltpetre
nor 1. for 'normal' (conversion of a branched-chain amino acid (e.g. valine) to an unbranched amino acid with the same number of C-atoms (5) norvaline (no longer IUPAC)
2. identical to 'demethyl' in subtractive nomenclature, e.g. 8,9,10-trinorbornane ($-3CH_2$)

oestro see estro
oligo from the Greek *oligos* few
ornithine from the Greek *ornis* bird
ortho from the Greek *orthos* correct, straight
ozone from the Greek *ozo* smell

p(ara) from the Greek *para* by, next
phenol from the Greek *phaino* gleam, shine + Latin oleum oil
phloroglucin from the Greek *phloios* bark + *rhiza* root + *glykys* sweet
phosphorus from the Greek *phaos* light + *phero* carry
pi (16th letter of the Greek alphabet), locant in histidine (from the Greek *pros* near, refers to the relative side-chain position)
picric acid from Greek *pikros* bitter
poly from the Greek *polys* many
polymer see above and . .*mer*
porphyrin from the Greek *porphyreos* purple colour
propionic acid from the Greek *protos* first + *pion* fat (the lowest member of the fatty acid series, which is similar to higher members of the series)
psi (23rd letter of the Greek alphabet) end-group in the carotenes; short for pseudo (trivial) from the Greek *pseudos* lie, deception
purine from the Latin *purus* pure + *ur*. . (q.v.)
pyridin pyrimidine see pyro
pyro from the Greek *pyr* fire, *pyretos* heat, fever (cf. antipyrine R, pyramidon R)

pyrolyse see pyro and . .lyse (break down by heating, dry distillation), e.g. pyruvic acid

pyrrole from the Greek *pyrros* flame-coloured, yellowish red (on account of the red colour produced by HCl on spruce wood)

quinine from the Indian *quina* chinchona bark

racemic, racemate from the Latin *racemus* grape, grape juice (from the racemic tartaric acid found in wine, a model for optically inactive mixtures formed from equal amounts of optical opposites)

retro from the Latin *retro* back, backwards

riboflavin see . .flavin

sarcosine from the Greek *sarx* flesh (*N*-methylglycine)

scopolamine after Giovanni Scopoli 1723–1788, Italian scientist

sec- from the Latin *secundus* second, next (secondary C-radical $R-\underset{\bullet}{C}H-R'$)

seco from the Latin *secare* to cut

semi from the Latin *semi* half

serine from the Latin *serum* whey

silicon from the Latin *silex* pebble, flint

stereo from the Greek *stereos* solid, fixed

stiba from the Latin *stibium*, Greek *stibi*, for antimony in, for example, the Hantzsch–Widman system

stilbene from the Greek *stilbo* shine, gleam

tau (19th letter of the Greek alphabet) for the Greek tele distant, as locant in histidine (relative side-chain position)

taurine from the Latin *taurus*; Greek *tauros* bull; 2-aminoethanesulfonic acid, which was first discovered in bovine bile

tautomerism contraction of the Greek *to auto* the same + . .*mer* (see above)

thio from the Greek *theion* sulphur

thyroxin from the Greek *thryeos* shield (3,3′,5,5′-tetraiodothyronine)

tropine from the Greek *trope* movement, change (see atropine)

tyrosine from the Greek *tyros* cheese

ur. ., . .ur indicating urea derivatives, from the Latin *urina* urine

ursane parent hydrocarbon of ursolic acid which was found in 'bear-berry' leaves (from the Latin *ursus* bear)

vinyl from the Latin *vinum*, wine, for its component ethanol with C_2

xanthene from the Greek *xanthos* yellow (from the colour of the compound)

xylose from the Greek *xylon* wood (due to the extraction of the material from hemicellulose, e.g. from wood)

yl, ylene from the Greek *hyle* material

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