

Naming and Indexing of Chemical Substances for Chemical Abstracts™

2007 Edition



A publication of Chemical Abstracts Service

Published by the American Chemical Society

Naming and Indexing of Chemical Substances for Chemical Abstracts™

A publication of Chemical Abstracts Service
Published by the American Chemical Society

Copyright © 2008 American Chemical Society
All Rights Reserved.
Printed in the USA

Inquiries concerning editorial content should be sent to:
Editorial Office, Chemical Abstracts Service, 2540 Olentangy River Road, P.O. Box 3012, Columbus, Ohio 43210-0012 USA

SUBSCRIPTION INFORMATION

Questions about CAS products and services should be directed to:

United States and Canada:

CAS Customer Care
2540 Olentangy River Road
P.O. Box 3012
Columbus, Ohio 43210-0012 USA

Phone: 800-753-4227 (North America)
614-447-3700 (worldwide)
Fax: 614-447-3751
E-mail: help@cas.org

Japan:

JAICI (Japan Association for International
Chemical Information)
6-25-4 Honkomagome
Bunkyo-ku, Tokyo
Japan, 113-0021

Phone: 81-3-5978-3621
Fax: 81-3-5978-3600
E-mail: customer@jaici.or.jp

Countries not named above: Contact CAS Customer Care, 2540 Olentangy River Road, P.O. Box 3012, Columbus, Ohio 43210-0012 USA; Telephone 614-447-3700; Fax 614-447-3751; E-mail help@cas.org. For a list of toll-free numbers from outside North America, visit www.cas.org.

NAMING AND INDEXING OF CHEMICAL SUBSTANCES

101. Foreword. Although the account which follows describes in considerable detail the selection of substance names for *Chemical Abstracts (CA)* indexes, it is not a nomenclature manual. It has the more restricted aim of enabling a user of *CA* indexes to proceed from the structure of an individual chemical compound to the place in the current *Chemical Substance Index* where the particular index name and any associated index entries will be found. This is the identical operation performed by a *CA* indexer when assigning an index name to a new or previously unnamed substance. What follows, in fact, is a comprehensive summary of *CA* substance indexing policies, which cover not only conventional organic and inorganic compounds but other completely defined substances entered in the *Chemical Substance Index* and given CAS Registry Number® identifiers. These substances include specific chemical elements, alloys, minerals, mixtures, polymers, enzymes, polysaccharides, and elementary particles.

The chemical nomenclature used by Chemical Abstracts Service (CAS) has developed in parallel and generally in accordance with the rules published by the International Union of Pure and Applied Chemistry (IUPAC). Although these rules provide unambiguous text equivalents for the great majority of substances, equally acceptable alternative rules within the present IUPAC system often lead to two or more unambiguous names. This causes no difficulty in normal scientific communication, but is totally unacceptable in a formal, rigidly controlled, alphabetic listing such as the *Chemical Substance Index*. Here the names must be not only unambiguous, unique, and totally reproducible, but selected so as to bring the names of structurally related substances into juxtaposition in the alphabetical listing. They must be equally derivable by index users searching for information about individual substances and by those who prepare the index. It is also desirable that both should be able to use mechanical aids in name generation and retrieval.

A major revision of *CA* index names was carried out in 1972 as the Ninth Collective Index period began. Most trivial names were dropped; exceptional treatment for various classes of substances was discontinued. Where, because of the stereochemical complexity of a natural product name, a trivial name was retained as a "stereoparent" (see ¶ 202), diagrams were furnished in the *Chemical Substance Index* to aid interpretation of index entries. The 1972 nomenclature revision and the reasons for its adoption are set forth in greater detail in the Ninth Collective Index Guide and in a journal article (*J. Chem. Doc.* **1974**, **14**(1), 3-15).

The preferred *CA* index names for most chemical substances have been continued unchanged since that date. Changes in name-selection policies for the Twelfth (1987-1991) and Thirteenth (1992-1996) Collective Index periods affect alloys, carbohydrates (lactams), coordination compounds, formazans, index name selection (multiplicative names), inorganic compounds (line formulas of clusters, intermetallic compounds), molecular addition compounds (common components; hydrates), nitrilimines, onium compounds (free radicals), peptides, phosphonium ylides, phosphoryl halides and halogenoids, polymers (block, graft, and hydrolytic), ring systems (list of common systems), salts (lists of common anions), stereochemistry (sign of optical rotation), and

zwitterions (inner salts, sydnones). The changes for the Fourteenth (1997-2001) Collective Index period affect coordination nomenclature, stereochemical practices, and stereoparents. The most recent changes (2007) involve locants, tautomers, and stereoparents. These changes, as well as the changes made in 1972, and in the Tenth (1977-1981) and Eleventh (1982-1986) Collective Index periods, are reviewed in Section G (¶¶ 225-293). The nomenclature of fullerenes is more fully documented in ¶ 163A of Section B.

The arrangement of sections is as follows:

- A. Nomenclature Systems and General Principles (¶¶ 103-139)
- B. Molecular Skeletons (¶¶ 140-163A)
- C. Principal Chemical Groups (Suffixes) (¶¶ 164-177)
- D. Compound Classes (¶¶ 178-201)
- E. Stereochemistry and Stereoparents (¶¶ 202-212)
- F. Specialized Substances (¶¶ 213-224)
- G. Chemical Substance Names for Retrospective Searches (¶¶ 225-293A)
- H. Illustrative List of Substituent Prefixes (¶ 294)
- J. Selective Bibliography of Nomenclature of Chemical Substances (¶¶ 295-308)
- K. Chemical Prefixes (¶¶ 309-311)
- L. Chemical Structural Diagrams from *CA* Index Names (¶¶ 312-318)
- M. Index

The arrangement within each of these sections is indicated by a key at the beginning of the section.

In the development of CAS policies for index names of chemical substances, no new nomenclature systems have been devised. Adaptation of current IUPAC rules to the specific needs of a highly ordered alphabetical index, not arbitrary coinage of new terms, has been the approach taken. It continues to be recognized by CAS that, while a unique name is needed for an index, and that this name, and the CAS Registry Number, are invaluable aids for substance identification, the use of this invariant index name for citation throughout every context in the scientific community is neither practicable nor desirable. But international agreement in chemical nomenclature, as embodied in the rules of IUPAC, IUB, and other organizations, continues to be of the greatest importance in restricting the *arbitrary* proliferation of substance names. References to individual rules which have formed the basis of CAS policies recorded in the sections that follow have not been cited, but the selective bibliography of the nomenclature of chemical substances which constitutes Section J contains a comprehensive list of current accepted rules.

102. Acknowledgement. CAS acknowledges the large contribution made by Cecil C. Langham in helping to develop and record *CA* name-selection policies for the Eighth Collective period (1967-1971) during the years immediately preceding his retirement in 1969. Dr. Langham's work constituted an invaluable starting point for the revised name-selection policies introduced in 1972.

A. NOMENCLATURE SYSTEMS AND GENERAL PRINCIPLES

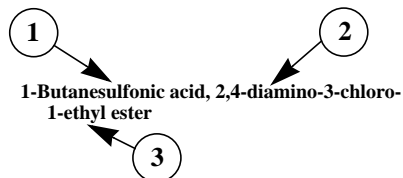
Introduction	¶ 103	Order of citation of derivative terms	¶ 113
Inversion of names	104	Locants	114
Name selection principles	105	for substituent suffixes	115
Order of precedence of compound classes	106	in substituent prefixes (radicals)	116
Spelling	107	for substituents on parents and parent radicals	117
Punctuation	108	in multiplicative nomenclature	118
Enclosing marks	109	for functional derivatives	119
Multiplicative prefixes	110	for indefinite compounds	120
"Mono"	111	Alphabetization	121
Functional derivatives	112		

Tautomeric compounds	¶ 122	Substituent suffixes	¶ 131
Additive nomenclature	123	Substituent prefixes	132
Conjunctive nomenclature	124	Compound radical names	133
Multiplicative nomenclature	125	Carbonyl radicals	134
Radiocofunctional nomenclature	126	Indicated hydrogen	135
Replacement ("a") nomenclature	127	Added hydrogen	136
Replacement prefixes	128	Numbering of molecular skeletons	137
Replacement nomenclature for functions	129	Index name selection	138
Substitutive nomenclature	130	Subtractive nomenclature	139

103. Introduction. Many names may be employed in scientific publications for a single compound. Even so simple a compound as $\text{H}_2\text{NCH}_2\text{CH}_2\text{OH}$ can be named 2-Aminoethanol, 2-Aminoethyl alcohol, 2-Hydroxyethylamine, β -Hydroxyethylamine, 2-Hydroxyethanamine, 1-Amino-2-hydroxyethane etc., all of which describe it unambiguously; often, the less systematic ("trivial") name Ethanolamine may be encountered. For more complex compounds, the number of possible names increases exponentially.

In these circumstances, selection rules are essential if a single preferred name for citation in an index of chemical names is to be determined for each identifiable substance; lacking such a single name, information regarding the substance becomes scattered in the index. Beyond this, it is desirable that the selection rules bring chemically related substances close together in the index, and that they should be as consistent and as free from exceptions as possible.

104. Inversion of names. Ordering in the *Chemical Substance Index* is based on the *index heading parent* (1), which is often made up of a basic skeleton name, e.g., "**Butane**," plus a suffix denoting the principal function, e.g., "**-sulfonic acid**." A locant, e.g., "**1-**," fixing its position is also often necessary. Following a comma (the *comma of inversion*) the substituents (2) are expressed in alphabetical order, e.g., "**2,4-diamino-3-chloro-**" and the *modification* (3), now printed in boldface, completes the name by citing any derivatives of the principal function, e.g., "**ethyl ester**," and stereochemical information (see ¶ 203) if appropriate. The uninverted name of the *acid* is 2,4-diamino-3-chloro-1-butanefulfonic acid, and of the ester, ethyl 2,4-diamino-3-chloro-1-butanefulfonate. The latter appears in the *Chemical Substance Index* as follows:



Also appearing in the boldface headings of certain very well-known substances are subdivision terms describing properties, etc., of the compound itself, or classifying certain derivatives of it, e.g., **reactions, esters**.

105. Name selection principles (see also ¶ 138). In choosing **1-Butanesulfonic acid** as the heading parent in the example above, rather than, for example, 1,3-Butanediamine, an order of precedence of chemical functions and compound classes (¶ 106) was followed. In this hierarchy, sulfonic acids are ranked higher than amines. In the example cited, so-called substitutive nomenclature (¶ 130) was the type of nomenclature used. Generally, a preferred index name is determined by proceeding as follows until a decision is reached:

- determine the most senior compound class;
- determine the type of nomenclature that is appropriate;
- determine the preferred index heading parent;
- name the remainder of the structure as substituents, and/or as functional derivatives by modification phrases;
- choose between alternatives where more than one unambiguous name is still possible.

The remainder of Section IVA is devoted to detailing the application of these rules.

106. Order of precedence of compound classes, in descending order:

- Free radicals and compounds for which substituent prefixes are unavailable, e.g., **Sulfur diimide** (¶ 200).
- Cationic compounds: coordination cations, onium, aminium, ylium cations.
- Neutral coordination compounds, including metallocenes.
- Anionic compounds, e.g., **Borate(1-)**.
- Acids: peroxy acids, expressed as principal groups, in the order of the parent acids; acids, expressed as principal groups, in the order carbon,¹ sulfur, selenium, tellurium; acids, expressed as functional parent compounds (¶ 130), in the order carbon (including **Carbonic acid** and **Formic acid**; see ¶ 183), chalcogen, nitrogen, phosphorus, arsenic, antimony, silicon, and boron.
- Acid halides and related species, first in the order of the parent acid (see (e), above); then, for each acid, in the order fluoride, chloride, bromide, iodide, azide, isocyanate, isothiocyanate, isocyanide, cyanide (for non-carbon acid residues only).
- Amides, in the same order as the parent acids (see (e), above).
- Nitriles, in the same order as the parent acids (see (e), above).

- Aldehydes, Thiols, Selenals, Tellurals.
- Ketones, Thiones, Selones, Tellones.
- Alcohols and Phenols (of equal rank), Thiols, Selenols, Tellurols.
- Hydroperoxides.
- Amines.
- Imines. (This is the lowest compound class expressed by a functional suffix; all the following classes are considered to be nonfunctional. For the ranking of nonfunctional cyclic and acyclic skeletons, see ¶ 138.)

(o) Nitrogen compounds: heterocyclic; acyclic (other than "a"-named chains; see ¶ 127), e.g., **Triazane, Diazene, Hydrazine, Hydroxylamine, Thiohydroxylamine**.

(p) Phosphorus compounds: heterocyclic, acyclic (other than "a"-named chains; see ¶ 127), e.g., **Diphosphine, Phosphine oxide, Phosphine sulfide, Phosphine imide, Phosphorane, Phosphine**.

- Arsenic compounds (in similar order).
- Antimony compounds (in similar order).
- Bismuth compounds (in similar order).
- Boron compounds: carboranes, hetero polyboranes, polyboranes, heterocyclic, **Borane**.

(u) Silicon compounds: heterocyclic, acyclic (other than "a"-named chains; see ¶ 127), e.g., **Disiloxane, Disilathiane, Trisilane, Disilane**. Note that the order is determined first by the total number of skeletal atoms, then by the presence of oxygen, sulfur, etc; see ¶ 128.

- Germanium compounds (in similar order).
- Tin compounds (in similar order).
- Lead compounds (in similar order).
- Oxygen compounds other than "a"-named chains (see ¶ 127): heterocyclic; acyclic polyoxides, e.g., **Trioxide, Peroxide**.

(z) Sulfur compounds: heterocyclic; acyclic polysulfides and their oxides, e.g., **Trisulfone, Trisulfide, Disulfone, Disulfoxide, Disulfide**.

- Selenium and tellurium compounds (in similar order).
- Carbon compounds: carbocyclic
- Silane
- Carbon compounds: acyclic

107. Spelling. CAS accepts *Merriam-Webster's Collegiate® Dictionary*² as the primary authority for spelling; e.g. sulfur (not sulphur); aluminium (not aluminum). *Random House Webster's Unabridged Dictionary*³ is used for words not found in the *Collegiate Dictionary*. Elision of vowels is often practiced in combining the segments of names: e.g., in **Butanone** and disiloxanyl the final "e" of the basic skeleton name has been dropped; in **Oxazepine** an "a" has been omitted twice, after "oxa" and before "ep"; and "a" is often omitted before a multiplied "amine" or "one" suffix, as in **Benzenetetramine** and **Cyclohexanehexone**; the terminal "o" of acenaphtho, benzo, naphtho, and peroxy, and the terminal "a" of cyclobuta, etc., are elided before vowels, e.g., **Benz[cd]indole, 5H-Cyclobut[fi]ndene**. Other examples of elision are -imidic (not -imidoic) acids; -imidamides (not imidoamides); -thiones (not thioones); and -hydrazonamides (not -hydrazonoamides). Examples will be found in later paragraphs. In a few cases, the vowel "o" is added for euphony, e.g., **Carbonothioic acid** (not Carbothioic acid).

Elision of entire syllables is now uncommon. Remaining examples include methoxy, ethoxy, propoxy, butoxy, phenoxy (not methyloxy), etc.) radicals, and the thienyl (not thiophene-yl) radical. **Carbamic acid** is an elided form of Carbonamidic acid (¶ 183); **Sulfamic acid** is used in place of Sulfuramidic acid, and **Sulfamide** instead of Sulfuramide or Sulfuric diamide. The suffix "-carboxylic acid" undergoes various forms of elision in formation of replacement names, e.g., "-carbothioamide."

108. Punctuation in chemical names is frequently of great importance in removing ambiguities and in differentiating one substance from another. Lower case italic Roman letters are used in fusion prefixes (¶ 151) in ring system names, and in *as-* and *s-Indacene*; capital italics such as *N-*, *O-*, *P-*, *S-*, are locants indicating substitution on these hetero atoms; *H-* denotes indicated or added hydrogen (¶¶ 135, 136); italic Arabic numerals are locants for atoms in abnormal valency states (¶ 158) and for "labeled" atoms (¶ 220); italic words and syllables are used in modifications to express isomeric oxides, e.g., *thiono-*oxide at a thio acid heading parent, and in stereochemical descriptors (¶ 203), e.g., *erythro-*, *tetrahedro-*. The small capitals *D-*, *L-*, and *DL-*, are configurational descriptors (¶ 203); like italic letters, they are disregarded in placing chemical names in order until Roman letters have been alphabetized.

The "comma of inversion" has been mentioned above (¶ 104). Other commas are used between individual locants in index heading parents, substituents,

¹Acetic acid and Benzoic acid are ranked here as though they were named Ethanoic acid and Benzenecarboxylic acid, respectively.

²*Merriam-Webster's Collegiate® Dictionary*, 11th ed., Merriam-Webster, Springfield, MA, 2003.

³*Random House Webster's Unabridged Dictionary*, 2nd ed., Random House, N.Y., 2001.

and modifications. Different *types* of functional derivatives are separated by commas in the text of the modification.

Examples:

- (a) **hydrazone phenylhydrazone**
- (b) **diethyl ester, sodium salt**
- (c) **ethyl methyl ester, hydrochloride**

Hyphens at the end of the set of substituents in the inverted part of a bold-face heading signify that no space is intended when the name is uninverted for use in textual matter. Conversely, absence of a hyphen after substituents at headings such as **Disulfide**, **Hydroperoxide**, **Peroxide**, indicates that a space appears at that point in the uninverted name.

Examples:

Acetic acid, 2-chloro-	(index name)
2-Chloroacetic acid	(uninverted name)
Disulfide, bis(2-chloroethyl)	(index name)
Bis(2-chloroethyl) disulfide	(uninverted name)

Hyphens separate locants from the words and syllables of a name; when used between locants, the intention is to indicate that such locants refer to different parts of the name; e.g., in **Acetamide, N-2-naphthalenyl-**, the “N-” places the 2-naphthalenyl substituent on the nitrogen of the heading parent, **Acetamide**.

Periods separate ring size descriptors in Von Baeyer and spiro names, e.g., **Bicyclo[3.2.0]heptane**. Colons separate sets of locants already related to one another; if a further step is called for, semicolons are employed.

Examples:

1,4:5,6-Dimethanonaphthalene
Benzo[1',2':3,4;5',4':3',4']dicyclobuta[1,2-a:1',2'-a']diindene

109. Enclosing marks are placed around compound substituent radicals and around and within complex radicals (¶ 162). Their presence or absence frequently removes ambiguity, especially when locants are omitted through lack of precise structural information.

Examples:

MeSiH_2Cl	Silane, chloromethyl-
$\text{ClCH}_2\text{SiH}_3$	Silane, (chloromethyl)-
	Benzoic acid, 3-(chlorobenzoyl)-
	Benzoic acid, (3-chlorobenzoyl)-
	Benzoic acid, 3-(3-chlorobenzoyl)-

Parentheses are placed around compound substituents like “(chloromethyl)”, above; in a case like (chloromethylamino), it is to be understood that both the chlorine atom and the unsubstituted methyl group are substituents of the amino group, i.e., $\text{Cl}(\text{CH}_3)\text{N}-$. The alternative structure, $\text{ClCH}_2\text{NH}-$ is named [(chloromethyl)amino], which is a *complex* substituent prefix. Parentheses are used around simple radicals when they are preceded by “bis,” “tris,” etc. (¶ 110), e.g., bis(methylene), tris(decyl). They are used also to separate locants of the same kind which would otherwise be separated only by hyphens, to indicate the second atom involved in double-bond formation when it is not the next in the numbered pathway, to enclose parts of a heading parent, to set off added hydrogen, and to enclose multiplied terms in modifications, ion terms that would otherwise be ambiguous, Ewens-Bassett numbers (¶ 215), descriptive terms and ratios, and parts of synonym line formulas.

Examples:

Benzoic acid, 4-(2-naphthalenyl)-
Bicyclo[4.2.0]oct-1(6)-ene
Butane(dithioic acid) (see ¶ 165)
1(2*H*)-Naphthalenone
bis(inner salt)
(disulfate) (from Disulfuric acid)
iron(3+) salt
compd. with benzenamine (1:1)
acetate (salt)
Thiooxydiphosphoric acid ((HO)₂P(O)]₂S₂)

Brackets enclose complex substituent prefixes and derivative terms, as well as Von Baeyer and spiro ring size designations (already described above). They

are also employed around a ring-assembly name when it is followed by a principal-group suffix or forms part of a radical name.

Examples:

[1,2'-Binaphthalene]-2-carboxylic acid
[1,1'-biphenyl]-4-yl

Brackets enclose structural features of bridges or component rings when the enclosed locants are not applicable to the total system.

Examples:

4a,9a-[2]Butenoanthracene	(the “2” locates the double bond in the buteno bridge)
4<i>H</i>-[1,3]Oxathiol[5,4-<i>g</i>]benzoxazole	(formed by fusion of 1,3-oxathio with benzoxazole; in the total ring system, the oxygen and sulfur atoms of the oxathiole ring are in the 6- and 8-positions respectively)

When a multiplicative index name is uninverted, brackets are placed around the heading parent.

Examples:

Acetic acid, 2,2'-oxybis-	(index name)
2,2'-Oxybis[acetic acid]	(uninverted name)
Benzoic acid, 4,4'-methylenebis[2-chloro-	(index name)
4,4'-Methylenebis[2-chlorobenzoic acid]	(uninverted name)

Brackets are sometimes needed for functional terms in modifications, especially following locants or multiplicative prefixes.

Examples:

S-[(dodecylthio)methyl] ester
bis[(2,4-dinitrophenyl)hydrazone]

110. Multiplicative prefixes. Generally, prefixes derived from the Greek (di, tri-, etc.) are used, rather than the Latin (bi-, ter-, etc.); exceptions are nona- (not ennea-) for nine, and undeca- (not hendeca-) for eleven. (For lists of Latin and Greek prefixes, see ¶ 309.) The Latin prefixes bi-, ter-, etc., are used for ring assemblies.

The prefixes bis-, tris-, tetrakis-, etc., are used for compound and complex radicals and functional derivatives, and to avoid misunderstanding in other cases, especially with names beginning with replacement terms like “aza” or “oxa”, fusion prefixes like “benzo” or “naphtho”, or compound fusion prefixes like “cyclopentapyrido.” They are used always in multiplying a heading parent.

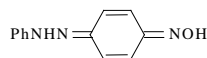
Examples:

bis(methylene)	tris(decyl)
bis(2-aminoethyl)	tetrakis(1-aziridinyl)
[1,2-ethanediylbis(oxymethylene)]	bis(benz[<i>a</i>]anthracen-1-yl)
bis(<i>O</i>-methyloxime)	Benzo[1,2-<i>c</i>:3,4-<i>c'</i>]bis[1,2,5]oxadiazole
bis(cyclohexanecetate)	Biscyclopenta[5,6]pyrido[4,3-<i>b</i>:3',4'-<i>c</i>]pyridine
tris(dihydrogen phosphate)	Benzoic acid, 2,2'-silylenebis-
bis(aziridinyl)	Phosphonic acid, <i>P,P'</i>-1,4-phenylenebis-
bis(2,1-diazenediyl)	
bis[(1,1'-biphenyl)-4-yl]	
bis(bicyclo[2.2.1]hept-2-yl)	

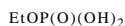
111. “Mono” is only rarely employed in index heading parents (an example is **Peroxymonosulfuric acid**) but is needed to express functional derivatives of polyfunctional heading parents and inner salts when needed. It is not used if a locant is necessary, or when only one functional group is present. Mono is used for esters of polybasic mononuclear acids having only one type of chalcogen atom, e.g. monoesters of carbonic acid, phosphonic acid, etc. The term “hydrogen” in an uninverted ester name precludes the use of “mono.”

Examples:

MeC(=NOH)Me	2-Propanone, oxime
MeOCO_2H	Carbonic acid, monomethyl ester
	1,2-Naphthalenediol, 2-acetate
EtOP(O)(OMe)_2	Phosphoric acid, ethyl dimethyl ester
	1,2,3-Oxadiazolium, 2-(dimethylamino)-4-(dimethylsulfonio)-5-hydroxy-, mono(inner salt)



**2,5-Cyclohexadiene-1,4-dione
1-(phenylhydrazone), 4-oxime**
(previously mono(phenylhydrazone),
oxime, but now locants are used.)



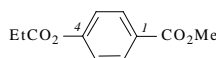
**Phosphoric acid
monoethyl ester**
(index name)

Ethyl dihydrogen phosphate
(uninverted name)

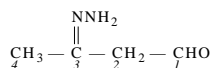
112. Functional derivatives of the principal reactive chemical groups of systematically-named index heading parents are cited in the modification; these derivatives, as defined for indexing purposes, are restricted to acyclic anhydrides, esters, hydrazides, hydrazones, and oximes. Other derivatives, such as semicarbazones, azines, acetals, and cyclic esters, are named in other ways, e.g., substitutively at the highest functional heading parent, as substituted hydrazones, etc., or as heterocycles, as detailed in Section D, below.

Functional derivatives of subsidiary functions (those not expressed by the suffix of the heading parent) are cited in the main boldface heading as compound or complex substituents.

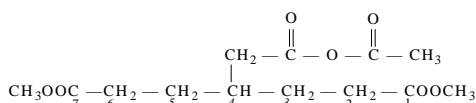
Examples:



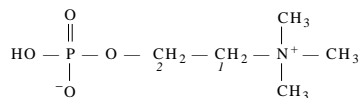
**Benzoic acid, 4-(1-oxopropano-
methyl ester** (not Benzoic acid,
4-hydroxy-, methyl ester,
propanoate)



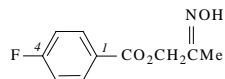
Butanal, 3-hydrazono- (not
Butanal, 3-oxo-, 3-hydrazone)



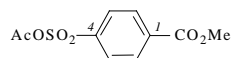
**Heptanedioic acid, 4-[2-(acetyloxy)-
2-oxoethyl]-
1,7-dimethyl ester** (not Hep-
tanedioic acid, 4-(carboxymeth-
yl)-, 4-anhydride with acetic
acid, dimethyl ester)



**Ethanaminium, N,N,N-trimethyl-2-
(phosphonoxy)-
inner salt** (not Ethanaminium,
2-hydroxy-N,N,N-trimethyl-,
dihydrogen phosphate
(ester), inner salt)



**Benzoic acid, 4-fluoro-
2-(hydroxyimino)propyl ester**
(not Benzoic acid, 4-fluoro-,
2-oxopropyl ester, oxime)



**Benzoic acid, 4-[(acetyloxy)-
sulfonyl]-
methyl ester** (not Benzoic acid,
4-sulfo-, S-anhydride with
acetic acid, methyl ester)

113. Order of citation of derivative terms in modifications. The normal order is:

- the term "inner salt";
- functional derivatives in the order: anhydrides, esters, hydrazides, hydrazones, oximes; multiplicative terms are cited before simple terms, e.g., 1,3-propanediyl dimethyl ester (with the appropriate locants), otherwise alphabetic order is followed;
- additive terms describing fragments covalently attached to the index heading compound, e.g., *N*-oxide;
- ionic terms, e.g., ion(1-), radical ion(1-), then ionic terms derived from separate structural fragments, e.g., chloride, acetate, or an "amminium" heading;
- metal salts, followed by other salts alphabetically, e.g., acetate, hydrochloride;

(f) other additive terms describing portions of the molecular structure not covalently attached, e.g., compd. with..., hydrate, mixt. with..., polymer with....

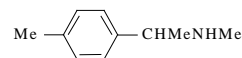
114. Locants. When a choice is necessary, italic Roman letters are placed before Greek letters, and Arabic numerals are placed last, e.g., *As*, *N*, *P*, *S*, α , β , γ , 1, 2, 3. (For the Greek alphabet see ¶ 310.)

Unprimed locants are followed by primed locants, then by doubly primed locants, etc., e.g., *N*, *N'*, *S*, α , 1', 2, 2', 3. Low numbering of indices (superscript Arabic numbers) and application of primes are not considered until regular numerical locants have been chosen.

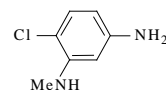
Examples:



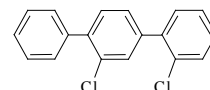
**Phosphonimidic diamide, N,N',N'',P-
tetramethyl-**



**Benzenemethanamine, N, alpha, 4-tri-
methyl-**



**1,3-Benzenediamine, 4-chloro-N³-
methyl-** (not 1,3-Benzenedi-
amine, 6-chloro-N¹-methyl-)



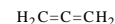
1,1':4',1''-Terphenyl, 2',2''-dichloro-
(not 1,1':4',1''-Terphenyl,
2,3'-dichloro-)

Locants for unsaturation in compounds named as index heading parents are always cited when the compound contains three or more skeletal atoms, except for monocyclic hydrocarbons with one multiple bond and no suffix.

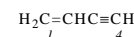
Examples:



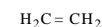
1-Triazene



1,2-Propadiene



1-Buten-3-yne



Ethene



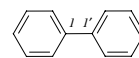
Cyclohexene



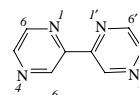
1,3-Cyclopentadiene

Locants denoting ring junctions of ring assemblies are always cited except for two-component assemblies of cycloalkenes, cycloalkadienes, etc.

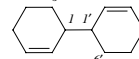
Examples:



1,1'-Biphenyl



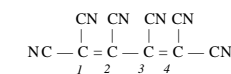
2,2'-Bipyrazine



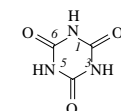
Bi-2-cyclohexen-1-yl

115. Locants for substituent suffixes of index heading parents are cited except for the following cases: mononuclear skeleton parents, a single substituent suffix on a homogeneous molecular skeleton with two skeletal atoms, or a single substituent suffix on benzene or a saturated homogeneous monocyclic ring. Locants are not cited for Geneva suffixes which terminate a chain, e.g., "oic acid", "dial".

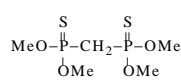
Examples:



**1,3-Butadiene-1,1,2,3,4,4-hexa-
carbonitrile**

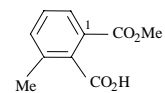
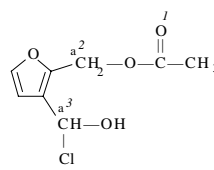
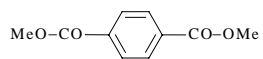


**1,3,5-Triazine-2,4,6(1H,3H,5H)-
trione**

$\text{HO}_2\text{CNHSiH}_2\text{NHC}_2\text{O}_2\text{H}$	Carbamic acid, <i>N,N'</i>-silylenebis-
MeSMe	Methane, 1,1'-thiobis-
$\text{HOSiH}_2\text{CH}_2\text{SiH}_2\text{OH}$	Silanol, 1,1'-methylenebis-
$\text{H}_2\text{NSiH}_2\text{CH}_2\text{SiH}_2\text{NH}_2$	Silanamine, 1,1'-methylenebis-
$\text{ClCH}_2\text{COO}(\text{CH}_2)_2\text{OCOCH}_2\text{Cl}$	Acetic acid, 2-chloro-, 1,1'-(1,2-ethanediyl) ester
	Phosphonothioic acid, <i>P,P'</i>-methylenebis-, <i>O^P,O^P,O^{P'},O^{P'}</i>-tetramethyl ester

119. Locants for functional derivatives are always cited when there is more than one occurrence of the principal functional group.

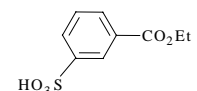
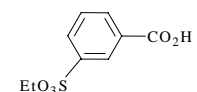
Examples:

	1,2-Benzenedicarboxylic acid, 3-methyl-, 1-methyl ester
	2,3-Furandimethanol, α^3-chloro-, α^2-acetate
$\text{MeOP}(\text{O})_p(\text{OH})\text{OP}(\text{O})_p(\text{OH})\text{OMe}$	Diphosphoric acid, <i>P,P'</i>-dimethyl ester
$\text{HO}_2\text{C}(\text{CH}_2)_2\text{CONHNH}_2$	Butanedioic acid, 1-hydrazide
$\text{MeC}(\text{=NOH})\text{CMe}=\text{NNHPh}$	2,3-Butanedione, 2-(phenylhydrazone), 3-oxime
	1,4-Benzenedicarboxylic acid, 1,4-dimethyl ester

Locants are cited for esters of compounds named at an alcohol parent. Examples:

$\text{H}_2\text{N}-(\text{CH}_2)_2\text{OCOCH}_3$	Ethanol, 2-amino-, 1-acetate (the term ester is not cited because a locant is present.)
$\text{PhCH}_2\text{CH}_2\text{OCOCH}_3$	Benzeneethanol, 1-acetate (for a conjunctive name, the ring locant is used.)

Locants are used in modifications for index headings that express the same (or similar) functions in both the index parent and the substituents when the latter are not derivatized. This avoids confusion with former CA index names. Examples:

	Benzoic acid, 3-sulfo-, 1-ethyl ester
	Benzoic acid, 3-(ethoxysulfonyl)- (formerly Benzoic acid, 3-sulfo-, 3-ethyl ester)

The locant for an additive term such as "oxide" is an Arabic number when a nitrogen, phosphorus, sulfur, etc., atom of a ring in the index heading parent is involved; otherwise a letter locant (*N*-, *S*-, etc.) is employed.

Locants are not employed for ionic modification terms, e.g., salts such as "sodium salt," "hydrochloride."

120. Locants for indefinite compounds must often be omitted. In addition, such compounds can sometimes be named only by departing from the regular name selection policies, e.g., by citation of the principal group in the modification instead of as a suffix of the heading parent, citation of a functional derivative in the modification rather than as a substituent, use of "mono" instead of the (unknown) locant, replacement of a numerical locant by the indefinite aromatic locant "*ar*-" or inclusion of question marks in a set of otherwise known locants.

Examples:

Benzenediamine
Benzoic acid, dichloro-naphthalene, 2,2'-(1,4-phenylene)bis-, disulfo deriv.
Benzenoacetic acid, 2-carboxy-, monomethyl ester
1,2-Ethanediol, 1-phenyl-, monocarbamate
Naphthalene, *ar*-chloro-1,2,3,4-tetrahydro-
Benzenemethanol, *ar*-amino-[1,1'-Biphenyl]-*ar,ar'*-dicarboxylic acid
Benzene, 1,2,?-trimethyl-

The italic word "*or*" is used with substituent prefixes (but never with index heading parents) when the number of alternative structures cannot be misinterpreted.

Examples:

Quinoline, 2-chloro-3(or 4)-methyl-Naphthalene, 1(or 2)-ethyl-2(or 1)-methyl-

When one or more substituent prefixes are in known positions and the remainder in unknown positions, lowest locants are used for the former.

Example:

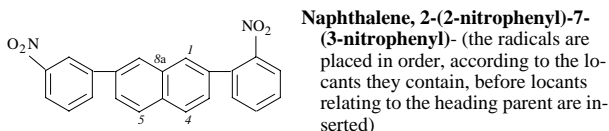
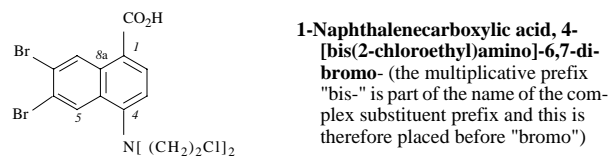
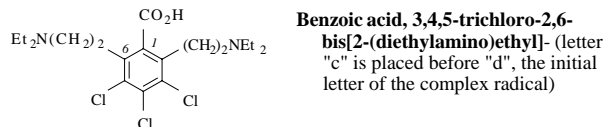
Naphthalene, chloro-2-methyl-

An indefinite name like **Piperidine, 2(or 4)-bromo-4(or 2)-chloro-** cannot be used because this name could be held to include the 2-bromo-2-chloro- and 4-bromo-4-chloro-isomers; in such cases locants are usually omitted.

121. Alphabetization of substituent prefixes affects the position in the index where an inverted chemical substance name will be found. Simple prefixes are placed in alphabetic order according to their names; only then are multiplicative prefixes (*di*-, *tri*-, etc.) placed in front of each as required, and locants inserted; e.g., an index compound in which two nitro groups, three bromine atoms, and a chlorine atom are present receives the substituent name "tribromo-chlorodinitro," and the substituents so arranged will be found together with an appropriate index parent, such as **Naphthalene**, alphabetized in accordance with *all* the Roman letters in the complete name. The total name with locants, e.g., **Naphthalene, 2,5,8-tribromo-3-chloro-1,6-dinitro-**, will be preceded in the list of index entries by both **Naphthalene, nitro-** and **Naphthalene, tetra-chloro-**.

Compound and complex substituent prefixes (radicals) are constructed on similar alphabetic principles and then arranged by their first letters (which may have been derived from multiplicative prefixes within the radicals) in the total name. This name is then placed in the index as described above, *all* letters being alphabetized. When the letters are all identical, arrangement depends on locants.

Examples:



122. Tautomeric compounds. Index names are normally based on the precise structures shown or described in the author's original document. Tautomerism (ready interconvertibility of isomers) in certain types of compounds causes a serious problem in index-name selection, the issue here being not which name to select for a given molecular structure but which diagram to name for a given tautomeric system if scattering at different names of information about what is essentially a single substance is to be avoided.

Common (trivial) names for most nitrogenous tautomeric systems are cross-referred to preferred systematic names.

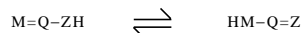
Examples:

Adenine.	See <i>9H-Purin-6-amine</i>
Barbituric acid.	See <i>2,4,6-(1H,3H,5H)-Pyrimidinetrione</i>
Caffeine.	See <i>1H-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl-</i>
Carbostyryl.	See <i>2(1H)-Quinolinone</i>
Cytosine.	See <i>2(1H)-Pyrimidinone, 4-amino-</i>
Guanine.	See <i>6H-Purin-6-one, 2-amino-1,9-dihydro-</i>
Hydantoin.	See <i>2,4-Imidazolidinedione</i>
Melamine.	See <i>1,3,5-Triazine-2,4,6-triamine</i>
Theophylline.	See <i>1H-Purine-2,6-dione, 3,9-dihydro-1,3-dimethyl-</i>
Uracil.	See <i>2,4(1H,3H)-Pyrimidinedione</i>
Uric acid.	See <i>1H-Purine-2,6,8(3H)-trione, 7,9-dihydro-</i>
Xanthine.	See <i>1H-Purine-2,6-dione, 3,9-dihydro-</i>

The necessity for many tautomeric structures to be redrawn to agree with selected CA index names is obviated by computer "normalization" algorithms in the CAS Registry System. In the normalization process, the different structural diagrams for a single tautomeric system (of one of the types expressed in the cross-references above) are recognized as equivalent and stored in identical machine-language representations. They share a single unique CAS Registry Number and CA Chemical Substance Index name.

The structural requirements for the normalization process and the rules for selecting unique CA Chemical Substance Index names are as follows:

I. Requirements for normalization of structures. Tautomeric structures represented by the following equilibrium:



are normalized, i.e., recognized as equivalent in the CAS Registry System, when the following requirements are met:

(a) Q = C, N, S, P, Sb, As, Se, Te, Br, Cl or I with any acceptable valency for the individual elements.

(b) M and Z = any combination of trivalent N and/or bivalent O, S, Se or Te atoms.

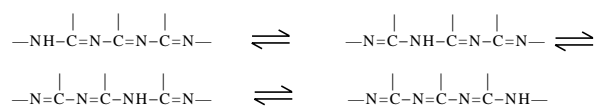
(c) The bonds involved in tautomerization may be in an acyclic chain or in a ring system or partly in both.

(d) The end-points, M and Z, may be in adjacent rings of a fused ring system, but a nitrogen atom which occupies a fusion point in such a system cannot take part in tautomerization.

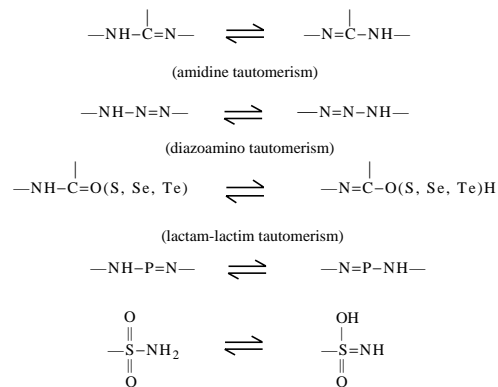
(e) The hydrogen atom of the tautomeric system may be replaced by deuterium or tritium.

(f) Two or more systems of the form shown above may be linked through a common atom, whereby a proton can be considered to migrate along the chain.

Example:

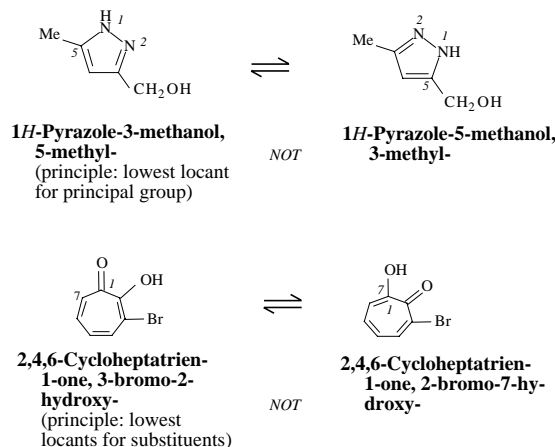


Replacement in the generalized formula above by specific elements affords normalized tautomeric systems such as the following:



A unique CA Chemical Substance Index name is selected for each compound containing a normalized tautomeric structure by application of the rules that follow (see II, below). For tautomeric pyrazole derivatives and for tropolones, CA selects a single preferred structure and index name, and assigns a single CAS Registry Number, even though these systems do not conform to the general equilibrium illustrated above and are not currently normalized by the CAS Registry System. Lowest locants are employed successively in index parents and substituents in these cases.

Examples:

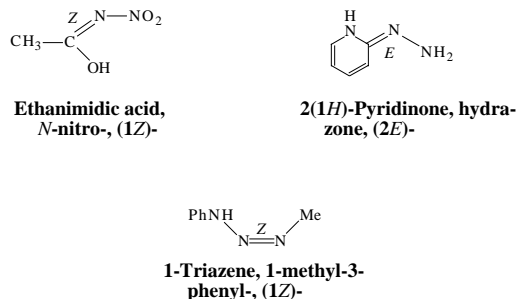


For phosphonic-phosphorous and phosphinic-phosphonous acid tautomers, see ¶ 197.

II. Rules for Choosing the Preferred Normalized Tautomer. These rules are used to select the particular structure of a tautomer from which the unique CA Chemical Substance Index name is then derived. They are applied in the order shown until a decision has been made.

Rule 1: The Stereo Retention Rule

When the original document reports the isolation of a normalized tautomer with an E or Z double bond connecting the central atom Q to a terminal N, the preferred tautomer retains the E or Z configuration.

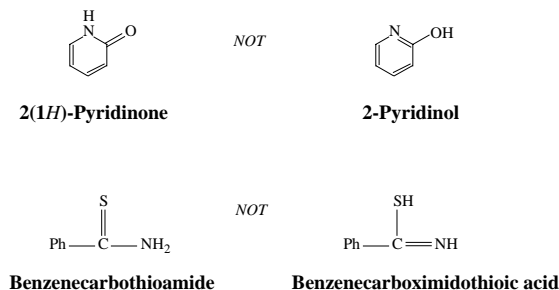


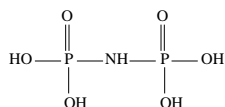
Rule 2: The Oxo Rule

For any tautomer mobile group, if M is a chalcogen and Z is N, the preferred tautomer has the mobile H on N; and if M and Z are both chalcogens, the preferred tautomer has the mobile H on the chalcogen of higher atomic number. The overall order of priority for attachment of the mobile H is then



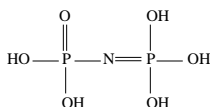
In other words, a double bond to oxygen is preferred above all others.





Imidodiphosphoric acid

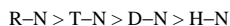
NOT

Phosphorimidic acid,
N-phosphono-1H-Phosphole, 1-selenyl-,
1-oxide

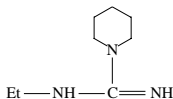
NOT

1H-Phosphole, 1-hydroxy-,
1-selenide**Rule 3: The Unsubstituted Imino Rule**

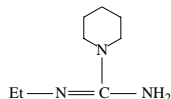
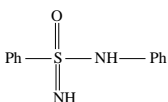
For an *acyclic* tautomer mobile group, if M and Z are both N, the order of priority for attachment of the mobile H is



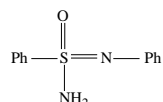
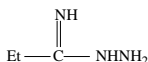
where R is any covalently attached atom or group other than H, D, or T. In other words, an unsubstituted imino group is preferred to a substituted one, and an unlabeled imino group is preferred to a labeled one.

1-Piperidinecarboximidamide,
N'-ethyl-

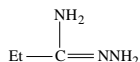
NOT

1-Piperidinecarboximidamide,
N'-ethyl-Benzenesulfonimidamide,
N-phenyl-

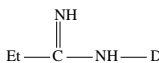
NOT

Benzenesulfonimidamide,
N'-phenyl-Propanimidic acid,
hydrazide

NOT

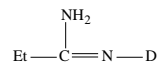


Propanehydrazonamide



Propanimidamide-N-d

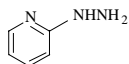
NOT



Propanimidamide-N'-d

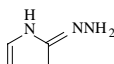
Rule 4: The Amino/Hydrazinyl Rule

For a tautomer mobile group in which M and Z are both N, but one N is in a ring and the other is attached to the ring, the preferred tautomer has the mobile H on the acyclic N.



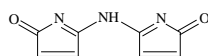
Pyridine, 2-hydrazinyl-

NOT

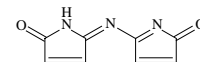
2(1H)-Pyridinone,
hydrazone

1H-Imidazol-2-amine

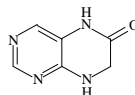
NOT

2H-Imidazol-2-imine,
1,3-dihydro-2H-Pyrrol-2-one, 5,5'-
iminobis-

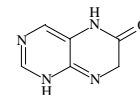
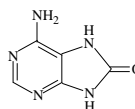
NOT

2H-Pyrrol-2-one, 1,5-dihydro-
5-[(2-oxo-2H-pyrrol-5-
yl)imino]-**Rule 5: The Alternating-Bond Rule**

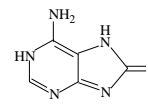
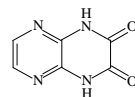
For a cyclic tautomer mobile group in which M and Z are both N and Q lies at the junction of two rings, the preferred tautomer has one N in a ring with alternating single and double bonds and the mobile H on the other N.

6(5H)-Pteridinone,
7,8-dihydro-

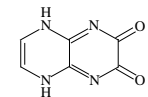
NOT

6(5H)-Pteridinone,
1,7-dihydro-8H-Purin-8-one, 6-amino-
7,9-dihydro-

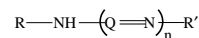
NOT

8H-Purin-8-one, 6-amino-
1,7-dihydro-Pyrazino[2,3-b]pyrazine-2,3-
dione, 1,4-dihydro-

NOT

Pyrazino[2,3-b]pyrazine-2,3-
dione, 5,8-dihydro-**Rule 6: The Tautomer CIP Rule**

For the isolated ($n = 1$) or extended ($n > 1$) tautomer



in which

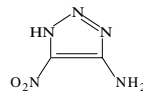
- R and R' are any covalently attached atoms or groups, and
- both terminal N's (those attached to R and R') are acyclic or both are in a ring,

the preferred tautomer has the mobile H on the terminal N of higher priority based on the Cahn-Ingold-Prelog (CIP) sequence rule, the one used to assign absolute configuration [R. S. Cahn, C. K. Ingold, and V. Prelog, *Angew. Chem. Int. Ed. Engl.*, **1966**, 5, 385-415 (errata: **1966**, 5, 511); V. Prelog and G. Helmchen, *ibid.*, **1982**, 21, 567-583.

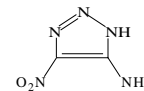
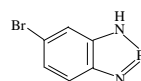
For each tautomer, a tree diagram is constructed for the terminal N bearing the mobile H. Then the following CIP-based rules are used:

Subrule 6.1: The Element Subrule

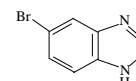
Under subrule 6.1, at the first point of difference, the element with the higher atomic number has priority. The terminal N for that branch is then assigned the mobile H in the preferred tautomer.

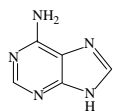
1H-1,2,3-Triazol-4-amine,
5-nitro-

NOT

1H-1,2,3-Triazol-5-amine,
4-nitro-1H-1,3,2-Benzodiazaphosphole,
6-bromo-

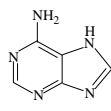
NOT

1H-1,3,2-Benzodiazaphosphole,
5-bromo-

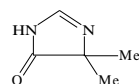


9H-Purin-6-amine

NOT

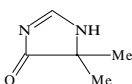


7H-Purin-6-amine

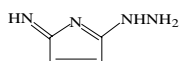


4H-Imidazol-4-one, 3,5-dihydro-5,5-dimethyl-

NOT

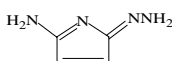


4H-Imidazol-4-one, 1,5-dihydro-5,5-dimethyl-

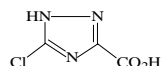


2H-Pyrrol-2-imine, 5-hydrazinyl-

NOT

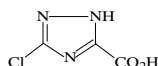


2H-Pyrrol-2-one, 5-amino-, hydrazone



1H-1,2,4-Triazole-3-carboxylic acid, 5-chloro-

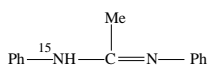
NOT



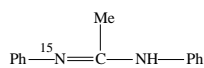
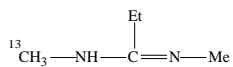
1H-1,2,4-Triazole-5-carboxylic acid, 3-chloro-

Subrule 6.2: The Isotope Subrule

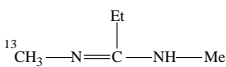
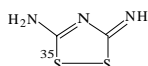
If a comparison of atomic numbers fails to reveal a difference in the tree diagrams, the CIP rule then compares mass numbers. Under subrule 6.2, at the first point of difference, the atom with the higher mass number has priority:

Ethanimidamide-*N*-¹⁵N, *N,N'*-diphenyl-

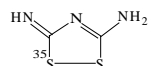
NOT

Ethanimidamide-*N'*-¹⁵N, *N,N'*-diphenyl-Propanimidamide, *N'*-methyl-*N*-(methyl-¹³C)-

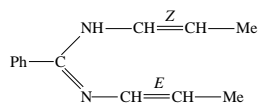
NOT

Propanimidamide, *N*-methyl-*N'*-(methyl-¹³C)-3H-1,2,4-Dithiazol-1,3⁵S-5-amine, 3-imino-

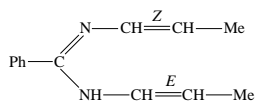
NOT

3H-1,2,4-Dithiazol-2-3⁵S-5-amine, 3-imino-**Subrules 6.3-6.5: The Stereo Subrules**

If a comparison of mass numbers also fails to reveal a difference, the CIP-based rule then compares stereo elements. For example, under subrule 6.3, a *Z* double bond has priority over an *E* one if the structure is X-CH=CH-Y, where X and Y are any covalently attached atoms or groups:

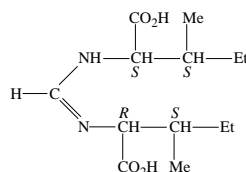
Benzenecarboximidamide, *N'*-(1*E*)-1-propen-1-yl-*N*-(1*Z*)-1-propen-1-yl-

NOT

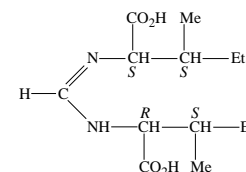
Benzenecarboximidamide, *N*-(1*E*)-1-propen-1-yl-*N'*-(1*Z*)-1-propen-1-yl-

Under subrule 6.4, a like pair of chiral centers (*R,R* or *S,S*) has priority over an

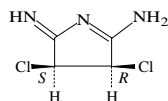
unlike pair (*R,S* or *S,R*):

L-Isoleucine, *N*-[[[(1*R*,2*S*)-1-carboxy-2-methylbutyl]imino]methyl]-

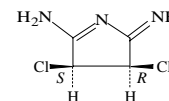
NOT

L-Isoleucine, *N*-[[[(1*R*,2*S*)-1-carboxy-2-methylbutyl]amino]methylene]-

And finally, under subrule 6.5, an *R* chiral center has priority over an *S* one:

2H-Pyrrol-5-amine, 3,4-dichloro-3,4-dihydro-2-imino-, (3*S*,4*R*)-

NOT

2H-Pyrrol-5-amine, 3,4-dichloro-3,4-dihydro-2-imino-, (3*R*,4*S*)-

123. Additive nomenclature embraces molecular structures whose several component parts are considered to be added together without replacement (substitution) of atoms (usually hydrogen). It includes coordination names (¶ 215), conjunctive nomenclature (¶ 124) and binary names of inorganic compounds (¶ 219).

Examples:

Copper, dichlorobis(methanamine)-Benzeneethanol
Sodium chloride (NaCl)

The construction of additive names often involves indicated or added hydrogens (¶¶ 135, 136) in that part of the molecule known as the heading parent, the addition of hydro "substituents", or the use of additive terms such as "oxide" or "sulfide" in the modification. In a few cases, the additive term becomes a part of the heading parent.

Examples:

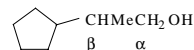
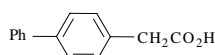
9(10H)-Anthracenone
Naphthalene, 1,2,3,4-tetrahydro-Pyridine, 1-oxide
Phosphine imide

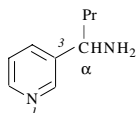
For salts and molecular addition compounds, see ¶¶ 192, 198.

124. Conjunctive nomenclature allows a cyclic molecular skeleton to be included as a part of the heading parent name even though the principal chemical group is separated from the ring by an acyclic chain. Larger molecules may be named thereby as heading parents and more compounds of similar structure can be collected at a given ring system name. Moreover, the major requirement of substitutive nomenclature, that the principal group be expressed in the heading parent as a suffix, is fulfilled.

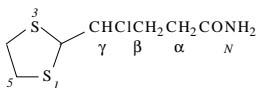
A conjunctive name is employed when any ring system (including a polyhedral borane) is attached by single bonds to one or more saturated acyclic hydrocarbon chains, each of which bears only one functional substituent corresponding to the principal chemical group of the compound. When a second or third such substituent is present on the chain, a conjunctive name may still sometimes be employed so long as the resulting index heading parent does not express more than a single function in each chain and other principles are not violated (see the final example below). It is always implied that the chemical functional group is at one end of the acyclic chain and the ring system is at the other.

Examples

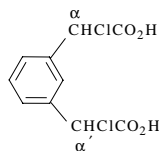
**Benzenemethanol****Cyclopentaneethanol, β-methyl-****[1,1'-Biphenyl]-4-acetic acid**



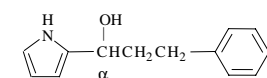
3-Pyridinemethanamine,
 α -propyl-



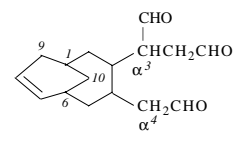
1,3-Dithiolane-2-butanamide,
 γ -chloro-



1,3-Benzenediacetic acid,
 α^1, α^3 -dichloro-



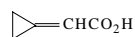
1H-Pyrrole-2-methanol, α -(2-phenylethyl)- (the heading parent which expresses the preferred ring system, not the preferred acyclic chain, is chosen)



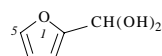
Bicyclo[4.3.1]dec-7-ene-3,4-diacetaldehyde, α^3 -(2-oxoethyl) (not Bicyclo[4.3.1]dec-7-ene-3-propanal, β -formyl-4-(2-oxoethyl)-; the preferred heading parent expresses the maximum number of principal groups and, because it also expresses a ring system, is preferred to **Butanedial**)

A conjunctive name is not permissible under the following conditions and the regular rules of substitutive nomenclature apply: 1) when a *double* bond joins the ring to the functional acyclic chain; 2) when a conjunctive index parent would express two or more functional groups in a single acyclic chain; 3) when the acyclic chain is unsaturated, or contains hetero atoms; and 4) when a conjunctive name would fail to express the maximum number of principal chemical groups.

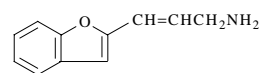
Examples:



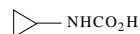
Acetic acid, 2-cyclopropylidene-



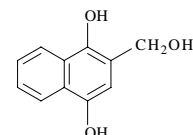
Methanediol, 1-(2-furanyl)-



2-Propen-1-amine, 3-(2-benzofuranyl)-



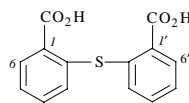
Carbamic acid, N-cyclopropyl-



1,4-Naphthalenediol, 2-(hydroxymethyl)-

125. Multiplicative nomenclature employs polyvalent radicals by which a multiplicity of occurrences of an index heading parent in a compound may be expressed.

Example:

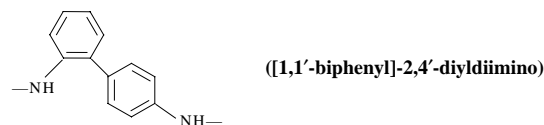
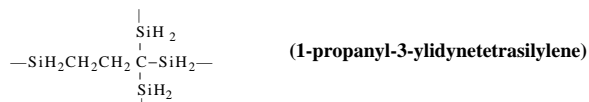
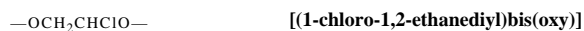
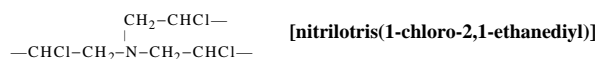
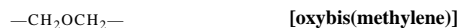


Benzoic acid, 2,2'-thiobis-

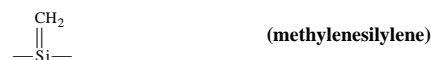
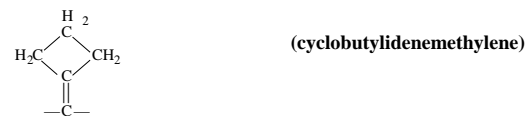
In the example above, a simple one-part polyvalent radical, thio, was employed as a multiplier; other such radicals are oxy, -O-; methylene, -CH₂-; 1,4-phenylene, -1,4-C₆H₄-; imino, -NH-; nitrilo, -N=; and 1,3-disiloxanediyl, -SiH₂OSiH₂-. In general, any simple multivalent radical may be used as a multiplicative radical, and may itself be substituted; e.g., (methylimino), -N(CH₃)-; (1-methyl-1,3-propanediyl), -CH(CH₃)CH₂CH₂-.

Multicomponent radicals may be used as multipliers if they contain a central one-part multivalent radical (simple, compound, or complex) around which all other multivalent radicals are so arranged that the sequence of atoms and bonds in each path is identical as one proceeds outwards. There is no restriction in the number of components that may comprise the total multiplying radical, so long as their use results in an unambiguous total name.

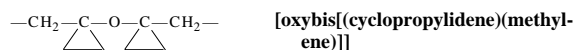
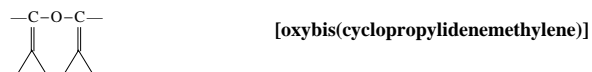
Examples of permissible multiplying radicals:



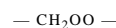
The requirement for total symmetry in multiplication allows the use of "ylidene" in combination with other bivalent radicals.



Enclosing marks are used to distinguish certain combinations of multivalent radicals which would otherwise be ambiguous.



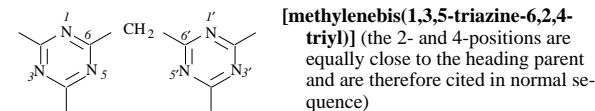
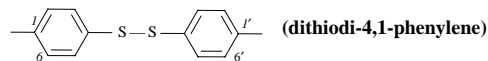
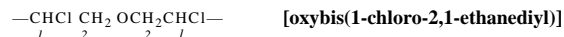
Examples of combinations of multivalent radicals which are not used as multipliers:



The naming of multiplying radicals is accomplished by citing first the central unit. This is followed by a prefix, e.g., "di" or "bis", denoting the number of "radial" series generated by the central unit. The remaining terms of the name, in the form of radicals, are cited in appropriate enclosing marks as necessary. The entire multiplying radical is set off by further enclosing marks,

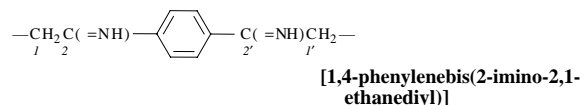
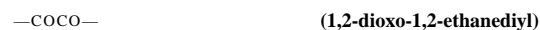
which are preceded by locants "placing" the radical at the proper point of attachment on each index heading parent. Multivalent radicals other than central units are numbered (if there is a choice) from the heading parents towards the center of the complete radicals, and the locant relating to the position closest to the heading parent is cited last.

Examples:



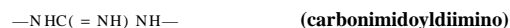
Carbonyl groups which are part of carbon chains are expressed as oxo substituents; chalcogen, imino, and hydrazono analogs are expressed as thioxo, selenoxo, telluroxo, imino, and hydrazono substituents.

Examples:



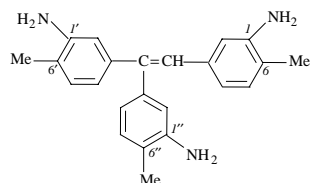
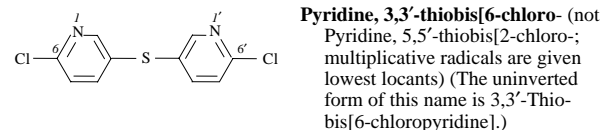
When carbonyl groups and their analogs are not part of a larger acyclic carbon chain, the names carbonyl, carbonothioyl, carbonimidoyl, etc., are employed.

Examples:



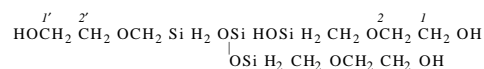
Valid multiplying radicals are used only when the entire compound is symmetrical around the central unit of such a radical; i.e., the radical must be attached to the heading parent by bonds of the same type (single, double, or triple) and at equivalent positions, and this parent must be identical with regard to positions of principal groups (and their functional derivatives) and other substituents. Whether or not such other substituents are present, the terms "bis," "tris," etc., are employed after the multiplying radical, not "di," "tri," etc. If other substituents are present, they are cited as regular substitutive radicals after an opening bracket (which, perforce, is left unclosed).

Examples:



The principles of multiplicative nomenclature are applied only after the index heading parent has been chosen, and after other principles, e.g., centrality (¶ 138), have been applied. When more than one multiplicative name is possible, that one is used which multiplies the greatest number of index heading parents, and then, if a choice is still necessary, that one which appears earliest in the alphabetic sequence of index entries. The number of occurrences of the parent is not increased by arbitrary breaking of the skeleton from which the multiplying radical is derived.

Example:



Ethanol, 2,2'-[[[3-[[[(2-hydroxyethoxy)methyl]silyloxy]-1,5-trisiloxanediyl]bis(methyleneoxy)]bis-(not Ethanol, 2,2',2''-[silylidynetris(oxy)silylenemethyleneoxy)]tris-)

126. Radicofunctional nomenclature is used by CA in only a few cases, for disulfides, hydroperoxides, and peroxides (¶ 200, 196). Radicofunctional names express the compound type, e.g., "peroxide," usually as a separate word. When inverted, the substituents are not followed by a hyphen unless multiplicative nomenclature (¶ 125) is used with **Hydroperoxide**; e.g., **Disulfide, ethyl methyl; Hydroperoxide, 1-methylethyl; Hydroperoxide, cyclohexylidenebis-**.

127. Replacement nomenclature ("a" nomenclature) is used for certain heterocyclic ring systems (¶ 146) and also, sometimes, for heteroorganic acyclic compounds. This nomenclature is limited to cases in which carbon atoms have been replaced in chains and rings by nonmetals and/or elements of which the hydrides are CA index heading parents, i.e., P, As, Sb, Bi, Si, Ge, Sn, Pb, and B.

Requirements for its use in expressing acyclic chains are as follows:

(a) A minimum of four hetero units must be present, none of which may be all or a part of a functional chemical group to be expressed in the index heading parent as the preferred functional compound class (i.e., as a functional suffix or as a functional index compound such as **Carbonic** or **Phosphonic acid**). A hetero unit is defined as an isolated hetero atom or a series of consecutive hetero atoms, alike or different, that may be expressed as a unit, such as by a bivalent radical name. Examples: -S- (thio); -S-S- (dithio); -N=N- (1,2-diazenediyl); -SiH₂-O-SiH₂- (1,3-disiloxanediyl); -SiH₂-NH-SiH₂- (1,3-disilazenediyl). The above are all single hetero units, but -HP-NH-, -S-O-, and -O-SiH₂-O-, are not.

(b) The "a" name must not be lower in order of precedence than the name obtained by regular substitutive nomenclature, i.e., it must express at least as many principal functions of at least equal rank.

(c) All hetero atoms must be in their standard valency state, or else the abnormal valency must be expressible unambiguously by use of "oxide," etc., terms.

(d) The chain may be terminated only by C, P, As, Sb, Bi, Si, Ge, Sn, Pb, or B.

Acyclic "a" nomenclature is employed for organic chains containing silicon or metal atoms, polyesters, anhydrides, amides, polyamides, polyalkylene glycols, and condensed carbonic acid derivatives. It is not used for peptides or polymers, or (if it can be avoided) for chains containing no carbon atoms. Otherwise, if the above criteria are met, an "a" name is always selected.

128. Replacement prefixes for the elements most frequently found in carbon chains are set out in descending order of precedence in Table I. (The order is the reverse of that shown in ¶ 215 for coordinated elements.)

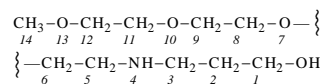
TABLE I
REPLACEMENT PREFIXES IN DESCENDING ORDER OF PRECEDENCE

Element	Substitutive Valence	Prefix
Oxygen	II	Oxa
Sulfur	II	Thia
Selenium	II	Selena
Tellurium	II	Tellura
Nitrogen	III	Aza
Phosphorus	III	Phospha
Arsenic	III	Arsa
Antimony	III	Stiba
Bismuth	III	Bisma
Silicon	IV	Sila
Germanium	IV	Germa
Tin	IV	Stanna
Lead	IV	Plumba
Boron	III	Bora

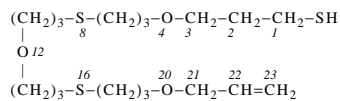
The replacement prefixes are placed in descending order of precedence ahead of the name of the carbon skeleton with locants to indicate the positions of the atoms replaced. Lowest locants are assigned to functional groups if present, otherwise to the hetero atoms.

Replacement nomenclature is also employed for acyclic substituent prefixes (radicals) when the above requirements are fulfilled. In this case, lowest locants are assigned to free valency positions; i.e., the "a" names are based on the carbon chain radical names, but the free valency locant ("1") is always cited.

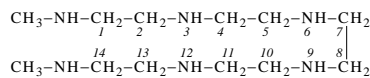
Examples:



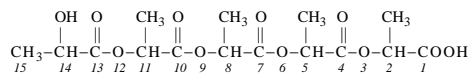
7,10,13-Trioxa-4-azatetradecan-1-ol



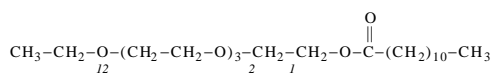
4,12,20-Trioxa-8,16-dithiatricos-22-ene-1-thiol



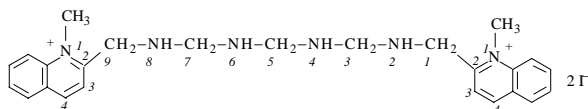
3,6,9,12-Tetraazatetradecane-1,14-diamine, N¹,N¹⁴-dimethyl-



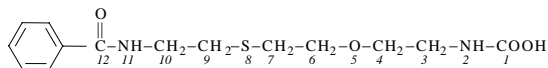
3,6,9,12-Tetraoxapentadecanoic acid, 14-hydroxy-2,5,8,11-tetramethyl-4,7,10,13-tetraoxo-



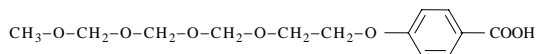
Dodecanoic acid 3,6,9,12-tetraoxatetradec-1-yl ester



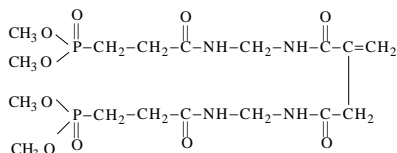
Quinolinium, 2,2'-(2,4,6,8-tetraazanonane-1,9-diyl)bis[1-methyl-, iodide (1:2)]



5-Oxa-8-thia-2,11-diazadodecanoic acid, 12-oxo-12-phenyl-



Benzoic acid, 4-(3,5,7,9-tetraoxadec-1-yloxy)-



Phosphonic acid, P,P'-(8-methylene-3,7,10,14-tetraoxo-4,6,11,13-tetraazahexadecane-1,16-diyl)-bis-, P,P,P',P'-tetramethyl ester

129. Replacement nomenclature for functions is a method of describing the replacement of hydroxyl and oxo functional groups by nitrogen, chalcogens, halogens, or halogenoids such as isocyanato. The replacement may be carried out in substituent suffixes, e.g., -thioic acid from -oic acid; in substituent prefixes, e.g., carbonimidoyl (¶ 134) from carbonyl, and phosphinothioyl from phosphinyl (¶ 197); and in functional parent compounds (¶ 130), e.g., **Phosphonimidodithioic acid** from **Phosphonic acid**.

Replacement of hydroxyl in compounds and radicals is denoted by the following affixes (the final "o" is often elided): amido (for -NH₂), azido (for -N₃), chlorido (for -Cl) (and similarly for other halo atoms), cyanatido (for -OCN), hydrazido (for -NHNH₂), isocyanatido (for -NCO), (isothiocyanatido) (for -NCS), and (thiocyanatido) (for -SCN). Seleno and telluro analogs are named analogously.

Replacement of oxo is denoted by the affixes hydrazono (for =NNH₂), imido (for =NH), thio (for =S), etc. Replacement of a hydroxyl and an oxo together

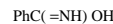
by =N is denoted by nitrido. Peroxy acids are named by use of the affixes peroxy, (thio)peroxy, and (dithio)peroxy.

These affixes are combined, in alphabetical order, with the functional suffix of compound names based on molecular skeletons. The systematic names **Benzenecarboxylic**, **Ethanoic**, and **Methanoic acids**, not the trivial names **Benzoic**, **Acetic**, and **Formic acids**, are used as the parents for functional replacement nomenclature.

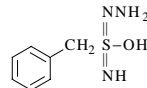
Examples:



Ethane(dithioic) acid (not Acetic acid, dithio-)



Benzenecarboximidic acid (the tautomeric **Benzamide** is preferred, except for esters and anhydrides; see ¶ 122)



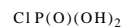
Benzenemethanesulfonylhydrazonimidic acid (derived from the conjunctive name **Benzenemethanesulfonic acid**)



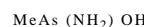
Ethane(dithioperoxy) acid

In replacement names from phosphorus and arsenic functional parent compounds (¶ 197), all the affixes except hydrazono may be employed as part of the suffix. For **Carbonic acid** and its relatives (¶ 183) all but hydrazido and nitrido may be used.

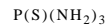
Examples:



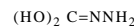
Phosphorochloridic acid



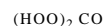
Arsanamidous acid, As-methyl-



Phosphorothioic triamide



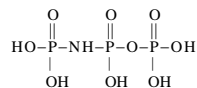
Carbonohydrazonic acid



Carbonodiperoxy acid

In replacement names from other mononuclear acids and from condensed nuclear acids (anhydrides), the affixes are used as nondetachable prefixes cited at the beginning of the heading parents. Because multiplicative prefixes are rarely used for thio and other chalcogen prefixes, ambiguity is resolved by synonym line formulas in the boldface index headings.

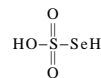
Examples:



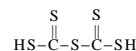
Imidotriphosphoric acid



Imidodicarbonic acid



Selenosulfuric acid (H₂SO₃Se)



Thiodicarbonic acid ((HS)C(S))₂S

Nondetachable prefixes are used in a few other cases.

Examples:



Chlorosulfuric acid



Imidosulfamide



Thiourea



Thiohydroxylamine



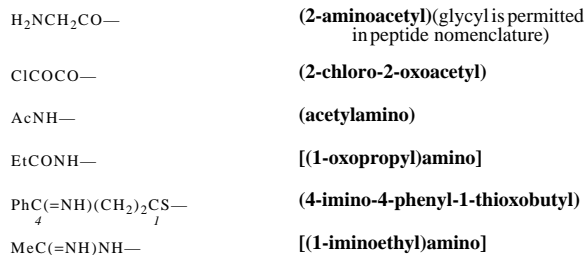
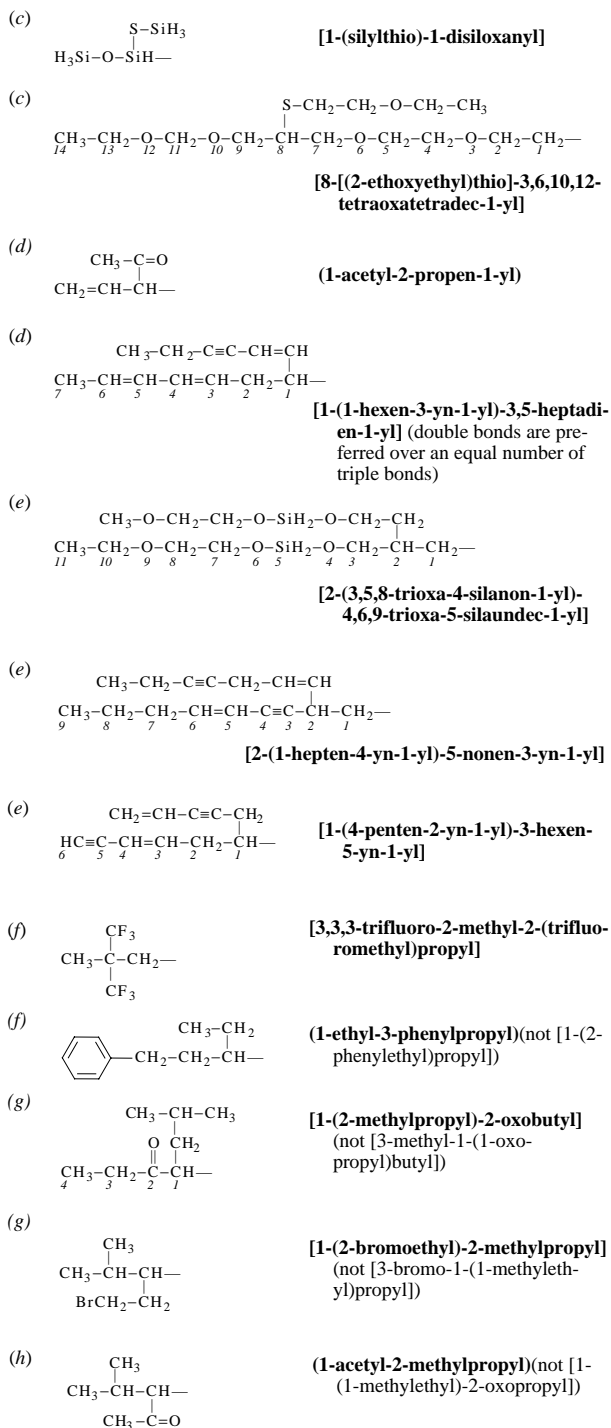
Thioperoxide, diacetyl



Thiohydroperoxide, O-ethyl

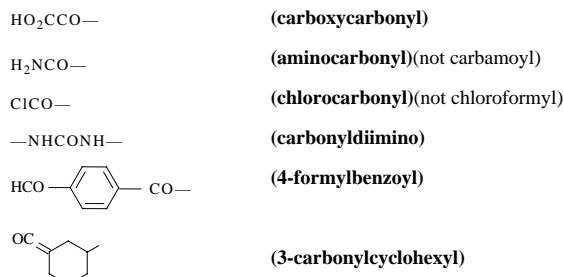
130. Substitutive nomenclature, in which hydrogen atoms are replaced by other atoms or chemical groups, is of paramount importance among nomenclature systems because of its versatility. *Substitutive parent compounds*, which are real or hypothetical compounds whose names imply the presence of replaceable hydrogen atoms, are of two kinds:

(a) *Functional parent compounds* have names which express a chemical function but are not based on a molecular skeleton. Substitutive examples include **Arsonic acid**, **Imidodicarbonic acid**, **Carbamic acid** and **Phosphonamidic chloride**. Their substituents are always expressed as prefixes, never as suffixes.



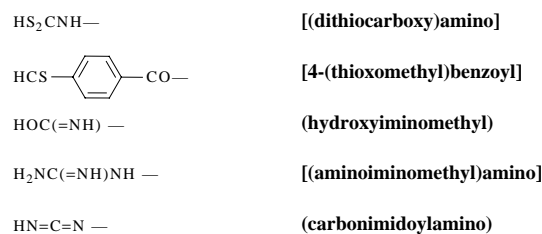
Isolated carbonyl radicals, other than carboxy, are expressed as carbonyl (as a doubling radical, or when both free valencies are attached to a single atom), formyl (if unsubstituted), benzoyl (if attached to a phenyl group which is not itself attached to another phenyl), or as a compound radical in which carbonyl is the parent.

Examples:

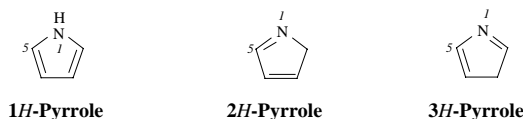


Replacement analogs of isolated carbonyl groups (other than chalcogen analogs of carboxy) are named as thioxo, imino, etc., derivatives of methyl, unless both free valencies are attached to a single atom, or the radical is being used multiplicatively (§ 125), in which case carbonimidoyl, carbonohydrazoneyl, carbonothioyl, etc., are employed.

Examples:



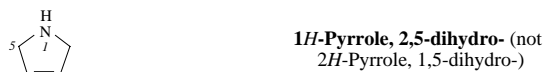
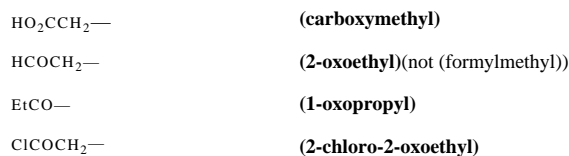
135. Indicated hydrogen is a designation comprising a locant followed immediately by an italic capital *H* placed before a ring system name to express the position of each of the saturated atoms necessary for formation of a definable, stable ring system. Thus, Pyrrole always has one saturated atom (an atom not connected to either of its neighbors by a double bond) and, according to the position of this atom, the compound is named as follows:



In the *Chemical Substance Index* only a single illustrative structural diagram is provided for each ring system, viz., the diagram which shows the saturated center(s) in the lowest-numbered nonangular position(s).

Tetrahydropyrrole has the trivial name **pyrrolidine**; dihydropyrroles are named as derivatives of that pyrrole which has indicated hydrogen at the lowest numbered position consistent with the structure. Other monocyclic hetero systems are named in the same way. Hydrogen on a single ring atom between two bivalent hetero atoms is not indicated in the name.

Examples:



134. Carbonyl radicals which form part of a carbon chain are expressed by oxo substituents on the chain; the only exceptions are carboxy (-C(O)OH) and acetyl (-C(O)CH₃) radicals. The latter is used whenever (1-oxoethyl) would otherwise be called for. All chalcogen, imido and hydrazinylidene analogs of carbonyl in a chain are treated similarly by use of thioxo, selenoxo, telluroxo, imido, and hydrazinylidene radicals, except for chalcogen analogs (but not imido, etc., analogs) of carboxy; e.g., (HS(S)C-) is named (dithiocarboxy). Replacement analogs of acetyl are named (1-iminoethyl), (1-thioxyethyl), etc. Acyl radical names other than acetyl and benzoyl, e.g., propanoyl, are not used for substituents; neither are amido radicals, e.g., acetamido.

Examples:



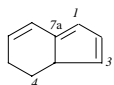
2*H*-Pyran, tetrahydro- (not *4H*-Pyran, tetrahydro-)



4*H*-1,3-Dithiin (not *2H,4H*-1,3-Dithiin)

The lowest locants for nonangular positions of fused ring systems are normally cited for indicated hydrogen.

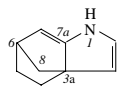
Example:



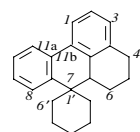
4*H*-Indene, 3*a*,5-dihydro- (not *3aH*-Indene, 4,5-dihydro- or *5H*-Indene, 3*a*,4-dihydro-)

Indicated hydrogen is assigned to angular or nonangular positions when needed to accommodate structural features, e.g., a bridge, spiro junction or ring-assembly junction, if that form of the ring system can exist.

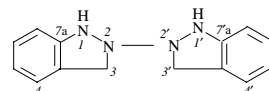
Examples:



3*a*,6-Methano-3*aH*-indole, 1,4,5,6-tetrahydro-



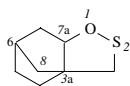
Spiro[7*H*-benz[de]anthracene-7,1'-cyclohexane], 4,5,6,6*a*-tetrahydro-



2,2'-Bi-2*H*-indazole, 1,1',3,3'-tetrahydro-

When a bridge requires hydrogen to be added, but indicated hydrogen of the parent system cannot be used for that purpose, the lowest locant, or a locant to accommodate a principal function, is chosen for the parent ring, and *additional indicated hydrogen* is cited in the name ahead of the bridge designation.

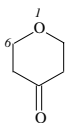
Example:



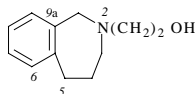
4*H*-3*a*,6-Methano-3*H*-1,2-benzoxathiole, tetrahydro- (*3aH*-1,2-Benzoxathiole cannot exist; the lowest available locant is therefore cited and the "extra" hydrogen for the bridge cited as additional indicated hydrogen, not in the "added" hydrogen form (see below), *3a(4H)*,6-Methano....)

After structural requirements have been met, indicated hydrogen is chosen to accommodate principal functions or (in a cyclic radical) free valencies, so long as the number of indicated hydrogens cited equals or exceeds the number of principal groups or free valencies that must be accommodated. For the usual case of a ring which requires a single indicated hydrogen for its existence, a single principal function or free valency is accommodated, but a polyfunctional compound is named at the ring system with lowest nonangular indicated hydrogen. (Functions on bridges are disregarded in applying this rule.)

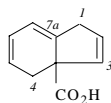
Examples:



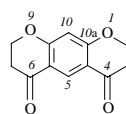
4*H*-Pyran-4-one, tetrahydro-



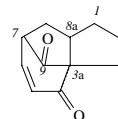
2*H*-2-Benzazepine-2-ethanol, 1,3,4,5-tetrahydro-



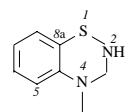
3*aH*-Indene-3*a*-carboxylic acid, 1,4-dihydro-



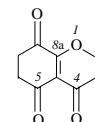
4*H*,6*H*-Benzo[1,2-*b*:5,4-*b'*]dipyran-4,6-dione, 2,3,7,8-tetrahydro-



4*H*-3*a*,7-Methanoazulene-4,9-dione, 1,2,3,7,8,8*a*-hexahydro- (not *1H*-3*a*,7-Methanoazulene-4,9-(*7H*)-dione, 2,3,8,8*a*-tetrahydro-) (the ketone function on the bridge is ignored in choosing indicated hydrogen to accommodate the single remaining function)

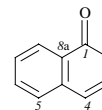


(2,3-dihydro-4*H*-1,2,4-benzothiadiazin-4-yl)(not *2H*-1,2,4-benzothiadiazin-4(3*H*)-yl)



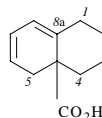
2*H*-1-Benzopyran-4,5,8-trione, 6,7-dihydro- (not *4H*-1-Benzopyran-4,5,8-trione, 2,3,6,7-tetrahydro-)

136. Added hydrogen is hydrogen which is added to a ring system in the same operation as, but in a position different from, hydrogen added to accommodate structural features of a ring system, e.g., bridges, or spiro or ring-assembly junctions, or principal groups of a heading parent, or free valencies of a parent radical, when indicated hydrogen (¶ 135) is either not needed for the ring system itself or cannot be chosen to accommodate them. It differs from indicated hydrogen in being expressed as a locant and capital italic *H* in parentheses immediately following the locant for the principal function or other accommodated structural feature, e.g., "2(1*H*)-." Use of added hydrogen permits expression of a principal function, etc., in a heading parent instead of as a substituent. Thus, **1-Naphthalenone** cannot exist without partial hydrogenation of the naphthalene ring system; a name such as **Naphthalene, 1,2-dihydro-1-oxo-** violates the rule that the principal function be expressed as a suffix. Therefore, two hydrogen atoms are added in one operation to provide the name **1(2*H*)-Naphthalenone**, in which the "added" (or "extra") hydrogen is at the 2-position.

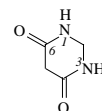


When principal functions or free valencies require added hydrogen, it is assigned to the lowest-numbered available angular or nonangular position; e.g., **1(2*H*)-Naphthalenone, 3,4-dihydro-** (not 1(4*H*)-Naphthalenone, 2,3-dihydro-); **2(4*H*)-Naphthalenone, 5,6,7,8-tetrahydro-**. When the ring system requires indicated hydrogen and it cannot be assigned to accommodate a principal group or free radical, it has preference over added hydrogen for lowest locants. When a *pair* of principal groups, e.g., "-dione," are expressed by a heading parent, added hydrogen is not cited unless necessary, it being understood that only sufficient hydrogen has been added to accommodate the functions.

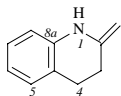
Examples:



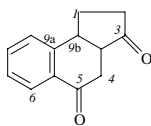
4*a*(2*H*)-Naphthalenecarboxylic acid, 1,3,4,5-tetrahydro- (a 4*a*(1*H*)-isomer cannot exist)



4,6(1*H*,5*H*)-Pyrimidinedione, dihydro-



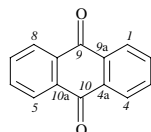
(3,4-dihydro-2(1H)-quinolinylidene)
(not (1,4-dihydro-2(3H)-quinolinylidene))



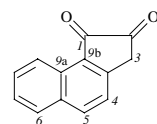
1H-Benz[e]indene-3,5(2H,4H)-dione, 3a,9b-dihydro-



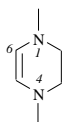
2H-Pyran-3(4H)-one, dihydro-
(3H-Pyran cannot exist)



9,10-Anthracenedione (not 9,10-(9H,10H)-Anthracenedione)



1H-Benz[e]indene-1,2(3H)-dione
(not 3H-Benz[e]indene-1,2-dione)
(low numbering of indicated hydrogen is observed, even if added hydrogen must then be cited)

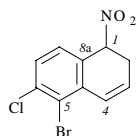


(2,3-dihydro-1,4-pyrazinediyl) (not (1,4(2H,3H)-pyrazinediyl))

Added hydrogen cited when hydrogen is required elsewhere for spiro and ring-assembly junctions is assigned (in descending order of preference) (a) to accommodate another spiro or ring-assembly junction, (b) to accommodate principal groups or free valencies, or (c) to lowest-numbered available positions.

137. Numbering of molecular skeletons. Lowest locants for a set of principal groups, substituents, etc., are always preferred. The set, e.g., 5,6,1,2,1 is compared with another (alternative) set, e.g., 1,2,5,6,5, by rearranging them both in ascending numerical sequence: 1,1,2,5,6 and 1,2,5,5,6. The set which contains the lowest locant at the first point of difference when all sets are compared term by term is the lowest, i.e., 1,1,2,5,6 is lower than 1,2,5,5,6.

Example:

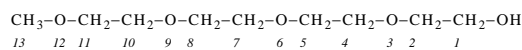


Naphthalene, 5-bromo-6-chloro-1,2-dihydro-1-nitro- (not Naphthalene, 1-bromo-2-chloro-5,6-dihydro-5-nitro-)

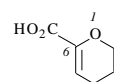
Lowest locants for various kinds of structural features in cyclic and acyclic molecular skeletons are assigned, in order, to:

- hetero atoms (except for "a"-named radicals, see ¶¶ 127, 161);
- indicated hydrogen;
- principal groups or (for radicals) free valencies;
- multiple bonds;
- substituent prefixes;
- the substituent prefix cited earliest in the name.

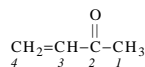
Examples:



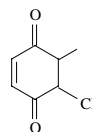
3,6,9,12-Tetraoxatridecan-1-ol



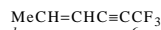
2H-Pyran-6-carboxylic acid, 3,4-dihydro- (not 4H-Pyran-2-carboxylic acid, 5,6-dihydro-)



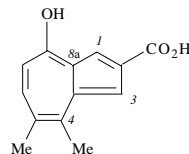
3-Buten-2-one (not 1-Buten-3-one)



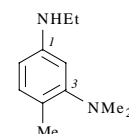
(6-chloro-2,5-dioxo-3-cyclohexen-1-yl)



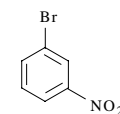
2-Hexen-4-yne, 6,6,6-trifluoro-
(double bond given preference over triple bond)



2-Azulenecarboxylic acid, 8-hydroxy-4,5-dimethyl-



1,3-Benzenediamine, N¹-ethyl-N³, N³,4-trimethyl- (not 1,3-Benzenediamine, N³-ethyl-N¹, N¹,6-trimethyl-; see ¶ 114)



Benzene, 1-bromo-3-nitro- (not Benzene, 3-bromo-1-nitro-)

138. Index name selection. Most organic compounds have names based on molecular skeletons, e.g., **Propanoic acid** (from propane); **1,3-Dioxan-2-amine** (from 1,3-dioxane). Procedures for selecting the preferred name of this kind for index use are described in this section (see also ¶ 105).

Selection of a heading parent name based on a molecular skeleton is made by successive application of the following principles until a decision is reached.

- Greatest number of the principal chemical functional group.
- Preferred atomic content of the molecular skeleton in accordance with the order of precedence of compound classes (¶ 106). The heading parent should express at least one occurrence of an atom appearing earliest in the following list: N, P, As, Sb, Bi, B, Si, Ge, Sn, Pb, O, S, Se, Te. (This principle is used to decide between a cyclic and an acyclic parent, but is not applied to choices between ring systems. When acyclic and cyclic skeletons of the same compound class are present, a cyclic parent is preferred.)
- Preferred ring system. The choice between ring systems for use as heading parents is based on the following criteria, applied successively until a decision is reached. The senior ring system should:
 - be a nitrogenous heterocycle;
 - be a heterocycle;
 - contain the largest number of rings;
 - be a cyclic system occurring earliest in the following list of systems; spiro, bridged fused, bridged nonfused (Von Baeyer), fused;
 - contain the largest individual ring (applies to fused carbocyclic systems);
 - contain the greatest number of ring atoms;
 - contain the greater number of ring atoms common to two or more rings (applies to Von Baeyer ring systems); thus



is senior to



- contain lowest locants for bridges;
 - contain the largest number of hetero atoms;
 - contain the most preferred hetero atom other than nitrogen, according to the order in Table I, ¶ 128, i.e., O, S, Se, Te, N, P, As, Sb, Bi, Si, Ge, Sn, Pb, B.
 - possess the most linear arrangement of rings (thus, **Anthracene** is senior to **Phenanthrene**);
 - possess the lowest locants for hetero atoms assigned according to the rules (¶¶ 146, 152);
 - express the lowest state of hydrogenation; thus, **Benzene** is preferred over **Cyclohexane**, **Pyridine** over **Piperidine**;
 - express the lowest locant for indicated hydrogen.
- Note: These criteria differ from those employed in selecting base components for fused systems (¶ 150).
- Greatest number of acyclic hetero atoms.
 - Largest index heading parent.

(f) Greatest number of most preferred acyclic hetero atoms, according to the order of precedence in ¶ 128, above; i.e., O, S, Se, Te, N, P, As, Sb, Bi, Si, Ge, Sn, Pb, B.

(g) Greatest number of multiple bonds.

(h) Lowest locants in the heading parent successively for hetero atoms, principal groups (suffixes), all multiple bonds, double bonds.

If the preferred heading parent occurs more than once in the total compound, further principles must be applied, as follows:

(i) Centrality. For three or more occurrences of the heading parent, at least one of which must be nonterminal, the basis of the name is the central occurrence (or one of the central pair—both, when multiplicative nomenclature is permitted—if the total number is even) in the linear arrangement which comprises all or part of the maximum number of occurrences.

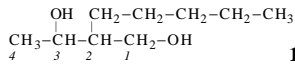
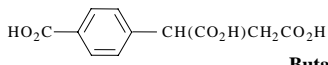
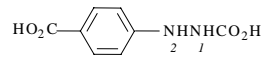
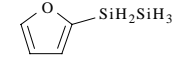

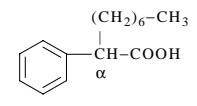
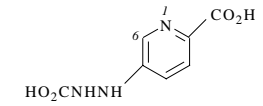
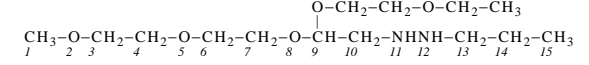
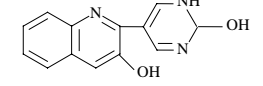
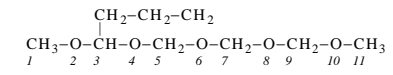
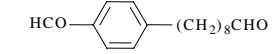
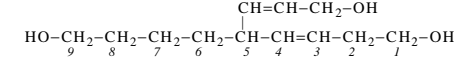
(j) Maximum number of substituent prefixes.

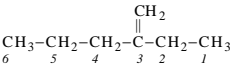
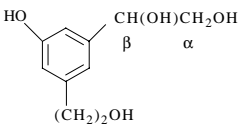
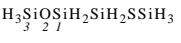
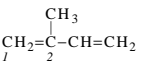
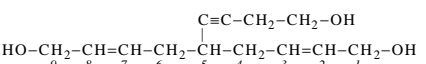
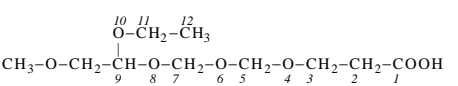
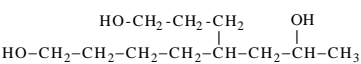
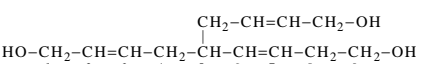

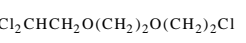
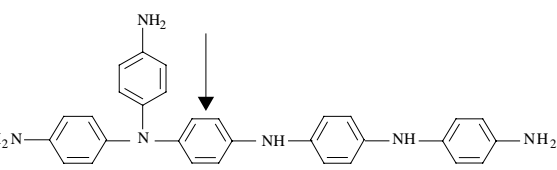
(k) Lowest locants for substituents on the heading parent.

(l) Multiplication of heading parents; when there is a choice of multiplicative names, that one is chosen which multiplies the largest number of occurrences of the index heading parent.

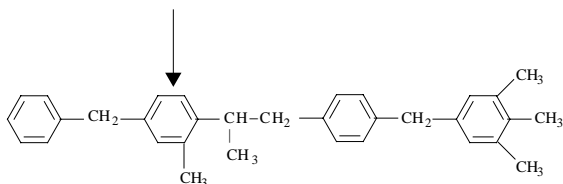
(m) Earliest index position of the total name.

Examples (the italic letters on the left indicate the particular rules (above) that are exemplified):

- (a)  **1,3-Butanediol, 2-pentyl-**
- (a)  **Butanedioic acid, 2-(4-carboxyphenyl)-**
- (b)  **Hydrazinecarboxylic acid, 2-(4-carboxyphenyl)-**
- (b)  **Disilane, 2-furanyl-**
- (b)  **Diazene, phenyl-** (not Benzenamine, *N*-imino-) (homogeneous hetero chains are never broken to obtain a higher function or more preferred parent)
- (b)  **Benzeneacetic acid, α -heptyl-** (not Nonanoic acid, 2-phenyl-)
- (b)  **2-Pyridinecarboxylic acid, 5-(2-carboxyhydrazino)-** (the number of preferred hetero atoms in the cyclic and acyclic chains is disregarded)
- (b)  **2,5,8-Trioxa-11,12-diazapentadecane, 9-(2-ethoxyethoxy)-**
- (c)  **3-Quinolinol, 2-(1,2-dihydro-2-hydroxy-5-pyrimidinyl)-**
- (d)  **2,4,6,8,10-Pentaoxaundecane, 3-propyl-**
- (e)  **Benzenonanal, 4-formyl-** (not Benzaldehyde, 4-(9-oxononyl)-)
- (e)  **3-Nonene-1,9-diol, 5-(3-hydroxy-1-propen-1-yl)-** (not 2,5-Octadiene-1,8-diol, 5-(4-hydroxybutyl)-)

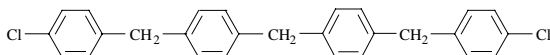
- (e)  **Hexane, 3-methylene-** (not 1-Pentene, 2-ethyl-)
- (e)  **1,3-Benzenediethanol, β , 5-dihydroxy-** (see ¶ 124)
- (f)  **Disiloxane, 1-disilathianyl-**
- (g)  **1,3-Butadiene, 2-methyl-**
- (g)  **2,7-Nonadiene-1,9-diol, 5-(4-hydroxy-1-butyn-1-yl)-** (double bonds are preferred over an equal number of triple bonds)
- (h)  **4,6,8,10-Tetraoxadodecanoic acid, 9-(methoxymethyl)-** (not 3,5,7,9-Tetraoxadodecan-12-oic acid, 4-(methoxymethyl)-)
- (h)  **1,7-Octanediol, 5-(3-hydroxypropyl)-** (not 1,8-Octanediol, 4-(2-hydroxypropyl)-)
- (h)  **2,6-Nonadiene-1,9-diol, 5-(4-hydroxy-2-buten-1-yl)-** (not 2,7-Nonadiene-1,9-diol, 5-(4-hydroxy-1-butenyl)-)
- (i)  **Benzene, 1,4-bis(phenylmethyl)-**
- (i)  **Ethane, 1-(2-chloroethoxy)-2-(2,2-dichloroethoxy)-**
- (i)  **1,4-Benzenediamine, N^1,N^1 -bis(4-aminophenyl)- N^4 -[4-(4-aminophenyl)amino]phenyl-**

(i,j)



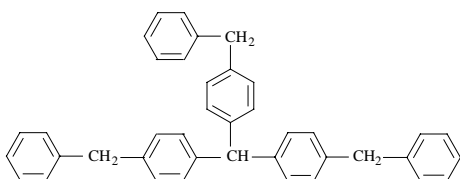
Benzene, 2-methyl-1-[1-methyl-2-[4-[(3,4,5-trimethylphenyl)methyl]phenyl]ethyl]-4-(phenylmethyl)- (of the two central occurrences of the preferred heading parent, the one with the maximum number (three) of substituents is chosen; note that the centrality principle prevents choice of the tetrasubstituted parent on the right)

(i,l)



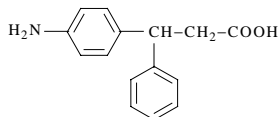
Benzene, 1,1'-methylenebis[4-(4-chlorophenyl)methyl]-

(i,l)



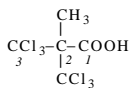
Benzene, 1,1',1''-methylidyne-tris[4-(phenylmethyl)- (when multiplication of the heading parent is permitted, occurrences directly attached to the central connecting radical are included in the same operation if possible)

(j)



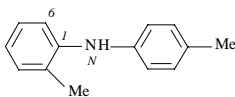
Benzenepropanoic acid, 4-amino-beta-phenyl-

(j)



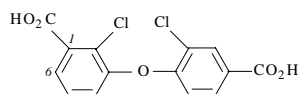
Propanoic acid, 3,3,3-trichloro-2-methyl-2-(trichloromethyl)- (not Propanoic acid, 2,2-bis(trichloromethyl)-) (like treatment of like groups is discontinued (¶ 255))

(k)



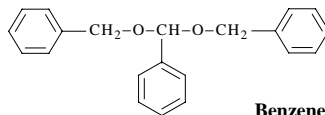
Benzenamine, 2-methyl-N-(4-methylphenyl)-

(k)



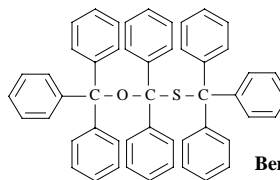
Benzoic acid, 3-(4-carboxy-2-chlorophenoxy)-2-chloro-

(l)



Benzene, 1,1'-[(phenylmethylene)bis(oxymethylene)]bis- (note that all occurrences of benzene are terminal and that the principle of centrality is therefore not applicable)

(l,m)



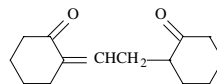
Benzene, 1,1',1''-[[[diphenyl(triphenylmethoxy)methyl]thio]methylidene]tris- (not Benzene, 1,1',1''-[[[diphenyl(triphenylmethyl)thio]methylidene]tris-])

(m)



Propanoic acid, 2,3,3,3-tetrafluoro-2-(trichloromethyl)- (not Propanoic acid, 3,3,3-trichloro-2-fluoro-2-(trifluoromethyl)-)

(m)



Cyclohexanone, 2-[2-(2-oxocyclohexyl)ethylidene]- (not Cyclohexanone, 2-[2-(2-oxocyclohexylidene)ethyl]-)

139. Subtractive nomenclature employs the suffixes “-ene” and “-yne” to signify removal of hydrogen pairs from saturated molecular skeletons; removal of hydrogen atoms from an aromatic system is denoted by “dehydro.”

Examples:



Bicyclo[2.2.1]hepta-2,5-diene



Pyridine, 2,3-didehydro- (not Pyridyne)

Functional class names such as “anhydride,” “ester,” “oxime,” imply loss of water and may strictly be regarded as subtractive terms. Prefixes such as “deoxy,” “nor,” and “anhydro,” are sometimes employed in names for classes of stereoparents (see Section E), but never in general index nomenclature.

B. MOLECULAR SKELETONS

Introduction	¶ 140
Acyclic hydrocarbons	141
Organic hetero chains	142
Homogeneous hetero chains	143
Heterogeneous hetero chains	144
Monocyclic hydrocarbons	145
Monocyclic hetero systems	146
Polycyclic systems	147
Fundamental fused carbocycles	148
Fundamental fused heterocycles	149
Selection of a base component	150
Index names for fused systems	151
Orientation and numbering of fused systems	152

Replacement ("a") nomenclature for fused systems	¶ 153
Bridged fused systems	154
Von Baeyer nomenclature	155
Spiro systems	156
Ring assemblies	157
Hetero atoms with abnormal valencies	158
Boron molecular skeletons	159
"Hetero" polyboranes	160
Substituent prefixes from molecular skeletons	161
Compound and complex radicals	162
Molecular skeletons as index heading parents	163
Fullerenes	163A

140. Introduction. A molecular skeleton is defined for purposes of name selection as a chain or ring of atoms in which the number of hydrogen atoms attached to each skeletal atom is (usually) implied or (occasionally) explicitly stated by citation of the substitutive valency and bonding of the skeletal atoms. Monoatomic hydrides of Group IVA and VA elements (except nitrogen) are also treated as molecular skeletons; so are boron hydrides, but because of their unusual nature these are discussed separately (¶ 159).

Examples:

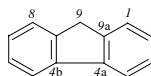
CH ₄	Methane
AsH ₅	Arsorane
H ₃ SiOSiH ₂ OSiH ₂	Trisiloxane
H ₃ SnSnH ₃	Distannane
$\text{CH}_3\text{-CH}_2\text{-O-CH}_2\text{-CH}_2\text{-O-CH}_2\text{-CH}_2\text{-O-CH}_2\text{-CH}_2\text{-O-CH}_2\text{-CH}_2\text{-O-CH}_2\text{-CH}_3$ <small>14 13 12 11 10 9 8 7 6 5 4 3 2 1</small>	3,6,9,12-Tetraoxatetradecane



Benzene



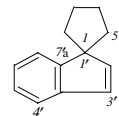
Pyrrolidine



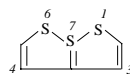
9H-Fluorene



Bicyclo[2.2.1]hept-2-ene



Spiro[cyclopentane-1,1'-[1H]-indene]



7λ⁴-[1,2]Dithiolo[1,5-b][1,2]dithiole

Molecular skeletons are nonfunctional substitutive parent compounds. Substituents denoting a preferred compound class are generally cited as suffixes and other substituents as prefixes. Molecular skeletons, alone or in combination with a substituent suffix, are *index heading parents*.

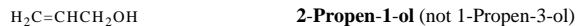
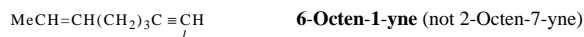
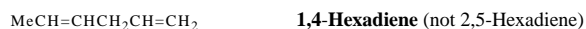
This part of the manual deals with the formation of index names for structures that consist solely of one or more molecular skeletons.

141. Acyclic hydrocarbons. Saturated unbranched alkanes containing one through four carbon atoms are named **Methane**, **Ethane**, **Propane**, and **Butane**. Higher members of the class are named by adding the termination "-ane" to the appropriate multiplicative term, as **Nonane** for C₉H₂₀, **Hexadecane** for C₁₆H₃₄, **Eicosane** for C₂₀H₄₂, **Heneicosane** for C₂₁H₄₄, and **Tritriacotane** for C₃₃H₆₈.

Unsaturated unbranched acyclic hydrocarbons (unbranched alkenes, alkadienes, alkynes, etc.) are named by replacing the ending "-ane" by "-ene" (for a single double bond), "-adiene" for two double bonds, "-yne" for a single triple bond, etc. Combinations, e.g., "-enynes," "-trienediyne," are employed when both bond types are present. Low numbering (¶ 137) is employed for the

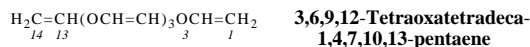
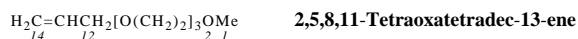
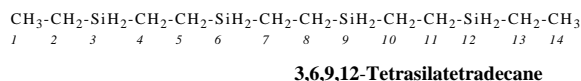
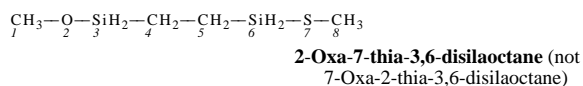
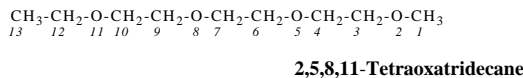
set of multiple bonds; when there is a choice, double bonds are preferred over triple bonds. When principal groups (functional suffixes) are present, these and not the multiple bonds are preferred for low numbering.

Examples:



142. Organic hetero chains containing at least four hetero units (¶ 127) are given "a" names, i.e., replacement names based on the hydrocarbon skeleton by use of "oxa," "thia," etc., prefixes. Lowest locants (¶ 137) are assigned to all hetero atoms regardless of type and then to preferred hetero atoms (Table I, ¶ 128). Locants for functional suffixes take precedence for low numbering.

Examples:



143. Homogeneous hetero chains are considered to include the mononuclear hydrides **Phosphine** (PH₃), **Phosphorane** (PH₅), **Arsine** (AsH₃), **Arsorane** (AsH₅), **Stibine** (SbH₃), **Bismuthine** (BiH₃), **Silane** (SiH₄), **Germane** (GeH₄), **Stannane** (SnH₄), and **Plumbane** (PbH₄). Chains composed of two or more of these hydride residues are named by prefixing the hydride name with "Di," "Tri," etc.

Examples:



Saturated nitrogen chains are named **Hydrazine** (not Diazane) for H_2NNH_2 , **Triazane** for H_2NNHNH_2 , **Tetrazane** for $H_2NNHNHNH_2$, etc.

Unsaturation is denoted by use of the subtractive suffixes “-ene” and “-yne.” Locants are employed as for hydrocarbon chains (¶ 114, 141).

Examples:

$HA_s=AsH$	Diarsene
$H_2Si=SiH_2$	Disilene
$H_2NN=NNH_2$	2-Tetrazene
$HN=NN=NH$	1,3-Tetrazadiene

144. Heterogeneous hetero chains in which any one of the Group IVA elements (silicon, germanium, tin, or lead) alternates with chalcogen are given “oxane,” “thiane,” etc. names.

Examples:

$H_3SiOSiH_2OSiH_3$ <small>1 2 3 4 5</small>	Trisiloxane
$H_3GeSeGeH_3$ <small>1 2 3</small>	Digermaselenane
$H_3SnSSnH_2SSnH_3$ <small>1 2 3 4 5</small>	Tristannathiane

Chains of alternating atoms of a Group IVA element and nitrogen, e.g., SiH_3NHSiH_3 , SnH_3NHSnH_3 , are not named Disilazane, Distannazane, etc. Instead, the amine function is recognized; thus, Disilazane is indexed at **Silanamine**, *N-silyl*-. However, substituent radicals derived from such heterogeneous chains containing nitrogen, e.g., 1-disilazanyl for SiH_3NHSiH_2- , are employed in the presence of higher functions (see ¶ 161).

“A” names for hetero chains are avoided unless carbon substituents can be included in the chain. Otherwise the preferred parent is a homogeneous hetero chain, hydride, or element name.

Examples:

$H_3GeOSiH_2SPbH_3$	Silane, (germyloxy)(plumbylthio)-
$H_3GeOPbH_2SeMe$ <small>1 2 3 4</small>	2-Oxa-4-selena-1-germa-3-plumbapentane

145. Monocyclic hydrocarbons (cycloalkanes, cycloalkenes, etc.) are named by attaching the prefix “cyclo” to the name of the acyclic hydrocarbon with the same number of carbon atoms. Unsaturation is expressed by use of “-ene” and “-yne” in place of “-ane” as for the acyclic analogs. No locant is employed for a single multiple bond; lowest locants (¶ 137) are cited when two or more multiple bonds are present. The trivial name **Benzene** is used for 1,3,5-Cyclohexatriene.

Examples:



Cyclohexane



1,3-Cyclopentadiene



Cyclohexene



1,3-Cyclohexadien-5-yne (not Benzyne)

146. Monocyclic hetero systems.

(a) Rings of three through ten members containing nonmetallic hetero atoms (except silicon) are named systematically by the (extended) Hantzsch-Widman system or at trivial names. Table II supplies the stems for the systematic names, which are completed by adding replacement prefixes for the hetero atoms in the order set out in Table I, ¶ 128, e.g., oxa, thia, aza, together with locants and multiplicative prefixes denoting the position and number of each. A locant for a single hetero atom is not cited. The preferred hetero atom is numbered “1.” This means the *set* of locants may not be the lowest possible, as defined in ¶ 137. The letter “a” of replacement prefixes is elided before another vowel in Hantzsch-Widman names; e.g., **Dioxazole**, not Dioxazole.

Examples:



Oxirene



Aziridine



Phosphorin



Oxazole (not 1,3-Oxazole, because the 1,2-isomer has the trivial name Isoxazole)



1,2-Oxathiolane (all locants are placed ahead of the name; cf. ¶ 146(c), below)



2H-1,5,2-Dithiazine (not 1H-2,4,1-Dithiazine; not 6H-1,3,6-Dithiazine; not 4H-1,5,4-Dithiazine) (The numbering must begin with a sulfur atom and proceed in the direction that gives lowest numbers to the remaining hetero atoms.) (The “2H” signifies indicated hydrogen (see ¶ 135)).

TABLE II
HANTZSCH-WIDMAN STEMS FOR MONOCYCLIC HETERO SYSTEMS OF THREE THROUGH TEN MEMBERS¹

No. of members in the ring	Rings containing nitrogen		Rings containing no nitrogen	
	Unsaturated ²	Saturated	Unsaturated ²	Saturated
3	-irine	-iridine	-irene	-irane
4	-ete	-etidine	-ete	-etane
5	-ole	-olidine	-ole	-olane
6	-ine ³	4	-in ³	-ane ^{5,6}
7	-epine	4	-epin	-epane
8	-ocine	4	-ocin	-ocane
9	-onine	4	-onin	-onane
10	-ecine	4	-ecin	-ecane

¹The symbols denoting the ring sizes for 3, 4, 7, 8, 9, 10 members are derived from numerical prefixes as follows: “ri” from *tri*; “et” from *tetra*; “ep” from *hepta*; “oc” from *octa*; “on” from *nona*; and “ec” from *deca*.

²Corresponds to the maximum number of noncumulative double bonds when the hetero atoms have the substituent valencies given in Table I, ¶ 128.

³When the Hantzsch-Widman prefixes “phospha,” “arsa,” or “stiba” are immediately followed by the Hantzsch-Widman stems “-in” or “-ine,” they are replaced by the prefixes “phosphor,” “arsen,” or “stibin,” respectively.

⁴Saturation is expressed by detachable prefixes such as “tetrahydro-,” “hexahydro-,” etc. The prefix “perhydro-” is not used.

⁵This stem is not used for saturated hetero systems based on the elements silicon, germanium, tin, or lead. Saturation of these rings is indicated by detachable prefixes such as “tetrahydro-,” “hexahydro-,” etc., when Hantzsch-Widman names are used.

⁶Saturation of six-membered hetero systems based on the elements boron or phosphorus is denoted by the stem “-inane.”

Table II indicates those cases in which special endings are employed for fully saturated monocyclic hetero systems: e.g., **Azetidine**, not Azete, tetrahydro-. Special names for *partially* saturated ring systems are discontinued.

Example:



Azete, 1,2-dihydro- (not 2-Azetine)

Certain five- and six-membered monocyclic hetero systems, both saturated and unsaturated, are indexed at trivial names. These names are set out in Table III in the order of the corresponding Hantzsch-Widman names, which are *not* used for indexing. Fully hydrogenated five-membered rings are given “-olidine” names, as for systematically named systems. Special names for partially hydrogenated five-membered rings e.g., **2-Pyrroline**, were discontinued in 1972; they are now named as dihydro derivatives of the fully unsaturated rings. Indicated hydrogen (see ¶135) is necessary in some rings to describe the location of the saturated skeletal atom, e.g., **1H-Pyrrole**, **2H-Pyrrole**, **3H-Pyrrole**. Presence of a triple bond in addition to the maximum number of noncumulative double bonds is expressed by the subtractive prefix “dihydro-.”

Example:



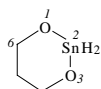
Pyridine, 2,3-didehydro-

TABLE III
MONOCYCLIC HETERO SYSTEMS
WITH TRIVIAL NAMES

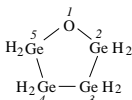
Hantzsch-Widman name	Index name
Azine	Pyridine
Azine, hexahydro-	Piperidine
Azole	Pyrrole (1H-, 2H-, or 3H-)
Azolidine	Pyrrolidine
1,2-Diazine	Pyridazine
1,3-Diazine	Pyrimidine
1,4-Diazine	Pyrazine
1,4-Diazine, hexahydro-	Piperazine
1,2-Diazole	Pyrazole (1H-, 3H-, or 4H-)
1,3-Diazole	Imidazole (1H-, 2H-, or 4H-)
1,2-Diazolidine	Pyrazolidine
1,3-Diazolidine	Imidazolidine
2H-1,4-Oxazine, tetrahydro-	Morpholine
1,2-Oxazole	Isoxazole
Oxin	Pyran (2H- or 4H-)
Oxole	Furan
1,2-Selenazole	Isoselenazole
Selenole	Selenophene
Tellurole	Tellurophene
2H-1,4-Thiazine, tetrahydro-	Thiomorpholine
1,2-Thiazole	Isothiazole
Thiole	Thiophene
1,3,5,2,4,6-Triazatriborine, hexahydro-	Borazine
1,3,5,2,4,6-Trioxatriborinane	Boroxin
1,3,5,2,4,6-Trithiatriborinane	Borthiin

(b) Rings of three through ten members containing antimony, tin, lead, germanium or bismuth atoms in addition to carbon atoms are indexed at Hantzsch-Widman names. Partially saturated and fully saturated six-membered ring systems of this type containing germanium, lead or tin are named on the basis of the unsaturated rings. Heterocycles containing metallic atoms other than the above five are indexed by coordination nomenclature (¶ 215).

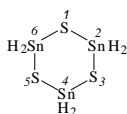
Examples:



4H-1,3,2-Dioxastannin, dihydro-



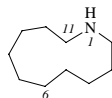
Oxatetragermolane



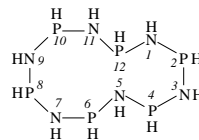
1,3,5,2,4,6-Trithiatristannin

(c) Rings of more than ten members not containing silicon atoms are indexed at organic replacement (“a”) names. Unsaturation is indicated by “-ene” and “-yne” suffixes.

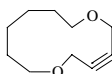
Examples:



Azacycloundecane



1,3,5,7,9,11-Hexaaza-2,4,6,8,10,12-hexaphosphacyclododecane



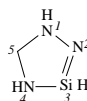
1,6-Dioxacyclododec-3-yne

(d) Rings containing silicon in general are indexed at replacement (“a”) names based on the cyclic hydrocarbons. Systems comprising only silicon atoms or silicon atoms alternating with nitrogen or one of the chalcogens are given “Cyclosila-” names.

Examples:



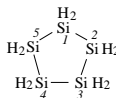
Silacyclopropane



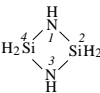
1,2,4-Triaza-3-silacyclopent-2-ene



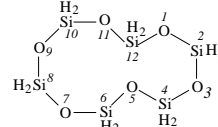
Silabenzene



Cyclopentasilane



Cyclodisilazane



Cyclohexasiloxane

147. Polycyclic systems may be subdivided into four classes as follows:

(a) *Fused systems* contain at least two rings of five or more members and only “ortho-” or “ortho- and peri-” fusions (see below).

(b) *Bridged systems* are monocyclic or fused systems with valence bonds, atoms, or chains connecting different parts of the structure.

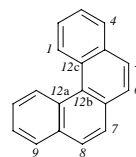
(c) *Spiro systems* have pairs of rings (or ring systems) with only one common atom.

(d) *Ring assemblies* have pairs of rings (or ring systems) connected by single bonds.

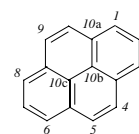
In the following sections, methods of naming ring systems of all these types will be described. The names of more complicated cases are built up from base components which may be described as “fundamental” systems.

148. Fundamental fused carbocycles with ortho-fusions only, e.g., **Naphthalene**, have adjoining rings with only two atoms in common; they thus have *n* common faces and *2n* common atoms. An ortho- and peri-fused system contains a ring which has two, and only two, atoms in common with each of two or more rings, the total system containing *n* common faces and *fewer than 2n* common atoms.

Examples:



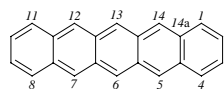
An ortho-fused system
(3 common faces; 6 common atoms)



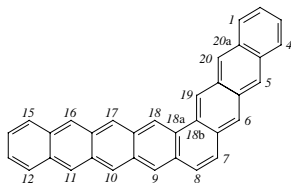
An ortho- and peri-fused system
(5 common faces; 6 common atoms)

Systems of five or more ortho-fused benzene rings are named by the "acene" system if the arrangement is linear, by the "phene" system if one central angular site is present.

Examples:



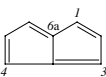
Pentacene



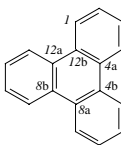
Octaphene

Names ending in "-alene" are employed for bicyclic fused systems, and in "-phenylene" for systems built up from benzene rings fused to alternate sides of a monocyclic hydrocarbon. (Analogous "-naphthylene" names have been used for corresponding 2,3-fusion systems of naphthalene.)

Examples:



Pentalene



Triphenylene

Table IV lists the names of trivially-named fundamental fused carbocycles in ascending order of preference for adoption as base components in the naming of more complex fused hydrocarbon systems. Also included are some of the names discussed immediately above. (The order is based on the rules described in ¶138, 150.) The ring analyses describe the number of component rings and the number of atoms each ring contains. Diagrams of these rings, which show the preferred orientation and numbering, are displayed in the *Ring Systems Handbook*. Diagrams justified by current entries are also provided in the semiannual and collective *Chemical Substance Indexes*.

The following ring systems require citation of indicated hydrogen (¶135) to complete the name: **Indene**, **Fluorene**, **Phenalene**, **Trindene**.

TABLE IV
FUNDAMENTAL FUSED CARBOCYCLES IN
ASCENDING ORDER OF PRECEDENCE FOR
USE AS BASE COMPONENTS IN FUSED
SYSTEMS

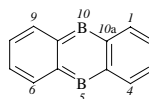
Name	Ring analysis
Pentalene	C ₅ -C ₅
Indene	C ₅ -C ₆
Naphthalene	C ₆ -C ₆
Azulene	C ₅ -C ₇
Heptalene	C ₇ -C ₇
Biphenylene	C ₄ -C ₆ -C ₆
<i>as</i> - Indacene	C ₅ -C ₅ -C ₆
<i>s</i> - Indacene	C ₅ -C ₅ -C ₆
Acenaphthylene	C ₅ -C ₆ -C ₆
Fluorene	C ₅ -C ₆ -C ₆
Phenalene	C ₆ -C ₆ -C ₆
Phenanthrene	C ₆ -C ₆ -C ₆
Anthracene	C ₆ -C ₆ -C ₆
Trindene	C ₅ -C ₅ -C ₅ -C ₆
Fluoranthene	C ₅ -C ₆ -C ₆ -C ₆
Acephenanthrylene	C ₅ -C ₆ -C ₆ -C ₆
Aceanthrylene	C ₅ -C ₆ -C ₆ -C ₆
Triphenylene	C ₆ -C ₆ -C ₆ -C ₆
Pyrene	C ₆ -C ₆ -C ₆ -C ₆
Chrysene	C ₆ -C ₆ -C ₆ -C ₆
Naphthacene	C ₆ -C ₆ -C ₆ -C ₆
Pleiadene	C ₆ -C ₆ -C ₆ -C ₇
Picene	C ₆ -C ₆ -C ₆ -C ₆ -C ₆
Perylene	C ₆ -C ₆ -C ₆ -C ₆ -C ₆
Pentaphene	C ₆ -C ₆ -C ₆ -C ₆ -C ₆
Pentacene	C ₆ -C ₆ -C ₆ -C ₆ -C ₆
Tetraphenylene	C ₆ -C ₆ -C ₆ -C ₆ -C ₈
Hexaphene	C ₆ -C ₆ -C ₆ -C ₆ -C ₆ -C ₆
Hexacene	C ₆ -C ₆ -C ₆ -C ₆ -C ₆ -C ₆

Rubicene
Coronene
Trinaphthylene
Heptaphene
Heptacene
Pyranthrene
Ovalene

C₅-C₅-C₆-C₆-C₆-C₆-C₆
C₆-C₆-C₆-C₆-C₆-C₆-C₆
C₆-C₆-C₆-C₆-C₆-C₆-C₆
C₆-C₆-C₆-C₆-C₆-C₆-C₆
C₆-C₆-C₆-C₆-C₆-C₆-C₆
C₆-C₆-C₆-C₆-C₆-C₆-C₆
C₆-C₆-C₆-C₆-C₆-C₆-C₆
C₆-C₆-C₆-C₆-C₆-C₆-C₆

149. Fundamental fused heterocycles often have trivial names, e.g., **Cinnoline**, **Xanthene**. Others belong to one or another semisystematic system. A linear set of three fused six-membered rings with the same hetero element in both unfused positions of the central ring are given "-anthrene" names.

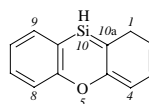
Example:



Boranthrene

A similar set with different hetero elements in these positions is given a "Pheno-" name containing the organic replacement terms in the usual order (Table I, ¶128) and the ending "-in" (or "-ine" if nitrogen, phosphorus or arsenic is included).

Example:



1H-Phenoxasilin

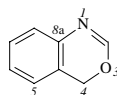
An exception is **Phenazine** for the analog that contains nitrogen in *both* central positions.

Arsenic and phosphorus analogs of fused nitrogen heterocycles (**Indole**, **Quinoline**, etc.) are named as follows: **Arsindole**, **Isoarsindole**, **Arsinoline**, **Isoarsinoline**, **Phosphindole**, **Isophosphindole**, **Phosphinoline**, **Isophosphinoline**, **Arsanthridine**, **Acridarsine**, **Acridophosphine**, **Phenarsazine**, **Phenophosphazine**.

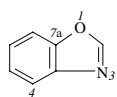
The replacement of the oxygen in **Xanthene** by sulfur or selenium has been denoted by the appropriate chalcogen functional replacement prefix: **Thioxanthene**, **Selenoxanthene**.

In the "benzo" system, bicyclic fused heterocyclic systems containing a benzene ring and a ring named by the Hantzsch-Widman system are indexed by prefixing the latter name by "Benz-" or "Benzo-." Indicated hydrogen, if necessary, and locants are placed in front of the complete name. Similar names are used when benzene is fused to a monocycle with a trivial name (unless the bicyclic system itself has a trivial name).

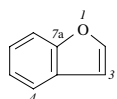
Examples:



4H-3,1-Benzoxazine (not *4H*-Benz-[d]oxazine)



Benzoxazole (locants are not cited; the isomers are named 1,2- and 2,1-Benzisoxazole)

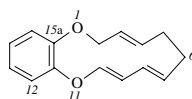


Benzofuran (the isomer is named Isobenzofuran)

Such "benzo" names are not usually adopted as base components of fused systems when only hydrocarbon rings are fused to the benzene portion.

When benzene is fused to a heterocyclic ring containing more than ten skeletal atoms, "Benzo-" or "Benz-" is placed ahead of the replacement ("a") name of the saturated ring and the ending changed to "-in" (or "-ine" if nitrogenous) to indicate the maximum number of noncumulative double bonds. (Saturated positions other than those occupied by indicated hydrogen are denoted by hydro substituents.)

Example:



2H-1,11-Benzodioxacyclotridecin, 5,6-dihydro-

Trivially named fundamental fused hetero systems are listed in Table V. Also included are some of the systems discussed immediately above, as well as a selection of monocyclic hetero systems to help illustrate the ascending order of priority for adoption as base components in complex fused systems.

Fused systems containing only silicon and carbon skeletal atoms are indexed at "Sila-" replacement names if the corresponding hydrocarbon has a fundamental name (Table IV, ¶148).

TABLE V
FUNDAMENTAL HETEROCYCLES IN
ASCENDING ORDER OF PRECEDENCE FOR
USE AS BASE COMPONENTS IN FUSED
SYSTEMS¹

Index Name	Ring Analysis
Isoarsindole ²	C ₄ As-C ₆
Arsindole ²	C ₄ As-C ₆
Isoarsinoline	C ₅ As-C ₆
Arsinoline	C ₅ As-C ₆
Arsanthridine	C ₅ As-C ₆ -C ₆
Acridarsine	C ₅ As-C ₆ -C ₆
Arsanthrene	C ₄ As ₂ -C ₆ -C ₆
Isoosphindole ²	C ₄ P-C ₆
Phosphindole ²	C ₄ P-C ₆
Isoosphinoline	C ₅ P-C ₆
Phosphinoline	C ₅ P-C ₆
Tellurophene	C ₄ Te
Selenophene	C ₅ Se
Selenanthrene	C ₄ Se ₂ -C ₆ -C ₆
Thiophene	C ₄ S
Thianthrene	C ₄ S ₂ -C ₆ -C ₆
Furan	C ₄ O
Pyran ²	C ₅ O
Isobenzofuran	C ₄ O-C ₆
Xanthen ²	C ₅ O-C ₆ -C ₆
Phenoxastibinin	C ₄ OsB-C ₆ -C ₆
Phenoxarsine ²	C ₄ AsO-C ₆ -C ₆
Phenoxaphosphine ²	C ₄ OP-C ₆ -C ₆
Phenoxatellurin	C ₄ OTe-C ₆ -C ₆
Phenoxaselenin	C ₄ OSe-C ₆ -C ₆
Phenoxathiin	C ₄ OS-C ₆ -C ₆
Pyrrole ²	C ₄ N
Imidazole ²	C ₂ N ₂
Pyrazole ²	C ₃ N ₂
Isothiazole	C ₃ NS
Isoxazole	C ₃ NO
Pyridine	C ₅ N
Pyrazine	C ₄ N ₂
Pyridazine	C ₄ N ₂
Pyrrolizine ²	C ₄ N-C ₄ N
Indolizine	C ₄ N-C ₅ N
Isoindole ²	C ₄ N-C ₆
Indole ²	C ₄ N-C ₆
Indazole ²	C ₃ N ₂ -C ₆
Purine ²	C ₃ N ₂ -C ₄ N ₂
Isoquinoline ³	C ₅ N-C ₆
Quinoline ³	C ₅ N-C ₆
Quinolizine ³	C ₅ N-C ₅ N
Phthalazine	C ₄ N ₂ -C ₆
Naphthyridine ⁴	C ₅ N-C ₅ N
Quinoxaline	C ₄ N ₂ -C ₆
Quinazoline	C ₄ N ₂ -C ₆
Cinnoline	C ₄ N ₂ -C ₆
Pteridine	C ₄ N ₂ -C ₄ N ₂
Carbazole ²	C ₄ N-C ₆ -C ₆
Phenanthridine	C ₅ N-C ₆ -C ₆
Acridine	C ₅ N-C ₆ -C ₆
Perimidine ²	C ₄ N ₂ -C ₆ -C ₆
Phenanthroline ⁵	C ₅ N-C ₅ N-C ₆
Phenazine	C ₄ N ₂ -C ₆ -C ₆
Anthridine	C ₅ N-C ₅ N-C ₅ N
Phenarsazine	C ₄ AsN-C ₆ -C ₆
Phenophosphazine ²	C ₄ NP-C ₆ -C ₆
Phenotellurazine ²	C ₄ NTe-C ₆ -C ₆
Phenoselenazine ²	C ₄ NSe-C ₆ -C ₆
Phenothiazine ²	C ₄ NS-C ₆ -C ₆
Phenoxazine ²	C ₄ NO-C ₆ -C ₆
Thebenidine	C ₅ N-C ₆ -C ₆ -C ₆
Quindoline ²	C ₄ N-C ₅ N-C ₆ -C ₆
Quinindoline ²	C ₄ N-C ₅ N-C ₆ -C ₆
Phthaloperine ²	C ₅ -C ₄ N ₂ -C ₆ -C ₆ -C ₆
Acridoline ²	C ₄ N-C ₅ N-C ₆ -C ₆ -C ₆
Triphenodithiazine	C ₄ NS-C ₄ NS-C ₆ -C ₆ -C ₆

Triphenodioxazine

Phenanthrazine

Anthrazine

C₄NO-C₄NO-C₆-C₆-C₆

C₄N₂-C₆-C₆-C₆-C₆-C₆-C₆

C₄N₂-C₆-C₆-C₆-C₆-C₆-C₆

¹The order of precedence is based first on the presence or absence of nitrogen, then upon the nature of the (other) hetero atoms (see Table I, ¶ 128). For fused heterocycles, this order (for base-component selection) is distinct from that used to determine seniority of a total ring system in an index name (¶ 138).

²Citation of indicated hydrogen (¶ 135), e.g., *1H-Pyrrole*, *2H-Pyrrole*, is necessary when these component names are used alone.

³Because of established usage, *Quinolizine* is favored over *Isoquinoline* and *Quinoline* as a base component.

⁴*Naphthyridine* requires the locants **1,5-**, **1,6-**, **1,7-**, **1,8-**, **2,6-** or **2,7-** to define the position of the nitrogen atoms.

⁵*Phenanthroline* requires the locants **1,7-**, **1,8-**, **1,9-**, **1,10-**, **2,7-**, **2,8-** or **2,9-** to define the positions of the nitrogen atoms.

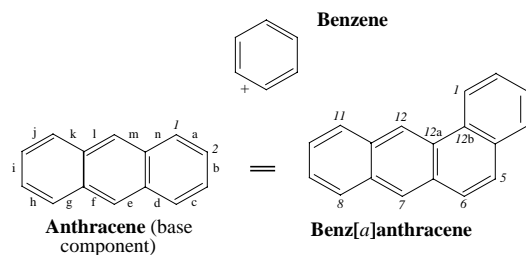
150. Selection of a base component is facilitated by use of Tables IV, ¶ 148 and V, ¶ 149; the appropriate component listed *latest* in these Tables is used. The system must contain at least two rings of five or more atoms, although such rings need not be directly fused to one another; i.e., they may be joined by a smaller ring, as in *Cyclobutadicyclopentene*. The criteria for base components differ markedly (in the case of heterocyclic systems) from those described (¶ 138) for a preferred ring system in a compound containing more than one. A base component of lower preference is used if the fusion procedure is not possible on the preferred component; as a last resource, an organic replacement ("a") name based on the fused hydrocarbon is employed.

The preferred base component should:

- be a heterocycle;
- be a nitrogenous heterocycle;
- be a nonnitrogenous heterocycle containing a hetero atom of highest precedence (see Table I, ¶ 128);
- contain the greatest number of rings;
- contain the largest individual ring; **Benzindene** (not Cyclopentanaphthalene) is an exception based on established usage;
- contain the greatest total number of hetero atoms;
- contain the greatest variety of hetero atoms, e.g., one nitrogen and one oxygen rather than two nitrogens;
- contain the greatest number of hetero atoms of highest precedence;
- possess the most linear structure;
- have the lowest locants for hetero atoms (before fusion).

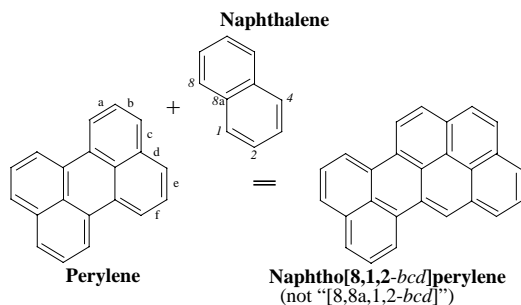
151. Index names for fused systems, other than fundamental systems which possess their own names (Tables IV, ¶ 148 and V, ¶ 149), are formulated from the names of the components. Cycloalkanes may be adopted as base components by invariant use of the "-ene" suffix. This denotes a maximum number of noncumulative double bonds; e.g., *Cyclooctene* as part of a fused system is not meant to imply the presence of a *single* double bond; instead, *saturated* carbon atoms are indicated by "hydro" prefixes. *Fusion locants* for the base component comprise lower case italic letters assigned sequentially to all sides, beginning with the side "1,2" as denoted by the usual peripheral locants. (See the *Ring Systems Handbook* for a complete set of ring system diagrams, including base components, complete with such locants.) If more than twenty-six letters are required, subsequent alphabets of the form *a*₁, *b*₁, *c*₁,... etc., are adopted. Locants for the fusion prefixes (derived from the less preferred fundamental ring systems) comprise the normal peripheral numerical locants. When a choice is possible, lowest alphabetic and numerical locants are cited. When one or both types of locants are unnecessary they are usually omitted. Numerical and letter locants are separated by a hyphen, and the locant set is bracketed.

Example:



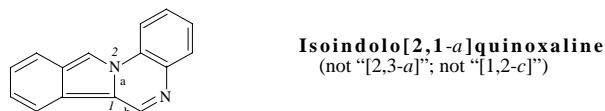
In this example, a locant defining the fusion site on **Benzene** is unnecessary. The "1,2" side of **Anthracene** is lettered "a" and the lettering proceeds around every side back to the 1-position. The fused system is then oriented (¶ 152) and renumbered.

Angular positions of base components involved in fusion are not cited.
Example:



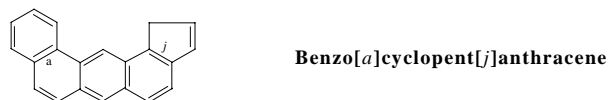
When a hetero atom is shared by two or more rings, it is expressed in all the components. When the order of lettering of the base component proceeds in the direction opposite to numbering in the fusion-prefix component, numerical locants for the latter are reversed.

Example:



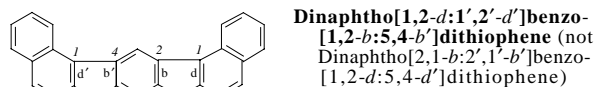
Fusion prefixes are placed in alphabetical order and the earliest cited prefix is given preference for lowest letter locant. When two or more fusion prefixes are identical, as in “Dibenzo-” systems, the letter locants are separated by commas, e.g., “[*a,j*]”.

Example:



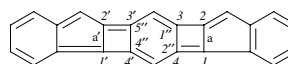
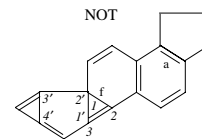
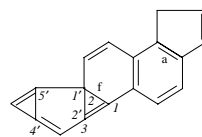
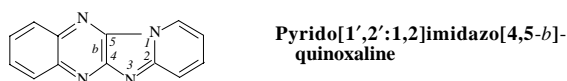
A form of multiplicative name is employed for fused systems different from that described for general substitutive nomenclature. Multiplication proceeds in steps, with “di,” “tri” repeated as necessary (not “bis,” “tris,” etc., except to avoid ambiguity). Serially primed letters are used for fusion sites on the second, third, etc., base components and the locant sets are separated by colons. When a base component is fused to a central component and to another component, lowest letters (when a choice must be made) relate to the central fusion site.

Examples:



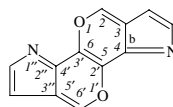
Ring systems fused to base components are designated primary components; a ring system (other than a base component) fused only to a primary component is a secondary component, and primed numerical locants are used to denote its fusion sites. Primed and unprimed locant sets are separated by colons. Lowest locants are used for the site closest to (or fused directly to) the base component. Doubly primed locants are needed (a) when the secondary component is centrally located with identical primary and base components on both sides, and (b) when tertiary components are present.

Examples:



Cyclopenta[*a*]cyclopropa[4',5']-cyclopenta[1',2':2,3]cyclopropa[1,2-*f*]naphthalene (not Cyclopenta[*a*]cyclopropa[3',4']-cyclopenta[2',1':1,3]cyclopropa[2,1-*f*]naphthalene.) (The locants 1,2 in the preferred name are lower than 2,1 in the incorrect name. It should be noted that the use of 1',2' requires that the cyclopentane ring be numbered the long way around.)

Benzo[1'',2'':3,4;5'',4'':3',4']dicyclobuta[1,2-*a*:1',2'-*a*]diindene (Note that a semicolon separates locant sets which already contain colons.)

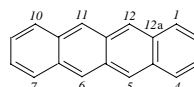


Pyrrolo[2'',3'':4',5']pyrano[2',3':5,6]pyrano[4,3-*b*]pyrrole

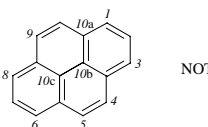
152. Orientation and numbering of fused systems.

(a) *Hydrocarbons.* The component rings are normally drawn as regular polygons. The cyclopropane ring may point left or right, and cyclopentane and cycloheptane rings may point up or down. The total system is oriented so that (a) a maximum number of rings are in a horizontal row, and (b) a maximum number are above and to the right. If further choice is necessary, then (c) a minimum number of rings should be in the lower left quadrant. Numbering begins at an atom not engaged in fusion in the most counterclockwise position of the uppermost ring furthest to the right. Angular positions are not counted; their locants, when needed, are derived from those of the preceding nonangular positions by addition of the lower-case Roman letters, “a,” “b,” etc. Interior atoms are numbered last by addition of letters to the highest available numerical locant in a continuous pathway, a clockwise route being followed whenever a choice presents itself; any remaining interior atoms are then numbered similarly from the next highest available numerical locant.

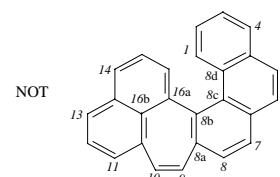
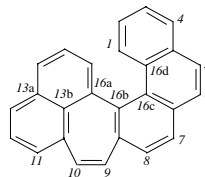
Examples:



Naphthacene



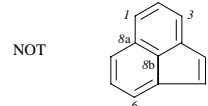
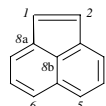
Pyrene



Naphtho[1',8':3,4,5]cyclohepta[1,2-*c*]phenanthrene

When a further choice is needed for orientation and numbering, carbon atoms at angular positions are assigned lowest numbers.

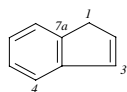
Examples:



Acenaphthylene (Note: 2a,5a,8a,8b is lower than 3a,5a,8a,8b)

Indicated hydrogen is assigned the lowest locant.

Example:

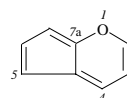


1H-Indene (not 3H-Indene)

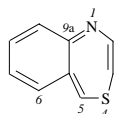
The following fused carbocyclic compounds have special numbering systems: **Anthracene**, **Phenanthrene**, **Cyclopenta[*a*]phenanthrene** (steroid numbering) and the **Cyclopropacyclopenta[*a*]phenanthrenes**.

(*b*) **Heterocycles**. The ring systems are oriented as for hydrocarbons. When a choice is necessary, lowest locants are assigned to (*a*) all hetero atoms; (*b*) most preferred hetero atom (Table I, ¶ 128); (*c*) carbon atoms common to two or more rings; (*d*) positions bearing indicated hydrogen; (*e*) an angular rather than a nonangular atom of the same hetero element. The ring is then numbered as for hydrocarbons, except that hetero atoms common to two or more rings are counted. Interior atoms are numbered last, following the shortest path from the highest previous number.

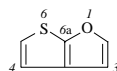
Examples:



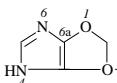
Cyclopenta[*b*]pyran



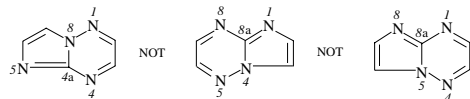
4,1-Benzothiazepine



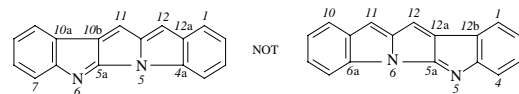
Thieno[2,3-*b*]furan



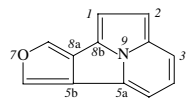
4H-1,3-Dioxolo[4,5-*d*]imidazole



Imidazo[1,2-*b*][1,2,4]triazine



Pyrrolo[1,2-*a*:5,4-*b'*]diindole

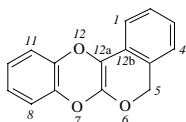


Furo[3,4-*a*]pyrrolo[2,1,5-*cd*]indolizine**

The following heterocyclic systems have special numbering systems: **Acridine**, **Carbazole**, **Purine**, **Xanthene**, and Epoxy- and Epithiocyclopenta[*a*]phenanthrenes (steroid numbering).

Indicated hydrogen for fused carbocyclic and heterocyclic systems is normally cited, if there is a choice, at the lowest nonangular position, unless a saturated angular atom is required to accommodate a principal function or free valency (see ¶ 135). Indicated hydrogen of component systems is ignored in constructing a fused ring name, and is reassigned if it is still needed in the final system.

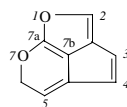
Example:



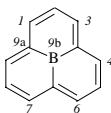
5H-[2]Benzopyrano[3,4-*b*][1,4]-benzodioxin (Note: The locants "2" and "1,4," which relate to the components, are bracketed to indicate that they do not conform to the peripheral numbering of the total system)

153. Replacement ("a") nomenclature for fused systems is employed when fusion names fail to express all interfaces (fusion sites) between component systems. This occurs when two or more components that are expressed as prefixes are fused to one another as well as to the base component. "A" names are also used for silicon replacement in a carbocycle that has a trivial name. Indicated hydrogen of the parent carbocycle is ignored, but is cited, if needed for the "a" name, ahead of the replacement prefixes.

Examples:



6H-1,7-Dioxacyclo[*cd*]indene (not 1,7-Dioxa-6H-cyclopent[*cd*]indene)



9b-Boraphenalene



1-Silanaphthalene, 3,4-dihydro-

Saturation of double bonds in fused systems is denoted by hydro prefixes which are given lowest locants; e.g., **Naphthalene, 1,2,3,4(not 5,6,7,8)-tetrahydro-**. Triple bonds are indicated by "didehydro."

154. Bridged fused systems are fused ring systems that possess atomic bridges or valence bonds which connect two or more parts of the system without creating or extending a fused system. They are named by adding bridge prefixes (in alphabetical order if different types are present) to the fused system names.

Simple bivalent bridges include methano (–CH₂–), ethano (–CH₂–CH₂–), etheno (–CH=CH–), propano (–CH₂CH₂CH₂–), 2-buteno (–CH₂CH=CHCH₂–), and benzeno (–C₆H₄–). Trivalent bridges, e.g., metheno (–CH=), 1-propanyl-3-ylidene (–CH₂CH₂CH=), and tetravalent bridges are also employed; locants for positions of attachment on the fused system are cited in the same order as free-valency locants of the radicals. Bridges from monocyclic hydrocarbons other than benzene are named as for the fusion prefixes, except that "endo-" is used with them to avoid ambiguity, e.g., "endo-cyclopenta." Simple hetero bridges include epoxy (–O–), epithio (–S–), imino (–NH–), epidioxy (–O–O–), and -silano- (–SiH₂–). Heterocyclic rings may also be used as bridges.

Example:



3,4-furano (cf. "furo" for the fusion prefix)

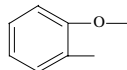
When locants are used for the bridge itself, e.g., 2-buteno, 3,4-furano-, they are placed in brackets within the bridged system name.

Compound bridges are named by combination of simple bridges beginning at the terminal position which gives the preferred (*a*) cyclic bridge (¶ 138), (*b*) hetero atom (Table I, ¶ 128), (*c*) chain, (*d*) alphabetic order.

Examples:

–NH(CH₂)₂– (iminoethano)

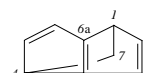
–OSO– (epoxythioxy)



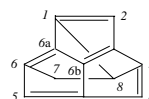
(epoxy[1,2]benzeno)

Indicated hydrogen of a fused system is cited, if possible, to accommodate a bridge. When this is unnecessary or impossible, the lowest-numbered nonangular indicated hydrogen is cited for the fused system, and additional indicated hydrogen, when needed, is cited ahead of the bridge locants.

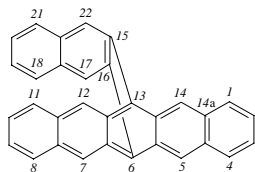
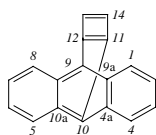
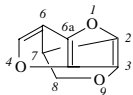
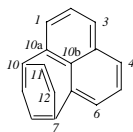
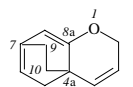
Examples:



1,4-Methanopentalene, 1,4-dihydro-

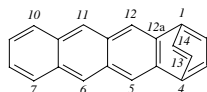
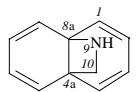
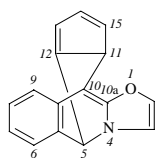


6,1,3-Ethanylylidencyclopenta[*cd*]pentalene

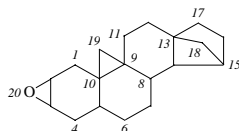
**6,13[2',3']-Naphthalenopentacene****9,10[1',2']-endo-Cyclobutanthracene****3,2,6-(Epoxyethanylylidene)furo-[3,2-b]furan****7,10-Ethenocyclohepta[de]-naphthalene****5H-4a,7-Ethano-2H-1-benzopyran**
(4aH-1-Benzopyran cannot exist)

Numbering of bridged fused systems is based on the regular numbering of the parent fused system. Lowest locants are assigned to bridgehead positions and the bridge atoms are numbered from the end nearest the highest numbered position of the parent fused system. In cyclic bridges, e.g., benzeno, *endo*-cyclobuta, the shorter bridge is first numbered, and then the rest of the ring in the same direction. If possible, hetero atoms in bridges are numbered low.

Examples:

**1,4-Ethenonaphthalene****8a,4a-(Iminomethano)naphthalene**
(not 4a, 8a-(Iminomethano)-naphthalene)**11H-5,10[1',2']-endo-Cyclopent-5H-oxazolo[3,2-b]isoquinoline**

The exceptional numbering employed for bridged cyclopenta[*a*]phenanthrenes is shown in the following example. Steroid numbering is used for positions 1 through 17. When the methyl groups normally numbered 18 and 19 are transformed into methano bridges, their locants are retained. Other bridges are numbered 20 and upward.



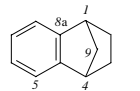
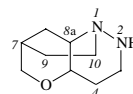
Criteria for the naming of bridged fused systems are applied successively as follows:

(a) The unbridged system contains the maximum number of (i) rings, (ii) skeletal atoms.

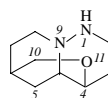
(b) The bridges are as simple as possible; e.g., two simple bridges are preferred to one compound bridge, and saturated bridges are preferred to unsaturated ones.

(c) The unbridged system has the highest precedence according to ¶ 138(c).

Examples:

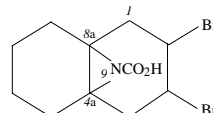
**1,4-Methanonaphthalene, 1,2,3,4-tetrahydro-**
(not 1,3-Ethano-1H-indene, 2,3-dihydro-)

NOT

**1,7-Ethano-1H-pyrano[3,2-c]-pyridazine, octahydro-** (not 4,6-(Epoxyethano)-1H-pyrano[1,2-b]pyridazine, octahydro-)(The fused ring system **Pyranopyridazine** is preferred to **Pyridopyridazine**; see ¶ 138.)

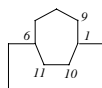
Fused carbocyclic and nonnitrogenous heterocyclic systems with simple imino bridges are named by use of the termination “-imine” with appropriate locants. Such a name requires addition of a regular functional suffix when appropriate. (Nitrogen heterocycles with imine bridges are named as bridged fused heterocycles in the usual manner.)

Example:

**Naphthalen-4a,8a-imine-9-carboxylic acid, 2,3-dibromo-octahydro-**

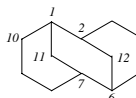
155. Von Baeyer nomenclature. This was first developed to name alicyclic hydrocarbons containing two rings. It has been extended to all bridged systems which cannot be treated as fused or bridged fused systems. Von Baeyer names for hydrocarbons are formed by prefixing to the name of the acyclic hydrocarbon with the same number of carbon atoms “Bicyclo-,” “Tricyclo-,” etc., terms, followed by a set of numerals, separated by periods and bracketed, which describes in descending sequence the number of atoms in each bridge. The system is numbered from one bridgehead *via* the other bridgehead(s) and back, always choosing the longest route. The system is numbered along the same route, ending with the smallest bridge, numbered from the bridgehead with the highest locant.

Example:

**Bicyclo[4.3.2]undecane**

For tricyclo- and higher hydrocarbon systems, superscripts are employed to indicate the positions of secondary bridges.

Example:

**Tricyclo[5.3.1.1^{2,6}]dodecane**

When more than one Von Baeyer name is possible for a hydrocarbon, the choice is determined by the following principles, applied successively until a decision is reached.

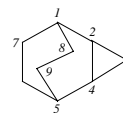
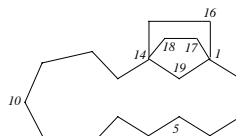
(a) The main ring contains the maximum number of atoms, two of which must serve as bridgeheads for the main bridge.

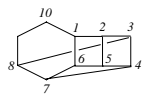
(b) The main bridge is as large as possible.

(c) The main ring is divided as symmetrically as possible by the main bridge.

(d) Lowest superscripts (regardless of order of citation) are cited.

Examples:

**Tricyclo[3.2.2.0^{2,4}]nonane** (not Tricyclo[2.2.2.1^{2,3}]nonane)**Tricyclo[3.2.1.0^{2,7}]octane** (not Tricyclo[2.2.2.0^{2,6}]octane)**Tricyclo[12.2.2.1^{1,14}]nonadecane****Tricyclo[4.4.1.1^{1,5}]dodecane**
(not Tricyclo[5.3.1.1^{1,6}]dodecane)



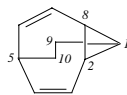
Pentacyclo[4.4.0.0^{2,2}.0^{3,8}.0^{4,1}]decane
(not Pentacyclo[4.4.0.0^{4,9}.0^{5,8}.0^{1,10}]decane; not Pentacyclo[4.4.0.0^{2,5}.0^{3,10}.0^{4,9}]decane; not Pentacyclo[4.4.0.0^{2,9}.0^{3,8}.0^{7,10}]decane)

Unsaturation is denoted by “-ene” and “-yne” suffixes. A second locant in parentheses is cited for a double bond at a bridgehead when it does not proceed to the next atom in the numbered path. Multiple-bond locants are determined by the following criteria applied successively:

- (a) The numbering proceeds in a clockwise sequence.
(b) The cases in which both locants for a double bond are cited are minimized.

(c) Lowest locants are employed.

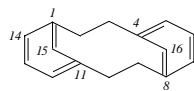
Examples:



Tricyclo[3.3.2.0^{2,8}]deca-3,6-diene



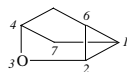
Bicyclo[4.2.0]oct-6-ene (not Bicyclo[4.2.0]oct-1(8)-ene)



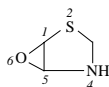
Tricyclo[9.3.1.1^{4,8}]hexadeca-1-(15),4,6,8(16),11,13-hexaene (not Tricyclo[9.3.1.1^{4,8}]hexadeca-4,6,8-(16),11(15),12,14-hexaene)

Von Baeyer names for *heterocyclic systems* are formed from the hydrocarbon names by use of replacement (oxa, thia, aza, etc.) prefixes and lowest locants for hetero atoms in the order of Table I, ¶ 128. Unsaturation is denoted as for hydrocarbons.

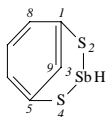
Examples:



3-Oxatricyclo[2.2.1.0^{2,6}]heptane
(not 5-Oxatricyclo[2.2.1.0^{2,6}]heptane; not 2-Oxatricyclo[2.2.1.0^{3,5}]heptane) (low numbering for bridge takes precedence over hetero atom)



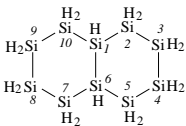
6-Oxa-2-thia-4-azabicyclo[3.1.0]hexane (not 6-Oxa-4-thia-2-azabicyclo[3.1.0]hexane)



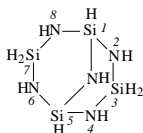
2,4-Dithia-3-stibabicyclo[3.3.1]nona-1(9),5,7-triene (not 2,4-Dithia-3-stibabicyclo[3.3.1]nona-1(8),5(9),6-triene)

Saturated bridged systems containing only silicon atoms, or silicon atoms alternating with nitrogen or one of the chalcogens, are given Bicyclosilazane, Tricyclosiloxane, etc., names. Regular Von Baeyer numbering is employed.

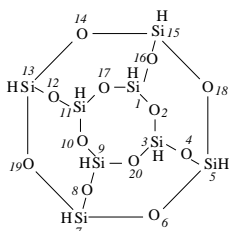
Examples:



Bicyclo[4.4.0]decasilane



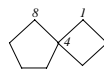
Bicyclo[3.3.1]tetrasilazane



Pentacyclo[9.5.1.1^{3,9}.1^{5,15}.1^{7,13}]octasiloxane

156. Spiro systems contain pairs of rings or ring systems having only one atom (a “spiro atom”) in common. In the simplest monospiro systems, in which two alicyclic rings share an atom, the name is formed by prefixing to the acyclic hydrocarbon name the term “Spiro” and numerals (separated by periods) in ascending sequence to define the number of atoms in each ring linked to the spiro atom. The numbering begins at the atom *next* to the spiro atom in the smaller ring and proceeds around that ring, through the spiro atom and around the larger ring.

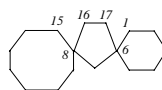
Example:



Spiro[3.4]octane

This system is extended to dispiro and higher systems. Numbering begins next to a terminal spiro atom and proceeds in such a way as to give the spiro atoms lowest locants.

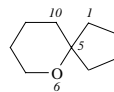
Example:



Dispiro[5.1.7.2]heptadecane (note that the numbering path corresponds to the bracketed sequence)

Heterocyclic analogs are named by “a” nomenclature. The hetero atoms are given locants as low as are compatible with the ring numbering.

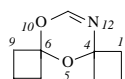
Example:



6-Oxaspiro[4.5]decane

Unsaturation is expressed by “-ene” and “-yne” suffixes.

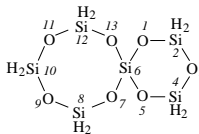
Example:



5,10-Dioxo-12-azadispiro[3.1.3.3]-dodec-11-ene

Saturated spiro systems containing only silicon atoms or silicon atoms alternating with nitrogen or one of the chalcogens are given Spirosilazane, Spirosiloxane, etc., names.

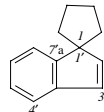
Example:



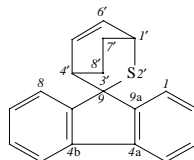
Spiro[5.7]hexasiloxane

Monospiro systems containing at least one fused or bridged component are named by placing the component names in brackets in alphabetical order and prefacing them with “Spiro.” The position of the spiro atom is denoted by two locants, separated by a comma, related to the two components. Primes are used for the component cited second. Indicated hydrogen (¶ 135) is assigned, where possible, to accommodate the spiro unions. Locants related to the components but not to the total spiro system are bracketed to avoid ambiguity.

Example:



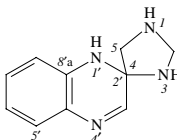
Spiro[cyclopentane-1,1'-(1H)-indene] (not Spiro[cyclopentane-1,1'-1'H-indene])



Spiro[9H-fluorene-9,3'-(2)thiabicyclo[2.2.2]oct[5]ene]

Added hydrogen (¶ 136) is cited in parentheses in the usual way, but with a primed locant if it does not relate to the component cited first. It is assigned the lowest available locant unless a different one can be used to accommodate a principal group.

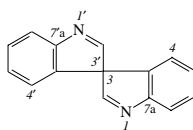
Example:



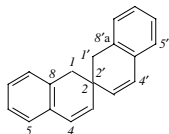
Spiro[imidazolidine-4,2'-(1'H)-quinoxaline]

Monospiro systems containing identical fused components are given "Spiro-" names. The component name is bracketed if it is preceded by locants or is itself made up of fusion components. Added hydrogen is cited in parentheses following the spiro locants.

Examples:



3,3'-Spiro[3H-indole]

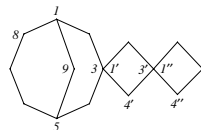


2,2'(1H,1'H)-Spirobinaphthalene

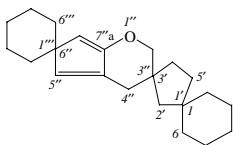
Di-, tri-, etc., spiro systems containing at least one fused or bridged component are named by extension of these policies. If terminal components are identical, citation is determined by earliest index position of the complete name. Serially primed locants are used for successive components.

"Branched" polyspiro systems in which a single component is surrounded by three or more identical components are named by citing the central component (which is assigned plain locants) first and multiplying the identical (terminal) components. When two terminal components of a "branched" spiro system are identical, and one different, they are cited in alphabetical order (as usual) and the term "bis" is applied as appropriate.

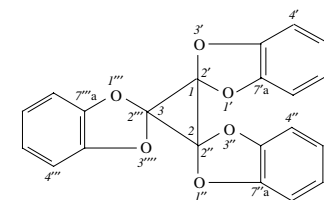
Examples:



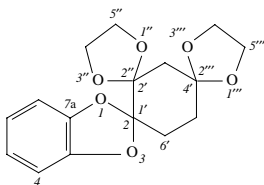
Dispiro[bicyclo[3.3.1]nonane-3,1'-cyclobutane-3',1''-cyclobutane]



Trispiro[cyclohexane-1,1'-cyclopentane-3',3''(2''H)-cyclopentab]pyran-6''(4''H),1'''-cyclohexane]



Trispiro[cyclopropane-1,2':2,2'':3,2'''-tris[1,3]benzodioxole]

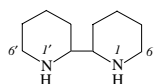


Trispiro[1,3-benzodioxole-2,1'-cyclohexane-2',2'':4',2'''-bis[1,3]dioxolane]

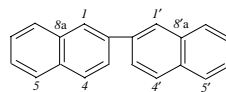
157. Ring assemblies contain a multiplicity of the same cyclic system joined by single bonds, not necessarily in equivalent positions. They are treated as molecular skeletons in substitutive nomenclature and rank just above the component ring. Except for assemblies of benzene, and two-component assemblies of cycloalkanes, cycloalkenes, and hetero systems with "cyclo" names (see below), they are named by prefixing the component names with the terms Bi-, Ter-, Quater-, Quinque-, Sexi-, Septi-, Octi-, Novi-, Deci-, Undeci-, etc.

Locants are placed ahead of the name to define the points of attachment. These locants are as low as possible, compatible with fixed numbering (expressed or implied) of the components, including "-ene" and "-yne" suffixes.

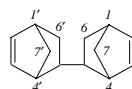
Examples:



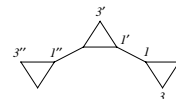
2,2'-Bipiperidine



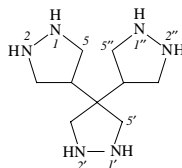
2,2'-Binaphthalene



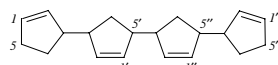
5,5'-Bibicyclo[2.2.1]hept-2-ene (not 2,2'-Bibicyclo[2.2.1]hept-5-ene)



1,1':2',1''-Tercyclopropane



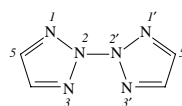
4,4':4',4''-Terpyrazolidine



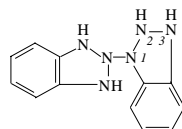
3,3':5',3'':5'',3'''-Quatercyclopentene

Indicated hydrogen (¶135) is assigned, where possible, to points of attachment. When indicated hydrogen is cited in different positions for different components, a ring-assembly name is not used. Added hydrogen (¶ 135) is cited immediately after the locant to which it relates.

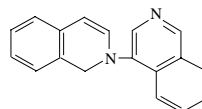
Example:



2,2'-Bi-2H-1,2,3-triazole



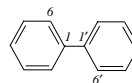
1H-Benzotriazole, 1-(1,3-dihydro-2H-benzotriazol-2-yl)-2,3-dihydro- (not 1H-Benzotriazole, 2-(2,3-dihydro-1H-benzotriazol-1-yl)-2,3-dihydro-; not 1(3H),2'-Bi-2H-benzotriazole, 1',3'-dihydro-)



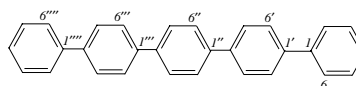
2(1H),4'-Bisquinoline

Linear benzene assemblies (*polyphenyls*) are named by prefixing "phenyl" with the appropriate term (Bi-, Ter-, etc.). Arabic numeral locants are cited in all cases for points of attachment. Two-component assemblies of monocyclic hydrocarbons and of hetero systems with "cyclo" names, e.g., **Cyclopentastannane**, **Cyclotrisiloxane**, and monocycles with one silicon using "sila" names, are named from the *radicals*, and locants for the points of attachment are cited only when the radical has no locant for the free valency. Two-component ring-assembly names from unsaturated ("enyl") radicals are formed only when the unsaturation is symmetrical with respect to the points of attachment.

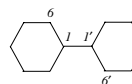
Examples:



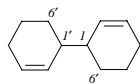
1,1'-Biphenyl



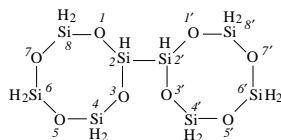
1,1':4',1'':4'',1''':4''',1''''-Quinquephenyl



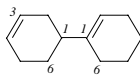
1,1'-Bicyclohexyl (not Bicyclohex-1-yl)



Bi-2-cyclohexen-1-yl (not 1,1'-Bi-2-cyclohexen-1-yl)

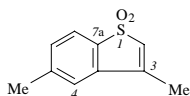


Bicyclotetrasiloxan-2-yl

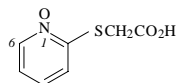


Cyclohexene, 1-(3-cyclohexen-1-yl)- (not Cyclohexene, 4-(1-cyclohexen-1-yl)- (lowest locant for the substituent prefix is preferred (¶ 138)))

158. Nonstandard heteroatoms in CA ring nomenclature. Additive terms are used to describe oxides, sulfides, selenides, and tellurides of ring heteroatoms:



Benzo[b]thiophene, 3,5-dimethyl-1,1-dioxide

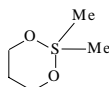


Acetic acid, 2-[(1-oxido-2-pyridinyl)thio]-

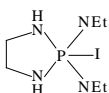
For all other neutral ring heteroatoms with nonstandard bonding numbers (hereafter referred to as nonstandard heteroatoms), the IUPAC lambda convention (*Pure Appl. Chem.* **1984**, 56, 769-778) is used, regardless of the heteroatom in question, its bonding number, or the kinds of bonds joining it to other skeletal atoms.

The rules are as follows:

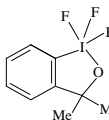
- The λ term is prefixed to the name for the ring parent, preceded by the locant for the nonstandard heteroatom—in a fusion name, that locant is for the fused ring system, not a component ring—and followed by a superscript denoting the nonstandard valence. (In the IUPAC recommendations, the λ is usually inserted within the ring name, after the locant for the nonstandard heteroatom.)



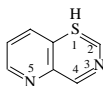
2 λ^4 -1,3,2-Dioxathiane, 2,2-dimethyl-



2 λ^5 -1,3,2-Diazaphospholidine-2,2-diamine, N,N,N',N'-tetraethyl-2-iodo-

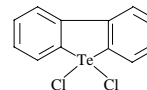


1 λ^5 -1,2-Benziodoxole, 1,1,1-trifluoro-1,3-dihydro-3,3-dimethyl-



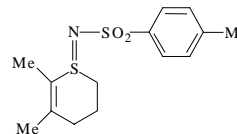
1 λ^4 -Pyrido[2,3-e]-1,3-thiazine

- For a ring parent with the maximum number of noncumulative double bonds, indicated hydrogen is used with a nonstandard heteroatom if that atom is joined to other skeletal atoms only by single bonds—unless the other atoms are divalent, in which case indicated hydrogen is not used. Indicated hydrogen always precedes the λ term.

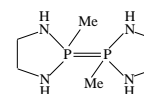


5H-5 λ^4 -Dibenzotellurophene, 5,5-dichloro-

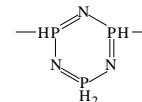
- A radical is formed according to the established rules—including the use of added hydrogen to accommodate an “ylidene” radical—when the free valence is on the nonstandard heteroatom.



Benzenesulfonamide, N-(3,4-dihydro-5,6-dimethyl-1 λ^4 -thiopyran-1(2H)-ylidene)-

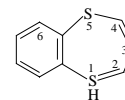


2 λ^5 -1,3,2-Diazaphospholidine, 2-methyl-2-(2-methyl-2 λ^5 -1,3,2-diazaphospholidin-2-ylidene)-



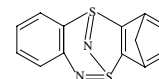
2 λ^5 ,4 λ^5 ,6 λ^5 -1,3,5,2,4,6-triazatriphosphorine-2,4-diyl

- After the established rules for low numbering have been applied—for heteroatoms, indicated hydrogen, an onium center, and so on—low numbering is assigned to a nonstandard heteroatom in preference to the same heteroatom with the standard bonding number.



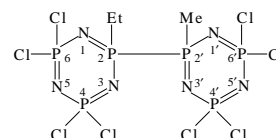
1 λ^4 -1,5-Benzodithiepin

- In a bridged fused ring system, the name of the bridge (including its locants and any indicated hydrogen required by the bridge) is prefixed to the fusion name with its λ term.

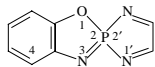


1,4-Methano-5,11-nitrilo-11H-5 λ^4 ,11 λ^4 -dibenzo[c,f][1,5,2]dithiazepine

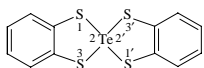
- In a ring assembly or spiro name, the component name is always cited with its own λ term.



2,2'-Bi-2 λ^5 ,4 λ^5 ,6 λ^5 -1,3,5,2,4,6-triazatriphosphorine, 4,4,4',4',6,6,6',6'-octachloro-2-ethyl-2'-methyl-



Spiro[2λ⁵-1,3,2-benzoxazaphosphole-2,2'-[2H-2λ⁵-1,3,2]diazaphosphole]



2,2'-Spirobi[2λ⁴-1,3,2-benzodithiatellurole]

- In a replacement name for a saturated ring parent, both the lambda convention and subtractive suffixes are used to describe a nonstandard heteroatom joined to cumulative double bonds.

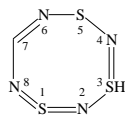


1λ⁴-1-Thia-4-silacyclohexa-1,6-diene

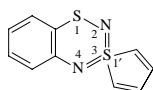
- To describe all other nonstandard heteroatoms joined to cumulative double bonds, the lambda convention is used together with the IUPAC delta convention (*Pure Appl. Chem.* **1988**, 60, 1395-1401). The terms are combined into a single expression, prefixed by the locant for the nonstandard heteroatom. The number of cumulative double bonds to the nonstandard heteroatom is specified by a superscript Arabic numeral after the δ.



1λ⁴δ²-1,2,3-Thiadiazole



1λ⁴δ²,3λ⁴-1,3,5,2,4,6,8-Trithiatetrazocine



Spiro[3λ⁶δ²-1,3,2,4-benzodithiadiazine-3,1'-[1H-1λ⁶]thiophene]

159. Boron molecular skeletons. Because the number of hydrogen atoms in neutral and anionic boron hydrides often bears no simple relationship to the number of boron atoms, borane names must express the number of both. (The single exception is **Borane** itself, which represents BH₃.) The *Ring Systems Handbook* should be consulted for structural diagrams of the neutral polyboranes of established structure. Diagrams justified by current index entries are displayed in the *Chemical Substance Indexes*. (In these diagrams, the lines do not represent electron-pair bonds but indicate the geometry of the structures.) Neutral boron hydrides, real or hypothetical, are treated as molecular skeletons in substitutive nomenclature. **Borane** and the diboranes as heteroacyclic compounds, and the higher hydrides as heterocyclic compounds. **Borane(1)** is BH, **Borane(2)** is BH₂. In higher boranes, the number of boron atoms is expressed by multiplicative prefixes.

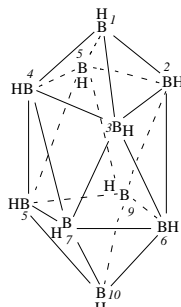
Examples:

B ₂ H ₄	Diborane(4)
B ₂ H ₆	Diborane(6)
B ₃ H ₇	Triborane(7)
B ₄ H ₁₀	Tetraborane(10)
B ₅ H ₉	Pentaborane(9)
B ₆ H ₁₀	Hexaborane(10)
B ₁₀ H ₁₄	Decaborane(14)

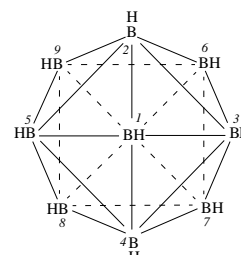
Until structures have been determined, author terms such as “*iso*” and “*neo*” are cited in index modifications to differentiate isomers.

Numbering of polyboranes in CA indexing is based on “Nomenclature of Boron Compounds” adopted by the American Chemical Society, and “Nomenclature of Inorganic Boron Compounds”, published by the International Union of Pure and Applied Chemistry,¹ which may be consulted for further details. For “closed” polyboranes (those whose boron skeletons are polyhedra with triangular faces throughout) the numbering begins with the boron atom at the head of the largest axis of highest order, then proceeds sequentially to the planes which intersect this axis. Boron atoms in each plane are numbered clockwise unless lowest locants for substituents demand anticlockwise numbering. On succeeding planes, numbering begins at the boron atom immediately “below” the lowest-numbered one on the previous plane, or the one nearest to it in the direction of numbering.

Example:



Decaborane(10)

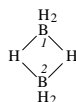


planar projection

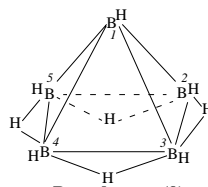
(Note that atom “6” (in the lower plane) is nearest to atom “2” in the direction of numbering.)

For “open” polyboranes (those with incomplete polyhedral boron skeletons) the rules are more complex. A planar projection, as viewed from the open side, is numbered so that interior boron atoms have lowest locants, beginning at the “center” or “apex.” Each atom set is numbered in the same direction.

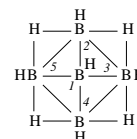
Examples:



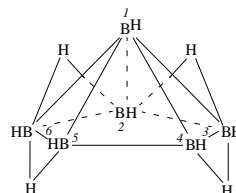
Diborane(6)



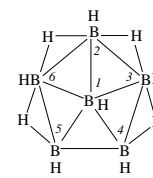
Pentaborane(9)



planar projection



Hexaborane(10)



planar projection

Some polyboranes can be named as derivatives of simpler polyboranes. Thus, a bimolecular polyborane, i.e., a two-component “ring” assembly in which both skeletons are identical, can be named as follows:

1,1'-Bipentaborane(9)

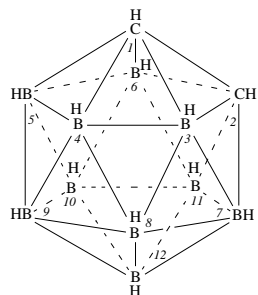
When the various parts of the structure are not identical, the general principles of substitutive nomenclature are applied, and a polyborane radical is used for the less preferred skeleton, e.g., **Decaborane(10), 2-octaboran(8)-1-yl-**.

Polyboranes joined along an edge, or with a triangular face in common, are named like fused ring systems; e.g., **Decaborano(14)[5',6':5,6]decaborane(14), Undecaborano[2',7',11':1,2,3]dodecaborane(17)**.

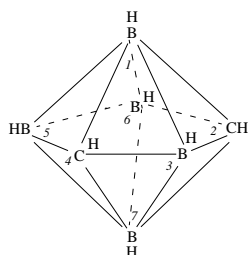
¹*Inorg. Chem.* **1968**, 7(10), 1945-65; *Pure Appl. Chem.* **1972**, 30(3-4), 683-710.

160. "Hetero" polyboranes are boron hydride skeletons in which boron atoms have been replaced by those of other elements, notably carbon. Replacement prefixes, e.g., "carba," "phospha," are employed with the polyborane name, and the number of hydrogen atoms attached to the skeleton expressed in parentheses after the name. Structural diagrams for compounds of established structure can be found in the *Ring Systems Handbook* and, when justified by current entries, in the *Chemical Substance Index*. Numbering is as for the parent polyboranes, with lowest compatible locants assigned to the replacement atoms.

Examples:



1,2-Dicarbadodecaborane(12)



2,4-Dicarbaheptaborane(7)

161. Substituent prefixes (radicals) derived from molecular skeletons are used very frequently in substitutive nomenclature. Their names are based on the skeleton names and may be classified accordingly as radicals from (a) monoatomic skeletons, (b) hydrocarbon chains, (c) organic hetero ("a"-named) chains, (d) homogeneous hetero chains, (e) heterogeneous hetero chains, (f) carbocycles, (g) heterocycles, (h) ring assemblies, (i) polyboranes. Combination of simple radicals to form compound and complex radicals is performed by application of principles described earlier (¶ 133). (See also "Illustrative List of Substituent Prefixes," which constitutes Section H (¶ 294).

(a) *Monoatomic radicals* from borane, methane, silane, germane, stannane, and plumbane are named by replacing "-ane" by "-yl," "-ylene," and "-ylidene" to denote the loss of one, two, or three hydrogen atoms. The final "e" of the hydrides arsorane and phosphorane may be replaced by "-yl," "-ylidene," and "-ylidene." Stibine and bismuthine may have the "-ine" ending replaced by "-ino," "-ylene," and "-ylidene." Phosphine and arsine may have the "-ine" replaced by "-ino," "-inidene," and "-inidyne." The -tetrayl suffixes indicate loss of all hydrogen from Group IVA monoatomic hydrides.

Examples:

H ₂ B-	boryl	HC≡	methylidyne
H ₂ C=	methylene	HSi≡	silylidyne
=Sn=	stannanetetrayl	HAs=	arsinidene
H ₂ P-	phosphino	As≡	arsinidyne
HP=	phosphinidene	H ₂ Sb-	stibino
P≡	phosphinidyne	HSb=	stibylene
H ₄ P-	phosphoranyl	Sb≡	stibylidyne
H ₃ P=	phosphoranylidene	H ₂ Bi-	bismuthino
H ₂ P≡	phosphoranylidyne	HBi=	bismuthylene
H ₂ As-	arsino	Bi≡	bismuthylidyne

(b) *Acyclic hydrocarbon radicals* are named from the skeletons by replacing "-ane," "-ene," and "-yne" suffixes by "-yl," "-enyl," and "-ynyl," (for monovalent radicals); by "-diyl," "-triyl," "-enediyl," "-ynediyl," etc., for divalent radicals with hydrogen removed at more than one position; and by "-ylidene" and "-ylidene" to indicate two or three hydrogen atoms lost at one position. (Methylene is an exception.) Locants are not cited for monovalent radicals (the free valency position is always "1"), but unsaturated positions are always indicated for chains of three or more atoms. Free valencies (single or

multiple) in one or two positions of an acyclic chain are always terminal, otherwise a compound radical name is employed. When three or more positions have free valencies, two of them must be terminal.

Examples:

MeCH ₂ -	ethyl
H ₂ C=CHCH ₂ -	2-propen-1-yl (not allyl)
EtCH=	propylidene
PrC≡	butylidyne
H ₂ C=C=	ethenylidene
H ₂ C=CHCH=	2-propen-1-ylidene
MeC≡CCH ₂ CH=CHCH=	2-hepten-5-yn-1-ylidene
-(CH ₂) ₂ -	1,2-ethanediyl
-CH ₂ CH=	1-ethanyl-2-ylidene
-CH=CH-	1,2-ethenediyl
-(CH ₂) ₃ -	1,3-propanediyl
=C=C=C=	1,2-propadiene-1,3-diylidene
-CH ₂ CHCH ₂ -	1,2,3-propanetriyl
-CH ₂ CCH ₂ -	1,3-propanediyl-2-ylidene

(c) *Organic heteroacyclic ("a") radicals* are used when the requirements (¶ 127) are met. The numbering of the parent radical is retained. A single free valency is hence always in the 1-position, and *this locant is always cited*. When there is still a choice, lowest locants are assigned to hetero atoms, then to most preferred hetero atoms (Table I, ¶ 128), then to unsaturation (with double bonds preferred).

Examples:

Me[O(CH ₂) ₂] ₃ OCH ₂ CH ₂ -	3,6,9,12-tetraoxatridec-1-yl (not [2-[2-[2-(2-methoxyethoxy)-ethoxy]ethoxy]ethyl])
MeSi ₁₀ H ₉ CH ₂ SiH ₇ CH=CHSiH ₄ CH ₂ SiH ₂ CH=	2,4,7,9-tetrasiladec-5-en-1-ylidene
-CH ₂ CH ₂ [S(CH ₂) ₂] ₂ SCH=CHNHCH ₂ CH ₂ -	3,6,9-trithia-12-azatetradec-10-ene-1,14-diyl

(d) *Homogeneous heteroacyclic radicals* are named analogously to acyclic hydrocarbon radicals, except that only the "e" of "ane" suffixes of heteroacyclic skeleton names is replaced by "-yl."

Examples:

HN=N-	diazanyl (also used for the substituted radical, rather than azo)
H ₂ NNHNH-	triazanyl
HN=NNH-	2-triazen-1-yl
H ₂ NN=NN=N-	1,3-pentazadien-1-yl
H ₂ PPH-	diphosphinyl
-PPPH-	1,2-diphosphinediyl
=AsAs=	1,2-diarsinediylidene
-Sb=Sb-	1,2-distibenediyl
H ₂ NNH-	hydrazinyl (not hydrazino)
H ₂ NN=	hydrazinylidene (not hydrazono)
-NHN=	1-hydrazinyl-2-ylidene
-NHNH-	1,2-hydrazinediyl (not hydrazo or hydrazi)
-N=N-	1,2-diazenediyl (not azo or azi)
=NN=	1,2-hydrazinediylidene (not azino)









(e) *Heterogeneous heteroacyclic radicals* are named analogously to hydrocarbon radicals.

Examples:

$\text{H}_3\text{SiOSiH}_2-$	1-disiloxanyl
$\text{H}_3\text{SiOSiH}=\text{}$	1-disiloxanylidene
$\text{H}_3\text{SnOSn}=\text{}$	1-distannoxanylidene
$-\text{SiH}_2\text{NHSiH}_2-$	1,3-disilazanediy
$-\text{SiH}_2\text{OSiHOSiH}_2-$	1,3,5-trisiloxanetriyl

(f) *Cyclic hydrocarbon radicals*. Loss of one or two hydrogen atoms from a single cycloalkane carbon atom is denoted by replacement of "ane" of the ring name by "-yl" and "-ylidene," respectively. The implied locant ("1" in all cases) is not expressed. In radicals from cycloalkenes, cycloalkadienes, etc., only the final "e" is replaced by the radical suffix, and locants for unsaturation and the free valency (always "1") are all cited. Loss of hydrogen at more than one position is expressed by the suffixes "-diyl" (not "-ylene"), "-diylidene," "-enylylidene," etc. All locants are cited, and locants for free valencies are assigned lowest locants.

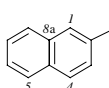
Examples:

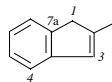
	cyclohexyl
	2-cyclopropen-1-yl
	2,4-cyclopentadien-1-yl
	1,5-cyclohexadien-3-yn-1-yl
	2,4-cyclohexadien-1-ylidene
	1,3-cyclopentenediy (not 1,3-cyclopentylene)
	1-cyclohexanyl-2-ylidene (not 1-cyclohexyl-2-ylidene)
	6-cyclohexen-1-yl-2-ylidene

Radicals from *benzene* are named phenyl (C_6H_5-), 1,2-, 1,3-, and 1,4-phenylene ($-\text{C}_6\text{H}_4-$), 1,2,3-benzenetriyl, 1,2,3,4-benzenetetrayl, etc.

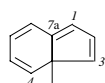
Fused hydrocarbon radicals are assigned the lowest locants compatible with the fixed numbering of the ring system. Indicated hydrogen (¶ 135) necessary for the existence of the ring is assigned to the lowest nonangular position unless it can be located to accommodate a monovalent radical in an angular position or an "ylidene" radical in a nonangular position. Added hydrogen (¶ 136) is cited immediately after the radical locant and is assigned the lowest available angular or nonangular position.

Examples:

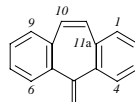
	2-naphthalenyl (not 2-naphthyl)
---	---------------------------------



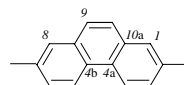
1H-inden-2-yl



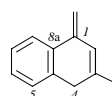
3aH-inden-3a-yl (a hydro derivative would be named, e.g., 2,3-dihydro-3aH-inden-3a-yl, not 2H-inden-3a(3H)-yl)



5H-dibenzo[a,d]cyclohepten-5-ylidene



2,7-phenanthrenediyl



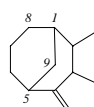
3-naphthalenyl-1(4H)-ylidene (not 2-naphthalenyl-4(1H)-ylidene)

Von Baeyer and spiro radicals follow similar principles. Free valency locants are assigned lowest locants compatible with ring-system numbering and are preferred over locants for unsaturation.

Examples:



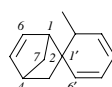
bicyclo[2.2.2]oct-5-en-2-yl (not bicyclo[2.2.2]oct-2-en-5-yl)



bicyclo[3.3.1]nonane-2,3-diyl-4-ylidene



dispiro[4.1.4.1]dodec-2-yl



spiro[bicyclo[2.2.1]hept-5-ene-2,1'-[3,5]cyclohexadien]-2'-yl (note: lowest locants are assigned, in order, to spiro atoms, free valencies, all multiple bonds, double bonds)

(g) *Heterocyclic radicals* from ring systems not named by organic replacement ("a") nomenclature are named analogously to fused-hydrocarbon radicals (above). The shortened form thienyl is used for thiophene radicals and all their fused derivatives; selenophenyl (not selenophenyl) is the name of the seleno analog.

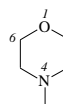
Examples:



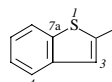
3-pyridinyl (not 3-pyridyl)



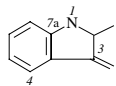
1(2H)-pyridinyl



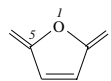
4-morpholinyl (not morpholino)



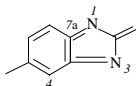
benzo[b]thien-2-yl (not benzo[b]-thiophen-2-yl)



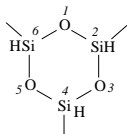
3*H*-indol-2-yl-3-ylidene (a hydro derivat would be named, e.g., 1,2-dihydro-3*H*-indol-3-ylidene, not 1*H*-indol-3(2*H*)-ylidene)



2,5-furandiylidene



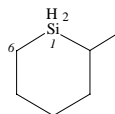
2*H*-benzimidazol-5-yl-2-ylidene



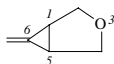
cyclotrisiloxane-2,4,6-triyl

“A”-named cyclic radicals are named like the hydrocarbon parents from which they have been derived by atom replacement. The hetero atoms receive lowest locants (cited or implied), then the free valencies (cited just ahead of the radical suffix).

Examples:



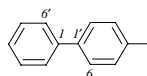
silacyclohex-2-yl (not 2-silacyclohexyl)



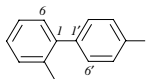
3-oxabicyclo[3.1.0]hex-6-ylidene

(*h*) *Ring-assembly radicals* are derived by bracketing the assembly name, eliding a final “e” if “y” is to follow, and appending the radical endings “-yl,” “-ylidene,” “-diyl,” etc., as appropriate. The free valencies need not be on the terminal rings of the assembly.

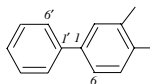
Examples:



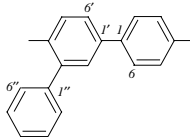
[1,1'-biphenyl]-4-yl (not 4-biphenyl)



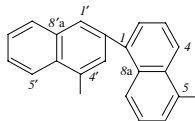
[1,1'-biphenyl]-2,4'-diyl (not 2,4'-biphenylene)



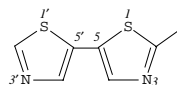
[1,1'-biphenyl]-3,4-diyl (not (4-phenyl-1,2-phenylene))



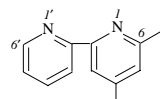
[1,1':3',1''-terphenyl]-4,4'-diyl (not (2-phenyl[1,1'-biphenyl]-4,4'-diyl))



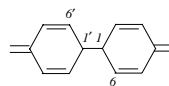
[1,2'-binaphthalene]-4',5-diyl



[5,5'-bithiazol]-2-yl (not [5-(5-thiazolyl)-2-thiazolyl])



[2,2'-bipyridine]-4,6-diyl (not [6-(2-pyridinyl)-2,4-pyridinediyl])



[bi-2,5-cyclohexadien-1-yl]-4,4'-diylidene

(*i*) *Polyborane radicals* are formed from polyborane and hetero polyborane names by citing the usual radical suffixes after the parenthetical designation of the number of hydrogen atoms, with elision of the final “e” before “y.” Requirements for locant citation with diborane radicals are the same as for the analogous acyclic hydrocarbon radicals.

Examples:

diboran(4)yl 1-pentaboran(9)yl

diboran(6)yl 1,2-dicarbododecaboran(12)-1-yl

diboran(4)ylidene 6,9-decaborane(10)diyl

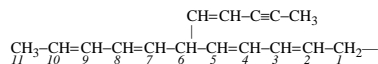
1,2-diborane(4)diyl

162. Compound and complex radicals from molecular skeletons are named by principles described earlier (¶ 133).

Examples:

Me₂CH– (1-methylethyl)

H₂C=CMe– (1-methylethenyl) (the unsaturated parent radical is preferred)



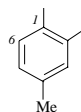
[6-(1-penten-3-yn-1-yl)-2,4,7,9-undecatetraen-1-yl]

PhCH=CH– (2-phenylethenyl) (not styryl)

PhC≡ (phenylmethylidyne) (not benzylidyne)



(2-methylphenyl) (not *o*-tolyl)

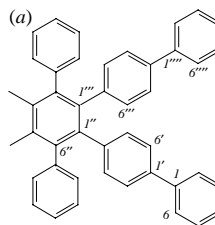


4-methyl-1,2-phenylene) (not 4-methyl-*o*-phenylene)

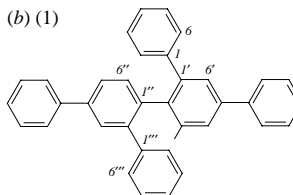
Radicals from branched polyphenyls are chosen by application of the following principles successively until a decision is reached:

- longest chain of rings containing all of the free valencies, which need not be on terminal rings;
- lowest locants in the radical name for (1) ring junctions, and (2) free valencies;
- maximum number of substituent prefixes;
- lowest locants for substituent prefixes;
- earliest index position of the radical name.

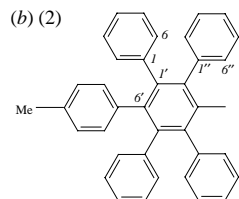
Examples (the letters on the left refer to the principles above):



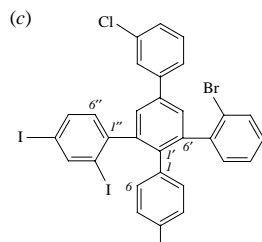
(3'',6''-diphenyl[1,1':4',1'':2'',1''':-4''',1''''-quinquephenyl]-4'',-5''-diyl)



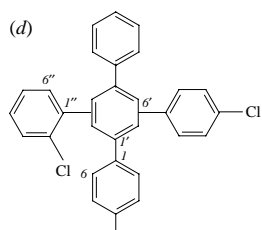
(4'',5'-diphenyl[1,1':2',1'':2'',1''':-quaterphenyl]-3'-yl)



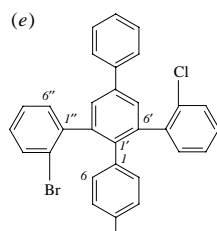
[6'-(4-methylphenyl)-4',5'-diphenyl-
[1,1':2',1''-terphenyl]-3'-yl]



[6'-(2-bromophenyl)-4-(3-chloro-
phenyl)-2'',4''-diiodo[1,1':2',1''-
terphenyl]-4-yl]



[2''-chloro-6'-(4-chlorophenyl)-4'-
phenyl[1,1':2',1''-terphenyl]-4-yl]



[2''-bromo-6'-(2-chlorophenyl)-4'-
phenyl[1,1':2',1''-terphenyl]-4-yl]
(not [6'-(2-bromophenyl)-2''-
chloro-4'-phenyl[1,1':2',1''-ter-
phenyl]-4-yl])

163. Molecular skeletons as index heading parents. These two entities coincide when no suffix, expressing a principal group, is added to the skeleton name, either because such a group is absent, or because it is attached to a hetero atom of the skeleton which changes it from a functional into a nonfunctional group.

Examples:



Ethane



Benzene, nitro- ("nitro" is a mandatory prefix (¶ 132))



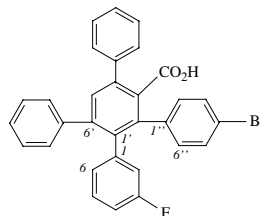
Piperidine, 1-hydroxy- ("hydroxy" is considered nonfunctional when attached to a hetero atom other than silicon)



Ethanone,1-(trimethylsilyl)-

Choice of a preferred index heading parent has already been described (¶ 138). In the case of a branched polyphenyl, the criteria are the same as for the derived radicals (¶ 162), except that principal groups replace free valencies.

Example:



**[1,1':2',1''-Terphenyl]-3'-carboxylic
acid, 4''-bromo-3-fluoro-4',6'-
diphenyl-** (a decision is reached by
choosing lowest locants for the
Terphenyl skeleton and then for the
principal group)

163A. Fullerenes. The even-numbered, closed spheroidal structures of 20 or more carbon atoms, in which every atom is bonded to three other atoms and of which the C_{60} "buckminsterfullerene" is the prime example, as known generically as "fullerenes".^{2,3} "Fullerene" has been adopted as the class name and to it are added ring sizes, number of carbon atoms, and point group symmetries to name specific members of the class. For example, in the name **[5,6]Fullerene- $\text{C}_{60}-I_h$** , "[5,6]" indicates the presence of ring sized 5 and 6, " C_{60} " the number of carbon atoms, and " I_h " the point group symmetry.⁴ When a fullerene is modified (e.g., by addition, replacement, or deletion of atoms), the ring sizes, the number of carbon atoms, and the point group symmetry remain those of the parent fullerene. Incompletely described fullerenes, i.e., where ring sizes and/or point group symmetries are not known or disclosed are named with only the number of carbon atoms, e.g., **Fullerene- C_{60}** . Existing nomenclature practices are followed as closely as possible when naming derivatives. Anions, cations, protonated fullerenes, and free radicals are named as follows:

[5,6]Fulleride(3-)- $\text{C}_{60}-I_h$

**[5,6]Fullerene- $\text{C}_{60}-I_h$
ion(1+)**

[5,6]Fulleren- $\text{C}_{60}-I_h-1(2H)$ -ylum

[5,6]Fulleren- $\text{C}_{60}-I_h-1(2H)$ -yl

Metallofullerenes are compounds in which one or more metals are either trapped inside the fullerene or located outside without bonding directly to it. They are given fullerene names, with the metals cited by name in alphabetical order

Example:

**[5,6]Fullerene- $\text{C}_{60}-I_h$
compd. with potassium (1:1), ion(1+)**

Partial hydrogenation of a fullerene is described by terms such as "hexatriacontahydro-", while full saturation is implied by the name "fullerane", e.g., **[5,6]Fullerane- $\text{C}_{60}-I_h$** .

Fullerenes containing substituents require that hydrogen be added before the substituents can be named.⁵ For example, $\text{C}_{60}\text{F}_{60}$ is named **[5,6]Fullerane- $\text{C}_{60}-I_h$, hexacontafluoro-** (the hydrogen being part of the parent name). C_{60}Br_2 is named as a dibromodihydrofullerene, and $\text{C}_{60}\text{H}_6\text{Ph}_6$ is named as a dodecahydrohexaphenylfullerene.

Addition of hydrogen is not necessary when a fullerene contains two functional groups, as in **[5,6]Fullerene- $\text{C}_{60}-I_h-1,60$ -diamine**.

Modification of the fullerene network such that some carbon atoms no longer have a connectivity of 3 are named by using "homo", "nor", and "seco", e.g., **1,2(2a)-Homo[5,6]fullerene- $\text{C}_{60}-I_h-2a$ -carboxylic acid**.

Replacement of a carbon atom by a trivalent hetero atom such as boron or nitrogen results in a free radical, e.g., **1-Bora[5,6]fullerene- $\text{C}_{60}-I_h-2$ -yl**.⁵

²Science 1988, 242, 1017-22; 1139-1145.

³"Fullerene" has also been defined as a closed, hollow network of 12 pentagonal and m hexagonal faces for a C_{20+2m} molecule (Science 1991, 254, 1768-1770), but CAS also includes structures with 3-, 4-, and 7- through 10-sided faces as fullerenes for purposes of naming.

⁴"Character Tables for Chemically Important Symmetry Groups". In: F. A. Cotton, Chemical Applications of Group Theory. 3rd ed., John Wiley & Sons, 1990. Appendix IIA, pp. 426-435.

⁵International Union of Pure and Applied Chemistry, Nomenclature of Organic Chemistry, Sections A,B,C,D,E,F, and H, 1979 ed., Pergamon Press, Oxford (England), 1979. Rules C-0.1 and C-32.

C. PRINCIPAL CHEMICAL GROUPS (SUFFIXES)

Introduction	¶ 164	Amides	¶ 171
Acids expressed as substituent suffixes	165	Nitriles	172
Acyclic acids with cyclic substituents	166	Aldehydes	173
Order of precedence of acids	167	Ketones	174
Acid radicals	168	Alcohols (and phenols)	175
Functional derivatives of acids	169	Amines	176
Acid halides	170	Imines	177

164. Introduction. In substitutive nomenclature, a principal chemical group is that substituent of a molecular skeleton which is selected for expression as a suffix. Only one kind of substituent may be cited as a suffix, viz., the most senior one as determined by the Order of Precedence of Compound Classes (¶ 106); all other substituents are expressed as prefixes (radicals) which may be simple, compound, or complex (¶¶ 132, 133). For functional compounds, the molecular skeleton name together with its suffix constitutes an index *heading parent*. The locants for suffixes are placed in front of the heading parent name unless locants for indicated hydrogen, hetero atoms (in "a" names), unsaturation, fusion sites, etc., are present, in which case they are placed just before the suffix.

In the following paragraphs, compound classes expressed as substituent suffixes are discussed in descending order of precedence.

165. Acids expressed as substituent suffixes on molecular skeletons include carboxylic, sulfonic, sulfinic, selenonic, and telluronic acids and their functional replacement analogs, such as peroxy, imidic and thio acids. For **Carbamic acid** and its relatives (including **Carbamic acid** and **Formic acid**) see ¶ 183.

(a) *Carboxylic acids* are named by the Geneva ("oic") or "-carboxylic" system. The "-oic acid" suffix is employed for acyclic mono- and dicarboxylic acids of carbon chains, including "a"-named acids; the "-carboxylic acid" suffix is used for acyclic polycarboxylic acids and compounds in which the carboxyl group is attached to a ring, a monoatomic hydride, or a heterocyclic chain. The trivial names **Acetic acid** and **Benzoic acid** are retained for these two acids and their substituted derivatives. (The amides, acid chlorides, etc., are named similarly, but organic replacement analogs are named systematically, e.g., **Benzenecarboximidic acid** (not Benzimidic acid).)

Examples:

MeCH₂CO₂H **Propanoic acid** (not Propionic acid)

Me(CH₂)₃CO₂H **Pentanoic acid** (not Valeric acid)

H₂C=CHCO₂H **2-Propenoic acid** (not Acrylic acid)

Me(CH₂)₄CH=CHCH₂CH=CH(CH₂)₇CO₂H
18 **9,12-Octadecadienoic acid**

HO₂CCO₂H **Ethanedioic acid** (not Oxalic acid)

HO₂C(CH₂)₃CO₂H **Pentanedioic acid** (not Glutaric acid)

H₃C-CH₂-O-CH₂-CH₂-O-CH₂-CH₂-O-CH₂-CH₂-O-CH₂-CH₂-O-CH₂-CH= }
23 **12,15,18,21-Tetraoxatricos-9-enoic acid**
21 (lowest locants are assigned to
18 functional suffixes, not replacement
15 prefixes)

COOH
1
HOOC-CH₂-CH-CH₂-COOH
1 **1,2,3-Propanetricarboxylic acid**
2 (numbering excludes the carboxyl
3 groups)

(HO₂C)₂C=C(CO₂H)₂ **1,1,2,2-Ethenetetracarboxylic acid**

HO₂CNHNHCO₂H **1,2-Hydrazinedicarboxylic acid** (not
1 Bicarbamic acid)

H₂PCO₂H **Phosphinecarboxylic acid** (not
Formic acid, phosphino-)

HO₂C-SnH₂-O-SnH₂-CO₂H
1 **1,3-Distannoxanedicarboxylic acid**

H₂B **Diborane(6)-1-carboxylic acid**
H

CO₂H
6 **2,6-Cyclohexadiene-1,2-dicarboxylic acid**
1 (lowest locants for principal
groups are preferred)

CO₂H
8 **1-Anthracenecarboxylic acid**
9 9a 1
5 10a 10 4a

8a **4-Quinolinecarboxylic acid**
5 4 CO₂H

5 **Spiro[1,3-dioxolane-2,2'(1'H)-**
3 **naphthalene]-5'-carboxylic acid**
2 1' 8'a 5'

HO₂C **[1,1'-Biphenyl]-2,2'-dicarboxylic acid**
6 1' 6' CO₂H

CO₂H **1,4(4H)-Pyridinedicarboxylic acid**
6 1 (the added hydrogen is expressed
after the final locant but relates to
the 1-carboxyl group; see ¶ 136)

HO₂C **1,2-Dicarbadoecaborane(12)-1,2-**
1 2 **dicarboxylic acid** (the 1,2-bond
does not possess single-bond
character)

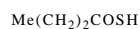
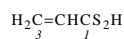
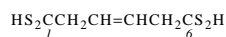
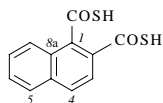
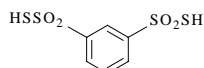
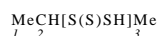
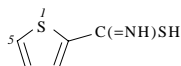
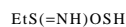
(b) *Sulfonic, sulfinic and sulfenic acids* and their selenium and tellurium analogs are expressed by appending the appropriate suffix to the name of the molecular skeleton. Mono- and diacids of these series, unlike "-oic acids," above, do not need to occupy terminal positions on a chain.

Examples:

EtSO₃H **Ethanesulfonic acid**

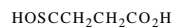
SO₃H
1
CH₃-CH₂-CH₂-CH-CH₃ **2-Pentanesulfonic acid**
5 4 3 2 1

Examples:

**Butanethioic acid****2-Propene(dithioic) acid****Benzenecarbothioic acid** (not Benzoic acid, thio-)**1-Piperidinecarbodithioic acid****Propanebis(thioic) acid****3-Hexenebis(dithioic) acid****1,2-Naphthalenedicarbothioic acid****1,3-Benzenedisulfonothioic acid****2-Propanesulfino(dithioic) acid****Methanesulfenothioic acid****2-Thiophenecarboximidothioic acid****Ethanesulfonimidothioic acid**

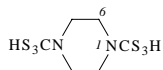
When different numbers of sulfur atoms replace oxygen in the functional groups of polyacids, the groups of higher sulfur content are expressed as substituent prefixes.

Examples:

**Propanoic acid, 3-(thiocarboxy)-****Acetic acid, 2-ethoxy-2-thio-**

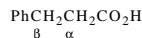
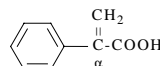
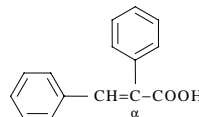
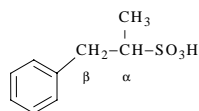
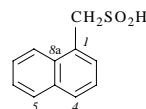
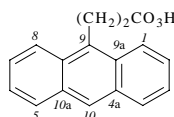
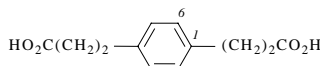
Thio peroxy acids are named by similar principles; the replacement affixes "(thioperoxy)" and "(dithioperoxy)" are placed, in alphabetic order with other terms such as "imido" and "hydrazono," in the "-oic," "carboxylic," "sulfonic," etc., suffixes of the appropriate parent acids.

Examples:

**Ethane(dithioperoxy) acid****Benzenecarboximido(thioperoxy) acid****1,4-Piperazinedicarbo(dithioperoxy)-thioic acid****Benzenesulfono(dithioperoxy) acid****1-Piperidinesulfeno(dithioperoxy) acid****2-Propanesulfeno(thioperoxy) acid****Ethaneselenoic acid****Benzenecarbosenoethioic acid**

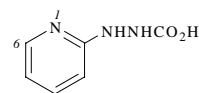
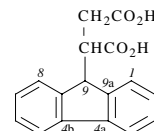
166. Acyclic acids with cyclic substituents may usually be named by conjunctive nomenclature (¶ 124).

Examples:

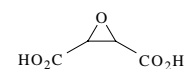
**Benzenepropanoic acid** (not Hydrocinnamic acid)**Benzenoacetic acid, α-methylene-** (not Atropic acid)**Benzenoacetic acid, α-(phenylmethylene)-** (not Benzene-2-propenoic acid, α-phenyl-; conjunctive nomenclature is not used with unsaturated acyclic acids (¶ 124))**Benzenoethanesulfonic acid, α-methyl-****1-Naphthalenemethanesulfonic acid****9-Anthracenepropaneperoxoic acid****1,4-Benzenedipropanoic acid**

When conjunctive names are impermissible, e.g., for unsaturated and polyfunctional acyclic acids, acids attached to rings by a double bond, and acids of noncarbon chains, the cyclic group is expressed as a substituent.

Examples:

**Hydrazinecarboxylic acid, 2-(2-pyridinyl)-****Butanedioic acid, 2-(9H-fluorene-9-yl)-**

Epoxy derivatives of acids are named as oxirane and oxetane derivatives. Example:

**2,3-Oxiranedicarboxylic acid** (not Butanedioic acid, 2,3-epoxy-)

167. Order of precedence of acids. Acid suffixes are the most preferred principal group of all non-cationic substituent suffixes (¶ 106), but only one type of acid suffix may be expressed in a heading parent. Less preferred acid functions are cited as substituent prefixes. The choice is made in accordance with the following hierarchy, listed in order of descending precedence:

(a) Peroxy acids. (Among peroxy acids, the choice depends on the nature of the parent acid as described in (b) through (i), below.) (See also the separate ranking of peroxy carbonic and peroxy phosphorus acids at ¶ 183, 197.)

(b) Carboxylic acids, followed by thio, seleno, and telluro analogs, in that order. The preferred acid group contains the maximum number of preferred chalcogens, oxygen being the most preferred. (For **Carbonic acid**, **Formic acid**, etc., see ¶ 183.)

(c) Carbohydrazonic acids, followed by chalcogen analogs (see (b)).

(d) Carboximidic acids, likewise.

(e) Sulfonic acids, followed by chalcogen and nitrogen analogs in the order of (b), (c), and (d).

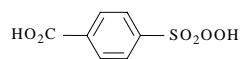
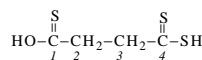
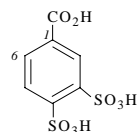
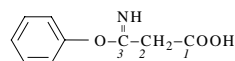
(f) Sulfonic acids, likewise.

(g) Sulfenic acids, likewise.

(h) Selenonic, seleninic, and selenenic acids, as for sulfonic acids.

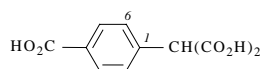
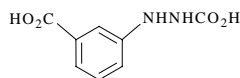
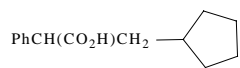
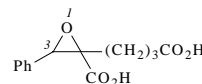
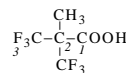
(i) Telluronic, tellurinic, and tellurenic acids, likewise.

Examples:

**Benzenesulfonoperoxoic acid, 4-carboxy-****Propanethioic acid, 3-(dithiocarboxy)-****Benzoic acid, 3,4-disulfo-****Propanoic acid, 3-imino-3-phenoxy-**

When two or more like acid groups are attached to different molecular skeletons, or when one or more are attached to a branched skeleton, the preferred index name is selected according to the usual rules (¶ 138).

Examples:

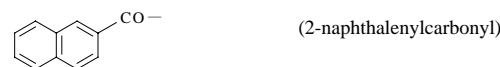
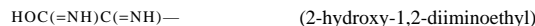
**Propanedioic acid, 2-(4-carboxyphenyl)-** (principle: maximum number of the principal group)**Hydrazinecarboxylic acid, 2-(3-carboxyphenyl)-** (principle: hetero acyclic parent preferred)**Benzeneacetic acid, alpha-(cyclopentylmethyl)-** (principle: preferred ring system)**2-Oxiranebutanoic acid, 2-carboxy-3-phenyl-** (principle: largest heading parent)**Propanoic acid, 3,3,3-trifluoro-2-methyl-2-(trifluoromethyl)-** (principle: maximum number of substituent prefixes)

Aldehydic, amic, anilic, hydroxamic, hydroximic, nitrolic, and nitrosolic acids are indexed as compounds of mixed function (see ¶ 228). So are trivially named hydroxy and oxo acids, e.g., Glycolic acid, Acetoacetic acid, and amino acids, e.g., Sulfanilic acid, other than those which are of biological significance (¶ 205).

168. Acid radicals derived, by removal of hydroxyl groups, from acids expressed as suffixes are named as compound and complex radicals. Acyl radicals, e.g., propionyl, naphthoyl, acetimidoyl, are no longer used as substituent prefixes; the only exceptions in general index nomenclature are acetyl (CH₃CO-) and benzoyl (C₆H₅CO-). Amino acid radicals, e.g., glycyl, L-alanyl, are restricted to use in peptide and decapeptide names (¶ 206).

Radicals derived from monocarboxylic acids are in general named as (1-oxoalkyl) or (arylcabonyl); carboximide acids afford (1-iminoalkyl) and (aryliminomethyl) radicals; carbothioic acids give (1-thioalkyl) and (arylthioxomethyl) radicals (carbonimidoyl and carbonothioyl are used only as multiplicative radicals (¶ 125) and in cases where both bonds are attached to the same atom); sulfonic, sulfinic, and sulfenic acid radical names are based on the parent radicals "sulfonyl," "sulfinyl," and "thio."

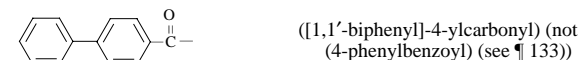
Examples:



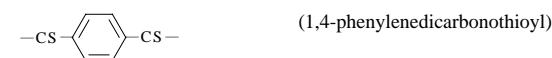
(2-naphthalenylcarbonyl)



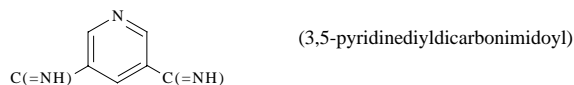
(1,2-phenylenedicarbonyl)



([1,1'-biphenyl]-4-ylcarbonyl) (not 4-phenylbenzoyl) (see ¶ 133)



(1,4-phenylenedicarbonothioyl)

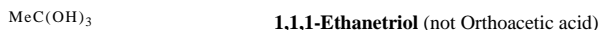


(3,5-pyridinediylcarbonimidoyl)



169. Functional derivatives of acids. In the absence of higher functions or more preferred compound classes (¶ 106), *esters* are indexed in the modification, usually at the acid name, sometimes at the alcohol (see ¶ 185). *Hydrazides* are likewise indexed at the acid name (¶ 189). *Hydrazones, azines, and semicarbazones* are named at hydrazonic acid parents (RC(OH):NNH₂) (¶ 165). *Oximes* of carboxylic acids are given *N*-hydroxy imidic acid names; *hydrates* and *acetals* (ortho carboxylic acids and their diesters) are indexed as alcohols (or thiols).

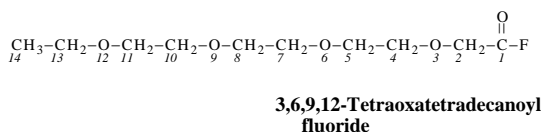
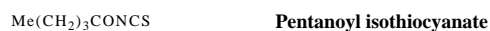
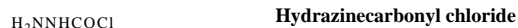
Examples:

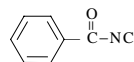


170. Acid halides. In this category are now included the halogenides, in which the hydroxyl groups of acids are replaced by -NC, -NCO, -NCS, -NCTe, -N₃, and (in acids other than carbon acids) -CN groups. They are named by placing the halide (etc.) term in the heading as a separate word following an acid term which ends as follows for various acid classes:

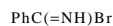
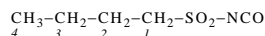
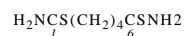
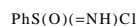
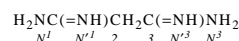
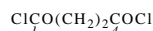
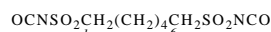
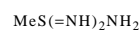
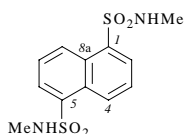
Acid suffix	Acid halide suffix
-carboxylic	-carbonyl
-carbohydrazonic	-carbohydrazonoyl
-carbothioic	-carbothioyl
-carboximidic	-carboximidoyl
-oic	-oyl
-hydrazonic	-hydrazonoyl
-thioic	-thioyl
-imidic	-imidoyl
-sulfonic	-sulfonyl
-sulfonylimidic	-sulfonylimidoyl

Examples:

**3,6,9,12-Tetraoxatetradecanoyl fluoride**

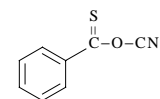
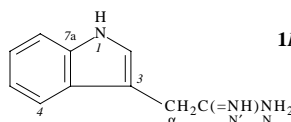
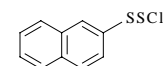
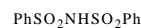
**Benzoyl isocyanide**

Examples:

**Benzenecarboximidoyl bromide****Acetamide****Benzenecarbothiyl chloride****Diazene-carboxamide****1-Butanesulfonyl isocyanate****Hexanedithioamide****Benzenesulfonimidoyl chloride****Propanediimidamide****Butanedioyl dichloride (not Butanedioyl chloride)****Benzenecarbohydrazonamide****1,6-Hexanedisulfonyl diisocyanate****Methanesulfonodiimidamide****Benzenepropanoyl azide****1,5-Naphthalenedisulfonamide, N,N'-dimethyl-**

Halides, etc., of peroxy acids are generally indexed as anhydrides, anhydrosulfides, etc., with halogen or halogenoid "oxo" acids such as **Hypochlorous** or **Thiocyanic acid**. Halides, etc., of (thio peroxy)sulfenic acids are indexed at **Disulfide**.

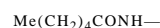
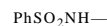
Examples:

**Carbonochloridothioic acid, anhydrosulfide with thiohypochlorous acid****Benzenecarbothioamide, N-phenyl-****Benzenecarbothioic acid, anhydride with cyanic acid****1H-Indole-3-ethanimidamide****Disulfide, chloro 2-naphthalenyl****Acetamide, N-acetyl- (not Diacetamide)****Benzenesulfonamide, N-(phenylsulfonyl)- (not Dibenzenesulfonamide)**

Amides of peroxy acids and thio peroxy acids are indexed as azanyl esters (¶ 193).

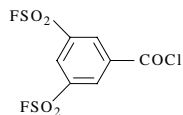
Amide radicals are named as compound or complex radicals based on "amino" or "imino," with acid radicals (¶ 168) as substituents.

Examples:

**(acetyl-amino) (not acetamido)****(benzoylimino)****[(1-oxohexyl)amino] (not hexanamido)****[(phenylsulfonyl)amino] (not benzenesulfonamido)****[(iminophenylmethyl)amino]**

When more than one acid halide residue is present in a compound, only one type is named in the heading parent. This is chosen by consideration first of the hierarchy of the parent acids (¶ 167) and then, if a further choice is necessary, of the following list of halides and halogenides (in descending order of precedence): -F, -Cl, -Br, -I, -N₃, -NCO, -NCS, -NCS₂, -NCTe, -NC, -CN.

Examples:

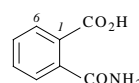
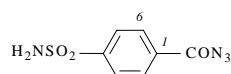
**Benzoyl chloride, 3,5-bis(fluorosulfonyl)-****Butanoyl fluoride, 4-iodo-4-oxo-**

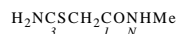
Functional derivatives of acid chlorides are indexed similarly to those of the parent acids (¶ 169).

171. Amides are named by modification of the parent acid suffixes, thus:

-oic acid	becomes	-amide
-carboxylic acid	becomes	-carboxamide
-carbohydrazonic acid	becomes	-carbohydrazonamide
-carbothioic acid	becomes	-carbothioamide
-carboximidic acid	becomes	-carboximidamide
-sulfonic acid	becomes	-sulfonamide

Secondary and tertiary amides are named as primary amides with *N*-substituents. Anilides, toluidides, etc., are indexed as *N*-aryl amides.

**Butanoic acid, 4-amino-4-oxo-****Benzoic acid, 2-(aminocarbonyl)-****Benzoyl azide, 4-(aminosulfonyl)-**



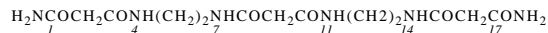
Propanamide, 3-amino-N-methyl-3-thio-



Acetamide, N-(phenylsulfonyl)-

Replacement (“a”) nomenclature is employed where applicable (¶ 127) for naming polyamides, but not peptides (¶ 206).

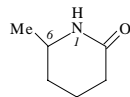
Example:



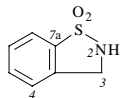
4,7,11,14-Tetrazaheptadecanediarnide, 3,8,10,15-tetraoxo-

Amides incorporated in a ring system are indexed at the ring name and ranked according to the nature of the suffix, if any (¶ 106), not as amides.

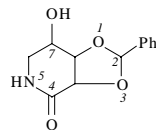
Examples:



2-Piperidinone, 6-methyl- (ranked as a ketone)



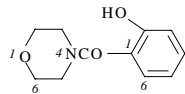
1,2-Benzisothiazole, 2,3-dihydro-1,1-dioxide (ranked as a non-functional cyclic nitrogen skeleton)



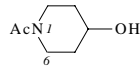
1,3-Dioxolo[4,5-c]pyridin-4(3aH)-one, tetrahydro-7-hydroxy-2-phenyl-

Amides of which only the nitrogen atom forms part of a ring, formerly referred to as “unexpressed amides”, are named according to the highest function present.

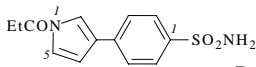
Examples:



Methanone, (2-hydroxyphenyl)-4-morpholinyl-



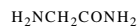
Ethanone, 1-(4-hydroxy-1-piperidinyl)-



Benzenesulfonamide, 4-[1-(1-oxopropyl)-1H-pyrrol-3-yl]-

Amides of amino acids with trivial names are named systematically except in peptide nomenclature (¶ 206).

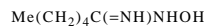
Example:



Acetamide, 2-amino- (not Glycinamide)

Oximes of amides (amidoximes) (R-C(=NOH)NH₂) are tautomeric with N-hydroxy carboximidamides (R-C(=NH)NHOH) and are indexed at imidamide names:

Example:



Hexanimidamide, N-hydroxy-

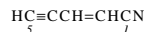
172. Nitriles (RC≡N) are indexed at names derived from “-carboxylic” and “-oic” acid names by use of “-carbonitrile” and “-nitrile” suffixes, respectively.

The zwitterionic nitrilimines[±] (RC≡N–N–R’) are named as substituted hydrazinium inner salts (¶¶ 201, 267).

Examples:



Acetonitrile



2-Penten-4-yne nitrile



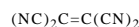
Ethanedinitrile (not Cyanogen)



Germanecarbonitrile



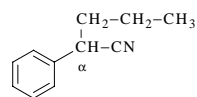
Hydrazinecarbonitrile



1,1,2,2-Ethenetetracarbonitrile



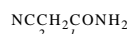
Benzonitrile



Benzenecetonitrile, α-propyl-

In the presence of higher functions, nitriles are always expressed as cyano radicals.

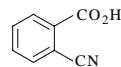
Examples:



Acetamide, 2-cyano- (not Propanamide, 3-nitrilo-)



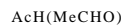
Propanoyl chloride, 2-cyano-



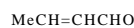
Benzoic acid, 2-cyano-

173. Aldehydes, RCHO, are named from “-carboxylic” and “-oic” acids by use of “-carboxaldehyde” and “-al” suffixes, respectively.

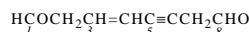
Examples:



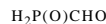
Acetaldehyde



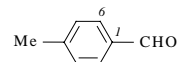
2-Butenal



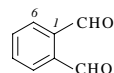
3-Octen-5-ynedial



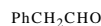
Phosphinecarboxaldehyde oxide



Benzaldehyde, 4-methyl-



1,2-Benzenedicarboxaldehyde



Benzenecetaldehyde

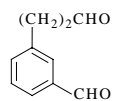
Chalcogen analogs of aldehydes are given “-thial,” “-selenal,” “-carbothioaldehyde,” etc., names.

In the presence of more highly ranked compound classes (¶ 106) or more preferred aldehydes, the -CHO group is expressed by formyl (if it does not form part of an acyclic carbon chain) or by a terminal oxo radical. For thioaldehydes, the equivalent radicals are (thioxomethyl) and a terminal thioxo radical.

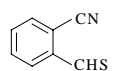
Examples:



Propanoic acid, 3-oxo-



Benzenepranal, 3-formyl-
(principle: largest heading parent)

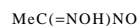


Benzonitrile, 2-(thioxomethyl)-

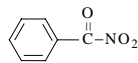


Butanethial, 4-telluroxo-

Substitution of the aldehydic hydrogen atom is not permitted.
Examples:



Ethanone, 1-nitroso-, oxime
(not Acetonitrosolic acid)



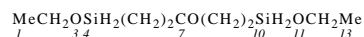
Methanone, nitrophenyl-
(not Benzaldehyde, α-nitro-)

174. Ketones, RC(:O)R', and their chalcogen analogs are named by use of the characteristic suffixes -one, -thione, -selone, and -tellone. (The last two classes must be differentiated from selenones and tellurones, which contain the noncarbon groups -SeO₂- and -TeO₂-, respectively.) The carbonyl group may be attached to carbon or other elements with the exception of hydrogen and those that could form an acid, acid derivative, or amide name. Conjunctive names are not employed for acyclic ketones attached to ring systems; instead, the cyclic portion is expressed as a substituent of the acyclic ketone parent (in which the oxo group may occupy the 1-position). When an acyclic ketone with two cyclic substituents consists only of a single carbon atom with a chalcogen attached, the heading parents **Methanone**, **Methanethione**, **Methaneselone** and **Methanetellone** are employed.

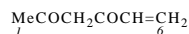
Examples:



2-Propanone (not Acetone)



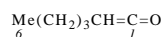
3,11-Dioxa-4,10-disilatridecan-7-one



5-Hexene-2,4-dione (not 1-Hexene-3,5-dione)



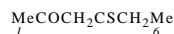
Ethenone (not Ketene)



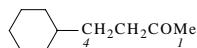
1-Hexen-1-one



2-Butaneselone



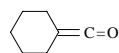
2-Hexanone, 4-thioxo- (not 2,4-Hexanedione, 4-thio-)



2-Butanone, 4-cyclohexyl-



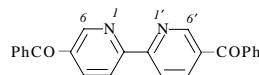
1-Hexanone, 1-phenyl- (not Hexanal, 1-phenyl-)



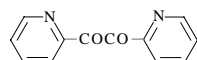
Methanone, cyclohexylidene-



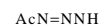
Methanone, diphenyl- (not Benzophenone)



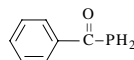
Methanone, 1,1'-[2,2'-bipyridine]-5,5'-diylbis[1-phenyl]- (a multiplicative name (¶ 125))



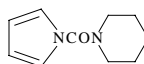
1,2-Ethanedione, 1,2-di-2-pyridinyl-



Ethanone, 1-(1-triazen-1-yl)-



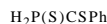
Methanone, phenylphosphino-



Methanone, 1-piperidinyl-1H-pyrrol-1-yl-



1-Propanone, 1-(hydroxysilyl)-



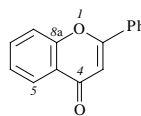
Methanethione, phenylphosphinothioyl-

Cyclic ketones (including those with neighboring hetero atoms) are named by appending "-one," "-thione," etc., suffixes to the ring names. Indicated hydrogen (required to form the ring system itself) is often chosen (where possible) to accommodate a single ketone group (¶ 135). In other cases, added hydrogen (¶ 136) is introduced at some other position of the ring system when the ketone suffix is attached.

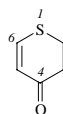
Examples:



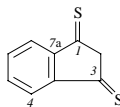
3-Cyclohexen-1-one



4H-1-Benzopyran-4-one, 2-phenyl-
(not flavone)



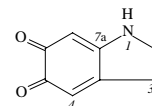
4H-Thiopyran-4-one, 2,3-dihydro-
(not 2H-Thiopyran-4(3H)-one)



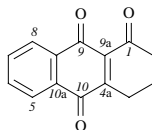
1H-Indene-1,3(2H)-dithione



4-Thiazolidinone



1H-Indole-5,6-dione, 2,3-dihydro-
(the two oxo substituents can be added as a pair without hydrogen being added elsewhere to the ring system)



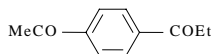
1,9,10(2H)-Anthracenetrione, 3,4-dihydro-
(the added hydrogen is cited in the lowest-numbered available position)

In the presence of higher functions or more preferred ketones, oxo, thioxo, selenoxo, and telluroxo radicals, are used. The =CO group, when not part of an acyclic chain or a ring, is expressed as carbonyl; the chalcogen analogs (carbonothioyl, carbonoselenoyl, and carbonotelluroyl) are used when they are not part of a chain, and when, in addition, they are either bonded to a single atom or used as multiplicative radicals. The trivially named radicals benzoyl, for (oxophenylmethyl), and acetyl, for (1-oxoethyl), are used when appropriate.

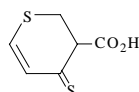
Examples:



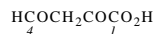
Butanoyl bromide, 3-oxo-
(not Acetyl bromide, acetyl-)



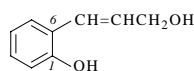
1-Propanone, 1-(4-acetylphenyl)-



2H-Thiopyran-3-carboxylic acid, 3,4-dihydro-4-thioxo-



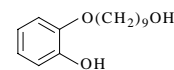
Butanoic acid, 2,4-dioxo- (not Propanoic acid, 3-formyl-2-oxo-)



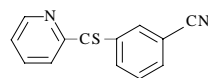
Phenol, 2-(3-hydroxy-1-propen-1-yl)- (not 2-Propen-1-ol, 3-(2-hydroxyphenyl)-)



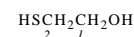
Hydrazinecarboxylic acid, 2-(cyclopropylcarbonyl)-



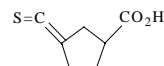
Phenol, 2-[(9-hydroxynonyl)oxy]- (principle: a cyclic parent is preferred (¶ 138))



Benzonitrile, 3-(2-pyridinylthio-methyl)- (not Benzonitrile, 3-(2-pyridinylcarbonothioyl)-)



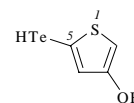
Ethanol, 2-mercapto-



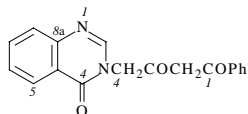
Cyclopentanecarboxylic acid, 3-carbonothioyl-

Hydroxy derivatives of thiophene, selenophene, and tellurophene are indexed at **Thiophene-ol**, etc., (the final "e" of the parents being left unelided to avoid confusion with chalcogen analogs of **Phenol**). The locant is placed immediately before the suffix.

Example:



Thiophene-3-ol, 5-telluryl-



1,3-Butanedione, 4-(4-oxo-3(4H)-quinazolinyl)-1-phenyl- (principle: maximum number of the principal chemical functional group (¶ 138))

Hydroxy, mercapto, selenyl, and telluryl groups attached to hetero atoms other than silicon are always expressed as prefixes (unless they form part of an acid functional parent compound (¶ 130)). "Esters" of such groups are also expressed as prefixes.

Examples:



Hydrazine, mercapto-



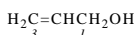
Boric acid, B,B-dimethyl-

175. Alcohols (and phenols) and their chalcogen analogs (thiols, selenols, and tellurols) are expressed by the suffixes -ol, -thiol, -selenol, and -tellurol, attached to a carbon or silicon atom of a molecular skeleton name. The only trivial name employed in CA indexes for a compound of this class is **Phenol** (for Benzenol). Phenols as a class are treated precisely like alcohols, the choice of index name for a compound containing alcoholic and phenolic groups depending on the usual rules (¶ 138). Alcoholic groups and their analogs are expressed as hydroxy, mercapto, selenyl, and telluryl prefixes on more preferred heading parents.

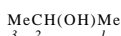
Examples:



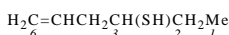
Ethanol (not Ethyl alcohol)



2-Propen-1-ol (not Allyl alcohol)



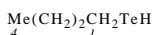
2-Propanol (not Isopropyl alcohol)



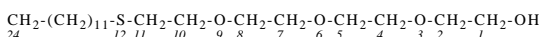
5-Hexene-3-thiol



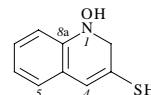
Silanol, 1-methyl-



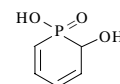
1-Butanetellurol



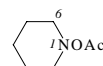
3,6,9-Trioxa-12-thiatetracosan-1-ol



3-Quinolinethiol, 1,2-dihydro-1-hydroxy-



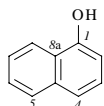
2-Phosphorinol, 1,2-dihydro-1-hydroxy-, 1-oxide



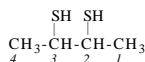
Acetic acid, 1-piperidinyl ester (not Piperidine, 1-(acetyloxy)-)



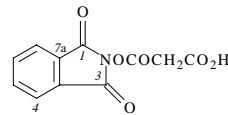
Benzeneselenol



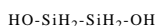
1-Naphthalenol (not 1-Naphthol)



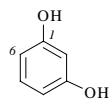
2,3-Butanedithiol



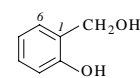
Propanedioic acid, 1-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl) ester (not Propanoic acid, 3-[(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)oxy]-3-oxo-)



1,2-Disilanediol



1,3-Benzenediol



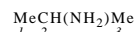
Benzenemethanol, 2-hydroxy- (not Phenol, 2-(hydroxymethyl)-) (principle: largest parent)

176. Amines are always named as primary amines, RNH_2 , or their *N*-derivatives, by attaching the suffix "-amine" to the name of a molecular skeleton, cyclic or acyclic. Attachment may be at a carbon or hetero atom. Trivial names, e.g., Aniline, and radicofunctional names, e.g., Methylamine, are not used.

Examples:



Methanamine (not Methylamine)



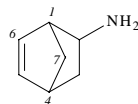
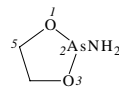
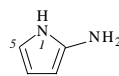
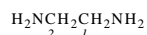
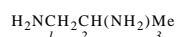
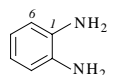
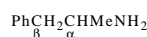
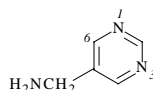
2-Propanamine (not Isopropylamine)



3-Buten-2-amine

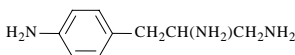
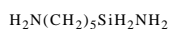
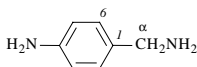
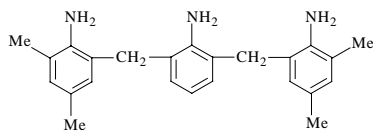


Plumbanamine

**Diphosphinamine****Benzenamine** (not Aniline)**Bicyclo[2.2.1]hept-5-en-2-amine****Bismuthinediamine****1,3,2-Dioxarsolan-2-amine****1H-Pyrrol-2-amine****1,2-Ethanediamine** (not Ethylenediamine)**1,2-Propanediamine****1,2-Benzenediamine** (not 1,2-Phenylenediamine)**Benzeneethanamine, α -methyl-****5-Pyrimidinemethanamine**

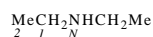
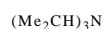
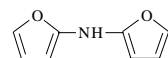
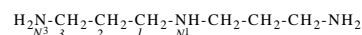
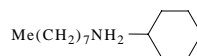
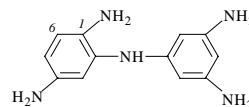
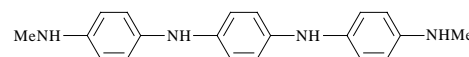
When higher functions (¶ 106) or more preferred amine parents are present, the prefix "amino" is employed.

Examples:

**1,2-Propanediamine, 3-(4-amino-phenyl)-** (principle: maximum number of the principal group)**Silanamine, 1-(5-aminopentyl)-** (principle: hetero atom parent preferred)**Benzenemethanamine, 4-amino-** (principle: largest heading parent)**Benzenamine, 2,6-bis[(2-amino-3,5-dimethylphenyl)methyl]-** (principle: centrality)

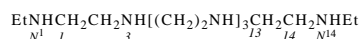
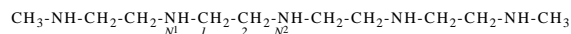
Secondary and tertiary amines, $RR'NH$ and $RR'R''N$, are named as derivatives of primary amines by application of the usual criteria (¶ 138).

Examples:

**Ethanamine, N-ethyl-** (not Diethylamine)**2-Propanamine, N,N-bis(1-methylethyl)-** (not Triisopropylamine)**2-Furanamine, N-2-furanyl-****1,3-Propanediamine, N¹-(3-aminopropyl)-****Silanamine, N-stannyl-** (principle: preferred hetero atom)**Cyclohexanamine, N-octyl-** (principle: a cyclic parent is preferred)**1,2,4-Benzenetriamine, N²-(3,5-diaminophenyl)-** (principle: lowest locants for principal groups)**Methanamine, N,N'-oxybis[N-methyl-]** (principle: multiplication)**1,4-Benzenediamine, N¹,N⁴-bis[4-(methylamino)phenyl]-** (principle: centrality)

Replacement names are employed for acyclic secondary and tertiary amines provided that the "-amine" suffix of the "aza" name expresses at least the same number of such groups as the conventional name and that other requirements (¶ 127), e.g., the presence of a minimum of four hetero units in the molecular skeleton, are satisfied.

Examples:

**3,6,9,12-Tetraazatetradecane-1,14-diamine, N¹,N¹⁴-diethyl-****1,2-Ethanediamine, N¹-[2-(methylamino)ethyl]-N²-[2-[(methylamino)ethyl]amino]ethyl]-** (not 3,6,9-Triazaundecane-1,11-diamine, N¹,N¹¹-dimethyl-; this organic replacement name expresses only three hetero units) (not 2,5,8,11,14-Pentaazapentadecane; this name does not express the amino groups as a substituent suffix)

Schiff bases (anils, azomethine compounds) contain the $-N=C-$ grouping and are therefore both amines and imines. They are indexed as amines in the absence of higher functions.

Example:

**Benzenamine, N-(phenylmethylene)-**

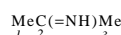
N-Hydroxy amines are named as such, not as hydroxylamine derivatives. Amine oxides are named by citation of the additive term "N-oxide" in the modification.

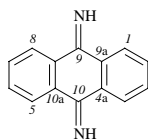
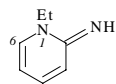
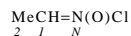
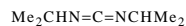
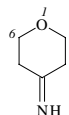
Examples:

**Benzenamine, N-hydroxy-****Ethanamine, N,N-diethyl-, N-oxide**

177. Imines are ranked as the lowest compound class named by use of a functional suffix. The "-imine" suffix is attached to a cyclic or acyclic molecular skeleton (at a carbon or hetero atom). Indicated and added hydrogen (¶¶ 135, 136) for cyclic imines are assigned as for the analogous ketones (¶ 174). N-Alkyl, N-aryl, etc., imines are indexed as amines (¶ 176). Conjunctive nomenclature is used for imines when the molecular skeleton to which a single function is attached is itself connected to a ring system by a single bond.

Examples:

**Ethanimine** (not Ethylideneimine)**2-Propanimine****Phosphinimine****2,4-Cyclopentadien-1-imine**



4H-Pyran-4-imine, tetrahydro- (not
2H-Pyran-4(3H)-imine, dihydro-)

Methanediimine (not Carbodiimide)

2-Propanamine, N,N'-methanetetraylbis- (not Methanediimine,
N,N'-bis(1-methylethyl)-)

**Ethanimine, N-chloro-,
N-oxide**

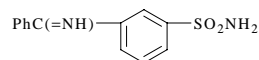
2(1H)-Pyridinimine, 1-ethyl-

9,10-Anthracenediimine

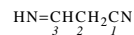
**Benzenemethanimine, N,N'-dithio-
bis[α-phenyl-** (principle: multipli-
cation of a conjunctive name)

In the presence of any other chemical function expressible as a suffix, imines are described by substituent prefixes. The =NH group is named imino; the =C=NH group is expressed as carbonimidoyl in a multiplying radical or when attached to a single atom; the -CH=NH group is named (iminomethyl) (not formimidoyl) unless the methyl group is part of an acyclic carbon chain.

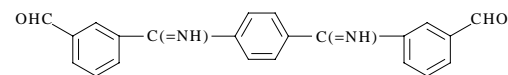
Examples:



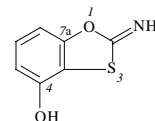
**Benzenesulfonamide, 3-(imino-
phenylmethyl)-**



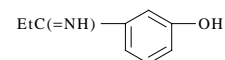
Propanenitrile, 3-imino-



**Benzaldehyde, 3,3'-(1,4-phenyl-
enedicarbonimidoyl)bis-**



1,3-Benzoxathiol-4-ol, 2-imino-



Phenol, 3-(1-iminopropyl)-

D. COMPOUND CLASSES

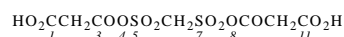
Introduction	¶ 178	Hydrazones	¶ 190
Anhydrides	179	Imides	191
Anions	180	Molecular addition compounds	192
Antimony and Bismuth compounds	181	Nitrogen compounds	193
Boron compounds	182	Organometallic compounds	194
Carbonic acid and relatives	183	Oximes	195
Cations	184	Oxygen compounds	196
Esters	185	Phosphorus and Arsenic compounds	197
Ester-anhydrides	186	Salts	198
Free radicals	187	Silicon, Germanium, Tin, and Lead compounds	199
Halogen and Halogenoid compounds	188	Sulfur, Selenium, and Tellurium compounds	200
Hydrazides	189	Zwitterionic compounds	201

178. Introduction. Previous sections have dealt with general principles and with the naming of specific compounds by combination of a molecular skeletal name with a suffix which describes the principal chemical function. The present section discusses nonfunctional compound classes (those that fall below imines in order of precedence (¶ 106)), and classes of compounds such as esters, free radicals, ions, addition compounds, oxo acids, and carbonic acid relatives, which are named by application of principles already discussed. The order is alphabetic by class.

179. Anhydrides of acid groups, at least one of which is expressed as a functional suffix ("oic acid," "carboxylic acid," "sulfonic acid," etc.), are indexed, if cyclic, at heterocycle names and, if acyclic, either at "a" names (¶ 127) or at acid heading parents with the term "anhydride" in the modification. (Acyclic anhydrides of certain mononuclear "oxo" acids, e.g., **Carbonic acid**, **Phosphonic acid**, are indexed at such headings as **Dicarbonic acid**, **Triphosphonic acid**.)

Replacement ("a") names are used for acyclic anhydrides when the suffix expresses no lower functionality than the heading parent of the regular substitutive name and the other requirements (¶ 127), e.g., that the molecular skeleton contain at least four hetero units, are satisfied.

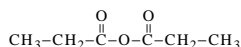
Example:



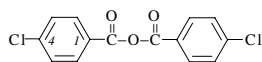
4,8-Dioxa-5,7-dithiaundecanedioic acid, 3,9-dioxo-, 5,5,7,7-tetraoxide

Symmetrical anhydrides of monobasic organic acids are indexed at the acid heading parent with the term "anhydride" in the modification. Locants are used when the parent is multiplied. Unsymmetrical anhydrides of monobasic acids, at least one of which is organic, are indexed at the name of the preferred acid (¶¶ 167, 138) with an "anhydride with" phrase in the modification. Anhydrides of **Hydrazinecarboxylic acid** and related compounds are given special treatment (see the final example below).

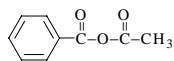
Examples:



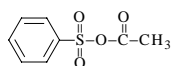
Propanoic acid, 1,1'-anhydride
(Locants are used because the parent is multiplied.)



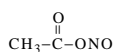
Benzoic acid, 4-chloro-, 1,1'-anhydride



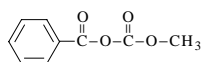
Benzoic acid, anhydride with acetic acid
(The parent is not multiplied so there are no locants.)



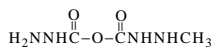
Acetic acid, anhydride with benzenesulfonic acid



Acetic acid, anhydride with nitrous acid



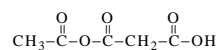
Benzoic acid, anhydride with methyl hydrogen carbonate (the ester name is given in its uninverted form (¶ 185); not Benzoic acid, anhydride with methoxyformic acid)



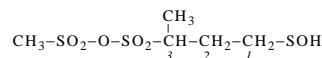
Dicarbonic dihydrazide, 2-methyl-
(see also ¶ 183)

Anhydrides of monobasic organic acids with polybasic acids are indexed at the name of the preferred acid. The terms "di," etc., are used to indicate the number of molecules of water lost in anhydride formation. Locants are cited for polybasic organic acids or when the parent is multiplied. A ratio is cited for anhydrides of an unmultiplied monobasic acid with an unmultiplied mononuclear polybasic acid and for anhydrides of two different unmultiplied polybasic mononuclear acids.

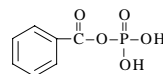
Examples:



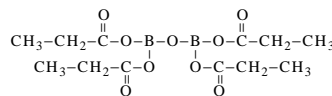
Propanedioic acid, 1-anhydride with acetic acid



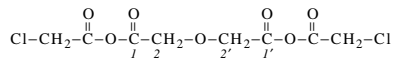
1,3-Butanedisulfonic acid, 3-anhydride with methanesulfonic acid (not "3-mono-anhydride with...")



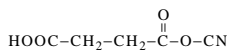
Benzoic acid, anhydride with phosphoric acid (1:1)



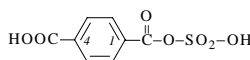
Propanoic acid, 1,1',1'',1'''-tetraanhydride with boric acid (H₃B₂O₅)



Acetic acid, 2,2'-oxybis-, 1,1'-dianhydride with 2-chloroacetic acid (principle: centrality (¶ 138))



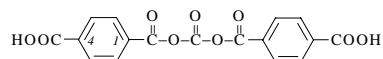
Butanedioic acid, 1-anhydride with cyanic acid



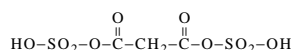
1,4-Benzenedicarboxylic acid, 1-anhydride with sulfuric acid

Acyclic anhydrides of different polybasic acids require locants.

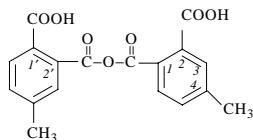
Examples:



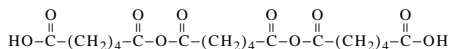
1,4-Benzenedicarboxylic acid, 1,1'-dianhydride with carbonic acid



Propanedioic acid, 1,3-dianhydride with sulfuric acid



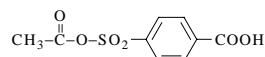
1,2-Benzenedicarboxylic acid, 4-methyl-, 1,2'-anhydride
(formerly bimol. 1,2'-monoanhydride)



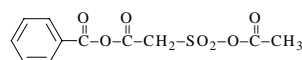
Hexanedioic acid, 1,1':6',1''-dianhydride
(formerly trimol. dianhydride)

When the acid group which has undergone anhydride formation would have been expressed (in its unmodified form) as a substituent of the preferred heading parent, the anhydride is likewise expressed as a (more complex) substituent of the same parent. Anhydride formation of an acid group expressed as a substituent in an "anhydride with" phrase is treated similarly.

Examples:



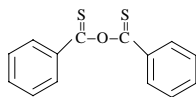
Benzoic acid, 4-[(acetyloxy)sulfonyl]-



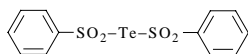
Benzoic acid, anhydride with 2-[(acetyloxy)sulfonyl]acetic acid

Chalcogen analogs of acyclic anhydrides are indexed like anhydrides. When the oxygen atom connecting the acid residues has been replaced, the terms "anhydrosulfide," "anhydroselenide," and "anhydrotelluride" are used, and the sulfur, selenium, or tellurium is indicated in the names of *both* acid components.

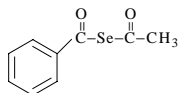
Examples:



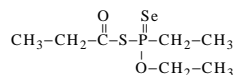
Benzenecarbothioic acid, 1,1'-anhydride (not "anhydrosulfide")



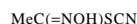
Benzenesulfonotelluric acid, 1,1'-anhydrotelluride



Benzenecarbosenoic acid, anhydroselenide with ethane-selenoic acid



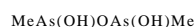
Propanethioic acid, anhydrosulfide with O-ethyl hydrogen P-ethylphosphonoselenothioate



Ethanimidothioic acid, N-hydroxy-, anhydrosulfide with thiocyanic acid

Symmetrical anhydrides of the monobasic "oxo" acids **Formic, Phosphinic, Arsenic, Phosphinous, and Arsinous acids** (and their substituted derivatives) are indexed by citation of the simple term "anhydride" in the modification. Symmetrical anhydrides of the dibasic "oxo" acids **Phosphonic, Arsonic, Phosphonos, and Arsonous acids** and their substituted derivatives are indexed at Di-, Tri-, etc., acid headings.

Example:



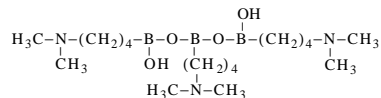
Diarsonous acid, dimethyl-

Anhydrides of boron acids are named as anhydrides.

Examples:



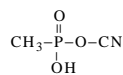
Boronic acid, B-methyl-B-phenyl-, B,B'-anhydride
(not Borane, oxybis[methylphenyl]-)



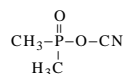
Boronic acid, B-[4-(dimethylamino)butyl]-, B,B':B',B'', dianhydride
(formerly Boronic acid, [4-(dimethylamino)butyl]-trimol. dianhydride)

Unsymmetrical anhydrides of "oxo" acids in general are indexed by use of "anhydride with" phrases at the preferred acid component heading parents, but cyanic acid anhydrides with mononuclear arsenic and phosphorus acids are expressed by means of "cyanato" replacement affixes or by the class term "cyanate."

Examples:



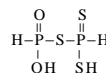
Phosphonocyanatidic acid, P-methyl-



Phosphinic cyanate, P,P-dimethyl-

Anhydrosulfides of "oxo" acids are generally named analogously by use of "anhydrosulfide" terms. Other chalcogens are treated similarly. When sulfur, etc., replaces oxygen in **Diphosphonic acid** and similar compounds, the non-detachable prefixes "Thio," etc., are employed. The number of sulfur atoms is not indicated in the name; instead, a synonym line formula is always cited.

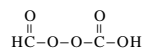
Example:



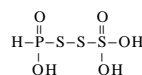
Thiodiphosphonic acid ((HO)HP(O)SHP(S)SH)

The peroxy analogs of this kind of "oxo" acid are indexed (with synonym line formulas) at such headings as **Thioperoxydiarsonic acid** ((HO)HAs(S)₂S₂). Anhydrides of mononuclear peroxy "oxo" acids are generally named at **Peroxide, Disulfide**, etc.

Examples:



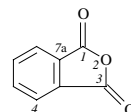
Peroxide, carboxy formyl



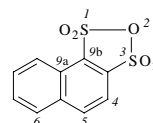
Disulfide, hydroxyphosphinyl sulfo

Cyclic anhydrides, anhydrosulfides, etc., are indexed like other heterocyclic compounds.

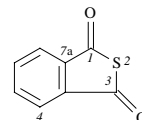
Examples:



1,3-Isobenzofurandione (not 1,2-Benzenedicarboxylic acid, cyclic anhydride)



Naphth[1,2-c][1,2,5]oxadithiole, 1,1,3,3-tetraoxide (not 1,2-Naphthalenedisulfonic acid, cyclic anhydride)



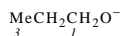
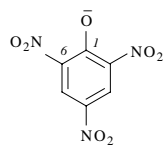
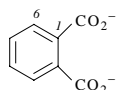
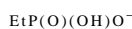
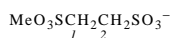
Benzo[c]thiophene-1,3-dione

180. Anions. Index names for anions are required as sole entries when anions themselves are being studied, and as additional entries in the indexing of salts (¶ 198). Anions are often expressed differently as modification terms at cationic heading parents.

Anions from unsubstituted **Ethyne, Arsine, Phosphine, Stibine, Silane** (Si⁴⁻ only), and **Hydrazine** are named **Acetylde, Arsenide, Phosphide, Antimonide, Silicide**, and **Hydrazide**. Synonym line formulas are used, e.g., **Acetylde** (C₂²⁻), except for **Hydrazide** (which is H₂NNH⁻) and **Silicide**, and for **Arsenide, Phosphide**, and **Antimonide** when all hydrogens have been lost.

Anions derived from compounds with names based on substitutive parent compounds (¶ 130) other than those just described are named at the heading parent for the neutral compound with a modification term such as "ion(1-)," "ion(2-)," or (if indefinite) "ion (neg)." Anions from esters of "oxo" acids are named similarly.

Examples:

**1,3-Cyclopentadiene, ion(1-)****1-Propanol, ion(1-)** (not Propoxide)**Phenol, 2,4,6-trinitro-, ion(1-)****1,2-Benzenedicarboxylic acid, ion(2-)****Arsine, dimethyl-, ion(1-)****Phosphonic acid, P-ethyl-, ion(1-)****Sulfuric acid, monophenyl ester, ion(1-)****1,2-Ethanedisulfonic acid, 1-methyl ester, ion(1-)**

Certain resonance-stabilized anions and cations containing hetero atoms are indexed by *CA* at names corresponding to preferred canonical structures. In the same manner as the analogous tautomeric compounds (¶ 122), anions are normalized, i.e., recognized as equivalent, by machine programs, regardless of how the structures are shown in the original documents. Each ion is assigned a single CAS Registry Number and a unique *CA* index name.

Resonance-stabilized anions of the general formula

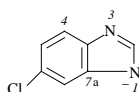


in which Q = C, N, S, P, Sb, As, Se, Te, Br, Cl, or I, and M and Z represent any combination of trivalent N and/or bivalent O, S, Se, or Te atoms are normalized in this way. The formula is analogous to that for normalized tautomeric compounds (¶ 122), with a negative charge replacing the hydrogen atom, and the requirements described for them apply equally to normalized anions. The names are derived by the same structural rules, and are identical except for addition of the index modification term "ion(1-)".

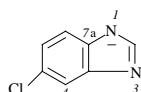
Examples:

**Propanamide, ion(1-)**

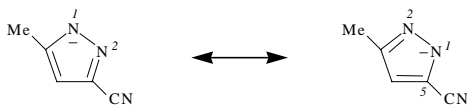
NOT

Propanimidic acid, ion(1-)**1H-Benzimidazole, 6-chloro-, ion(1-)**

NOT

**1H-Benzimidazole, 5-chloro-, ion(1-)**

Negative ions from tautomeric pyrazole and tropolone systems are not normalized by the CAS Registry System; their preferred structures and names are based on nomenclature rules, such as low numbering for principal functional groups, low numbering for substituents, etc.

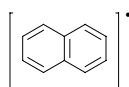
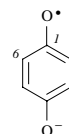
**1H-Pyrazole-3-carbonitrile, 5-methyl-, ion(1-)**

NOT

1H-Pyrazole-5-carbonitrile, 3-methyl-, ion(1-)

Radical ions are named at the neutral compound heading with "radical ion" terms in the modification.

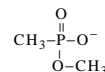
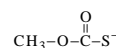
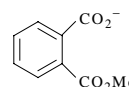
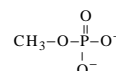
Examples:

**Naphthalene, radical ion(1-)****2,5-Cyclohexadiene-1,4-dione, radical ion(1-)**

At cationic index headings, e.g., **Ethanaminium** (see ¶ 184, 198), anions are expressed by "-ide" or "-ate" terms, as described below, or by "salt with" phrases. The "salt with" phrase is followed by a ratio, e.g., (1:1).

Modification terms for *unsubstituted* carbanions from acyclic and monocyclic hydrocarbons are derived by adding "-ide" to the hydrocarbon name after elision of the final "e," e.g., "benzenide," "cyclopentadienide." Unsubstituted acids expressed as principal groups (e.g., carboxylic and sulfonic acids) afford anions which are named by "-ate" terms in the modification, e.g., "acetate," "1,2-benzenedicarboxylate." **Phosphonic acid, Carbamic acid**, and other substitutive functional parent acids, whether substituted or not, also provide anions which are named in modifications by means of "-ate" terms, e.g., "phosphonate," "dimethylcarbamate." Similar terms are used for anions from partial esters of polybasic "oxo" acids.

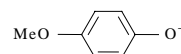
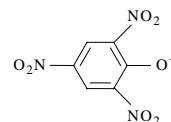
Examples:

**P-methyl O-methylphosphonate****O-methyl carbonothioate****1-methyl 1,2-benzenedicarboxylate****P-methyl phosphate**

Anions from the *unsubstituted* alcohols and phenols **Methanol, Ethanol, 1-Propanol, 1-Butanol**, and **Phenol** are named by "-oxide" terms, e.g., "propoxide," "phenoxide". Loss of hydrogen from the mercapto group of unsubstituted **Benzenethiol** is expressed as "benzenethiolate".

In all other cases, anion names at cation headings are replaced by "salt with" phrases; it is to be understood that, in a complete salt name, a ratio would always be added when known.

Examples:


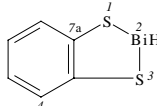
**salt with 4-methoxyphenol** (not "4-methoxyphenoxide")**salt with benzenamine****salt with 2,4,6-trinitrophenol** (not "picrate")

181. Antimony and Bismuth compounds, are conveniently discussed together because of the close similarity in the indexing treatment of their derivatives. Antimony and bismuth are metals (¶ 215), and their salts are named as such, not as cyclic or acyclic molecular skeletons. (Prior to *CA* Volume 95 (see ¶ 101), antimony was classed as a nonmetal for indexing purposes; now, it and bismuth are treated alike.)

Hydrides of trivalent antimony and bismuth are named **Stibine** and **Bismuthine**, respectively; polymolecular saturated and unsaturated hydride chains have names such as **Distibine, Distibene, Tribismuthine**. The mononuclear oxide heading parents **Stibine oxide** and **Bismuthine oxide** are employed, as are also the analogous names for the sulfides, etc., and imides. In heterocyclic compounds the valency is understood to be three unless an abnormal valency can be expressed in the name (¶ 158).

Examples:

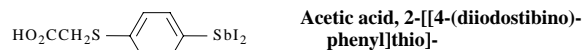
**Bismuthine, triethyl-**

EtSbCl ₂	Stibine, dichloroethyl-
Ph ₂ BiI	Bismuthine, iododiphenyl-
(F ₃ C) ₂ SbSbMe ₂ _{2 1}	Distibine, 1,1-dimethyl-2,2-bis-(trifluoromethyl)-
PhSb=SbPh	Distibene, 1,2-diphenyl-
Ph ₂ Sb(O)OH	Stibine oxide, hydroxydiphenyl-
H ₂ Sb(O)NH ₂ _{1 N}	Stibinamine, 1-oxide
EtBiH ₂ =NMe _{1 N}	Bismuthine imide, 1-ethyl-N-methyl-
	1H-Stibole
	1,3,2-Benzodithiabismole

Heterocyclic antimony and bismuth compounds without functional suffixes are ranked in accordance with the seniority of ring systems (¶ 138). Nonfunctional acyclic antimony substitutive parent compounds follow arsenic compounds in order of precedence (¶ 106) and are followed in turn by bismuth and then boron parents. Within each class the order is determined by the number of hetero atoms, then unsaturation, size and additive hetero atoms, as illustrated by the following descending order of antimony compounds: **Tristibine**, **Distibene**, **Distibine**, **Stibine oxide**, **Stibine sulfide**, **Stibine imide**, **Stibine**. In the presence of more preferred compound classes, the following substituent prefixes are employed. (The substituent prefixes stiboso (-SbO), stibo (-SbO₂), stibinico (=Sb(O)OH), and stibono (-Sb(O)(OH)₂) were used prior to CA Volume 95 (see ¶ 101).)

	<i>Substituent Prefix</i>		<i>Substituent Prefix</i>
-SbH ₂	stibino	-BiH ₂	bismuthino
=SbH	stibylene	=BiH	bismuthylene
≡Sb	stibylidyne	≡Bi	bismuthylidyne
-Sb=Sb-	1,2-distibenediyl		

Examples:



Trihydroxy and hydroxy oxo derivatives of **Stibine**, **Bismuthine**, **Stibine oxide**, **Bismuthine oxide** and their chalcogen analogs are given binary oxide, hydroxide, etc., names (with synonym line formulas) such as **Antimony hydroxide** (Sb(OH)₃), **Bismuth hydroxide** (Bi(OH)₃), **Antimony hydroxide oxide** (Sb(OH)O) and **Bismuth hydroxide oxide** (Bi(OH)O). (Antimonic acid headings were used prior to CA Volume 95 (see ¶ 101).)

Halo, alkoxy, and aryloxy derivatives of **Stibine**, **Bismuthine** and their oxides are so named; amino derivatives are named at **Stibinamine**, **Stibinediamine**, **Bismuthinamine**, etc.

Examples:

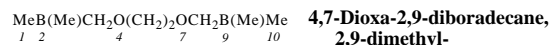


Arsenic compounds. See *Phosphorus and Arsenic compounds* (¶ 197).

182. Boron compounds. For the naming of neutral boron hydrides and replacement ("a") analogs (hetero polyboranes) see ¶¶ 159, 160. Except for hydroxyl groups attached to boron (¶ 175), principal groups on such hydrides are expressed as suffixes in the regular way, and conjunctive names are adopted with those known to have closed polyhedral structures; e.g., **Diborane(4)-1,1,2,2-tetramine** and **1,2-Dicarbododecaborane(12)-1,2-diethanol**.

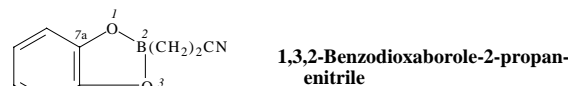
Acyclic carbon chains containing boron atoms are given "a" names if the requirements (¶ 127) are met.

Example:



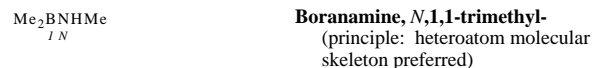
Heterocyclic boron compounds and their derivatives are named by the usual procedures (¶ 146). Intramolecular coordination bonds between boron atoms and other hetero atoms are ignored in naming; thus, a zwitterionic ring bond between boron and phosphorus in the last example below is disregarded, and the monocyclic system is named. (A monocycle entirely dependent on such a bond is named as an acyclic compound.)

Examples:



Boron molecular skeletons fall between nonfunctional bismuth and silicon compounds in the order of precedence of compound classes (¶ 106). Within the boron class, the descending order is carbapolyboranes, hetero polyboranes, polyboranes, heterocyclic boron compounds, and finally **Borane**. When more preferred groups or molecular skeletons are present, boron substituent prefixes (¶ 161) are used.

Examples:



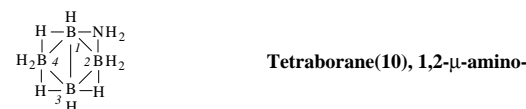
When the position of substituent suffixes or prefixes cannot be related to the accepted numbering of polyboranes and hetero polyboranes (as illustrated in the *Ring Systems Handbook* and current *Chemical Substance Index*), no numerical locants are used, but capital italic letters may be cited to denote substitution on a "hetero" atom in a hetero polyborane.

Examples:



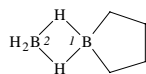
Substitution of *bridging hydrogen* of a polyborane or hetero polyborane is indicated by the prefix "μ" (mu); when necessary, the locants of the boron-atom bridgeheads are cited.

Examples:



Cyclic derivatives of polyboranes (other than **Diborane(4)**) and hetero polyboranes formed by replacement of non-bridging hydrogen atoms by bivalent radicals are named by citing such radicals as substituents.

Examples:



Diborane(6), 1,1-(1,4-butanediyl)-



1,2-Dicarbododecaborane(12), 1,2-[oxybis(methylene)]-

Hydroxy derivatives of **Borane** have acid names as follows:

$B(OH)_3$	Boric acid (H_3BO_3)
$HB(OH)_2$	Boronic acid
$H_2B(OH)$	Borinic acid

Boronic and borinic acids have replaceable hydrogen atoms attached to boron and are used as substitutive parent compounds. Their esters, anhydrides and salts are named in the usual way, but their acid halides, amides and hydrazides are named as **Borane**, **Boranamine**, and **Hydrazine** derivatives, respectively. Chalcogen analogs are named by use of affixes thio, seleno, and telluro.

Hydroxy derivatives of **Diborane(4)**, are now indexed at that index heading parent.

Examples:

$MeB(OMe)OEt$	Boronic acid, B-methyl-, ethyl methyl ester
$PhBMeOH$	Borinic acid, B-methyl-B-phenyl-
$PhB(SH)_2$	Boronodithioic acid, B-phenyl-
$AcOBMe_2$	Acetic acid anhydride with B,B-dimethylborinic acid
$PhB(NHNH_2)_2$	Hydrazine, 1,1'-(phenylborylene)bis-
$(HO)_2BB(OH)_2$	Diborane(4), 1,1,2,2-tetrahydroxy- (prior to CA Volume 95 the name Hypoboric acid was used)
$B(NH_2)_3$	Boranetriamine

Boric acid (H_3BO_3) is not a substitutive parent. Esters and anhydrides are indexed as functional derivatives; hydrazides are indexed at **Hydrazine**.

Examples:

$(HO)_2BOPr$	Boric acid (H_3BO_3), monopropyl ester
$(H_2NNH)_3B$	Hydrazine, 1,1',1''-borylidynetris-

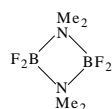
Addition compounds of neutral boranes are named as molecular coordination compounds (see ¶ 215). (Prior to CA Volume 95 (see ¶ 101), they were indexed at the component names (¶ 192).)

Example:

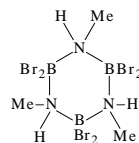
$[B(NMe_3)H_3]$	Boron, (N,N-dimethylmethanamine)trihydro-(T-4)- (preferred index name) (formerly indexed at Methanamine, N,N-dimethyl-, compd. with borane (1:1), and at Borane, compd. with N,N-dimethylmethanamine (1:1))
-----------------	--

Oligomeric boranamines which are linear or unspecified are indexed at the monomer name with "dimer," "trimer," etc., in the modification. Cyclic dimers are named as μ -derivatives of **Diborane(6)**. Monocyclic trimers, tetramers, etc., are given ring names in which the abnormal valencies of hetero atoms are expressed (see ¶ 158).

Examples:



Diborane(6), bis[μ -(dimethylamino)]tetrafluoro-



Borazine, 2,2,4,4,6,6-hexabromo-1,2,3,4,5,6-hexahydro-1,3,5-trimethyl-

Ionic boron compounds are indexed by coordination nomenclature (see ¶ 215) at such names as **Borate(2-)**, **decahydrodeca-** (for $[B_{10}H_{10}]^{2-}$), and **Boron(1+)**, **diamminedihydro-** (for $[BH_2(NH_3)_2]^{1+}$). Acidic polyboranes and hetero polyboranes are named as complex acids (¶ 215); e.g., **Borate(2-)**, **decahydrodeca-, hydrogen (1:2)** (not Decaborane(12)). Prior to the Eleventh Collective Index period, the special term "borata" denoted a tetrahedral borate anion attached to carbon atoms in a heterocyclic ring system. Now, compounds of this type are named by coordination nomenclature at such index headings as **Borate(1-)**.

183. Carbonic acid and relatives, with a few trivially named exceptions, are indexed by the principles of replacement nomenclature for functions (¶ 129), based on the names **Carbonic acid** (for $(HO)_2C=O$) and **Formic acid** (for HCO_2H). Trivial names employed in CA indexes are: Formyl halides and halogenides (except the cyanide, which is indexed at **Acetonitrile, 2-oxo-**), **Formamide, Formaldehyde, Hydrocyanic acid, Urea, Guanidine, Cyanic acid, Thiocyanic acid, Selenocyanic acid, and Tellurocyanic acid**. These trivially named compounds are ranked with the appropriate class (acid, amide, etc.) as **Carbonic acid** derivatives, which fall below derivatives of acids named as principal groups (carboxylic, sulfonic, etc.) and above inorganic "oxo" acids (**Hypochlorous acid, Phosphonic acid**, etc.) (see ¶ 106).

Examples:

$H-\overset{O}{\parallel}-NCO$	Formyl isocyanate
$H-\overset{O}{\parallel}-OCN$	Formic acid, anhydride with cyanic acid
$HCONHMe$	Formamide, N-methyl-

Analogs (imidic, hydrazonic, peroxy, chalcogen) of **Formic acid, Formamide**, etc., are named systematically as methanoic acid analogs, but are ranked as compounds related to **Formic acid**.

Examples:

$H-\overset{O}{\parallel}-O-OH$	Methaneperoxoic acid
$H-\overset{S}{\parallel}-SH$	Methane(dithioic) acid (not Formic acid, dithio-)
$HCSNH_2$	Methanethioamide (not Formamide, thio-)
$HC(=NH)NCO$	Methanimidoyl isocyanate
HCS_2CN	Methane(dithioic) acid, anhydrosulfide with thiocyanic acid
$HO-\overset{S}{\parallel}-CO_2H$	Formic acid, 1-(thiocarboxy)- (not Methanethioic acid, carboxy-)

Replacement of the nuclear hydrogen atom in formic acid compounds by radicals derived from molecular skeletons leads to carboxylic acids, carbothioamides, etc., expressed as suffixes on the skeleton names.

Formaldehyde analogs have systematic names based on **Methane**, e.g., **Methanimine** (for $CH_2=NH$) and **Methanethial** (for $CH_2=S$). (**Methanethione** (¶ 174) is employed only as the index heading parent for thio ketones with two cyclic substituents and for cyclic thio ketenes.) Replacement of hydrogen in formaldehyde by carbon skeletons leads to larger aldehydes and to ketones; they and their analogs are named by the usual principles of substitutive nomenclature (¶¶ 173, 174). Replacement by nitrogen, halogen, etc., leads to compounds which are often named as **Formic** or **Carbonic acid** derivatives.

Examples:

	3-Pyridinecarboxaldehyde
Ph_2CO	Methanone, diphenyl-
$PhC(=NH)Me$	Benzenemethanimine, α-methyl-
$HCONH_2$	Formamide
H_2NCOCl	Carbamic chloride
$Cl_2C=NH$	Carbonimidic dichloride

Carbonic acid analogs in which oxygen is replaced by halogen, halogenoid, chalcogen, or nitrogen atoms or groups (§ 129) (except cyano or a single hydroxyl) are given functional replacement names. The replacement of one hydroxyl by amino leads formally to Carbonimidic acid, $H_2NC(O)OH$, but it and its analogs are named at the approved abbreviated forms **Carbamic acid**, **Carbamothioic acid**, etc.

Examples:

$(HO)_2C=NH$	Carbonimidic acid (the tautomeric Carbamic acid is preferred in indexing unless both acid hydrogen atoms have been replaced.)
$H_2NC(=NH)OH$	Carbamimidic acid (not Carbonimidic acid) (Urea is preferred in indexing in the absence of a covalent acid derivative.)
$ClCO_2H$	Carbonochloridic acid
$NCCO_2H$	Carbonocyanidic acid
$(HO)_2C_2O$	Carbonodiperoxoic acid
$H_2NC(=NH)SSH$	Carbamo(dithioperox)imidic acid
Cl_2CS	Carbonothioic dichloride
$ClCOBr$	Carbonic bromide chloride

Carbonic diamide is named **Urea**, and its chalcogen analogs are indexed at **Thiourea** (not Urea, thio-), etc. The monohydrazide of carbonic acid is **Hydrazinecarboxylic acid**, but the dihydrazide is named **Carbonic dihydrazide**. The monocyanide of **Carbonic acid** is **Acetonitrile**, **2-oxo-**; the dicyanide is **Propanedinitrile**, **2-oxo-**; the trivial name **Guanidine** is employed for Carbonimidic diamide.

Examples:



Carbonic acid linear polyanhydrides are named at **Dicarbonic acid**, **Tricarbonic acid**, etc. Carbonimidic, carbonoperoxoic, and carbonimidoperoxoic acid anhydrides are named in the same manner. When all the anhydride oxygens have been replaced by -OO- or -NH- groups, nondetachable "peroxy-" and "imino-" prefixes are cited ahead of the name along with multiplicative prefixes. Chalcogen analogs are treated similarly, except that synonym line formulas form part of the name, and multiplicative prefixes are not cited. When both acid groups have been replaced by amide or acid halide functions, appropriate names are derived, but when only one hydroxyl group has been replaced, or different functions are present, choice of a simpler parent is made. Longer chains can often be indexed by replacement ("a") nomenclature (§ 127).

Examples:

$HO-C(=O)-O-C(=O)-OH$	Dicarbonic acid
$HO-C(=O)-O-C(=O)-O-C(=O)-OH$	Tricarbonimidic acid
$HO-O-C(=O)-O-C(=O)-O-OH$	Dicarbonodiperoxoic acid
HO_2COOCO_2H	Peroxydicarbonic acid
$HO-C(=O)-NH-C(=O)-NH-C(=O)-OH$	Diimidotricarbonimidic acid
$HO-C(=S)-S-S-C(=S)-OH$	Thioperoxydicarbonic acid ([(HO)C(S)] ₂ S ₂)
$Cl-C(=O)-O-C(=O)-Cl$	Dicarbonic dichloride
$Cl-C(=O)-NH-C(=O)-Br$	Imidodicarbonic bromide chloride
$H_2NNHCONHCONHNH_2$	Imidodicarbonic dihydrazide
$CICONHCO_2H$	Carbamic acid, N-(chlorocarbonyl)-
$NH_2-C(=O)-NH-C(=O)-NH-C(=O)-NH-C(=O)-NH_2$ <small>1 2 3 4 5 6 7 8 9</small>	2,4,6,8-Tetraazanonanediamide, 3,5,7-trioxo-

Carbonic acid and its relatives are placed in the order of precedence of compound classes just below acids expressed as suffixes attached to molecular skeleton names, e.g., sulfonic acids (§ 106). Within this subclass of acids, they are ranked by the following criteria, applied successively until a decision is reached: (a) number of acid groups; (b) number of nuclear carbon atoms; (c) precedence of atoms directly attached to nuclear carbon atoms (see Table I, § 128); (d) number of most preferred hetero atoms directly attached to nuclear carbon atoms; (e) order of priority of other atoms or groups attached to nuclear carbon atoms. A partial list in descending order is: **Peroxydicarbonic acid**, **Dicarbonic acid**, **Imidodicarbonic acid**, **Carbonoperoxoic acid**, **Carbonic acid**, **Carbonimidic acid**, **Carbonochloridic acid**, **Carbamic acid**, **Formic acid**, **Cyanic acid**, and **Thiocyanic acid**. (Chalcogen analogs of each acid immediately follow it in descending order of increasing replacement of oxygen by sulfur, selenium, and tellurium.) Acid chlorides, amides, etc., are ranked within their own classes in a similar order.

Carbamic acid derivatives with cyclic substituents are not assigned conjunctive names. In the presence of higher functions, including any acid expressed as a suffix, the carbamic acid residue is indicated by a (carboxyamino) radical. Its replacement analogs are named in the usual manner. Its hydrazides are indexed at **Hydrazinecarboxamide**.

Examples:

	Carbamic acid, N-2-naphthalenyl- (not 2-Naphthalenecarbamic acid)
	Carbamic acid, N,N'-1,4-phenylenebis- (not Carbamic acid, 1,4-phenylenebis- (see § 118))
Me_2NCS_2H	Carbamodithioic acid, N,N-dimethyl-
$PrNHC(=NH)OEt$	Carbamimidic acid, N-propyl-, ethyl ester
	Benzenesulfonic acid, 4-(carboxyamino)-

Cyanic acid and its chalcogen analogs are treated as mononuclear "oxo" acids; their esters and anhydrides are named in the usual way. Isocyanic acid and its analogs are not used in general index nomenclature; their esters and anhydrides are named like halogen compounds. The acids themselves, and their salts, are indexed at **Cyanic acid**, **Thiocyanic acid**, etc. The amide, H_2NCN , is named **Cyanamide**.

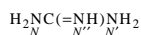
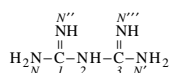
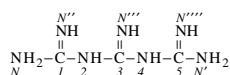
Examples:

$MeOCN$	Cyanic acid, methyl ester
$H_3CC(O)SCN$	Ethanethioic acid, anhydrosulfide with thiocyanic acid
	Benzoic acid, 4-cyanato-
$PhNCO$	Benzene, isocyanato- (not Isocyanic acid, phenyl ester)
$H_2C=CHCONCO$	2-Propenoyl isocyanate
$PhNHCN$	Cyanamide, N-phenyl- (not Benzene-carbamionitrile)

Numerical and italic letter locants are used with carbonic acid relatives to place substituents. Locants are employed with monosubstituted **Guanidine** and **Carbamimidic acid**.

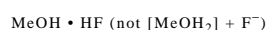
Examples:

$MeNHCONH_2$ <small><i>N</i> <i>N'</i></small>	Urea, N-methyl-
$MeNHCSNHMe$ <small><i>N</i> <i>N'</i></small>	Thiourea, N,N'-dimethyl-
$H_2NNHC(=NH)SEt$	Hydrazinecarboximidithioic acid, ethyl ester

**Carbonic dihydrazide****Guanidine****Imidodicarbonimidic diamide****Diimidotricarbonimidic diamide**

184. Cations, including carbonium ions (which possess an electron-deficient, tricoordinate carbon atom), “ium” ions (defined for index nomenclature purposes as resulting from addition of a proton to a saturated carbon atom or of one covalent substituent other than hydrogen to a fully substituted hetero atom), and radical cations related to these two classes are described here. (For salts of which they are components, see ¶ 198.) When a proton is added to a hetero atom, the resulting compound is named as a salt (if the anion is known) or by such modification phrases as “conjugate acid” or “conjugate monoacid” at the neutral component followed by the appropriate ratio.

Examples:

**Hydrofluoric acid, compd. with methanol (1:1)****Pyridine, conjugate acid (1:1)**

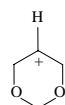
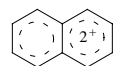
Carbon cations formally derived by *addition* of a proton to a saturated carbon atom are named at the molecular skeleton name by use of a modification term such as “protonated”.

Example:

**Ethane, protonated (1:1)**

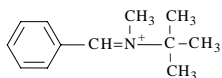
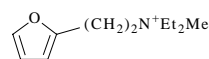
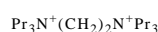
Orthodox carbonium compounds are named from the hydrocarbon (or other parent) *radical* by addition of “-ium.”

Examples:

**Ethylum****Ethylum, 1-methyl- (not 2-Propylum)****Ethylum, 1-oxo- (not Acetylium)****Methylum, cyclopropyloxo- (not Cyclopropylcarbonylium)****1,3-Dioxan-5-ylum****Naphthalenediylium, dihydro-**

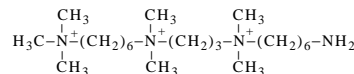
Acyclic *nitrogen cations* derived from amines attached to parent molecular skeletons are named by converting the preferred “-amine” name (¶ 176) to “-aminium” and expressing the remaining quaternizing groups as substituent prefixes.

Examples:

**Methanaminium, N,N,N-trimethyl-****Methanaminium, N-methyl-N-oxo-****2-Propanaminium, N,2-dimethyl-N-(phenylmethylene)- (principle: largest amine parent)****2-Furanethanaminium, N,N-diethyl-N-methyl- (from a conjunctively-named amine)****1,2-Ethanediaminium, N¹,N¹,N¹,N²,N²,N²-hexapropyl- (principle: maximum number of the preferred substituent suffix)****Methanaminium, N-ethylidyne-**

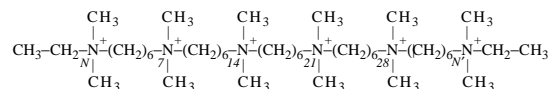
Quaternary ammonium cations not included in the heading parent are expressed as substituted ammonio, ⁺NH₃-, iminio, ⁺NH₂=, and nitrilio, ⁺NH≡, radicals.

Example:

**1,6-Hexanediaminium, N¹-[3-[(6-aminohexyl)dimethylammonio]propyl]-N¹,N¹,N⁶,N⁶,N⁶-penta-methyl- (principle: largest heading parent)**

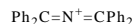
Aminium and diaminium names may be derived from amines named by replacement (“a”) nomenclature. In addition, cationic centers in the “a” name of a molecular skeleton may be expressed, if such a name is permitted (see ¶ 127), by use of the “azonia” replacement prefix.

Example:

**7,14,21,28-Tetraazoniatetracontane-1,34-diaminium, N¹,N³⁴-diethyl-N¹,N¹,N³⁴,N³⁴,7,7,14,14,21,21,28,28-dodecamethyl-**

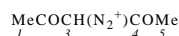
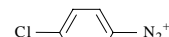
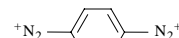
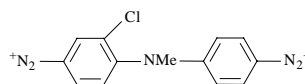
Iminium names are employed when the quaternary nitrogen atom is attached to one or more bivalent radicals derived from a molecular skeleton, and analogous monovalent radicals are absent. The names are derived from those of the preferred imines (¶ 177).

Example:

**Benzenemethaniminium, N-(diphenylmethylene)-α-phenyl-**

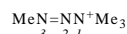
Diazonium compounds contain the $-\text{N}_2^+$ group attached to a substitutive parent compound. When such a parent is a molecular skeleton, the suffix “-diazonium” is employed; otherwise **Diazonium** is the heading parent. The corresponding substituent prefix is “diazonio.”

Examples:

**3-Pentanediazonium, 2,4-dioxo-****Benzenediazonium, 4-chloro-****1,4-Benzenebis(diazonium)****Diazonium, (methylamino)-****Benzenediazonium, 3-chloro-4-[(4-diazoniophenyl)methylamino]-**

Cations from acyclic nitrogen molecular skeletons are named in a similar manner by use of the “-ium” suffix. Lowest locants are given to cationic centers when a choice is necessary.

Examples:

**Hydrazinium, 1,1-dimethyl-1-phenyl-****Triazanium, 2,2-dimethyl-****2-Triazenium, 1,1,1,3-tetramethyl-****Hydrazinium, 1,1,1,2,2,2-hexamethyl-**

Acyclic cations from nonnitrogenous hetero atoms are indexed at **Phosphonium**, **Arsonium**, **Stibonium**, **Bismuthonium**, **Oxonium**, **Sulfonium**, **Iodonium**, etc. The corresponding substituent prefixes are phosphonio, arsonio, etc. **Diphosphine**, H_2P-PH_2 , affords **Diphosphinium**.

Examples:

$Me_3P^+(CH_2)_2P^+Me_3$	Phosphonium, 1,1'-(1,2-ethanediyl)bis[1,1,1-trimethyl- (analogous compounds with one or more noncarbon attachments to phosphorus are indexed at Phosphorus(1+) (see ¶ 215))
$Cl_2PP^+Me_3$	Diphosphinium, 2,2-dichloro-1,1,1-trimethyl-
Me_4As^+	Arsonium, tetramethyl-
Me_3S^+	Sulfonium, trimethyl- (the corresponding <i>S</i> -oxide is named Sulfoxonium, trimethyl-)
Ph_2I^+	Iodonium, diphenyl- (the corresponding <i>I</i> -oxide is named Iodonium, diphenyl-, I-oxide)

Cyclic cations from rings with "a" names are named by replacing the aza, oxa, thia, etc., terms by the cationic prefixes azonia, oxonia, thionia, etc. They are cited in the same order as the corresponding neutral terms (Table I ¶ 128); when the same element is present in neutral and cationic forms, alphabetic order of the terms is followed, but the cationic center is preferred for lowest locants if a choice is available.

Examples:

	5-Aza-2-azoniabicyclo[4.2.2]decane, 2,2-diethyl-
	2,6,7-Trioxa-1-phospha-4-phosphoniabicyclo[2.2.2]octane, 4-methyl-
	8-Thioniabicyclo[3.2.1]octane, 8-methyl-
	1-Oxa-4-azoniaspiro[4.4]nonane, 2,2,4,4-tetramethyl-
	5-Phosphoniaspiro[4.4]nonane

Cationic monocyclic and fused ring systems, other than those with "a" names, are indexed at heading parents derived from the heterocycle name by addition of an "-ium" suffix. Lowest locants are preferred for indicated hydrogen, e.g., **1H** (never **3H**)-**Benzimidazolium**; a cationic center is numbered lower than a neutral hetero atom of the same element if a choice is available.

Examples:

	Pyridinium, 1,3-dimethyl-
	Phenazinium, 3,7-dibromo-5-methyl- (not Phenazino-, 2,8-dibromo-10-methyl-)
	Piperazinium, 1,1,4,4-tetramethyl-
	Furanium, 1-ethyltetrahydro-

In all the examples above, the charge of the cationic atom was derived from an additional covalent substituent at a ring hetero atom already saturated to the covalency limit. Similar names are used (for rings other than those with "a" names) when the covalency limit is exceeded within the ring system itself, no "external" substitution being involved. The "-ium" name is derived from the uncharged heterocycle, indicated hydrogen, if present, being removed. If indicated hydrogen is needed for the cationic system, it is added at the lowest available nonangular position. The trivial names **Furylium**, **Pyrylium**, **Thiopyrylium** (and their benzo analogs), and **Xanthylium** (from **Xanthene**) are used. When other hetero atoms are present in the ring system, a locant before the "-ium" suffix defines the position of the cationic center.

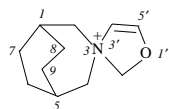
Examples:

	Quinolizinium
	Pyrylium, 4-methoxy- (from <i>2H</i> - or <i>4H</i> -Pyran)
	Dibenziodolium, 1,9-dimethoxy-
	1,3-Dioxol-1-ium, 2-methyl-
	Phenothiazin-5-ium, 3,7-bis(dimethylamino)-

Cationic heterocyclic monospiro compounds, other than those from "a"-named rings, have the "-ium" term placed in the name in accordance with the nature of the component rings. When the cationic hetero atoms are in nonspiro positions, the "-ium" suffix is appended to the appropriate component. If the spiro and cationic centers coincide, or if both component rings contain such a center, the "-ium" is attached only to the second component (if the components are different). For "a"-named components, "azonia," "oxonia," etc., terms are used as appropriate; in addition, an "-ium" suffix is attached to the second component if the spiro atom is cationic and the second component does not have an "a" name.

Examples:

	Spiro[benzothiazolium-4(5H),1'-cyclopentane], 6,7-dihydro-2,3-dimethyl-
	Spiro[1,3-dioxolane-2,6'(2'H)-isoquinolinium], 2',2'-dimethyl-
	Spiro[isoquinoline-2(1H), 2'-(2'H)pyrido[1,2-a]pyrazinium]
	Spiro[5H-dibenzophospholium]
	Spiro[3-azoniabicyclo[3.1.0]hexane-6,9'-(9H)fluorene], 3,3-dimethyl-



Spiro[3-azoniabicyclo[3.2.2]nonane-3,3'(2H)-oxazolium]

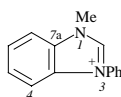
Dispiro compounds with other than "a"-named components and containing two cationic spiro atoms have the "ium" suffix appended to the terminal, i.e., the first and third, component names.

Several classes of *resonance-stabilized cations* containing nitrogen atoms are either normalized by the CAS Registry System or treated as though they were; i.e., to avoid scattering of information in CA indexes, each such cation, regardless of how its structure is drawn, is assigned a unique CAS Registry Number and unique CA *Chemical Substance Index* name (cf. ¶¶ 122, 180). A normalized cation is any cyclic cation with the substructure



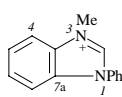
where (a) the terminal N's are in the same ring or adjacent rings (but not at a ring junction) and (b) the bonds to R and R' are not part of the ring.

Examples:

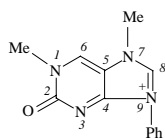


1H-Benzimidazolium, 1-methyl-3-phenyl-
(principle: positive charge on the CIP-preferred nitrogen)

NOT

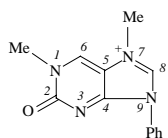


1H-Benzimidazolium, 3-methyl-1-phenyl-



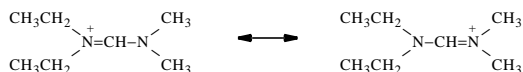
1H-Purinium, 2,7-dihydro-1,7-dimethyl-2-oxo-9-phenyl-
(principle: positive charge on the CIP-preferred nitrogen)

NOT



1H-Purinium, 2,9-dihydro-1,7-dimethyl-2-oxo-9-phenyl-

For resonance-stabilized cations that are not normalized, the unique CA *Chemical Substance Index* name is derived by regular nomenclature rules (see ¶ 138).



Ethanaminium, N-[(dimethylamino)methylene]-N-ethyl-
(principle: preferred index parent)

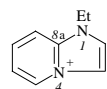
NOT

Methanaminium, N-[(diethylamino)methylene]-N-methyl-



Imidazo[1,2-a]pyridinium, 1-ethyl-
(principle: the neutral ring, quaternized by substitution, is preferred)

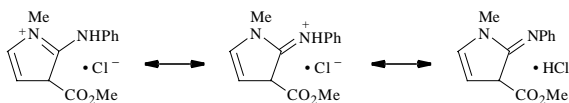
NOT



1H-Imidazo[1,2-a]pyridinium, 4-ium, 1-ethyl-

When at least one canonical form of a resonance-stabilized cation represents a *hydrogen atom* as being attached to a positively charged nitrogen atom, it is named as a neutral compound with an index modification term such as "conjugate acid" or (if the anion is known) as a salt such as "hydrochloride" followed by the appropriate ratios.

Example:



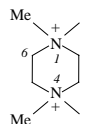
(The hydrochloride salt is the preferred structure.)

Cationic prefixes are used when more preferred compound classes (¶ 106) are present, or when different cations, or additional occurrences of the same cation, cannot be included in the heading parent. Heteroacyclic cationic prefixes are based on "onio" radicals such as ammonio and iminio (for singly and doubly bound nitrogen, respectively), diazonio, sulfonio, phosphonio, and iodonio. Cyclic cationic radicals from rings, not named by "a" nomenclature, containing a single hetero atom at which the free valency is located are named by changing the "ium" ending of the cation name to "io"; e.g., pyridinio, 2H-pyranio, phenanthridinio. In all other cases, heteroacyclic and heterocyclic cationic prefixes are derived from the cation name by adding "-yl," "-diyl," etc., to the "ium" suffix with locants (low-numbered if there is a choice) to indicate the points of attachment.

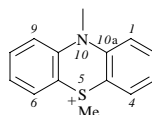
Examples:



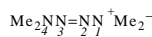
(1-methylpyridinium-2-yl)



(1,4-dimethylpiperazinium-1,4-diyl)



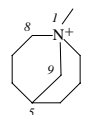
(5-methyl-10H-phenothiazinium-10-yl)



(1,1,4,4-tetramethyl-2-tetrazenium-1-yl)



piperidinium-1-ylidene



1-azoniabicyclo[3.3.1]non-1-yl

Carbon cationic prefixes are named by addition of "yl" to the cation name. Locants are cited (except for methane prefixes) for both the cationic center and the point of attachment, with lowest locants for the latter.

Examples:



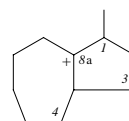
methyliumyl



1-ethylium-1-yl



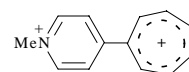
(tetrahydro-4H-pyran-4-yl)ium-4-yl)



(octahydro-8a(1H)-azulenium-1-yl)

Cationic compounds are ranked in the following descending order of precedence of elements: C, N, P, As, Sb, Bi, O, S, Se, Te, F, Cl, Br, I. When more than one cationic center is present, the general rules of substitutive nomenclature (¶ 138) are applied, the cationic centers being considered as principal chemical groups for this purpose.

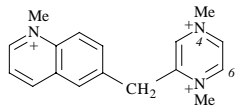
Examples:



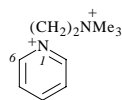
Cycloheptatrienylium, (1-methylpyridinium-4-yl)- (principle: carbon cation preferred)



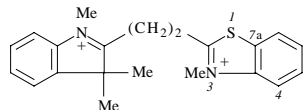
1-Propanaminium, 3-(dimethylsulfonio)-N,N,N-trimethyl- (principle: nitrogen cation preferred)



Pyrazinium, 1,4-dimethyl-2-[(1-methylquinolinium-6-yl)methyl]- (principle: maximum number of cationic centers)



Pyridinium, 1-[2-(trimethylammonio)ethyl]- (principle: ring parent preferred)

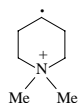


Benzothiazolium, 3-methyl-2-[2-(1,3,3-trimethyl-3H-indolium-2-yl)ethyl]- (principle: preferred ring)

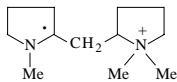
Cationic compounds of *indefinite structure* are named by use of alternative locants if possible, e.g., **Quinazolinium, 1(or 3)-methyl-, iodide (1:1)**; otherwise as molecular addition compounds of the neutral compounds with a term such as “compd. with iodomethane (1:1)” (not “monomethiodide”) in the modification.

Cationic free radicals from carbonium ions are named like the carbon cationic prefixes (above); e.g., **Methyliumyl; 4-Cyclohexylium-1-yl**. When the free radical and cationic centers are separated, the “-yl” suffix is preceded by a locant, if known. When the free radical and cationic center are in different parent molecular skeletons, the free radical supplies the heading parent.

Examples:



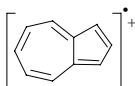
Piperidinium-4-yl, 1,1-dimethyl-



2-Pyrrolidinyl, 2-[(1,1-dimethylpyrrolidinium-2-yl)methyl]-1-methyl-

Delocalized radical cations are described at the index name of the corresponding neutral compound by the modification term “radical ion” followed by a cationic Ewens-Bassett number in parentheses.

Example:



Azulene, radical ion(1+)

Cationic free radicals formally derived by loss of an electron from a heteroatom of a molecular skeleton or of an isolated chalcogen atom are named similarly (¶ 270).

Example:



Methanamine, N,N-dimethyl-, radical ion(1+)

185. Esters, other than cyclic esters, of principal functions are named as such for indexing purposes, usually at the acid component name. Cyclic esters are named as heterocyclic ring system derivatives. Esters of hydroxy, mercapto, carboxy, sulfo, etc., groups expressed as substituents of heading parents are expressed as compound or complex substituents, not as modification terms at the same heading parent. To be recognized as an ester in CA indexing, a C-O, C-S, C-Se, or C-Te bond must be present. Thus, ethyl cyanate and ethyl perchlorate are considered to be esters, but ethyl azide, ethyl isocyanate, and ethyl chloride are not.

Examples:



Cyanic acid, ethyl ester



Perchloric acid, ethyl ester



Ethane, azido-



Ethane, isocyanato-



Ethane, chloro-

To permit information on esterified alcohols and thiols to be more readily found in the *Chemical Substance Index*, the usual rules of index name selection

are modified for esters. The chemical functionality (¶ 106) of certain very common acids (“Class I” acids) is disregarded for the purpose of naming their esters, unless the “alcoholic” component is also very common, and the entry is made instead at the uncommon alcohol, despite its lower functionality. The “Class I” acids comprise: **Acetic acid; Benzenesulfonic acid; Benzenesulfonic acid, 4-methyl-; Benzoic acid** and its monoamino, mononitro, and dinitro derivatives; **Boric acid (H₃BO₃); Carbamic acid; Carbamic acid, N-methyl-; Carbamic acid, N-phenyl-; Carbonic acid; Formic acid; Methanesulfonic acid; Nitric acid; Phosphoric acid; Phosphorodithioic acid; Phosphorothioic acid; Phosphorous acid; Propanoic acid; Sulfuric acid; and Sulfurous acid**. All other acids, including isotopically labeled forms of “Class I” acids, belong to “Class II.”

Esters of “Class I” monobasic acids with “Class II” alcohols and thiols are indexed at the latter. Esters of “Class I” acids with “Class I” alcohols and thiols are indexed at the acids. “Class I” alcohols are: **Benzenethanol; Benzenemethanol; 1-Butanol, 2-ethyl-; 2-Butanol; Cyclohexanol; 1-Decanol; 1-Dodecanol; Ethanol; Ethanol, 2-(diethylamino)-; Ethanol, 2-(dimethylamino)-; Ethenol; 1-Heptanol; 1-Hexanol, 1-Hexanol, 2-ethyl-; Methanol; 1-Nonanol; 1-Octadecanol; 1-Octanol; 1-Pentanol; Phenol** and its monochloro, monomethyl, and mononitro derivatives; **1-Propanol; 1-Propanol, 2-methyl-; 2-Propanol; 2-Propanol, 2-methyl-; and 2-Propen-1-ol**. The list of “Class I” thiols is completely analogous to the “Class I” alcohol list; the individual index names are also analogous, e.g., **Benzenethanethiol; 2-Propanethiol, 2-methyl-**; except that the **Phenol** analog is **Benzenethiol**. All selenols and tellurols belong to “Class II.”

Esters formed from hydroxy derivatives of nitrogen, phosphorus, arsenic, antimony, bismuth, germanium, tin and lead are named as such. They are always indexed at the acid regardless of the type of acid. The acyclic nitrogen radicals used in ester names are azanyl, diazanyl, diazenyl, triazanyl, etc.

Examples:



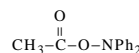
Acetic acid, 2-phenylethyl ester



Sulfuric acid, monomethyl ester (the uninverted name is methyl hydrogen sulfate)



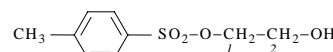
Phosphorodithioic acid, O-methyl S-phenyl ester



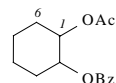
Acetic acid, diphenylazanyl ester

In each of the examples above, a “Class I” acid is esterified by a “Class I” alcohol or thiol. When the acid belongs to “Class I” and the alcohol or thiol to “Class II,” the entry is found at the alcoholic component name, except when the acid is polybasic and the alcohols differ from one another, in which case the acid heading is chosen. When the ester is named at the alcohol heading a locant is always cited for the “ate” or “ite” term. This eliminates the need for the parenthetical expression “(ester)”.

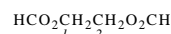
Examples:



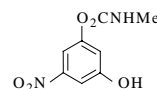
1,2-Ethanediol, 1-(4-methylbenzenesulfonate)



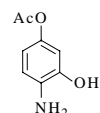
1,2-Cyclohexanediol, 1-acetate 2-benzoate



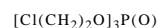
1,2-Ethanediol, 1,2-diformate (the uninverted name is 1,2-ethanediyl diformate)



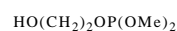
1,3-Benzenediol, 5-nitro-, 1-(N-methylcarbamate)



1,3-Benzenediol, 4-amino-, 1-acetate



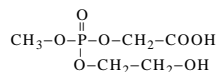
Ethanol, 2-chloro-, 1,1',1''-phosphate (3:1) (all the “Class II” alcoholic components are alike here; the ratio is necessary to indicate a neutral ester of known composition; the mono- and diesters are named with “**dihydrogen phosphate**” and “**hydrogen phosphate**”, respectively in the modification)



Phosphorous acid, 2-hydroxyethyl dimethyl ester (the entry is made at a “Class I” acid, not at the “Class II” alcohol **1,2-Ethanediol**, because the alcoholic components are unlike)

When an ester of the type illustrated immediately above has a more preferred acid residue present in the molecule, the "Class I" polybasic acid becomes a substituent.

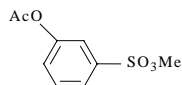
Example:



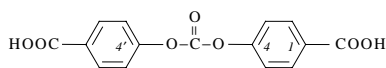
Acetic acid, 2-[[2-(2-hydroxyethoxy)-methoxyphosphinyl]oxy]- (not Acetic acid, hydroxy-, 2-hydroxyethyl methyl phosphate)

Esterified substituents of the index heading parent are expressed as substituents, not as modification phrases.

Examples:



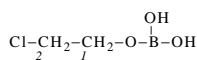
Benzenesulfonic acid, 3-(acetyloxy)-, methyl ester (not Benzenesulfonic acid, 3-hydroxy-, methyl ester acetate)



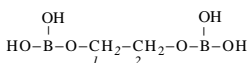
Benzoic acid, 4,4'-[carbonylbis-(oxy)]bis- (not Benzoic acid, 4-hydroxy-, carbonate (2:1))

The phrase "ester with" is usually avoided in general index nomenclature for compounds of known structure, even when the alcoholic component contains a function higher than alcohol, but it is employed when an acid which requires a line formula is cited in a modification; a ratio is included if the alcohol is monohydric and has a single occurrence, and locants are used if the alcohol is polyhydric or has multiple occurrences.

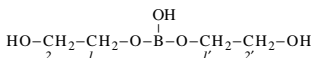
Examples:



Ethanol, 2-chloro, ester with boric acid (H₃BO₃) (1:1)



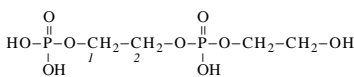
1,2-Ethandiol, 1,2-diester with boric acid (H₃BO₃)



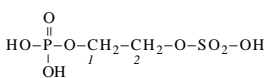
1,2-Ethandiol, 1,1'-diester with boric acid (H₃BO₃)

The word "hydrogen," with multiplicative prefixes if necessary, is used with an "-ate" (or "-ite") term derived from a polybasic acid cited in a modification to denote unesterified acid groups. One or more "hydrogen" terms may be replaced by radicals to denote further esterification not expressed in the heading parent. When all acid groups of a polybasic acid have been esterified, "hydrogen" cannot be cited; therefore, if the precise structure is known, a ratio is placed after the "-ate" term. If more than one such term is necessary, the complete "-ate" phrases are cited (without commas) in alphabetical order.

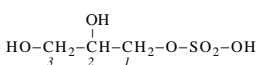
Examples:



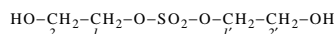
1,2-Ethandiol, 1-(dihydrogen phosphate) 2-(hydroxyethyl hydrogen phosphate) (principle: maximum number of functional derivatives)



1,2-Ethandiol, 1-(dihydrogen phosphate) 2-(hydrogen sulfate)



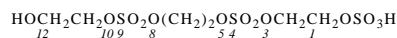
1,2,3-Propanetriol, 1-(hydrogen sulfate)



1,2-Ethandiol, 1,1'-sulfate

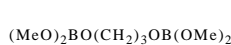
Esters are named by replacement ("a") nomenclature if the requirements (¶ 127) are met.

Example:



3,5,8,10-Tetraoxa-4,9-dithiadecane-1,12-diol, 1-(hydrogen sulfate), 4,4,9,9-tetraoxide

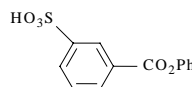
Multiplicative radicals in modifications are cited ahead of nonmultiplicative. Example:



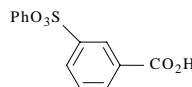
Boric acid (H₃BO₃), B,B'-(1,3-propanediyl) B,B,B'B'-tetramethyl ester

Although locants to differentiate between principal and subsidiary groups are strictly not necessary in ester modifications (because esterification of the latter is not expressed in the modification), they are nevertheless cited to preclude misinterpretation.

Examples:



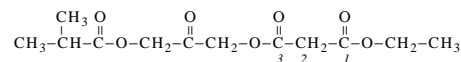
Benzoic acid, 3-sulfo-, 1-phenyl ester



Benzoic acid, 3-(phenoxy sulfonyl)-

Esterification of an alcoholic component cited in the index modification is expressed as a substituent of the esterifying radical.

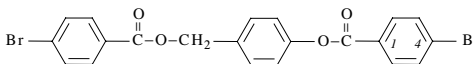
Example:



Propanedioic acid, 1-ethyl 3-[3-(2-methyl-1-oxopropoxy)-2-oxopropyl] ester (not Propanedioic acid, ethyl 3-hydroxy-2-oxopropyl ester, 2-methylpropanoate)

The choice of a preferred index name for a complex ester depends on the normal criteria (¶ 138), first on the preferred acid class (peroxyic, carboxylic, carboximidic, sulfonic, carbonic, etc.) then on the preferred heading parent and the particular occurrence of such a parent if it occurs more than once. If there are three or more occurrences, the principle of centrality is invoked; if there are only two, often the preferred name is the one appearing earliest in index sequence.

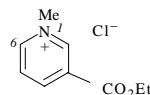
Example:



Benzoic acid, 4-bromo-, 4-[[4-(4-bromobenzoyloxy)methyl]phenyl]phenyl ester (not Benzoic acid, 4-bromo-, [4-[(4-bromobenzoyloxy)phenyl]methyl ester)

When functions higher in precedence than acids are present, all esters are expressed as substituents.

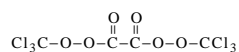
Example:



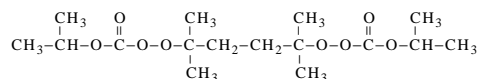
Pyridinium, 3-(ethoxycarbonyl)-1-methyl-, chloride (1:1)

Peroxy acid esters and their chalcogen analogs are named in the usual way, with "OO," "OS," "SeO," "SS," etc., locants used when necessary along with the usual "O," "S," etc., locants.

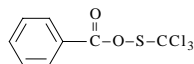
Examples:



**Ethanediperoxoic acid,
1,2-bis(trichloromethyl) ester**



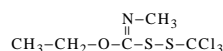
**Carbonoperoxoic acid,
OO',*OO'*-(1,1,4,4-tetramethyl-
1,4-butanediyl) *O'*,*O'*-bis(1-
methylethyl) ester**



**Benzenecarbo(thioperoxoic) acid,
OS-(trichloromethyl) ester**



**Ethanesulfeno(thioperoxoic) acid,
SO-methyl ester**



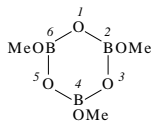
**Carbonyl(dithioperoxy)imidic acid,
N-methyl-,
O-ethyl *SS*-(trichloromethyl)
ester**

Esters of *boric acids* and their chalcogen analogs are indexed regularly, except for those of Hypoboric acid and cyclic metaboric acids, (HBO₂)_n, which are named as derivatives of the molecular skeletons.

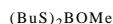
Examples:



**Diborane(4), 1,1-diethoxy-2,2-
dimethoxy-**



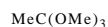
Boroxin, 2,4,6-trimethoxy-



**Thioboric acid ((HO)(HS)₂B),
S,S-dibutyl *O*-methyl ester**

Esters of *ortho acids* and their peroxy and chalcogen analogs are indexed like ethers, sulfides, peroxides, hydroperoxides, alcohols, etc. Ortho acid names are not used as heading parents.

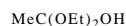
Examples:



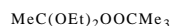
**Ethane, 1,1,1-trimethoxy- (not
Orthoacetic acid, trimethyl ester)**



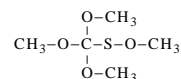
Benzene, [tris(methylthio)methyl]-



Ethanol, 1,1-diethoxy-



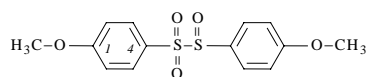
**Peroxide, 1,1-diethoxyethyl 1,1-
dimethylethyl**



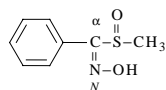
**Methanesulfenic acid, trimethoxy-,
methyl ester**

Oxides of thio esters are named not as ester derivatives but at the preferred molecular skeleton or other heading parent with sulfinyl or sulfonyl prefixes.

Examples:



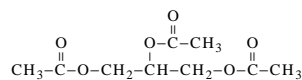
Benzene, 1-methoxy-4-[[[4-methoxyphenyl)sulfinyl]sulfonyl]-



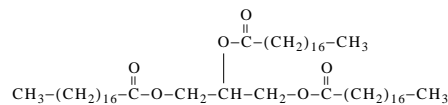
**Methanone, (methylsulfinyl)phenyl-,
oxime**

Glycerides, esters of **1,2,3-Propanetriol** (glycerol), are indexed at the name of the preferred acid unless only "Class I" acids are present.

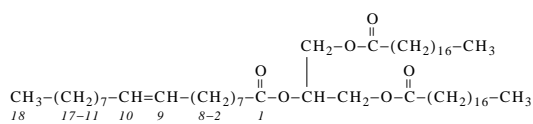
Examples:



**1,2,3-Propanetriol,
1,2,3-triacetate**



**Octadecanoic acid,
1,1',1''-(1,2,3-propanetriyl) ester**



**9-Octadecenoic acid,
2-[(1-oxooctadecyl)oxy]-1-
[[[(1-oxooctadecyl)oxy]methyl]-
ethyl ester (principle: unsaturated
acid preferred)**

Urethanes are esters of **Carbamic acid** and its derivatives. *Xanthic acids* are *O*-esters of **Carbonodithioic acid**.

Examples:



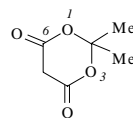
**Carbamic acid, *N*-phenyl-,
ethyl ester**



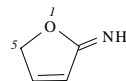
**Carbonodithioic acid,
O-phenyl ester**

Cyclic esters and lactones are indexed as heterocycles.

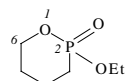
Examples:



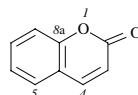
**1,3-Dioxane-4,6-dione, 2,2-di-
methyl-
(not Propanedioic acid, cyclic 1-
methylenehydride ester)**



**2(5*H*)-Furanimine (not 2-Buten-
imidic acid, 4-hydroxy-,
γ-lactone)**



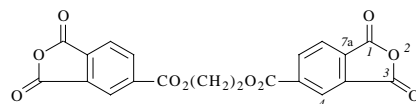
**1,2-Oxaphosphorinane, 2-ethoxy-,
2-oxide (not Phosphonic acid,
(4-hydroxybutyl)-, monoethyl ester,
δ-lactone)**



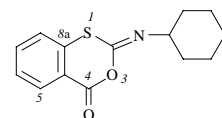
**2*H*-1-Benzopyran-2-one (not
Coumarin; not 2-Propenoic acid,
3-(2-hydroxyphenyl)-, δ-lactone)**

186. Ester-anhydrides are named by combining the policies for anhydrides and esters (§§ 179, 185). Cyclic anhydride and cyclic ester components are named in accordance with heterocyclic nomenclature. Anhydride terms precede ester terms where this can be done unambiguously (but see the last example, below). Esters cited in modifications are named in the uninverted form unless the acid is one for which a synonym line formula is required.

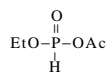
Examples:



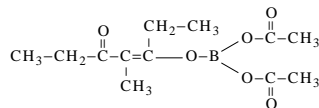
**5-Isobenzofurancarboxylic acid,
1,3-dihydro-1,3-dioxo-,
5,5'-(1,2-ethanediyl) ester**



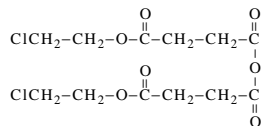
**4*H*-3,1-Benzoxathin-4-one,
2-(cyclohexylimino)- (not
Carbonimidithioic acid,
cyclohexyl-, anhydride with
2-mercaptobenzoic acid, cyclic
ester)**



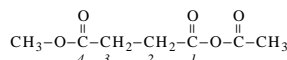
**Acetic acid,
anhydride with ethyl
hydrogen phosphonate**



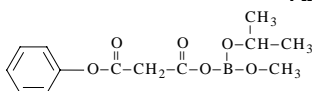
**Acetic acid,
anhydride with boric acid
(H₃BO₃) mono(1-ethyl-2-
methyl-3-oxo-1-penten-1-yl)
ester (2:1)**



**Butanedioic acid,
1,1'-anhydride, 4,4'-bis(2-
chloroethyl) ester**



**Butanedioic acid,
1-anhydride with acetic acid,
4-methyl ester**



**Propanedioic acid,
1-anhydride with boric acid
(H₃BO₃) monomethyl mono
(1-methylethyl) ester, 3-phenyl
ester**

187. Free radicals, highest in the order of precedence of compound classes (¶ 106) and functional groups, if present, are named as substituents. Most, but not all, free radical names coincide with the names of substituent prefixes (¶ 132, 133).

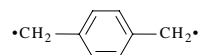
Examples:



Ethyl



Methyl, phenyl-



Methyl, 1,1'-(1,4-phenylene)bis-



Methylidyne, bromo-



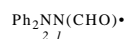
Ethyl, 2-ethoxy-1,2-dioxo- (not Acetyl, ethoxyoxo-)



Phosphino



Silylene, difluoro-



Hydrazinyl, 1-formyl-2,2-diphenyl-

Free radicals that might be considered as derived from **Borane** are indexed at **Borane(1)** and **Borane(2)**.

Examples:



Borane(2), fluoro- (not Boryl, fluoro-)



Borane(1), fluoro- (not Boron fluoride (BF))

Free radicals from ammonia, amides, or amines are named as **Amidogen**, H₂N•, **Imidogen**, HN•, and their derivatives.



Amidogen, difluoro- (not Nitrogen fluoride (NF₂))



Imidogen, (carboxyphenylmethyl)-

The heading parent **Nitroxide** is employed for the free radical H₂N-O•.

Example:



Nitroxide, dimethyl

Free radicals from hydroxyl and hydroperoxy groups that are attached to a molecular skeleton, including (acyloxy) radicals (see below), are indexed at “-oxy” and “-dioxy” heading parents with systematically named nondetachable prefixes. Chalcogen analogs are named similarly at “-thio” and “-dithio” heading parents.

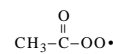
Examples:



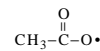
Methoxy (not Oxy, methyl-)



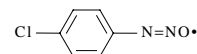
Methoxy, oxo- (not Formyloxy)



Ethyldioxy, 1-oxo-



Ethoxy, 1-oxo- (not Acetyloxy)



Diazenyloxy, 2-(4-chlorophenyl)-



Methylthio

Acyl free radicals (derived from aldehydes or acids) are named as α-oxo derivatives of the alkyl parents.

Examples:



Ethyl, 1-oxo- (not Acetyl)



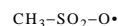
Methyl, cyclopropyloxy- (not Cyclopropylcarbonyl)



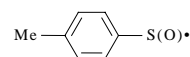
Methyl, aminooxo- (not Amino-carbonyl)

Free radicals from sulfonic and sulfinic acids are named as derivatives of alkyl and aryl sulfonyl and sulfinyl radicals and the analogous oxy radicals.

Examples:



(Methylsulfonyl)oxy



Phenylsulfinyl, 4-methyl-

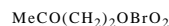
The following chalcogen hydride free radicals are employed: **Hydroxyl**, HO•; **Hydroperoxo**, HOO•; **Mercapto**, HS•; and **Selenyl**, HSe•.

188. Halogen and halogenoid compounds. (See also *Acid halides*, ¶ 170). The halogen and halogenoid “oxo” acids are hypohalous acids, HOX (e.g., **Hypochlorous acid**, HOCl); halous acids, HOXO; perhalic acids, HOXO₃; **Cyanic acid**, HOCN; and **Fulminic acid**, HONC. Their esters and anhydrides are named in the regular way. They rank below acids, e.g., carboxylic, sulfonic, expressed as suffixes on molecular skeleton names (¶ 106), and in their presence are expressed as cyanato, (iodyloxy), (chloryloxy), etc., radicals.

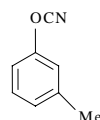
Examples:



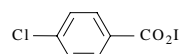
**Hypo-fluorous acid,
phenyl ester**



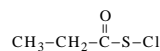
**Bromic acid,
3-oxobutyl ester**



**Cyanic acid,
3-methylphenyl ester**



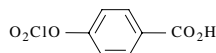
**Benzoic acid, 4-chloro-,
anhydride with hypoidous acid
(not Benzoyl hypoidite, 4-chloro-)**



**Propanethioic acid,
anhydrosulfide with thiohypo-
chlorous acid** (not Propanoyl thiohypochlorite)

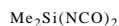


Acetic acid, 2-cyanato-

**Benzoic acid, 4-(chloroxy)-**

The groups $-X$, $-XO$, $-XO_2$, $-XO_3$, $-NC$, $-NCO$, $-N_3$, and their chalcogen analogs, e.g., $-XSe$; $-NCS$, are normally expressed as substituent prefixes when attached to a molecular skeleton; the radicals chloro, chlorosyl, chloryl, perchloryl, isocyano, isocyanato, isothiocyanato, azido, etc., are used (see the Illustrative List of Substituent Prefixes in Section H (¶ 294)).

Examples:

**Methane, trichloro-** (not Chloroform)**Benzene, iodyl-****Piperidine, 1-isocyano-****Silane, diisocyanatodimethyl-** (not Isocyanic acid, dimethylsilylene ester)

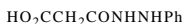
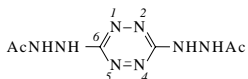
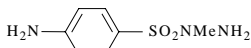
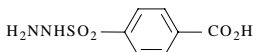
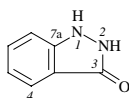
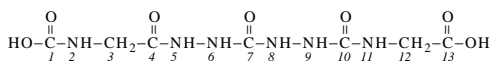
Groups such as $-I(OH)_2$, $-ClBr_2$, are not expressed by (dihydroxyiodo) and (dibromochloro) radicals; instead, coordination nomenclature (¶ 215) based on the central halogen atom is employed.

Example:

**Iodine, dihydroxyphenyl-**

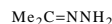
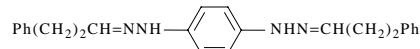
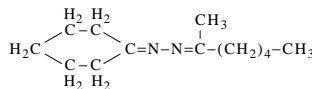
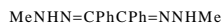
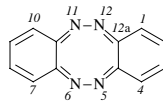
189. Hydrazides of principal acid groups are expressed by hydrazide terms in the index modification except for (a) sulfenic acid hydrazides, $R-S-NHNH_2$, which are indexed at **Hydrazine** with a "thio" substituent prefix; and (b) hydrazides of **Hydrazinecarboxylic acid**, for which the heading parent **Carbonic dihydrazide**, $(H_2NNH)_2CO$, (¶ 183) is employed. Hydrazides of subsidiary groups, e.g., of carboxyl substituents on aminium compounds, are indexed as substituents by use of hydrazino radicals. Cyclic hydrazides are indexed as heterocycles. Replacement ("a") names are used when the requirements (¶ 127) are satisfied.

Examples:

**Benzenecarbothioic acid, hydrazide****Acetic acid, 2-acetylhydrazide** (not Hydrazine, 1,2-diacetyl-)**Propanedioic acid, 1-(2-phenylhydrazide)** (not Propanoic acid, 3-oxo-3-(2-phenylhydrazino)-)**Acetic acid, 1,1'-[2,2']-(1,2,4,5-tetrazine-3,6-diyl)dihydrazide****Benzenesulfonic acid, 4-amino-, 1-methylhydrazide****Diazenecarboxylic acid, 2-(4-carboxyphenyl)-, 1-[2-(4-carboxyphenyl)hydrazide]** (principle: hetero acyclic parent preferred)**Benzoic acid, 4-(hydrazinylsulfonyl)-****3H-Indazol-3-one, 1,2-dihydro-** (not Benzoic acid, 2-hydrazino-, cyclic hydrazide)**2,5,6,8,9,11-Hexaazatridecanedioic acid, 4,7,10-trioxo-**

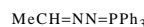
190. Hydrazones of ketone and aldehyde principal groups are expressed by hydrazone terms in the index modification, except for hydrazones of carbonyl groups of acids, acid halides, and amides; these are usually indexed as hydrazonic acids (¶ 169) and their halides and amides. Azines are indexed as "-ylidene" hydrazones; osazones as dihydrazones (of adjacent carbonyl groups); and cyclic hydrazones as heterocycles. In the presence of compound classes more preferred than the aldehyde or ketone bearing the hydrazone, a hydrazone substituent is cited.

Examples:

**2-Propanone, hydrazone****Benzenepropanal, 1,1'-[2,2']-(1,4-phenylene)dihydrazone****Cyclohexanone, 2-(1-methylhexylidene)hydrazone** (not 2-Heptanone, azine with cyclohexanone) (principle: ring preferred to chain)**Acetic acid, 2-[[2-(2-phenylhydrazinylidene)methyl]thio]-** (not Acetic acid, mercapto-, formate, phenylhydrazone)**1,2-Ethanedione, 1,2-diphenyl-, 1,2-bis(2-methylhydrazone)****Dibenzo[c,g][1,2,5,6]tetrazocine** (not 3,5-Cyclohexadiene-1,2-dione, bimol. cyclic azine)

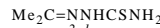
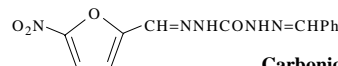
Phosphazines, which contain the fragment $=C=N-N=P$, are indexed as phosphoranylidene hydrazones.

Example:

**Acetaldehyde, 2-(triphenylphosphoranylidene)hydrazone**

Semicarbazones, **isosemicarbazones**, **carbohydrazones**, and **semioxamazones** of systematically named compounds are expressed, not by these modification terms or as substituted hydrazones, but by the general principles of substitutive nomenclature on the basis of the highest function present.

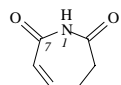
Examples:

**Hydrazinecarbothioamide, 2-(1-methylethylidene)-** (not 2-Propanone, thiosemicarbazone)**Hydrazinecarboximide, 2-(phenylmethylene)-, ethyl ester** (not Benzaldehyde, 3-ethylisosemicarbazone)**Carbonic dihydrazide, 2-[[5-nitro-2-furanyl)methylene]-2'-(phenylmethylene)-** (not 2-Furan-carboxaldehyde, 5-nitro, carbohydrazone with benzaldehyde)**Acetic acid, 2-amino-2-oxo-, 2-(phenylmethylene)hydrazide** (not Benzaldehyde, semioxamazone)

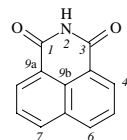
191. Imides are indexed as heterocycles with "-one" suffixes and are accordingly ranked as ketones; in the presence of higher ranking compounds, the

imide is expressed as a heterocyclic radical. The "diimide" of orthocarbonic acid, $\text{HN}=\text{C}=\text{NH}$ ("carbodiimide") is indexed at **Methanediiimide**, and its derivatives are often to be found at amine or amide headings.

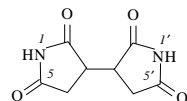
Examples:



1H-Azepine-2,7-dione, 3,4-dihydro-
(not 2-Hexenimide)



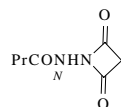
1H-Benz[de]isoquinoline-1,3-
(2H)-dione (not 1,8-Naphthalenedicarboximide)



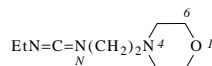
[3,3'-Bipyrrolidine]-2,2',5,5'-
tetrone (not 1,2,3,4-Butanetetracarboxylic 1,2:3,4-diimide)



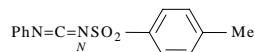
4H-1,3,2-Dithiazine, dihydro-,
1,1,3,3-tetraoxide (not 1,3-Propanedisulfonimide)



Butanamide, N-(2,4-dioxo-1-azetidiny)-



4-Morpholineethanamine, N-
(ethylcarbonimidoyl)-



Benzenesulfonamide, 4-methyl-
N-(phenylcarbonimidoyl)-

For sulfur imides, see ¶ 200; for **Phosphine imide**, see ¶ 197.

192. Molecular addition compounds of neutral components are generally indexed in the *Chemical Substance* and *Formula Indexes*. The preferred name appears at the formula of each component. (The formula headings used are those of the components.) Ratios are used in the name to express stoichiometry. Some common components are not indexed unless all other components are also "common" or cannot be related to compound classes described in the "Order of Precedence of Compound Classes" (¶ 106); however, unesterified acids in the following list are indexed when not components of salts with bases. These common components are:

Acetic acid
Acetic acid, 2,2,2-trifluoro-
Acetonitrile
Benzene
Benzene, methyl- *
Benzene, 1,3,5-trinitro-
1,3-Benzenediol, 2,4,6-trinitro-
Benzenesulfonic acid *
Benzenesulfonic acid, 4-methyl-
Benzoic acid
Borate(1-), tetrafluoro-, hydrogen (1:1)
Butanedioic acid, 2,3-dihydroxy- (all stereoisomers)
2-Butenedioic acid (of defined or undefined stereochemistry)
Carbamimidothioic acid, phenylmethyl ester *
Cyclohexanamine *
Cyclohexanamine, N-cyclohexyl-
Ethanamine, N,N-diethyl- *
Ethanedioic acid
Methane, dichloro- *
Methanesulfonic acid *
Phenol, 2,4,6-trinitro-
1,2,3-Propanetricarboxylic acid, 2-hydroxy-
3H-Pyrazol-3-one, 2,4-dihydro-5-methyl-4-nitro-2-(4-nitrophenyl)- *
Pyridine

* The preferred name is printed at the molecular formula for these compounds.

In addition, compounds with *water* and *ammonia* are not indexed at these names; they are expressed as "hydrate" and "ammoniate". Fractional hydrates and ammoniates, such as hemi- and sesquihydrate, are named by use of a ratio as hydrate (2:1) and hydrate (2:3), respectively. Other solvates are indexed as molecular addition compounds. Often the solvate component receives the only entry; e.g., **Ethanol, compd. with pyridine (1:1)**. Crystal forms of organic compounds containing solvents of crystallization are indexed only as the unsolvated species except when properties of the crystals themselves are being studied. "Hydrates" of carbonyl compounds are indexed as *gem*-diols; e.g., "acetaldehyde hydrate" is indexed as **1,1-Ethanediol**.

Ozonides of known structure are indexed by regular nomenclature; ozonides of unsaturated compounds are indexed at the compound headings with "ozonide" modification terms when the structures are unknown; "ozonides" of other compounds, e.g., phosphorus acid esters, are expressed as "compd. with ozone" and a ratio.

Bisulfite addition compounds are named as salts of specific hydroxy sulfonic acids when the structures are known or can reasonably be assumed, otherwise as a molecular addition compound of the carbonyl compound with a phrase such as "compd. with sodium hydrogen sulfite" and a ratio in the modification. (This is an exception; an "oxo" acid salt ranks higher than an aldehyde or ketone (¶ 106) and would normally receive the preferred index entry.)

Diels-Alder adducts (diene adducts) of unknown constitution are indexed like molecular addition compounds, except that the "compd. with" phrase is replaced by "adduct with."

Catena compounds (cyclic compounds with interlocking rings) are indexed at the components with a "catena compd. with" phrase and a ratio.

Rotaxane is the term given to a linear molecule threaded through a cyclic molecule. The cyclic molecule is usually large, and the linear molecule usually has bulky end groups that prevent unthreading. These are indexed at the component names with a "rotaxane compd. with" phrase and a ratio.

The "preferred" index name is the name given precedence in the CAS Registry System, and therefore the name which, after uninversion of the index heading if necessary, may be used among CA users in general discussions and reports. (To the index user in search of information, all the index names for an individual compound are of equal value.) For molecular addition compounds of stereoparents and their derivatives (¶ 203 I) with nonstereoparents, the preferred index entry appears at the former heading. In the absence of a stereoparent, the preferred index name is that which describes, in order of decreasing preference:

- a component other than a common component (see list above) selected according to the Order of Precedence of Compound Classes (¶ 106);
- a common component highest in the same order;
- a component which does not belong to any compound class described in the "Order of Precedence of Compound Classes," according to the earliest alphabetic position of the index name.

Examples ((a) is the preferred index name in each case):

- (a) **2,5-Cyclohexadiene-1,4-dione, 2,3,5,6-tetrachloro-, compd. with coronene (1:?)** (The question mark indicates an unknown ratio; a functional compound is preferred to cyclic hydrocarbon)
- (a) **Anthracene, compd. with 2,4,6-trinitrophenol (2:1)** (The cyclic hydrocarbon is preferred to a common compound of higher rank)
- (a) **Methane, 1,1'-sulfinylbis-, compd. with iodine (1:1)** (by "iodine," the molecular form I_2 is implied; atomic forms are indicated, when necessary, by phrases such as "compd. with at. chlorine (1:2)")

193. Nitrogen compounds. Cyclic nitrogen compounds, including lactams, sultams, and cyclic hydrazones, oximes, etc., are indexed at heterocyclic molecular skeletons (see *Section B*). Nitrogen-containing functional derivatives include imidic acids, amides, amines, imines, etc., for which the appropriate paragraph should be consulted. **Hydroxylamine** (see below) is a substitutive functional parent compound (¶ 130). Acyclic nitrogen skeletons, alone or with principal groups expressed as suffixes, are employed as heading parents for indexing purposes. Some groups, including azido, nitro, nitroso, and isocyanato, are always expressed as substituent prefixes (¶ 132). *aci*-Nitro, $\text{HON}(\text{O})=$, may be substituted; e.g., (propyl-*aci*-nitro) is $\text{CH}_3\text{CH}_2\text{CH}_2\text{ON}(\text{O})=$.

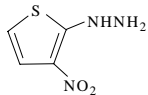
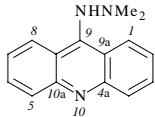
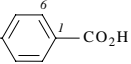
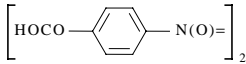
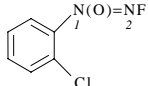
Diazene, $\text{HN}=\text{NH}$; **1-Triazene**, $\text{NH}=\text{N}-\text{NH}_2$; **Triazene**, $\text{NH}_2-\text{NH}-\text{NH}_2$, etc., are molecular skeleton heading parents to which the principal groups except hydroxy (and its chalcogen analogs), amino, and imino can be suffixed. **Hydrazine** is used as a trivial name for Diazene and its derivatives. Except for hydrazides (¶ 189) and hydrazones (¶ 190), alkyl and aryl are indexed at these nitrogen parents, which rank just below nitrogen heterocycles as the highest class of nonfunctional compounds (¶ 106). Within the class, seniority depends first on the number of hetero atoms, then on maximum unsaturation. When more preferred compound classes (including all those expressed by means of function suffixes) are present, the nitrogen skeletons are named as substituent prefixes, some of which have trivial names.

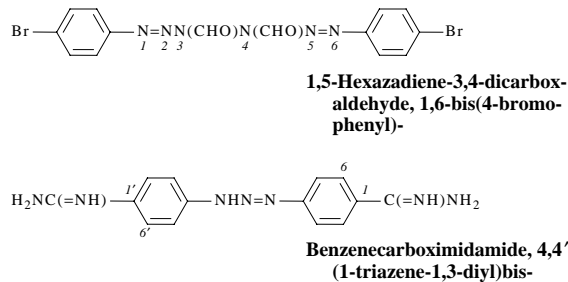
Examples (See also ¶ 161):

HN=N-	diazenyl
-N=N-	1,2-diazenediyl
-N=N(O)-	1-oxidodiazenyl
	2-oxidodiazenyl
H ₂ NNH-	hydrazinyl
H ₂ NN=	hydrazinylidene
-NHNH-	1,2-hydrazinediyl
-NHN=	1-hydrazinyl-2-ylidene
=NN=	1,2-hydrazinediylidene
H ₂ NNHNNH-	triazanyl
H ₂ NN=N-	1-triazen-1-yl
HN=NNH-	2-triazen-1-yl
-N=NNH-	1-triazene-1,3-diyl
H ₂ NNHNNHNNH-	tetrazanyl
=NNHNNH=	1,4-tetrazenediylidene

Hydrazides (¶ 189) and hydrazones (including azines) (¶ 190) are excluded from the following examples.

Examples:

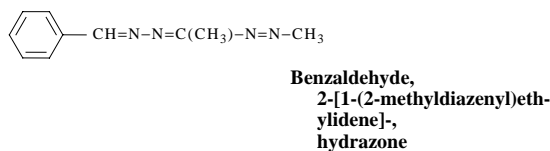
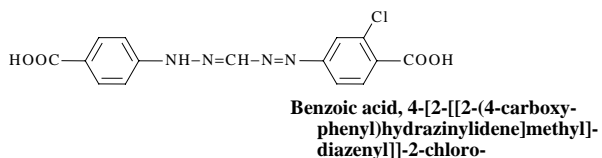
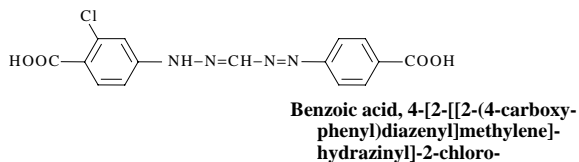
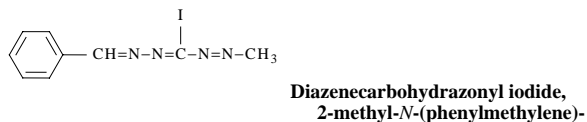
H ₂ NNHCO ₂ H _{2 1}	Hydrazinecarboxylic acid
HO ₂ CNHNHCO ₂ H _{1 2}	1,2-Hydrazinedicarboxylic acid
H ₂ NNHCONHMe _{2 1 N}	Hydrazinecarboxamide, N-methyl-
Et ₂ NNEt	Hydrazine, 1,1,2-triethyl-
H ₂ NNHOH	Hydrazine, hydroxy-
	Hydrazine, (3-nitro-2-thienyl)- (principle: preferred hetero atom in heading parent (¶ 138))
	Acridine, 9-(2,2-dimethylhydrazinyl)-
PhN=NSO ₃ H	Diazenesulfonic acid, 2-phenyl-
PhN=NCONH ₂ _{2 1 N}	Diazenecarboxamide, 2-phenyl-
PhN=N(O)- 	Benzoic acid, 4-(1-oxido-2-phenyldiazenyl)-
	Benzoic acid, 4,4'-(1,2-dioxido-1,2-diazenediyl)bis-
	Diazene, 1-(2-chlorophenyl)-2-fluoro-, 1-oxide
H ₂ NN=NAc	Acetic acid, 1-triazen-1-yl ester
MeSO ₂ NHNNHNC(=NH)Me _{3 2 1}	Ethanimine, 1-[3-(methylsulfonyl)triazanyl]-



Formazan is a trivial name that describes the tautomeric compound H₂N=N=CH-N=NH. Beginning with the Thirteenth Collective period, the use of formazan and its associated prefixes, formazano and formazanyl, has been discontinued and compounds containing the formazan residue are named systematically.

Examples:

H ₂ N=N=CH-N=NH	Diazenecarboxaldehyde, hydrazone (formerly Formazan)
H ₂ N=N=C(CH ₃)-N=N-CH ₃	Ethanone, 1-(2-methyldiazenyl)-, hydrazone
H ₂ N=N=C(CH ₂ OH)-N=N-CH ₃	Ethanone, 2-hydroxy-1-(2-methyldiazenyl)-, hydrazone



Hydroxylamine, H₂NOH; **Thiohydroxylamine**, H₂NSH, etc., are substitutive parent compounds; i.e., substituent prefixes but (usually) not substituent suffixes may be attached to them. *N*-Ylidene derivatives are oximes (¶ 195), imidic acid derivatives (¶ 165), etc.

In general, *N*-alkyl and *N*-aryl derivatives of **Hydroxylamine** are indexed as amines; *N*-acyl derivatives as amides; and *S*-amino derivatives of **Thiohydroxylamine** are indexed as sulfenamides. When the nitrogen atom is unsubstituted, *O*-derivatives are usually indexed at **Hydroxylamine**, etc.

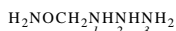
Examples:

H ₂ NOSO ₃ H	Sulfuric acid, monoazanyl ester
H ₂ NOAc	Acetic acid, azanyl ester
H ₂ NOCO ₂ H	Carbonic acid, monoazanyl ester
H ₂ NOCONH ₂	Carbamic acid, azanyl ester
BuONH ₂	Hydroxylamine, O-butyl-

**Hydroxylamine, *O,O'*-1,2-ethane-diybis-****Ethanesulfenamide****Benzenamine, *N*-hydroxy-****Acetamide, *N*-mercapto-****Carbamic acid, *N*-hydroxy-****Urea, *N*-hydroxy-****Benzenesulfonamide, *N*-hydroxy-**

Hydroxylamine and its chalcogen analogs rank lowest among the nonfunctional nitrogen parents. In the presence of more preferred compound classes, the radicals (aminoxy), (aminothio), (hydroxyamino), etc., are employed.

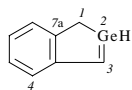
Examples:

**Acetic acid, 2-(hydroxyamino)-2-oxo-****Triazane, 1-[(aminoxy)methyl]-**

194. Organometallic compounds. Organic derivatives of germanium, tin, lead, antimony, and bismuth are indexed at hydride heading parents (see ¶ 181, 199).

Cyclic derivatives of these metals with standard substitutive valencies are indexed as heterocycles.

Example:

**1H-2-Benzogermole**

Acyclic metal derivatives, other than acetylides (¶ 219) and those indexed at metal hydride names, are indexed at the metal element name. Such names are ranked as neutral coordination compounds (¶ 215) and all functional compounds are expressed as substituent prefixes. When all metal atoms cannot be expressed by the heading parent, elements other than those of Groups IVA and VA are expressed as “-io” radicals, e.g., sodio, magnesio, aurio, lithio, when the metal replaces a single hydrogen. No hydrogen or other “substituent” is implied by these radical names, and atoms or groups attached to them must be expressed.

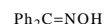
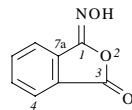
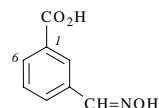
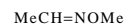
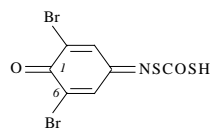
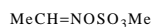
Examples:

**Lithium, phenyl-****Phosphonium, [3-(bromo-mercurio)-1-propen-1-yl]-trimethyl-, bromide (1:1)**

195. Oximes contain a bivalent hydroxylamine residue, =N-OH. When this residue has replaced oxygen in carboxylic acids, acid halides, and amides, the compounds are named as *N*-hydroxy derivatives of imidic acids (¶ 165), imidoaldehydes (¶ 170), and imidamides (¶ 171). Cyclic oximes are indexed at heterocyclic parents, e.g., **Isoxazole**.

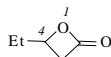
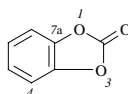
Acyclic oximes derived from aldehydes and ketones expressed as principal-group suffixes are expressed by “oxime” terms in the index modifications at the carbonyl-containing heading parents. When the carbonyl group is expressed as a substituent, it is replaced by the (hydroxyimino) radical, HO-N=. *O*-Alkyl, *O*-aryl, and *O*-acyl oximes are named as such in the modification or as an “-oxyimino” radical. Oximes derived from **Hydroxylamine-*O*-sulfonic acid** (¶ 193) are named as substituents of that heading parent.

Examples:

**Formaldehyde, oxime****Methanone, diphenyl-, oxime****1,3-Isobenzofurandione, monooxime****Benzoic acid, 3-[(hydroxyimino)-methyl]-****Acetaldehyde, *O*-methyloxime****2,5-Cyclohexadiene-1,4-dione, 2,6-dibromo-, 4-[S-(thiocarboxy)thiooxime]****Hydroxylamine-*O*-sulfonic acid, *N*-ethylidene-, methyl ester**

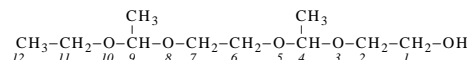
196. Oxygen compounds include a wide range of compound classes: acids, anhydrides, esters, alcohols, salts, metal oxides, etc. These are discussed in other sections and paragraphs. Cyclic oxygen compounds are indexed as heterocycles; these include cyclic esters, anhydrides, ethers, and oximes, as well as lactones, sulfones, etc.

Examples:

**Oxirane, 2,2-diethyl- (not Butane, 1,2-epoxy-2-ethyl-)****2-Oxetanone, 4-ethyl- (not Pentanoic acid, 3-hydroxy-, β-lactone; see ¶ 185)****1,3-Benzodioxol-2-one (not Carbonic acid, cyclic 1,2-phenylene ester; see ¶ 185)****7-Oxabicyclo[4.1.0]heptane (a Von Baeyer ring system; see ¶ 155)**

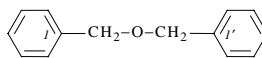
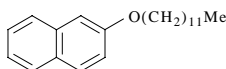
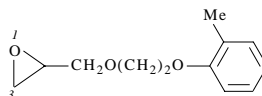
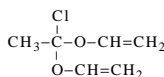
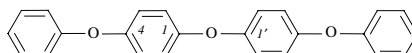
Acyclic ethers (including acetals and ortho esters) are indexed by replacement (“a”) nomenclature if the requirements (¶ 127) are satisfied.

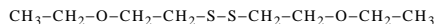
Example:

**3,5,8,10-Tetraoxadodecan-1-ol, 4,9-dimethyl- (not Acetaldehyde, 1,2-ethanediy ethyl 2-hydroxyethyl diacetal)**

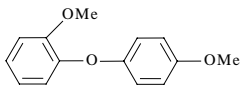
When “a” names are not permitted, acyclic ethers are indexed at heading parents (functional parent compounds, hydrocarbons, etc.) by use of “oxy” radicals, including the elided radicals (¶ 107) methoxy, ethoxy, propoxy, butoxy, and phenoxy.

Examples:

**Ethane, methoxy- (not Ether, ethyl methyl)****Ethane, 1,1'-oxybis- (not Ethyl ether)****Benzene, 1,1'-[oxybis(methylene)]bis-****Naphthalene, 2-(dodecyloxy)- (principle: ring preferred to chain (¶ 138))****Oxirane, 2-[[2-(2-methylphenoxy)-ethoxy]methyl]- (principle: preferred ring)****Ethene, 1,1'-[(1-chloroethylidene)-bis(oxy)]bis- (principle: unsaturation)****Benzene, 1,1'-oxybis[4-phenoxy]- (principles: centrality and multiplication)**



Disulfide, bis(2-ethoxyethyl) (an "a" name cannot be used; only three hetero units (¶ 127) are present)



Benzene, 1-methoxy-2-(4-methoxyphenoxy)- (principle: lowest locants for substituent prefixes)

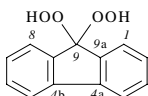
Hydroperoxides, ROOH, follow alcohols (including phenols) in order of precedence (¶ 106). They are indexed at the radicofunctional heading parent **Hydroperoxide**. No hyphen follows the substituent radical (¶ 108) unless the heading parent is being multiplied by a prefix such as "bis". In the presence of more preferred compound classes, or when the HOO- group is attached to a hetero atom other than silicon, a hydroperoxy radical is employed. The chalcogen analogs R-S-OH and R-S-SH are indexed as sulfenic acids and sulphenothioic acids, respectively (¶ 165). **Thiohydroperoxide** is the heading parent for R-O-SH compounds.

Hydrotrioxide, Hydrotetraoxide, etc., heading parents are treated in a similar manner, and hydrotrioxy and hydrotetraoxy radicals can be used as substituent prefixes.

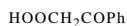
Examples:



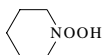
Hydroperoxide, ethyl (the uninverted name is Ethyl hydroperoxide)



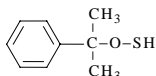
Hydroperoxide, 1,1'-(9H-fluoren-9-ylidene)bis-



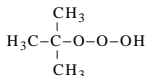
Ethanone, 2-hydroperoxy-1-phenyl-



Piperidine, 1-hydroperoxy-



Thiohydroperoxide, O-(1-methyl-1-phenylethyl)

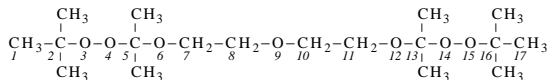


Hydrotrioxide, 1,1-dimethylethyl

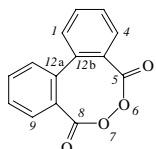
Acyl hydroperoxides are peroxy acids (¶ 165).

Peroxides, R-O-O-R' (R and R' = alkyl or acyl), are named at the radicofunctional heading parent **Peroxide** unless a replacement ("a") name (¶ 127) is appropriate. Cyclic peroxides are indexed as heterocycles and are ranked in accordance with the seniority of ring systems (¶ 138). Acyclic peroxides rank with the nonfunctional oxygen parents (¶ 106) and in the presence of a more preferred compound class are expressed by "dioxy" radicals. Acyl alkyl (and acyl silyl) peroxides are esters of peroxy acids. Symmetrical diacyl peroxides derived from "oxo" acids are named at acid, acid halide, etc., heading parents such as **Peroxydiphosphonic acid**. Dithio peroxides are indexed at **Disulfide** (¶ 200); R-S-O-R' compounds are named as esters of sulfenic acids (¶ 165). The corresponding diacyl compounds are indexed at **Thioperoxide**.

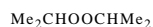
Examples:



3,4,6,9,12,14,15-Heptaaoxheptadecane, 2,2,5,5,13,13,16,16-octamethyl-



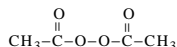
Dibenzo[d,f][1,2]dioxocin-5,8-dione



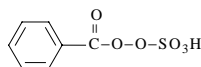
Peroxide, bis(1-methylethyl)



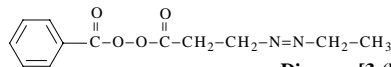
Peroxide, ethyl methyl (the uninverted name is Ethyl methyl peroxide)



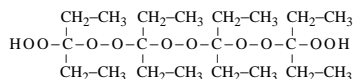
Peroxide, diacetyl



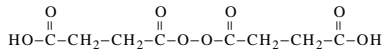
Peroxide, benzoyl sulfo



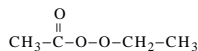
Diazene, [3-(benzoyldioxy)-3-oxopropyl]ethyl-



Hydroperoxide, 1,1'-[dioxybis(1-ethylpropylidene)dioxy(1-ethylpropylidene)]bis-



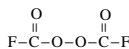
Butanoic acid, 4,4'-dioxybis[4-oxo-



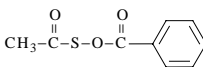
Ethaneperoxoic acid, ethyl ester



Peroxyhypofluorous acid, methyl ester



Peroxydicarbonic difluoride



Thioperoxide, S-acetyl O-benzoyl

The heading parents **Trioxide**, **Tetraoxide**, etc., are treated analogously and, in the presence of more preferred compound classes, radicals such as (methyltrioxy), $\text{CH}_3\text{-O-O-O-}$, are used.

Example:



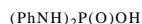
Trioxide, dimethyl

197. Phosphorus and arsenic compounds. The fundamental phosphorus and arsenic "oxo" acids are shown in Table VI. By use of replacement nomenclature (¶ 129) in which oxo and hydroxyl groups are replaced by other chalcogen atoms or nitrogen groups, a large number of acids, acid halides, amides, etc., can be named. **Phosphorous acid** is the heading parent when all three hydroxyl groups are involved in anhydride, ester, or salt formation; otherwise the tautomeric **Phosphonic acid** is the preferred heading parent. Similarly, **Phosphinic acid** is preferred over the tautomeric **Phosphonous acid**. **Metaphosphorous acid** is the name used for the unsubstituted acid and its ester and salts, but **Phosphenuous acid** is the fundamental name from which replacement analogs are derived. **Metaphosphoric** and **Phosphenic acids** stand in the same relationship, except that the special names **Metaphosphimic acid**, **Thiometaphosphimic acid**, etc., are used for $(\text{HO})\text{P}(\text{O})(=\text{NH})$ (or $(\text{HO})_2\text{P} \equiv \text{N}$) and its chalcogen analogs.

TABLE VI
FUNDAMENTAL MONONUCLEAR
PHOSPHORUS AND ARSENIC OXO ACIDS

"Trivalent" acids			
$(\text{HO})_3\text{P}$	Phosphorous acid	$(\text{HO})_3\text{As}$	Arsenous acid
$(\text{HO})_2\text{HP}$	Phosphonous acid	$(\text{HO})_2\text{HAs}$	Arsonous acid
$(\text{HO})\text{H}_2\text{P}$	Phosphinous acid	$(\text{HO})\text{H}_2\text{As}$	Arsinuous acid
HOPO	Phosphenuous acid Metaphosphorous acid (HPO₂)	HOAsO	Arsenenuous acid
"Pentavalent" acids			
$(\text{HO})_3\text{PO}$	Phosphoric acid	$(\text{HO})_3\text{AsO}$	Arsenic acid (H₃AsO₄)
$(\text{HO})_2\text{HPO}$	Phosphonic acid	$(\text{HO})_2\text{HAsO}$	Arsonic acid
$(\text{HO})\text{H}_2\text{PO}$	Phosphinic acid	$(\text{HO})\text{H}_2\text{AsO}$	Arsinic acid
HOPO_2	Phosphenic acid Metaphosphoric acid (HPO₃)	HOAsO_2	Arsenenic acid

Examples:



Phosphordiamidic acid, N,N'-di-phenyl-

$\text{Me}_2\text{NNHP(O)(OH)}_2$ _{2,1}	Phosphorohydrazidic acid, 2,2-dimethyl-
$\text{MeNHP(OH)(=NH)NHMe}$ _{N N' N''}	Phosphordiamidimidic acid, N,N'-dimethyl-
Ph_2AsOH	Arsinous acid, diphenyl-
EtNHAs(O)(OH)_2	Arsenamidic acid, N-ethyl-

Esters and anhydrides are indexed by the usual rules. **Phosphorous, Phosphoric, Phosphorothioic** and **Phosphorodithioic acids** are "Class I" acids; their esters with a single alcohol or thiol of "Class II" (¶ 185) are indexed at the alcohol name, but "mixed" esters are indexed at the phosphorus acid unless a more preferred compound class (e.g., carboxylic acid, aminium compound) is present. All cyclic esters are indexed as heterocycles.

Examples:

$(\text{EtO})_2\text{PO}(\text{CH}_2)_2\text{NH}_2$	Phosphorous acid, 2-aminoethyl diethyl ester
$[\text{Cl}(\text{CH}_2)_2\text{O}]_3\text{P}$	Ethanol, 2-chloro-, phosphite (3:1)
HP(O)(OH)OMe	Phosphonic acid, monomethyl ester
EtP(O)(OEt)SEt	Phosphonothioic acid, ethyl-, O,S-diethyl ester
$\begin{array}{c} \text{CH}_3 \quad \text{CH}_3 \\ \quad \\ \text{H}_3\text{C}-\text{As}-\text{S}-\text{As}=\text{S} \\ \\ \text{CH}_3 \end{array}$	Arsinodithioic acid, dimethyl-, anhydrosulfide with dimethyl-arsinothioic acid

Nonacidic mononuclear arsenic and phosphorus names are derived from the acid names in the usual way by expressing the highest function as a class term, e.g., "amide," "chloride," and the other replacement terms in alphabetical order within the main part of the name. The descending order of precedence for class terms is: hydrazide, halide (all considered equivalent, and cited in alphabetical order), azide, amide, cyanide, isocyanide, cyanate, thiocyanate (etc.), isocyanate, isothiocyanate (etc.), nitride, imide. Nonacidic analogs of phosphoric acid in which an oxo and hydroxyl group have been replaced by $\equiv\text{N}$, are named at **Phosphonitrile** headings.

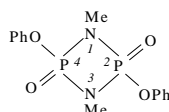
Examples:

$(\text{H}_2\text{N})_3\text{P}=\text{NH}$	Phosphorimidic triamide
$\text{Cl}_3\text{P}=\text{NH}$	Phosphorimidic trichloride
$(\text{H}_2\text{N})\text{Cl}_2\text{PS}$	Phosphoramidothioic dichloride
$(\text{H}_2\text{N})\text{BrClPO}$	Phosphoramidic bromide chloride
$(\text{OCN})\text{ClFPO}$	Phosphorisocyanatidic chloride fluoride
$(\text{H}_2\text{N})_2(\text{N}_3)\text{PO}$	Phosphordiamidic azide
$(\text{H}_2\text{N})_2(\text{NC})\text{PO}$	Phosphorocyanidic diamide
$(\text{H}_2\text{NNH})\text{F}_2\text{PO}$	Phosphorodifluoridic hydrazide
$(\text{H}_2\text{N})_3\text{P}$	Phosphorous triamide
Cl_3P	Phosphorous trichloride
ClF_2P	Phosphorous chloride difluoride
$(\text{NC})\text{H}_2\text{P}$	Phosphinous cyanide
$(\text{SCN})\text{H}_2\text{P}$	Phosphinous isothiocyanate
H_2NPS	Phosphenothious amide
$\text{ClP}=\text{NH}$	Phosphenimidous chloride
$(\text{H}_2\text{N})\text{ClHP}=\text{NH}$	Phosphenamidimidic chloride
$\text{Cl}_2\text{P}=\text{N}$	Phosphonitrile chloride (not Phosphoronitridic dichloride)
$(\text{H}_2\text{N})_3\text{AsO}$	Arsenic triamide
$(\text{H}_2\text{N})\text{ClHAs}=\text{NH}$	Arsenamidimidic chloride
$(\text{NCS})_2\text{HAsO}$	Arsenic dithiocyanate
$(\text{H}_2\text{N})\text{H}_2\text{As}=\text{NH}$	Arsinimidic amide
Cl_3As	Arsenous trichloride

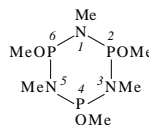
Cl_2HAs	Arsonous dichloride
$(\text{NC})\text{H}_2\text{As}$	Arsinous cyanide
$\text{ClAs}=\text{NH}$	Arsenenimidous chloride
BrAsO	Arsenenous bromide
Cl_3PO	Phosphoric trichloride
ClF_2PO	Phosphoric chloride difluoride
$(\text{OCN})_3\text{PO}$	Phosphoric triisocyanate
Cl_3PS	Phosphorothioic trichloride
$\text{OP}=\text{N}$	Phosphoric nitride

Esters and anhydrides of cyclic oligomers of metaphosphorus acids are indexed as heterocycles.

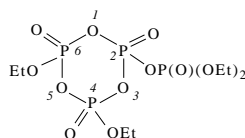
Examples:



1,3,2,4-Diazadiphosphetidine, 1,3-dimethyl-2,4-diphenoxy-, 2,4-dioxide



1,3,5,2,4,6-Triazatriphosphorine, 1,2,3,4,5,6-hexahydro-2,4,6-trimethoxy-1,3,5-trimethyl-



1,3,5,2,4,6-Trioxatriphosphorinane, 2-[(diethoxyphosphinyl)oxy]-4,6-diethoxy-, 2,4,6-trioxide

Phosphorus and arsenic molecular skeletons other than those named as acids and acid analogs are indexed as heterocycles or as acyclic hydride names: **Phosphine**, PH_3 ; **Arsine**, AsH_3 ; **Phosphorane**, PH_5 ; **Arsorane**, AsH_5 ; **Diphosphine**, $\text{H}_2\text{P}-\text{PH}_2$; **Triarsine**, $\text{H}_2\text{As}-\text{AsH}-\text{AsH}_2$; etc. Oxo, thio (etc.), and imino derivatives of **Phosphorane** and **Arsorane** are indexed at additive headings.

Examples:

H_3PO	Phosphine oxide
H_3AsSe	Arsine selenide
$\text{H}_3\text{P}=\text{NH}$	Phosphine imide
HPO_2	Phosphine oxide, oxo- (not Phosphorane, dioxo-)

Oxides, etc., of **Diphosphine**, **Diarsine**, **Triphosphine**, etc., are indexed by use of "oxide" and "sulfide" terms, with locants if necessary, in the modification. Acid derivatives of one of the phosphorus atoms are indexed at acid parents when names based on the phosphorus chains are impracticable.

Example:

PhPHP(O)H_2	Diphosphine, phenyl-, 2-oxide
$\text{Et}_3\text{P}(\text{Cl})\text{P(O)Cl}_2$	Phosphonic dichloride, P-(chlorotriethylphosphoranyl)-

Derivatives of **Phosphine** and other phosphorus and arsenic molecular skeleton parents are named substitutively by use of suffixes and prefixes.

Examples:

$(\text{HO})_2\text{P(O)CO}_2\text{H}$	Phosphinecarboxylic acid, 1,1-dihydroxy-, oxide
F_4PNHMe	Phosphoranamine, 1,1,1,1-tetrafluoro-N-methyl-
$\text{Me}_2\text{AsCO}_2\text{H}$	Arsinecarboxylic acid, 1,1-dimethyl-
$\text{EtAsMe}_2=\text{NH}$	Arsine imide, As-ethyl-As,As-di-methyl-

(EtO) ₅ P	Phosphorane, pentaethoxy-
Ph ₃ As(OAc) ₂	Arsorane, bis(acetyloxy)triphenyl-
HPO	Phosphine, oxo-
MeAsS	Arsine, methylthioxo-
MePPHMe	Diphosphine, 1,2-dimethyl-
(Me)(Ph)As–As(Ph)(Me)	Diarsine, 1,2-dimethyl-1,2-diphenyl-
MeAs=AsMe	Diarsene, 1,2-dimethyl-

Polyphosphorus acids (anhydrides of the mononuclear acids) and their replacement analogs do not follow the rules described for the mononuclear acids. They are given traditional inorganic names, and many cross-references will be found at mononuclear names (see also ¶ 219). (Polyarsenic acids are named analogously.)

Examples:

(HO) ₂ P(O)OP(O)(OH) ₂	Diphosphoric acid
(HO) ₂ P(O)P(O)(OH) ₂	Hypophosphoric acid
(HO)HP(O)OP(O)(OH) ₂	Isohypophosphoric acid
(HO) ₂ POP(O)(OH) ₂	Diphosphoric(III,V) acid
(HO) ₂ POP(OH) ₂	Diphosphorous acid
(HO) ₂ P(O)NHP(O)(OH) ₂	Imidodiphosphoric acid
(HO) ₂ P(O)OP(O)(OH)NHP(O)(OH)OP(O)(OH) ₂	P'-Imidotetraphosphoric acid
(H ₂ N) ₂ P(O)NHP(O)(OH) ₂	P,P-Diamidoimidodiphosphoric acid

Line formulas are used with thio, seleno, and telluro analogs of polyphosphorus acids to indicate the number and positions of sulfur (etc.) atoms. Thio, etc., prefixes are placed at the beginning of the name without multiplicative terms; e.g., **Thiodiphosphorous acid** ([(HO)₂P₁S₁]; **Thiodiphosphoric(III,V) acid** ([(HO)₂POP(S)(OH)₂]; **Thiooxydiphosphoric acid** ([(HO)₂P(S)₁S₂]; **Thioimidodiphosphoric acid** ([(HO)₂P(S)₁S₂NH₁].

When all acid groups have been replaced, the compounds are named as halides, amides, etc. The phosphoric halides and halogenoids are named by phosphoryl terms, the phosphoric amides by single-word heading parents. The phosphorous analogs of both classes are indexed at Phosphorous binary heading parents with a multiplicative prefix for the class term.

Examples:

Cl ₂ P(O)OP(O)Cl ₂	Diphosphoryl chloride (the phosphorous analog is named Diphosphorous tetrachloride)
(H ₂ N) ₂ POP(NH ₂) ₂	Diphosphorous tetraamide (the phosphoric analog is named Diphosphoramide)
$\begin{array}{c} \text{O} \quad \text{O} \quad \text{O} \\ \parallel \quad \parallel \quad \parallel \\ \text{H}_2\text{N}-\text{P}-\text{NH}-\text{P}-\text{NH}-\text{P}-\text{NH}_2 \\ \quad \quad \\ \text{NH}_3 \quad \text{NH}_3 \quad \text{NH}_3 \end{array}$	Diimidotriphosphoramide

In the order of precedence of compound classes (¶ 106), phosphorus and arsenic acids are functional heading parents, which fall below the acids expressed as principal functions (carboxylic, sulfonic, etc.) but above the highest nonacid group (acid halides). Phosphorus acids as a group rank just above arsenic acids. Within each group, seniority is dependent on (a) the greatest number of acid groups; (b) the greatest number of nuclear phosphorus or arsenic atoms; (c) the highest oxidation state (5+) of these atoms; (d) the most preferred atoms (Table I, ¶ 128) attached to the nuclear atoms; (e) the greatest number of such preferred atoms; (f) the nature of less preferred atoms. A partial list of acids in descending order of precedence is: **Triphosphoric, Diphosphoric, Imidodiphosphoric, Diphosphorous, Phosphoroperoxoic, Phosphoric, Phosphorothioic, Phosphorodithioic, Phosphorous, Phosphorochloridic, Phosphorohydrazidic, Phosphoramidic, Phosphonic, Phosphinic, Phosphinous acid**. (Chalcogen analogs of each acid immediately follow it in descending order of increasing replacement of oxygen by sulfur, selenium, and tellurium.) For the choice between tautomeric pairs such as **Phosphorous** and **Phosphonic acids**, also see above.

Nonacid analogs are ranked according to their class, e.g., halide, amide; then on the multiplicity of their class, e.g., a diamide is preferred over a monoamide; then on the remaining criteria set out above for the acids.

In the presence of more preferred compound classes, phosphorus and arsenic acids and hydrides are expressed by the following substituent radicals (*denotes a radical which requires bis, tris, etc., (and parentheses) instead of di, tri, etc., when more than one is present):

H ₂ P–	*phosphino	H ₂ As–	*arsino
H ₂ P(O)–	*phosphinyl	H ₂ As(O)–	*arsinyl
H ₂ P(S)–	phosphinothioyl	H ₂ As(S)–	arsinothioyl
H ₂ P(=NH)–	phosphinimyl	H ₂ As(=NH)–	arsinimyl
HP(≡N)–	phosphononitridyl	HAs(≡N)–	arsononitridyl
H ₄ P–	*phosphoranyl	H ₄ As–	*arsoranyl
HP=	phosphinidene	HAs=	arsinidene
HP(O)=	*phosphinylidene	HAs(S)=	arsinothioylidene
P(O)≡	*phosphinylidyne	As≡	arsinidyne

The above are substitutive; the following are not, and can be used only as simple radicals (¶ 132):

P(O)–	phosphoroso	As(O)–	arsenososo
P(O) ₂ –	phospho	As(O) ₂ –	arso
(HO) ₂ P(O)–	phosphono	(HO) ₂ As(O)–	arsono
–P(O)(OH)–	phosphinico (multiplying radical only)	–As(O)(OH)–	arsinico (multiplying radical only)

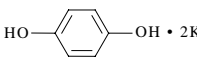
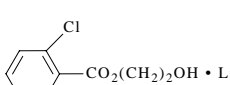
Radicals from polynuclear arsenic and phosphorus hydrides are formed like the carbon analogs.

Examples:

H ₂ PPH–	diphosphinyl
–PPH–	1,2-diphosphinediyl
=PP=	1,2-diphosphinediylidene
–P=P–	1,2-diphosphenediyl
–As=As–	1,2-diarsenediyl
–PH(PH) ₂ PH–	1,4-tetraphosphinediyl

198. Salts. *Metal salts* of acids and of other compounds having replaceable hydrogen on chalcogen atoms (whether expressed in the heading parent, in the substituents, or in a previous modification phrase) are indexed by use of salt terms in the modification. Ratios and Ewens-Bassett numbers are used, but locants are never cited. In the presence of hetero atom groups capable of forming chelate rings, salts of aluminum, beryllium, gallium, indium, magnesium, thallium, and the transition metals with acids (except polybasic hydroxy acids) are named by coordination nomenclature (¶ 215).

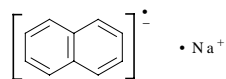
Examples:

AcOH • Na	Acetic acid, sodium salt (1:1)
	1,4-Benzenediol, potassium salt (1:2)
PhP(O)(OH)OEt • K	Phosphonic acid, P-phenyl-, monoethyl ester, potassium salt (1:1)
3 MeOH • Bi ³⁺	Methanol, bismuth(3+) salt (3:1)
	Benzoic acid, 2-chloro-, 2-hydroxyethyl ester, lithium salt (1:1)

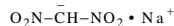
When a metal (except Sb³⁺, Bi³⁺, Ge⁴⁺, Sn⁴⁺, or Pb⁴⁺) has replaced hydrogen atoms attached to nitrogen, phosphorus, arsenic or antimony in molecular skeletons, they also are named as salts, e.g., **Piperidine, potassium salt (1:1); Acetamide, sodium salt (1:1); Phosphine, cyclohexyl-, lithium salt (1:1);** but unsubstituted **Hydrazine, Phosphine, and Arsine** afford the binary heading parents **Sodium hydrazide (NaN₂H₃); Lithium arsenide (LiH₂As); Aluminum phosphide;** etc.

Except for those cyclic derivatives of germanium, tin, lead, antimony, and bismuth which are treated as heterocycles (¶ 194), cyclic metal salts of two or more compounds, as well as mixed acyclic salts, are named by coordination nomenclature (¶ 215). Metal salts of radical anions and of certain delocalized structures, e.g., β -dicarbonyl compounds and nitro alkanes, are indexed by citing the ion term in the modification followed by the metal name and a ratio.

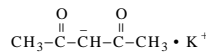
Examples:



Naphthalene, radical ion(1-), sodium (1:1)



Methane, dinitro-, ion(1-), sodium (1:1)



2,4-Pentanedione, ion(1-), potassium (1:1)

Uninverted names for metal salts of acids and esters depend on the structure and name of the acid or ester. The metal is cited first when there is a free acid group remaining in the parent that can take an "ate" or "ite" suffix. If there is no acid group available in the parent, e.g., all acid functions of the parent are esterified, the metal follows the acid name. When the acid is one that requires a line formula, the acid name is placed first.

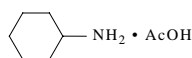
Examples:

sodium acetate (1:1)
potassium carbonate (1:1)
calcium ethyl phosphate (1:1)
zinc methyl sulfate (1:2)
1,4-diethyl 2-sulfobutanedioate sodium salt (1:1)
potassium 2-hydroxybenzoate (1:1)
calcium 4-aminobenzoate (1:2)
perboric acid (HBO(O₂)) sodium salt (1:1)

In uninverted names of alcohol or amine metal salts, the alcohol or amine is cited first, e.g., 2,6-dimethylphenol lanthanum(3+) salt (3:1) or 2-ethoxybenzamine sodium salt (1:1).

Amine, phosphine, etc., salts of acids, alcohols, thiols, etc., in general are indexed in the *Chemical Substance Index* at the preferred name. The preferred name is also cited at each of the component formulas in the Molecular Formula Index. Exceptions are salts of ammonia, indexed only as ammonium salts at the acid headings, and the "common components" of molecular addition compounds (¶ 192) together with the following common acids: hydriodic, hydrobromic, hydrochloric, hydrofluoric, nitric, nitrous, perchloric, phosphoric, phosphorous, sulfuric, and sulfurous. Entries are not made for these components except for salts that contain *only* "common components," in which case a single entry based on the rules for molecular addition compounds (¶ 192) is made. At the acid heading, a "compd. with" phrase appears in the modification.

Example:



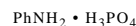
Acetic acid, compd. with cyclohexylamine (1:1)

At index headings for nitrogenous substances, and those containing trivalent phosphorus or arsenic, an "-ate", "-ite", or "-ide" term is normally cited in the modification, but when the acid has a synonym line formula, or is an acid ester indexed at a "Class II" alcohol name, a "compd. with..." phrase is used instead.

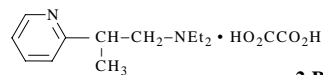
Examples:



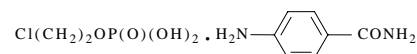
Arsine, dimethyl-, hydrochloride (1:1)



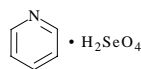
Benzenamine, phosphate (1:1)



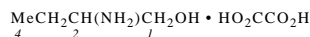
2-Pyridineethanamine, N,N-diethyl-beta-methyl-, ethanedioate (1:1)



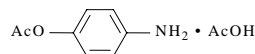
Benzenamide, 4-amino-, compd. with 2-chloroethyl dihydrogen phosphate (1:1)



Selenic acid, compd. with pyridine (1:1)



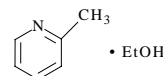
1-Butanol, 2-amino-, ethanedioate (1:1)



Phenol, 4-amino-, 1-acetate, acetate (1:1)

For salts of amines, etc., with alcohols and thiols, the phrase "compd. with" and a ratio are used.

Examples:



Ethanol, compd. with 2-methylpyridine (1:1)

Salts of aminium compounds and other substitutive cations are indexed by combining the "-ium" heading and the anion term, named according to the rules already described, (¶¶ 180, 184). The preferred name appears in the *Chemical Substance Index* and at each of the components in the *Formula Index* except for the following common anions:

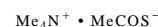
- halide and halogenide simple anions, e.g., bromide, cyanide, thiocyanate, azide;
- chalcogenide anions, e.g., hydroxide, sulfide;
- anions derived from acetic acid, benzenesulfonic acid, 4-methylbenzenesulfonic acid, 1,1,1-trifluoromethanesulfonic acid, methanesulfonic acid, carbonic acid, phosphoric acid, nitric acid, nitrous acid, sulfuric acid, sulfurous acid, and 2,4,6-trinitrophenol;
- methyl sulfate (MeOSO₃⁻), and ethyl sulfate (EtOSO₃⁻);
- tetrafluoroborate(1-) (BF₄⁻), tetraphenylborate(1-) (BPh₄⁻), and hexafluorophosphate(1-) (PF₆⁻).

Ternary salts of this kind are indexed by citing the terms in alphabetical order in the modification, cations first, then anions. In molecular addition compounds, the "-ium" salt is cited in uninverted form.

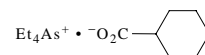
Examples:



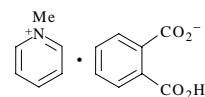
Methanaminium, N,N,N-trimethyl-, bromide (1:1)



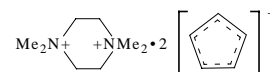
Methanaminium, N,N,N-trimethyl-, ethanethioate (1:1)



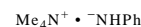
Arsonium, tetraethyl-, cyclohexanecarboxylate (1:1)



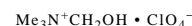
Pyridinium, 1-methyl-, 1,2-benzenedicarboxylate (1:1)



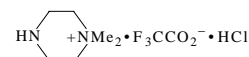
Piperazinium, 1,1,4,4-tetramethyl-, cyclopentadienide (1:2)



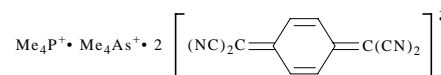
Methanaminium, N,N,N-trimethyl-, salt with benzenamine (1:1)



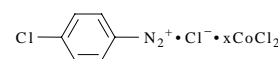
Methanaminium, 1-hydroxy-N,N,N-trimethyl-, perchlorate (1:1)



Piperazinium, 1,1-dimethyl-, 2,2,2-trifluoroacetate hydrochloride (1:1:1) (¶ 281A)



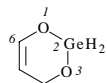
Phosphonium, tetramethyl-, tetramethylarsonium, salt with 2,2'-(2,5-cyclohexadiene-1,4-diylidene)bis[propanedinitrile] (1:1:2)



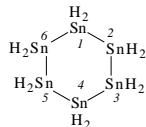
Benzenediazonium, 4-chloro-, chloride, compd. with cobalt chloride (CoCl₂) (1:1:?)

199. Silicon, germanium, tin, and lead compounds are indexed (a) as heterocyclic compounds, (b) as derivatives of acyclic hydride parents such as **Germane** or **Disilane**, (c) as special acyclic parents such as **Tristannathiane** or **Tetrasiloxane**, or (d) as silicic acids.

Heterocyclic compounds are indexed by the usual methods (¶¶ 146, 149).
Examples:



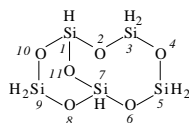
4H-1,3,2-Dioxagermin



Hexastannin, hexahydro-



Silacyclopentane



Bicyclo[5.3.1]pentasiloxane

Acyclic linear chains of tetravalent hydrides of silicon, germanium, tin, and lead are molecular skeletons with names derived from the mononuclear hydrides: **Silane**, **SiH₄**; **Germane**, **GeH₄**; **Stannane**, **SnH₄**; **Plumbane**, **PbH₄**.

Examples:

H ₃ SiSiH ₃	Disilane
H ₃ GeGeH ₂ GeH ₃	Trigermane
H ₃ Sn(SnH ₂) ₁₁ SnH ₃	Tridecastannane
H ₃ SiSiH ₂ SiH(SiH ₃)SiH ₂ SiH ₃	Pentasilane, 3-silyl-

When a single element of this series alternates with a single chalcogen in a linear acyclic chain, “-ane” names which express the nature of the alternating elements and number of silicon (etc.) atoms are employed.

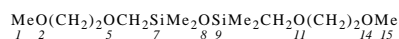
Examples:

(H ₃ Si) ₂ O	Disiloxane
(H ₃ Si) ₂ S	Disilathiane
(H ₃ Ge) ₂ Se	Digermaselenane
(H ₃ Sn) ₂ Te	Distannatellurane
(H ₃ SnO) ₂ SnH ₂	Tristannoxane
H ₃ Si(OSiH ₂) ₂ OSiH ₃	Tetrasiloxane

An acyclic chain of alternating silicon and nitrogen atoms is not named as a silazane; instead the functionality of the nitrogen is recognized. Thus, disilazane, H₃SiNHSiH₃, is indexed at **Silanamine**, *N*-silyl-. However, silazanyl radicals (see below) are employed in the presence of higher functions.

Replacement (“a”) names are used as parents when the chain contains carbon atoms and the other requirements (¶ 127) are met.

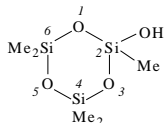
Example:



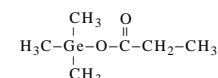
2,5,8,11,14-Pentaoxa-7,9-disilapentadecane, 7,7,9,9-tetramethyl-

Derivatives of all these parents are named by the usual substitutive methods except for silicic acids and germanium, tin, and lead hydroxides and salts (see below). A hydroxyl group on a germanium, tin, or lead atom is expressed as a hydroxy prefix, but by the suffix “-ol” on a silicon atom when it is a principal group. *O*-Acyl derivatives of silanols or of hydroxy germyl, stannyl, and plumbyl are named as esters.

Examples:

SiCl ₄	Silane, tetrachloro-
Me ₃ SiCN	Silane carbonitrile, trimethyl-
Me ₃ SnCN	Stannane carbonitrile, trimethyl-
Me ₃ SiOH	Silanol, 1,1,1-trimethyl-
Et ₃ SiOSiEt ₂ OH	1-Disiloxanol, 1,1,3,3,3-pentaethyl-
H ₃ GeNH ₂	Germanamine
(HOSiMe ₂) ₂ CH ₂	Silanol, 1,1'-methylenebis[1,1-dimethyl-]
	2-Cyclotrisiloxanol, 2,4,4,6,6-pentamethyl-

ClSnMe ₂ O ₂ SnMe ₂ Cl	Distannoxane, 1,3-dichloro-1,1,3,3-tetramethyl-
PhPb(O)OPb(O)Ph	Diplumbane, 1,3-dioxo-1,3-diphenyl-
(Me ₃ Si) ₂ Se	Disilaselene, 1,1,1,3,3,3-hexamethyl-
Me ₂ PbO	Plumbane, dimethoxy-
F ₃ SiSiH ₃	Disilane, 1,1,1-trifluoro-
Et ₃ PbPbEt ₃	Diplumbane, 1,1,1,2,2,2-hexaethyl-
PhPb(O)OH	Plumbane, hydroxyoxophenyl-
HOGeH ₂ OGeH ₂ OH	Digermoxane, 1,3-dihydroxy-
(MeO) ₃ SiMe	Silane, trimethoxymethyl-
Me ₃ SiOAc	Silanol, 1,1,1-trimethyl-, 1-acetate

**Propanoic acid, trimethylgermyl ester**

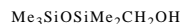
Substituent prefixes (radicals) from silicon, germanium, tin, and lead mononuclear hydrides are formed by adding the suffixes “-yl,” “-ylene,” and “-ylidene” to the appropriate stem, or “-tetrayl” to the hydride name: silyl, H₃Si-; germylene, H₂Ge=; stannylidene, HSn≡; plumbanetetrayl, =Pb=. Radicals from polynuclear hydrides and “oxanes,” etc., are derived as for hydrocarbons.

Examples:

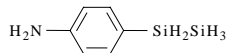
H ₃ SiSiH ₂ -	disilanyl
-GeH ₂ GeH ₂ -	1,2-digermanediyl (formerly digermanylene)
H ₃ SnSnH ₂ SnH=	tristannanylidene
≡SnSn≡	1,2-distannanediylidene
H ₃ SiOSiH ₂ -	1-disiloxanyl
H ₃ SiNHSiH ₂ -	1-disilazanyl
-PbH ₂ OPbH ₂ -	1,3-diplumbanediyl
-SiH ₂ OSiHOSiH ₂ -	1,3,5-trisiloxanetriyl

The nonfunctional germanium, tin, and lead hydrides fall (in that order) between boron and oxygen heading parents in order of precedence of compound classes (¶ 106). The heading parent Silane is an exception. It now ranks below cyclic carbon parents and above acyclic carbon parents. This ranking does not apply to any other silicon parents, cyclic or acyclic, functional or nonfunctional. When a principal group is expressed as a suffix, the compound is classed accordingly. **Silanol** is ranked with the alcohols, and is placed above all carbon-chain monohydric alcohols, cyclic or acyclic (¶ 138).

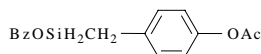
Examples:



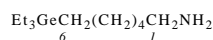
Methanol, 1-(1,1,3,3,3-pentamethyl-disiloxanyl)- (not 3-Oxa-2,4-disilapentan-1-ol, 2,2,4,4-tetramethyl-)



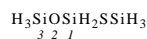
Benzenamine, 4-disilanyl-



Silanol, 1-[[4-(acetyloxy)phenyl]-methyl]-, 1-benzoate (not Phenol, 4-[[benzoyloxy)silyl]methyl]-, acetate)



1-Hexanamine, 6-(triethylgermyl)-



Disiloxane, 1-(silylthio)-

Silicic acids are silanes and siloxanes (and chalcogen analogs) in which all hydrogen atoms have been replaced by hydroxyl and oxo groups (or their chalcogen analogs). Their esters and anhydrides are named as usual. Cyclic derivatives are named as heterocycles.

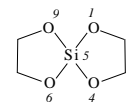
Examples:



Silicic acid (H_4SiO_4), tetraethyl ester



Thiosilicic acid ($\text{H}_4\text{SiO}_3\text{S}$), *O,O,O*-tris(1-methylethyl) ester



1,4,6,9-Tetraoxa-5-silaspiro[4.4]nonane (not 1,2-Ethanediol, cyclic diester with silicic acid (H_4SiO_4))

Germanium, tin, and lead analogs of silicic acids are named at binary hydroxide and hydroxide oxide heading parents. Symmetrical derivatives of **Germane**, **Stannane**, and **Plumbane**, in which all hydrogen atoms have been replaced by groups derived from alcohols, thiols, etc., or acids, are named as metal salts.

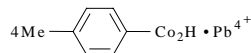
Examples:



Germanium hydroxide ($\text{Ge}(\text{OH})_4$)



Tin hydroxide oxide ($\text{Sn}(\text{OH})_2\text{O}$)

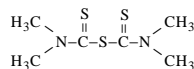


Benzoic acid, 4-methyl-, lead(4+) salt (4:1)

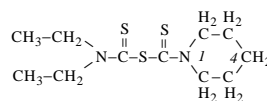
200. Sulfur, selenium, and tellurium compounds are often named similarly to oxygen compounds, but sometimes, e.g., in sulfonic and selenic acids (¶ 165), the sulfur, etc., acts as a nuclear atom in a functional group of which no oxygen analog is known. Because sulfur, selenium, and tellurium are treated identically, "thio," "sulfur," "sulfide," etc., in the following discussion may invariably be replaced by the corresponding selenium or tellurium term.

Cyclic sulfur compounds are named as heterocycles; sulfur alternating with silicon, germanium, tin, or lead atoms forms the silathianes, etc. (¶ 199). Sulfur analogs of anhydrides are usually named as anhydrosulfides, but the anhydrosulfides of acids named as functional parent compounds are often indexed at polynuclear acid headings, e.g., **Thiodicarbonyl acid**.

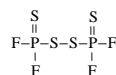
Examples:



Thiodicarbonyl diamide, ($(\text{H}_2\text{NC}(\text{S}))_2\text{S}$), *N,N,N',N'*-tetramethyl-



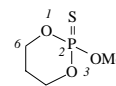
1-Piperidinecarbodithioic acid, anhydrosulfide with *N,N*-diethylcarbomodithioic acid



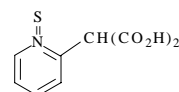
Thioperoxydiphosphoric tetrafluoride, ($(\text{F}_2\text{P}(\text{S})_2\text{S}_2)$)

The additive term "sulfide" is used in modifications when sulfur is attached to saturated Group VA elements in molecular skeletons. The locant relating to the parent is used when the parent contains the heteroelement sulfide; otherwise, an element symbol provides the locant.

Examples:



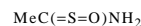
1,3,2-Dioxaphosphorinane, 2-methoxy-, 2-sulfide



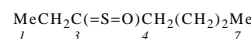
Propanedioic acid, (1-sulfido-2-pyridinyl)-

Oxides of doubly-bound sulfur atoms in principal groups are named in the modification with an "S" locant.

Examples:



Ethanethioamide, S-oxide

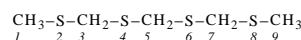


3-Heptanethione, S-oxide

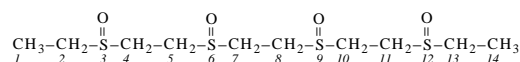
Phosphine sulfide, Arsine sulfide, and Stibine sulfide (¶¶ 181, 197) are substitutive parent compounds, but the sulfides of **Diphosphine**, **Triarsine**, etc., are named by modification terms.

Acyclic sulfides, sulfoxides, and sulfones, containing one or more isolated sulfur atoms, including thio acetals and thio ortho esters, are named (like ethers (¶ 196)) as substituents of hydrocarbons and other heading parents by use of thio radicals, unless a replacement ("a") name (¶ 127) is permissible. In the latter, oxide terms in the modification are employed to express sulfinyl ($-\text{S}(\text{O})-$) and sulfonyl ($-\text{S}(\text{O})_2-$) groups. The analogs of "thio" are "seleno" and "telluro"; those of "sulfinyl" are "seleninyl" and "tellurinyl"; those of "sulfonyl" are "selenonyl" and "telluronyl."

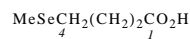
Examples:



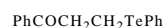
2,4,6,8-Tetrathianonane



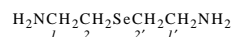
3,6,9,12-Tetrathiatetradecane, 3,6,9,12-tetraoxide



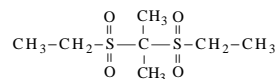
Butanoic acid, 4-(methylseleno)-



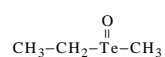
1-Propanone, 1-phenyl-3-(phenyltelluro)-



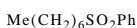
Ethanamine, 2,2'-selenobis-



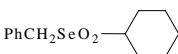
Propane, 2,2-bis(ethylsulfonyl)- (principle: largest heading parent (¶ 138))



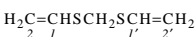
Ethane, (methyltellurinyl)- (principle: largest heading parent)



Benzene, (heptylsulfonyl)- (principle: ring preferred over chain)



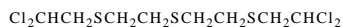
Benzene, [(cyclohexylselenonyl)methyl]- (principle: preferred ring system)



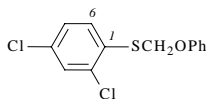
Ethene, 1,1'-[methylenebis(thio)]bis- (principles: largest heading parent and multiplication)



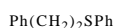
Ethene, [(1-ethoxyethyl)thio]- (principle: maximum number of unsaturated bonds)



Ethane, 1,1'-thiobis[2-[(2,2-dichloroethyl)thio]- (principles: centrality and multiplication)



Benzene, 2,4-dichloro-1-[(phenoxymethyl)thio]- (principle: maximum number of substituent prefixes)



Benzene, [(2-phenylethyl)thio]- (not Benzene, [2-(phenylthio)ethyl]-) (principle: earliest index position)

Hydrodisulfides are named as dithioperoxy acids, as sulfenothioic acids, or as thio analogs of mononuclear peroxy "oxo" acids. The oxides R-S(O)-SH and $\text{R-S(O)}_2\text{-SH}$ are named as sulfinothioic and sulfonothioic acids.

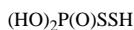
Examples:



Benzenecarbo(dithioperoxy) acid



Ethanesulfenothioic acid



Phosphoro(dithioperoxy) acid



Thioperoxymonosulfuric acid ((HO)(HSS)SO₂)

The compounds R-S-S-SH , R-S(O)-S-SH , $\text{R-S(O)}_2\text{-S-SH}$, are named as sulfeno(dithioperoxy) acids and their sulfino and sulfono analogs.

Example:



Benzenesulfeno(dithioperoxy) acid

Hydrotrisulfide is a radicofunctional heading parent for acyl derivatives, and **Hydrotetrasulfide**, etc., for alkyl and aryl derivatives.

Example:



Hydrotrisulfide, ethyl

Acyl substituted polysulfides are named as Ketones



Ethanone, 1-trithio-

Cyclic polysulfides are named as heterocycles; acyclic sulfides fulfilling the requirements (¶ 127) of replacement nomenclature are indexed at "thia" names. Other acyclic disulfides, trisulfides, etc., are indexed at **Disulfide** and similar heading parents unless they are esters of dithioperoxy acids or chalcogen analogs of peroxy condensed mononuclear acids. (Examples of these exceptions are illustrated below.) Hydrogen polysulfides in which both of the terminal hydrogen atoms have been replaced by sulfo groups constitute the polythionic acids; thus, **Tetrathionic acid** is $\text{HO}_3\text{S-S-S-SO}_3\text{H}$.

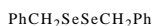
Examples:



6,9-Dioxa-3,7,8,12-tetrathiatetradecane



Disulfide, bis(1-methylethyl)



Diselenide, bis(phenylmethyl)



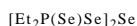
Disulfide, 1,1'-(1,2-ethanediy)bis[2-ethyl



Trisulfide, diphenyl



Ethanone, 1,1'-dithiobis-



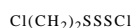
Triselenide, bis(diethylphosphinoselenoyl)



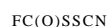
Disulfide, diethoxy



Ethanone, 1-(chlorodithio)-



Trisulfide, chloro 2-chloroethyl



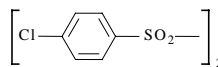
Disulfide, cyano fluorocarbonyl (not Formyl fluoride, (cyanodithio)-)

The heading parents **Disulfoxide**, **Trisulfone**, etc., are employed for chalcogen compounds in which the same number of oxygen atoms is attached to each skeletal atom. When all oxide atoms are on one sulfur, the compounds are named whenever possible as esters or anhydrides of thio analogs of sulfur acids. When different numbers of oxide atoms are attached to skeletal sulfur atoms, substitutive nomenclature is employed in which thio, sulfinyl, and sulfonyl radicals are cited separately.

Examples:



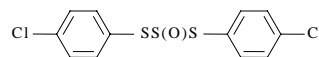
Disulfoxide, dimethyl



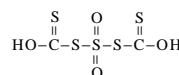
Disulfone, bis(4-chlorophenyl)



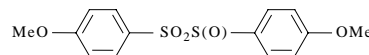
Benzenesulfonylthioic acid, S-phenyl ester



Thiosulfurous acid, (H₂S₃O), S,S-bis(4-chlorophenyl) ester



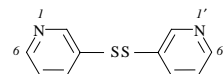
Carbonodithioic acid, bis(anhydrosulfide) with thiosulfuric acid (H₂S₃O₂)



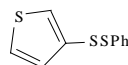
Benzene, 1-methoxy-4-[[4-methoxyphenyl)sulfinyl)sulfonyl]- (not Benzene, 1-methoxy-4-[[4-methoxyphenyl)sulfonyl)sulfinyl]-) (principle: earliest index position)

Cyclic sulfides, etc., are ranked according to the rules for ring systems; acyclic sulfur, selenium, and tellurium heading parents follow, in that order, the oxygen heading parents (**Peroxide**, etc.). Within each element group, the descending order is illustrated as follows: **Trisulfide**, **Disulfone**, **Disulfoxide**, **Disulfide**. In the presence of more preferred compound classes, dithio, trithio, diseleno, disulfonyl, etc., radicals are used as substituents.

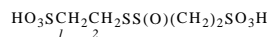
Examples:



Pyridine, 3,3'-dithiobis-



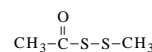
Thiophene, 3-(phenyldithio)- (principle: preferred ring system)



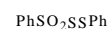
Ethanesulfonic acid, 2-[[2-sulfoethyl)sulfinyl]thio]- (not Ethanesulfonic acid, 2-[[2-sulfoethyl]thio]sulfinyl]-) (principle: earliest index position)

Acyl alkyl and acyl aryl disulfides are named as esters of either dithioperoxy acids or peroxy mononuclear "oxo" acids.

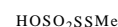
Examples:



Ethane(dithioperoxy) acid, methyl ester



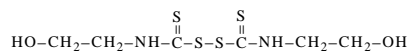
Benzenesulfonylthio(dithioperoxy) acid, phenyl ester



Thioperoxymonosulfuric acid, ((HO)(HSS)SO₂), SS-methyl ester

Symmetrical diacyl disulfides derived from polybasic mononuclear "oxo" acids (except **Sulfuric acid** and **Sulfurous acid**; see above) are named at Thioperoxy headings.

Example:



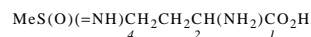
**Thioperoxydicarbonic diamide,
((H₂N)C(S)₂)₂, *N,N'*-bis(2-
hydroxyethyl)-**

Sulfilimine, H₂S=NH, and **Sulfoximine**, H₂S(O)=NH, are substitutive heading parents. The selenium and tellurium analogs are named **Selenilimine**, **Tellurilimine**, **Selenoximine** and **Telluroximine**. They are ranked just below imine suffix compounds (¶ 106). Higher functions in chalcogen-linked derivatives can be recognized by use of other chalcogen-nitrogen parents or by sulfonimidoyl, sulfonimidoyl, etc., radicals.

Examples:

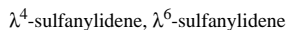


Sulfilimine, *S,S*-diethyl-

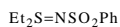


**Butanoic acid, 2-amino-4-(*S*-
methylsulfonimidoyl)-**

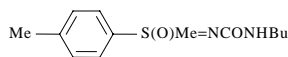
N-derivatives containing higher chemical functions are named at these functions by using the following newly introduced radical names:



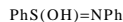
and their selenium and tellurium analogs



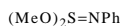
**Benzenesulfonamide, *N*-(diethyl-
 λ^4 -sulfanylidene)-**



Urea, *N*-butyl-*N'*-[methyl(4-methylphenyl)oxide- λ^4 -sulfanylidene]-



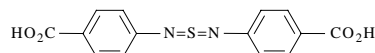
**Benzenesulfonimidic acid,
N-phenyl-**



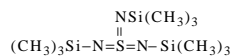
**Imidosulfurous acid, *N*-phenyl-
dimethyl ester**

Sulfur diimide, HN=S=NH, and **Sulfur triimide**, HN=S(=NH)=NH, are substitutive heading parents and are ranked with the sulfur parents. The above mentioned radical names are used when higher functions are present.

Examples:



Benzoic acid, 4,4'-(λ^4 -sulfanylidene)dinitrilo)bis-



**Silanamine, *N,N',N''*- λ^6 -sulfane-
trilylidenetris[1,1,1-trimethyl-**

Sulfimide, O₂S=NH, and **Thionyl imide**, OS=NH, are substitutive heading parents. They follow the imines in order of precedence (¶ 106) and, when necessary, are expressed by sulfonyl (O₂S=) (sulfinylamino) (OS=N-), etc., radicals.

Examples:



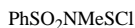
Methanamine, *N*-sulfonyl-



Benzenesulfonamide, *N*-sulfinyl-

Amidosulfonyl chloride (H₂N-S-Cl) is ranked with mononuclear "oxo" acid halides and can be expressed by (chlorothio) and [(chlorothio)amino] radicals when necessary.

Example:



**Amidosulfonyl chloride, *N*-methyl-
N-(phenylsulfonyl)- (not Benzene-
sulfonamide, *N*-(chlorothio)-*N*-
methyl-)**

Mixed sulfide-selenides, etc., with three contiguous chalcogen atoms are usually named by compound and complex radicals; e.g., [selenobis(thio)] for -S-Se-S-. When only two different contiguous chalcogen atoms are present, the compound is an ester of a sulenic (etc.) acid analog.

Example:



**Benzenesulfoselenoic acid,
phenyl ester**

Acyclic tetravalent and hexavalent sulfur compounds containing at least one substituent derived from a molecular skeleton (¶ 130) that cannot be named by general index nomenclature as described above, or as "oxo" acid derivatives, are given coordination names (¶ 215).

Examples:

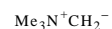


**Sulfur, pentafluorophenyl-,
(*OC*-6-21)-**

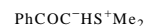


**Tellurium, dichlorodiphenyl-,
(*T*-4)-**

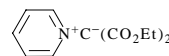
201. Zwitterionic compounds have internally compensating ionic centers. When the cationic center is known, the compound is named either as an "inner salt".



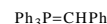
**Methanaminium, *N,N,N*-trimethyl-,
inner salt**



**Sulfonium, dimethyl(2-oxo-2-phenylethyl)-,
inner salt**



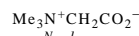
**Pyridinium, 1-[2-ethoxy-1-(ethoxycarbonyl)-
2-oxoethyl]-,
inner salt**



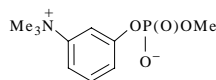
**Phosphorane, triphenyl(phenylmethylene)-
(preferred index name)**

Zwitterionic compounds are usually named at the "ium" heading with "inner salt" as the phrase in the modification. "Inner salt" (¶ 293A) indicates a compensating anion located in the same molecule as the cation. The expression "bis(inner salt)" at a "dium" heading indicates two compensating anions in the same molecule. A phosphonium compound of this type is indexed as a phosphonium inner salt only when such a zwitterionic structure is emphasized or discussed by the author. Otherwise only a neutral **Phosphorane** entry is made.

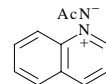
Examples:



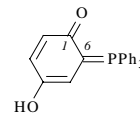
**Methanaminium, 1-carboxy-*N,N,N*-
trimethyl-,
inner salt**



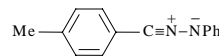
**Benzenaminium, 3-[(hydroxy-
methoxyphosphinyl)oxy]-*N,N,N*-
trimethyl-,
inner salt**



**Quinolinium, 1-(acetylamino)-,
inner salt**



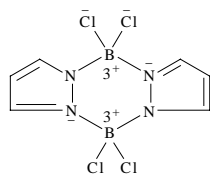
**2,4-Cyclohexadien-1-one, 4-
hydroxy-6-(triphenylphospho-
ranylidene)- (the alternative ionic
structure is named **Phosphonium**,
2,5-dihydroxyphenyl)tri-
phenyl-, inner salt)**



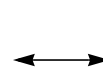
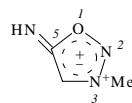
**Hydrazinium, 1-[(4-methyl-
phenyl)methylidene]-2-phenyl-,
inner salt**

Cationic "ium" compounds with internally compensating borate anions are named where possible by coordination nomenclature (¶ 215); the term "borata" is avoided.

Example:



Boron, tetrachlorobis[μ -(1*H*-pyrazolato- κ N¹: κ N²)]di- (not 4*H*,4*H*,8*H*,8*H*-7*a*,8*a*-Diazia-3*a*,4*a*-diazonia-4,8-diborata-*s*-indacene, 4,4,8,8-tetrachloro-)

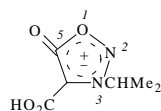


1,2,3-Oxadiazolium, 5-amino-3-methyl-, inner salt (formerly Sydnone imine, 3-methyl-)

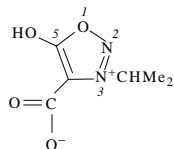
Meso-ionic compounds such as sydnone derivatives are named, if possible, at an “-ium” parent by use of the term “inner salt” in the modification.

Examples:

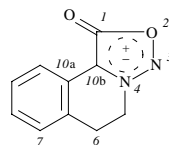
mesoionic form



preferred structure



1,2,3-Oxadiazolium, 4-carboxy-5-hydroxy-3-(1-methylethyl)-, inner salt (formerly Sydnone, 4-carboxy-3-(1-methylethyl)-)



[1,2,3]Oxadiazolo[4,3-*a*]isoquinolin-4-ium, 5,6-dihydro-1-hydroxy-, inner salt

E. STEREOCHEMISTRY AND STEREOPARENTS

Introduction	¶ 202
Stereochemistry	203
Alkaloids	204
Amino acids	205
Peptides	206
Proteins	207

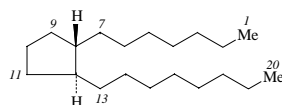
Carbohydrates	¶ 208
Cyclitols	209
Nucleosides and Nucleotides	210
Steroids	211
Terpenes	212

202. Introduction. A discussion of stereochemical descriptors for systematically named compounds, modified stereoparents, and coordination compounds follows this introduction. The remainder of Section E is directed to various classes of stereoparents. A stereoparent is an index heading parent the name of which implies specific stereochemical information. Illustrative structural diagrams for stereoparents that have received entries in current indexing are provided in the *Chemical Substance Index*; these diagrams indicate both the stereochemistry and the numbering systems from which locants are derived. The bond lengths and angles shown in these diagrams have been drawn in a standard format and do not necessarily represent the actual shape of the compounds.

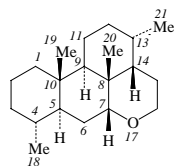
It is convenient to divide natural products into four classes according to the methods by which they are indexed. The classification has been most completely worked out for alkaloids, discussed more fully in ¶ 204, below.

Class A contains those substances, of little or no stereochemical complexity, which are indexed systematically rather than as stereoparents.

Class B stereoparents represent groups of natural products which have cyclic molecular skeletons in common. The base structure is derived by removal of all chemical functions but retention of hydrocarbon substituents and the pattern of hydrogenation; the name is derived from the trivial names of the related natural products, and author numbering is adopted if possible. General substitutive nomenclature, as illustrated in previous sections of this introduction, is used to convert the stereoparents into complete index names by addition of prefixes, suffixes and conjunctive terms. Examples of Class B stereoparents are **Prostane** and **Picrasane**:



Prostane ((1*S*,2*S*)-1-heptyl-2-octylcyclopentane)



Picrasane ((3*S*,3*aS*,6*aR*,7*aS*,8*R*,11*aS*,11*bR*,11*cS*)-hexadecahydro-3,8,11*a*,11*c*-tetramethylphenanthro[10,1-*bc*]pyran)

Class C stereoparents imply both stereochemistry and chemical functionality. Other functions (including higher functions) are expressed as substituents. Examples will be found in the discussion of alkaloids (¶ 204). Miscellaneous Class C stereoparents include **Leucomycin V**. Their derivatives are indexed like alkaloids.

Class D stereoparents possess incompletely elucidated structures. If sufficient information is available, they are named systematically and no stereochemical descriptor is assigned. When no systematic name is possible, the trivial name in the original document is used.

Because treatment of stereoparents by the general rules of substitutive nomenclature can sometimes lead to loss of stereochemical information, special rules for their derivatives are employed. Thus, esters and semicarbazones (and their chalcogen analogs) are named as derivatives of the stereoparents, not at "Class II" acid names or as **Hydrazinecarboxamide** derivatives. Esters formed by an acidic and an alcoholic stereoparent are indexed at the stereoparent that contains the highest chemical function.

Examples:

Androstan-17-ol, butanoate, (5 α ,17 β)-

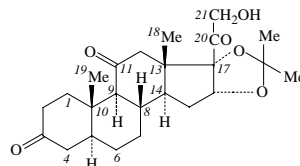
The preferred CA name is the one that employs the stereoparent in the index heading parent. Addition compounds and salts containing more than one stereoparent derivative are assigned a preferred index name based on chemical functionality of the stereoparents.

Example:

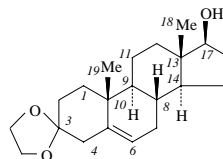
L-Proline, compd. with (8 α ,9*R*)-cinchonan-9-ol (1:1)

Acyclic *acetals* of functions expressed by "-one" suffixes or "oxo" substituents of stereoparents are indexed as dialkoxy derivatives. Cyclic acetals of stereoparent diols with formaldehyde are named as [methylenebis(oxy)] derivatives of the stereoparent; other cyclic acetals are named similarly if subsidiary functions of the stereoparent are involved, but by modification terms if a principal chemical function has been acetalized. Lactones of principal functions are also named in the modification.

Examples:



Pregnane-3,11,20-trione, 21-hydroxy-16,17-[(1-methylethylidene)bis(oxy)]-, (5 α ,16 α)-



Androst-5-en-3-one, 17-hydroxy-, cyclic 1,2-ethanediyl acetal, (17 β)-

When two or more stereoparents are covalently attached to one another the compound is normally indexed at the stereoparent that expresses (a) the largest number of highest chemical functions, (b) the most preferred skeleton.

Citation of additional and modified stereochemistry at stereoparent and stereoparent derivative names is discussed in the following section.

203. Stereochemistry is expressed in CA index names¹ by three methods: The stereochemistry for the heading parent of *systematically named* compounds, including some natural products with only one or two chiral centers, e.g., most carbohydrates with four or fewer carbon atoms, simple alkaloids and terpenes, and some steroid degradation products, is expressed in the modification, following all other structural information such as "ethyl ester," and ahead of descriptive terms related to a specific abstract, such as "spectrum of." Additional stereochemical expressions are included with the substituent and modification terms to which they refer. The terms used in this "systematic stereochemistry" are the main subject of the present section.

Natural products, especially those with a multiplicity of chiral centers, are conveniently indexed at fundamental trivial names (*stereoparents*) where they and their derivatives can be found at headings familiar to users in the alkaloid, carbohydrate, steroid, and terpene fields. The concept of stereoparents has been discussed above; the separate natural product classes to which it is applied are the subjects of ¶¶ 204-212.

Coordination compounds require specialized descriptors to describe the arrangement of ligands around the central atom. These are discussed in the final part of this paragraph.

I. Systematically named compounds. New rules have been adopted for systematic stereochemistry in CAS index nomenclature. These conventions have been applied since March 1997 to systematically named fragments of structures containing stereoparents. The new policy was expanded in June

¹For a more extensive discussion of the stereochemical descriptors found in CA index names, see J. E. Blackwood and P. M. Giles, Jr., *J. Chem. Inf. Comput. Sci.* **1975**, 15, 67-72; M. F. Brown, B. R. Cook, and T. E. Sloan, *Inorg. Chem.* **1975**, 14, 1273-1278; *ibid.* **1978**, 17, 1563-1568.

1998 (CA Volume 129) to all systematic organic compounds.

The methods described below are a simplification of previous CAS stereochemical practice. Rules that were in use since the beginning of the Ninth Collective Index period (1972) have now been thoroughly revised. The need for a single expression to describe the total stereochemistry of a molecule has been eliminated. Stereochemical terms are now placed within the parts of a chemical name to which the stereochemical information applies. Only the stereochemistry contained in the heading parent is expressed in the name modification following all other structural information.

In general, the new rules are consistent with IUPAC recommendations and produce CAS index names containing stereochemical information which can be readily interpreted.

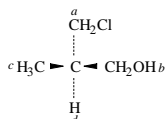
The terms *R* and *S* are employed for chiral elements possessing either absolute or relative stereochemistry. The term *rel* is used in conjunction with *R* and *S* for structures with only relative stereochemistry. *E* and *Z* are used primarily to describe geometrical isomerism about double bonds. The relative terms *cis*, *trans*, *endo*, *exo*, *syn*, *anti*, α , and β are used as alternatives to *R* and *S* in certain limited situations.

Assignment of the absolute terms *R* and *S* depends on the priority ranking of atoms or groups attached to the stereochemical element whose chirality ("handedness") is to be determined by the Cahn-Ingold-Prelog Sequence Rule.^{2,3} This ranking depends first on the descending order of atomic number of the atoms directly attached to the chiral center; thus, for bromochlorofluoriodomethane the order is I, Br, Cl, F. In the following diagrams these atoms are represented by *a*, *b*, *c*, and *d*, respectively. The least preferred atom or group, *d*, is represented by a dotted line to indicate it is to be considered to be below the plane of the paper, while *a*, *b*, and *c* are to be imagined to project toward the viewer at an angle. (The analogy of an automobile steering wheel with three radial bars is a useful one to visualize.) *R* is assigned to a clockwise (right-handed) sequence of *a*, *b*, *c*, while *S* denotes a counterclockwise (anticlockwise) sequence.



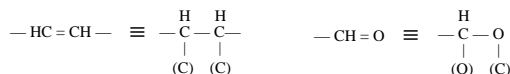
Alternative ways of drawing chiral diagrams are often more convenient: either (a) at most two bonds (as indicated by ordinary lines) are shown to be in the plane while one projects forward and one backward (as indicated by a wedge and a dotted line, respectively), or (b) two bonds are shown projecting forward and two backward, as in the diagram below. In both instances it must be remembered that the atom or group of lowest priority, *d*, must be oriented away from the viewer so that the clockwise or counterclockwise arrangement of *a*, *b*, and *c* is correctly observed.

In organic compounds it is generally necessary to compare the ranking of two or more carbon bonds. This is done by proceeding outward *one step at a time* until a decision is reached.



In the structure above, H clearly has the lowest priority, but it is necessary to establish the ranking of the three carbon groups. This is done by arranging the atomic numbers of the *most senior substituent* on each carbon in descending order: Cl, O, H. This elicits the absolute stereochemical descriptor *R*.

Branching, especially branching close to the chiral center, raises the priority ranking of alkyl groups. Multiple bonds of all kinds are handled by "duplicating" or "triplicating" both of the atoms connected by the bonds; thus:

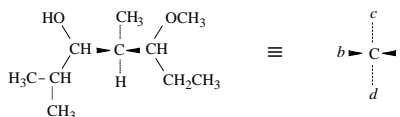


Only the immediate atoms are replicated; the procedure is not carried further. Aryl, e.g., phenyl, naphthalenyl, radicals are handled in a similar manner.

²International Union of Pure and Applied Chemistry. *Nomenclature of Organic Chemistry, Section, A, B, C, D, E, F and H*, 1979 ed., Pergamon Press, Oxford (England) 1979, Section E, Appendix 2, pp. 486-490.

³R. S. Cahn, C. K. Ingold, and V. Prelog, *Angew. Chem., Int. Ed. Engl.* **1966**, 5, 385-415 (errata: 1966, 5, 511). For a modification in the treatment of cyclic pathways, see V. Prelog and G. Helmchen, *ibid.* **1982**, 21, 567-583.

The following groups are arranged in descending order of Sequence Rule priority: —SCH_3 , —SH , —OCOCH_3 , $\text{—OCH}_2\text{CH}_3$, —OCH_3 , —OH , —NO_2 , $\text{—N(CH}_3)_2$, —NH_2 , —COOH , —COCH_3 , —CHO , $\text{—CH}_2\text{OH}$, $\text{—C}\equiv\text{N}$, $\text{—CH}_2\text{NH}_2$, $\text{—C}_6\text{H}_5$, $\text{—C(CH}_3)_2\text{CH}_2\text{CH}_3$, $\text{—C(CH}_3)=\text{CH}_2$, $\text{—CH(CH}_3)\text{CH}_2\text{CH}_3$, $\text{—CH}_2\text{CH}_2\text{CH}_3$, $\text{—CH}_2\text{CH}_3$, —CH_3 . It is essential to rank branched chains by a rigorous procedure if assignment errors are to be avoided. In



it can be immediately perceived that H has the lowest rank (*d*) and that of the three carbon bonds CH_3 has rank *c*. Proceeding outward to the left and right from the chiral center we observe that each carbon is attached to one oxygen, one carbon, and one hydrogen. The rule to be observed here is that we should now proceed *just one step along the senior (highest-priority) branches* (in this instance through the oxygens) to find H on the left, C (preferred) on the right. The fact that, in the *junior* branch, the priorities are reversed, with C attached to two C's and an H on the left, to only one C and two H's on the right, is disregarded, because this stage in the process is never reached. Only when a one-step search of the senior branches results in a tie is the junior branch inspected *to the same extent*. (This would have been necessary, with a consequent assignment of *S* instead of *R*, if —OCH_3 replaced —OH in the diagram, even if, at the same time, $\text{—OCH}_2\text{CH}_3$ replaced —OCH_3 on the right.)

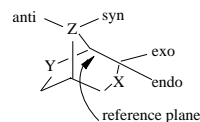
In complicated cases it is sometimes necessary to construct an exploration table or tree diagram in assigning *R* and *S* descriptors. A useful summary of Sequence Rule procedures is included in Section E of the IUPAC rules,² but consultation of the papers of Cahn, Ingold and Prelog, especially their 1966 paper,³ may be necessary for resolution of the most difficult cases.

Relative descriptors of various kinds are used as follows:

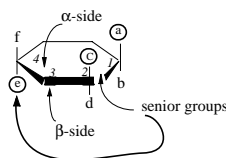
(A) *cis* and *trans* are restricted to cyclic structures with two achiral stereogenic atoms (an atom is stereogenic when interchange of two of the atoms or groups attached to it produces a nonidentical compound). An example is **1,3-Cyclobutanediol**. The *cis* isomer has the senior groups (as defined by the Sequence Rule) on the same side of the reference plane.

(B) *endo* and *exo* are used only for achiral ring positions on the X and Y bridges of bicyclo[X.Y.Z]anes (¶ 155) in which $X \geq Y > Z > 0$, and $X + Y < 7$. The *exo* isomer has the configuration in which the senior substituent is on the same side of the reference plane as the Z bridge (see diagram below).

(C) *syn* and *anti* are restricted to achiral ring positions on the Z bridge of a bicyclo[X.Y.Z]ane in which $X \geq Y > Z > 0$, and $X + Y < 7$. The *syn* isomer has the senior substituent oriented towards the X bridge.



(D) α and β are employed for ring positions of certain meso cyclic compounds. In the diagram below, the senior groups at the three stereogenic centers (by the Sequence Rule) are *a*, *c*, *e*; the junior groups are *b*, *d*, *f*. The α -side of the reference plane is that side on which the preferred substituent lies at the lowest-numbered stereogenic position; *c* lies on the same side as *a*, so both are assigned α descriptors; *e* lies on the opposite side of the reference plane and is assigned a β descriptor; hence: 1α , 2α , 4β . It should be noted that this usage differs from that for cyclic stereoparents (¶ 203II, below), in which " α -" means "below the plane" and denotes absolute configuration.



(E) *E* and *Z* (from German: "entgegen" (opposite) and "zusammen" (together)) are geometrical stereodescriptors for substances having achiral elements resulting from double bonds. In a compound



the double bond can be considered to be in a vertical plane, and *a*, *b*, *c*, and *d* in a horizontal plane. When the senior atom or group at X (*a*) and the senior

atom or group at Y (c) are on the same side of the vertical reference plane, the descriptor Z is cited; its isomer is assigned an *E* descriptor.⁴

(G) The (\pm) descriptor is only used for indicating stereoparents are racemic instead of absolute. The optical rotation descriptors (+) and (-) indicate the sign of rotation of plane-polarized light in the visible range (400-700 nm). The original literature should be consulted for the specific conditions under which the optical rotation was obtained.

These descriptors, alone or in combination, are employed to express the total stereochemical information for a chemical substance as follows:

(1) Stereochemistry for the index heading parent is cited at the end of the preferred (inverted) index name. Locants are used with all stereochemical terms, except *cis* and *trans*, relating to the parent.

(2) Stereochemistry for substituents and modifications of the parent are expressed at the beginning of each individual nomenclature fragment to which the stereochemical terms apply.

(3) The preferred stereo terms are *R*, *S*, *E*, and *Z*. Each is preceded by a locant, arranged in locant order, and separated by commas. The resulting stereochemical expression is enclosed in curves and followed by a hyphen, e.g., (1*R*,2*S*,3*R*,5*E*)-.

(4) For substances with only partially known stereochemistry, stereogenic elements of unknown configuration are ignored for nomenclature purposes. The term [*partial*] is no longer used.

(5) The term *rel* is used as a global expression to denote that the entire stereochemistry of a structure is relative only. Thus, *rel* appears at the end of the name modification following any stereochemical terms describing the parent.

(6) The sign of optical rotation, (+) or (-), follows the term *rel* when the complete relative configuration of a substance is defined but the absolute stereochemistry is unknown.

(7) When the substance has only one chiral element, not defined by the author, the sign of rotation is cited alone at the end of the inverted name.

(8) In the uninverted name (+), (-), *rel*, *rel*(+), or *rel*(-) appear at the beginning of the name, before any other terms.

(9) When the absolute configuration of a substance is unknown, either of two enantiomeric structures may be used to depict the relative configuration. Both the inverted and uninverted names will express that enantiomer which results in the first occurring *R* term in the inverted CAS index name.

(10) Stereogenic centers which cannot be expressed as *R* or *S* may be described using *endo*, *exo*, *syn*, *anti*, *cis*, *trans*, α , or β .

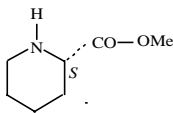
(11) Bicyclo[X.Y.Z]ane compounds in which $X \geq Y > Z > 0$, and $X + Y < 7$, and which contain achiral stereogenic elements are the only structures for which *endo*, *exo*, *syn*, and *anti* are used. These terms are each preceded by a locant which is followed by a hyphen with the resulting stereochemical expression enclosed in curves, e.g., (3-*endo*, 8-*anti*).

(12) The terms *cis* and *trans* are used for eight-membered or smaller rings substituted in only two achiral stereogenic positions. No locants or enclosing marks are used with single occurrences of these terms. Multiple terms for ring assemblies, e.g., bicyclohexyl, are cited in the order of unprimed, primed, double-primed, etc., rings and separated by commas and enclosed in curves.

(13) Use of α and β is restricted to cases not covered by the above rules. These terms are not cited in the same stereochemical expression in combination with other relative terms.

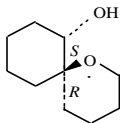
Examples:

C₇H₁₃NO₂
Stereo: absolute



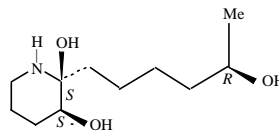
2-Piperidinecarboxylic acid, methyl ester, (2*S*)-

C₁₀H₁₈O₃
Stereo: relative



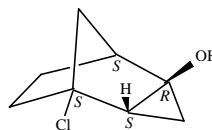
1-Oxaspiro[5.5]undecan-7-ol, (6*R*,7*S*)-*rel*-

C₁₁H₂₃NO₃
Stereo: absolute (-)



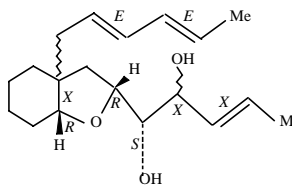
2,3-Piperidinediol, 2-[(5*R*)-5-hydroxyhexyl]-, (2*S*,3*S*)-

C₈H₁₁ClO
Stereo: relative



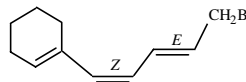
Tricyclo[3.2.1.0^{2,4}]octan-2-ol, 5-chloro-, (1*R*,2*S*,4*R*,5*R*)-*rel*-

C₁₀H₃₀O₃
Stereo: absolute partial



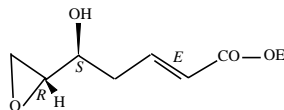
3-Pentene-1,2-diol, 1-[(2*R*,7*aR*)-3*a*-(2*E*,4*E*)-2,4-hexadienyloctahydro-2-benzofuranyl]-, (1*S*)-

C₁₁H₁₅Br
Stereo: relative



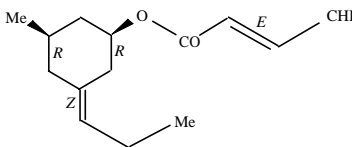
Cyclohexene, 1-[(1*Z*, 3*E*)-5-bromo-1,3-pentadienyl]-

C₉H₁₄O₄
Stereo: absolute



2-Pentenoic acid, 5-hydroxy-5-(2*R*)-2-oxiranyl-, (2*E*,5*S*)-

C₁₄H₂₀I₂O₂
Stereo: relative (+)

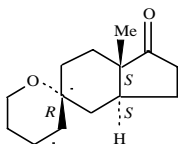


2-Butenoic acid, 4,4-diiodo-, (1*R*,3*R*,5*Z*)-3-methyl-5-propylidene-cyclohexyl ester, (2*E*)-*rel*-(+)-

(The *Z* double bond is cited on the atom closer to the parent.)

⁴J. E. Blackwood, C. L. Gladys, A. E. Petrarca, W. H. Powell, and J. E. Rush, "Unique and Unambiguous Specifications of Stereoisomerism about a Double Bond in Nomenclature and Other Notation Systems", *J. Chem. Doc.* **1968**, 8, 30-32.

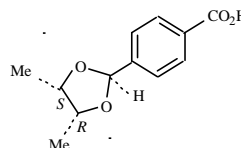
C₁₄H₂₂O₂
Stereo: absolute



Spiro[5*H*-indene-5,2'-[2*H*]pyran]-1(4*H*)-one, decahydro-7*a*-methyl-, (2'*R*,3*aS*,7*aS*)-

(The lower locant (2') is used to cite the *R* center.)

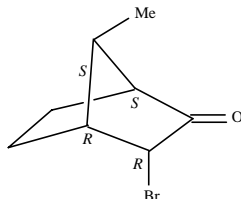
C₁₂H₁₄O₄
Stereo: relative



Benzoic acid, 4-[(2 α ,4 β ,5 β)-4,5-dimethyl-1,3-dioxolan-2-yl]-

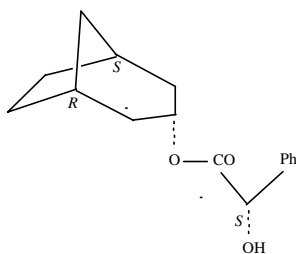
(The 2-position on the dioxolane ring is achiral stereogenic.)

C₈H₁₁BrO
Stereo: absolute



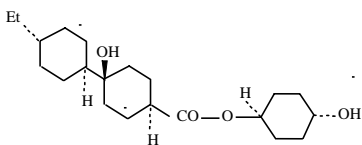
Bicyclo[2.2.1]heptan-2-one, 3-bromo-7-methyl-, (1*S*,3*R*,4*R*,7*S*)-

C₁₆H₂₀O₃
Stereo: absolute



Benzeneacetic acid, α -hydroxy-, (3-*endo*)-bicyclo[3.2.1]oct-3-yl ester, (α *S*)-

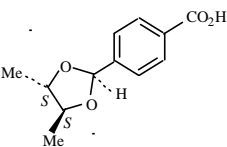
C₃₁H₃₆O₄
Stereo: relative



[1,1'-Bicyclohexyl]-4-carboxylic acid, 4'-ethyl-1-hydroxy-, *trans*-4-hydroxycyclohexyl ester, (*cis,trans*)-

(The unprimed ring is *cis* and the primed ring is *trans*.)

C₁₂H₁₄O₄
Stereo: absolute

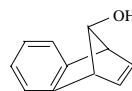


Benzoic acid, 4-[(4*S*,5*S*)-4,5-dimethyl-1,3-dioxolan-2-yl]-

(The 2-position on the dioxolane ring is non-stereogenic.)

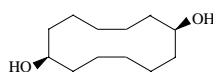
The stereochemistry of some compounds cannot be described completely by the rules above. The presence of stereochemical information in an original document is indicated in the index entries for such compounds by the modification term "stereoisomer."

Examples:



stereoisomer

[This achiral stereogenic system can only be described by *syn* or *anti*, but these descriptors are not allowed for this ring system.]



stereoisomer

[This achiral stereogenic system can only be described by the α / β system, which is not allowed in rings of this size. Had the system been chiral, *R* and *S* could have been used.]

Molecular addition compounds, mixtures and polymers of components with stereogenic elements have the stereochemical descriptors cited with the respective components; a descriptor for the entire addition compound, etc., is cited last, if known.

Examples:

Cyclohexanol, 4-amino-*trans*-, acetate (1:1)

2-Furancarboxylic acid, tetrahydro-2-methoxy-(2*R*)-, compd. with *rel*-methyl (1*R*,2*S*)-2-aminocyclobutanecarboxylate

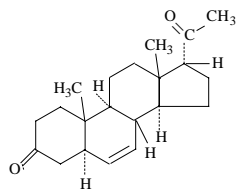
1,2-Cyclobutanedicarbonyl dichloride (1*R*,2*R*)-*rel*-, polymer with *rel*-(2*R*,5*S*)-2,5-dimethylpiperazine

Although the polymer in the final example above probably has *cis-trans* stereochemistry, these terms are not repeated at the monomer headings; the structural repeating unit entry (§ 222), however, would cite the descriptors in the order dictated by that heading.

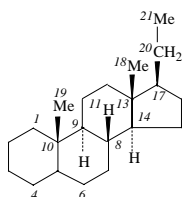
II. *Stereoparents* have been discussed in § 202.

A stereochemical descriptor is cited in an index modification at a stereoparent heading to express differences between the stereoparent illustrative diagram and the structure of the reported substance. In the diagrams the configurations on ring-system substituents are indicated by dotted lines for α and "wedges" for β . Variations for specific derivatives are indicated by citing appropriate α and β terms with the locants of the modified centers. Variant stereochemistry for acyclic, bridge and spiro centers is indicated by *E* and *Z* or by *R* and *S* as described for systematic stereochemistry, above. If a variation is not reported, the normal stereochemistry is considered to be retained. When the modified stereochemistry is unknown, e.g., indicated by a wavy line in a structural diagram, the descriptor *x* (*xi*) is assigned to that position. Descriptors are also cited for added configurations (when the stereoparent diagram shows no stereochemistry at a center). When the added stereochemistry is in a stereoparent substituent or modification, the descriptor is cited as a prefix, e.g., [(5 α ,16*E*)-androstane-16-ylidene]-. When the center is in a systematically named substituent or modification term, the descriptor is placed with the systematic nomenclature term, e.g., **Pregnane-3,20-dione, 5-hydroxy-6-[(1*Z*)-3-hydroxy-1-propenyl]-, (5 α ,6 β)-**.

Examples (the stereoparent diagram is compared with an author's diagram for a derivative in each case):

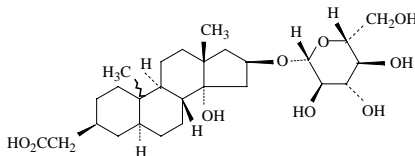


A pregnane derivative

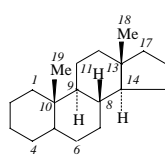


Pregnone (stereoparent)

(The configuration at positions 8, 9, 10, 13 and 14 correspond; position 5 has added stereochemistry; position 17 has modified stereochemistry. The stereochemical descriptor at **Pregn-6-ene-3,20-dione** is (5 α ,17 α)-.)



An androstane derivative



Androstane (stereoparent)

Positions 8, 9, and 13 are normal; position 14 is substituted, but has normal configuration. Position 10 has unknown modified stereochemistry; positions 3, 5 and 16 have added stereochemistry and the substituent at 16 is a stereoparent (β -D-glucopyranosyl radical).

The stereochemical descriptor is (3 β ,5 α ,10 ξ ,16 β)-. (The stereochemistry within the stereoparent radical is expressed by the substituent radical name.)

III. Coordination compounds. The stereochemistry of mononuclear complexes is expressed by special descriptors. The term "stereoisomer" is used for polynuclear coordination complexes when all the nuclear stereochemistry is known. When no nuclear stereochemistry is known, ligand stereochemistry is cited using the rules for systematic organic compounds. No ligand stereochemistry is cited unless all ligand stereochemistry is described. When more than one ligand is stereogenic, the stereochemistry for the complex is cited as if all ligand stereochemistry is in one organic ligand. The discussion that follows is necessarily brief; for a more detailed explanation the review by T. E. Sloan⁵ should be consulted.

For coordination numbers 1, 2, and 3, no nuclear stereochemistry is possible. Ligands are assigned systematic descriptors according to the rules in I above. If the chirality of a 3-coordinate tetrahedral complex is reported, it is described as *R* or *S* by application of the Sequence Rule as described above. The special coordination descriptors comprise:

(a) a *symmetry site term* to describe the molecular geometry about the nuclear atom;

(b) a *configuration number* to identify the atoms on each axis and plane of the system;

(c) a *chirality symbol* to differentiate members of enantiomeric pairs (when the structure has no reflection symmetry); and

(d) a *ligand segment* (when ligands have stereochemistry of their own) cited as described in ¶ 203I, above.

Symmetry site terms are comprised of one- to three-letter abbreviations to describe the geometry around the central atom combined with the coordination number. They are generally based on information reported by an author, but some assumptions are made in indexing: **square planar** for 4-coordinate Pd^{2+} , Pt^{2+} , Rh^+ , Ir^+ , Au^{3+} , Se^{2+} , and Te^{2+} ; **square pyramidal** for 5-coordinate nitrido complexes of all metals and oxo complexes of technetium (the nitrido and oxo ligands are assumed to be axial); **octahedral** for all 6-coordinate complexes unless the ligand constraints prohibit this geometry; or if an anionic nonmetallic coordination center contains six identical monodentate ligands; **tetrahedral** for 4-coordinate complexes of (a) all 4-coordinate metallic complexes except Mn, Fe, Ru, Os, Co, Rh, Ir, Ni, Pd, Pt, Cu, Ag, or Au; (b) any 4-coordinate complex of Fe^{2+} , Ru^{2+} , Os^{2+} , Co-, Rh-, Ir-, Ni^0 , Pd^0 , Pt^0 , Cu^+ , Ag^+ , or Au^+ ; (c) Ni^{2+} , Fe^{2+} , Fe^{3+} , or Mn^{2+} with four halides or pseudohalides; (d) Co^{2+} with four monodentate ligands; (e) all 4-coordinate nonmetallic complexes except Se^{2+} and Te^{2+} (tetrahedral descriptors are not cited for anionic nonmetallic complexes containing four identical monodentate ligands); and (f) substances indexed at **Antimony(1+)**, **Arsenic(1+)**, **Bismuth(1+)**, and **Phosphorus(1+)** (not **Phosphonium**, see ¶ 184). Americyl, neptunyl, plutonyl, and uranyl (Mo_2^{n+}) groups in 5, 6, 7, 8, and 9 coordinate complexes are assumed to be *trans*. Molybdenyl and tungstyl are assumed to have *cis* oxo groups. The amines are assumed to be *trans* in the Reineckate anion.

Planar ring systems, α -dioximes, 2,2':6',2''-terpyridine and 2,2',2''-nitrilotris[ethanol] as ligands impose their geometry on the central atom; thus, a zinc-porphine complex is square planar, not tetrahedral. Symmetry site terms

are not required for 4- and 6-coordinate anionic coordination complexes containing nonmetallic central atoms and identical monodentate ligands: they can be assumed to be tetrahedral and octahedral, respectively. The terms are omitted also when information is lacking.

T-4	tetrahedral
SP-4	square planar
TB-5	trigonal bipyramidal
SP-5	square pyramidal
OC-6	octahedral
TP-6	trigonal prismatic
PB-7	pentagonal bipyramidal
OCF-7	octahedral faced monocapped
TPS-7	trigonal prismatic square faced monocapped
CU-8	cubic
SA-8	square antiprismatic
DD-8	dodecahedral
HB-8	hexagonal bipyramidal
OCT-8	octahedral trans-bicapped
TPT-8	trigonal prismatic triangular faced bicapped
TPS-8	trigonal prismatic square faced bicapped
TPS-9	trigonal prismatic square faced tricapped
HB-9	heptagonal bipyramidal

Configuration numbers depend first upon application of the Sequence Rule to determine order of seniority (priority) of atoms coordinated to the central atom. When constitutionally equivalent atoms are present, the same priority number is assigned to each; thus in $\text{Ma}_2\text{b}_2\text{c}_2$, the order is 1,1,2,2,3,3. When a choice of configuration number is possible, preference is given to the atom of lower priority (higher numerical value). Tie-breaking is necessary with equivalent sets of polydentate ligand atoms. Chiral ligands, otherwise identical, are ranked with the *R*-form above the *S*-form. The chirality symbols *C*—for clockwise— and *A*—for anticlockwise (counterclockwise)—are used to denote absolute stereochemistry in coordination compounds, except that *R* and *S* are used for tetrahedral complexes, and Δ (delta) and Λ (lambda) for octahedral complexes containing *cis*-bis(monodentate)bis(bidentate) ligands and tris(bidentate) ligands, respectively. Chirality symbols are placed after configuration numbers, which are determined and cited as follows:

(a) *Tetrahedral complexes (T-4)* are assigned no configuration number. The chirality symbol *R* or *S* is assigned as for organic compounds with a single chiral center.

(b) *Square planar complexes (SP-4)* have the ligating atoms at the corners of a square. The rank number of the atom diagonally opposite the senior atom (1) is cited as the configuration number. Three isomers are possible when all four ligands are different.

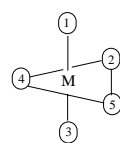
Example:



Configuration number	= 4
Stereochemical descriptor	= (SP-4-4)-
(No chirality symbol is required)	

(c) *Trigonal bipyramidal complexes (TB-5)*. The configuration number comprises the rank numbers for the atoms at the ends of the major axis cited without punctuation in descending order of priority. If the complex has no reflection symmetry, the order of atoms in the plane perpendicular to the axis is expressed by *C* (clockwise ascending sequence of numerals, equivalent to descending priority) or *A* (anticlockwise) as viewed from the highest priority ligand on the major axis.

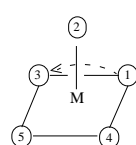
Example:



Configuration number	= 13
Chirality symbol	= A
Stereochemical descriptor	= (TB-5-13-A)-
(When all five coordinating atoms are different, 10 configurations are possible. Each is chiral, affording 20 possible stereoisomers.)	

(d) *Square pyramidal complexes (SP-5)* have a lone coordinating atom on the principal axis and four atoms in a square planar configuration at right angles to this axis. The first digit of the configuration number is the priority number of the lone atom; the second digit is the priority number of the atom situated *diagonally opposite* to the most senior coordinating atom in the plane. The chirality symbol is derived by viewing the plane from the position of the lone axial atom and tracing a path around the square plane from the most senior atom to the next most senior atom present. If this path is clockwise, *C* is the assigned chirality symbol; if anticlockwise, the symbol is *A*.

Example:



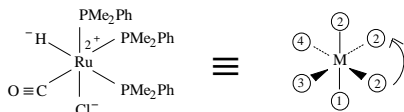
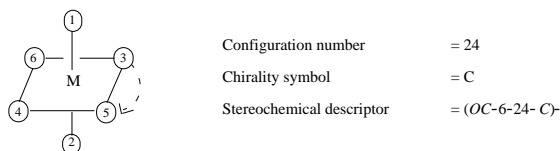
Configuration number	= 25
Chirality symbol	= A
Stereochemical descriptor	= (SP-5-25-A)-

(When all coordinating sites are unlike, 15 configurations are possible. Each is chiral, affording 30 possible stereoisomers.)

⁵T. E. Sloan in *Topics in Inorganic and Organometallic Stereochemistry*, G. Geoffroy, ed., John Wiley & Sons, Inc., New York, 1981, 1-36.

(e) Octahedral systems (OC-6) for which C and A can be used as chirality symbols (see above) have configuration numbers of which the first digit is derived from the priority number of the atom opposite to atom 1 and the second digit from the priority number opposite to the senior atom in the plane perpendicular to the axis containing atom 1. When no reflection symmetry is present, the chirality symbol is derived by viewing the plane from atom 1 and tracing a path clockwise (C) or anticlockwise (A) from the most senior atom to the next most senior atom.

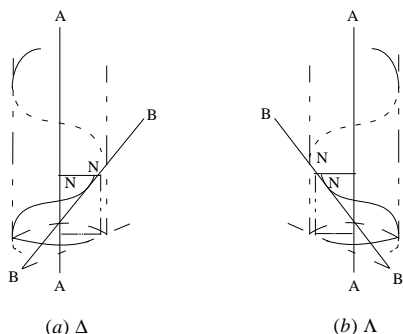
Examples:



(The priorities of the ligand atoms are determined by arranging their atomic numbers (17,15,6 and 1) in descending order thus: Cl,P,C and H. There are three identical ligands of order 2; one is on the main axis (opposite ligand 1), the others are in the transverse plane opposite 3 and 4; the higher number is cited. The transverse pathway from the preferred 2 to the neighboring (less preferred) 2 is clockwise when viewed from atom 1.)

Configuration number = 24
Stereochemical descriptor = (OC-6-24-C)-

For octahedral complexes with two or three bidentate ligands oriented in a skew configuration, the helicity symbols Δ and Λ are employed instead of chirality symbols, they are related to right-handed and left-handed spirals, respectively, as follows:

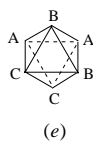


In diagram (a) above, BB is a tangent to the right-handed helix that has axis AA and radius NN; (b) shows its mirror image, a left-handed helix. Turning each diagram through 90 degrees in either direction results in the simplified diagrams (c) and (d), respectively.

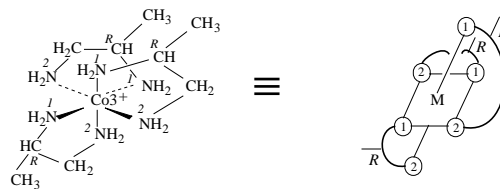


AA and BB have now lost their respective identities as axis and tangent and can be considered either as two tangents or as two segments of a double helix. BB is in front of AA in both diagrams; in (c), when AA is horizontal, BB descends to the right, in (d) to the left.

In the octahedral complex, pictured as a regular octahedron in (e) below, the lines AA and BB represent two bidentate ligands oriented as in (c) above and represented by the helicity symbol Δ . (A third bidentate ligand, if it were present at CC, would not affect the helicity.)

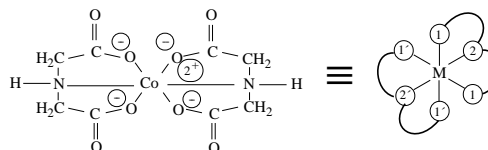


The helicity symbol replaces the chirality symbol in octahedral complexes of this type. In the complex named in abbreviated fashion as [Co(1,2-pn)₃]³⁺ the ligands themselves have chirality (denoted by R or S), and their geometry around the cobalt atom is described by use of "1" (for bonding to a secondary carbon) and "2" (for bonding to CH₂). The helicity can be seen to correspond to the diagram above and the symbol Δ is therefore appropriate.



Configuration number = 21
Chirality symbol = Δ
Stereochemical descriptor = (OC-6-21- Δ -(R),(R),(R))-

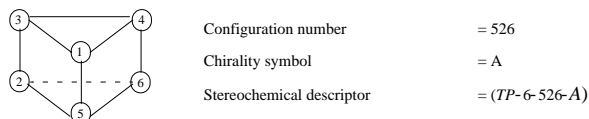
Octahedral complexes containing identical bis(tridentate) ligands are assigned geometric and chirality symbols in the same manner as normal octahedral complexes. However, in order to distinguish between enantiomers it is necessary to add primes to the donor atoms of one ligand. The primes are retained in the configuration number and this distinguishes between enantiomers.



Configuration number = 1'1'
Stereochemical descriptors = (OC-6-1'1'-)

(f) *Trigonal prismatic complexes (TP-6)*. The configuration number is obtained by citing the priority numbers of the three atoms opposite to (eclipsed by) the preferred triangular face, i.e., the face containing the maximum number of ligating atoms of highest priority (lowest numerals). These numbers are cited to correspond to the ascending numerical order of the respective eclipsing atoms. A chirality symbol, C or A, denotes the direction of numerical progression of the eclipsed atoms.

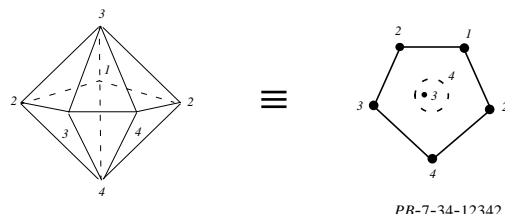
Example:



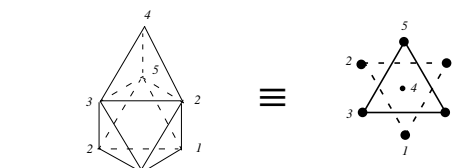
(g) Stereochemical descriptors were extended to 7-, 8-, and 9- coordinate complexes in 1977.⁶

In the following table, all 12 model polyhedra for 7-, 8-, and 9-coordinate complexes are shown, with examples of priority numbers for ligands from which configuration numbers are derived.

1. Pentagonal bipyramidal

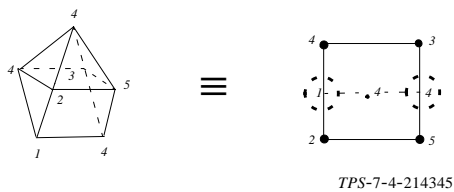


2. Octahedral faced monocapped

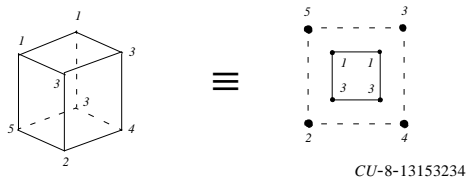


⁶ M. F. Brown, B. R. Cook, and T. E. Sloan, *Inorg. Chem.* **1978**, *17*, 1563-1568.

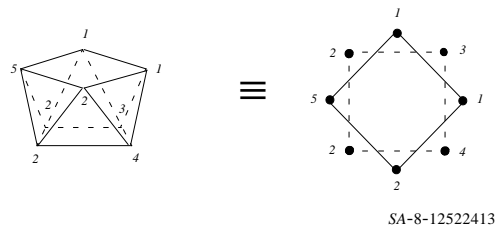
3. Trigonal prismatic square faced monocapped



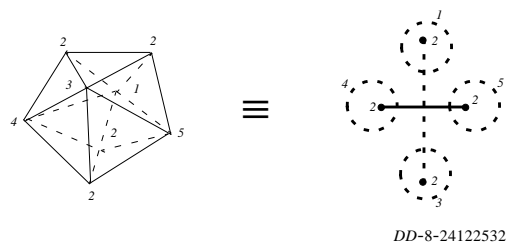
4. Cubic



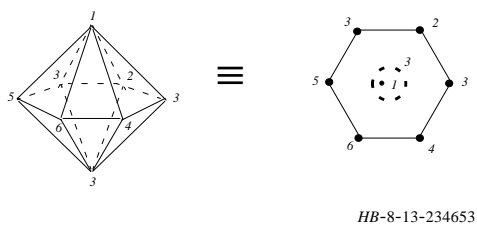
5. Square antiprismatic



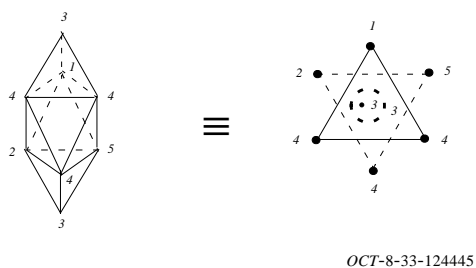
6. Dodecahedral



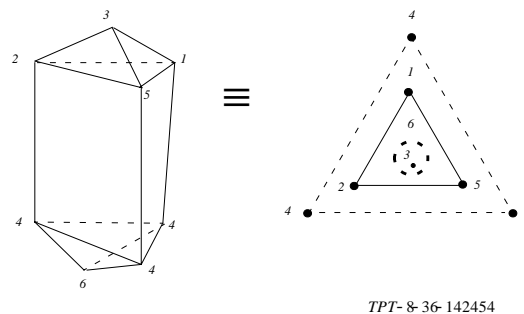
7. Hexagonal bipyramidal



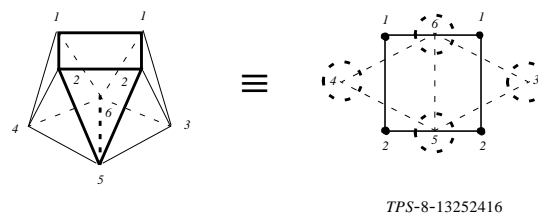
8. Octahedral trans-bicapped



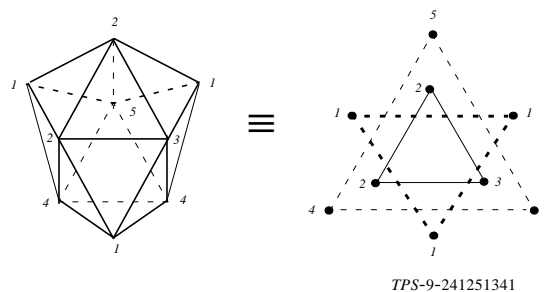
9. Trigonal prismatic triangular faced bicapped



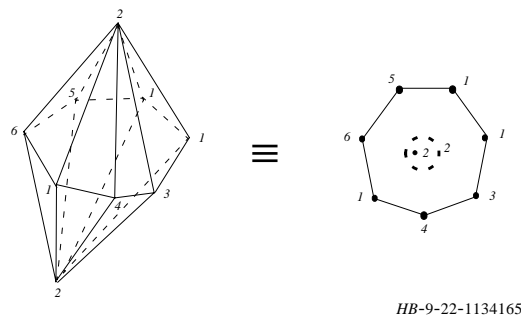
10. Trigonal prismatic square faced bicapped



11. Trigonal prismatic square faced tricapped



12. Heptagonal bipyramidal



The configuration number is assigned by orienting the model structure with the highest-order axis in the vertical plane. The model structure is then viewed from the highest priority ligating atom on the highest-order axis or from a point on the highest-order axis above the most preferred end or terminal plane perpendicular to the axis. The most preferred end or terminal plane is that end plane which either contains the greatest number of atoms, contains the greatest number of highest priority ligating atoms, or is adjacent to a plane containing the greatest number of highest priority ligating atoms. (Note that the *OCF-7* (octahedral faced monocapped), *TPS-7* (trigonal prismatic square faced monocapped), and *TPS-8* (trigonal prismatic square faced bicapped) model structures are of low symmetry and have only one correct orientation.)

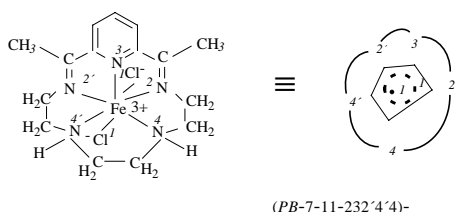
The configuration numbers for the model structures coded *PB-7*, *OCF-7*, *TPS-7*, *HB-8*, *OCT-8*, *TPT-8*, and *HB-9* begin with the priority numbers of the ligating atom(s) on the highest-order axis and are given in lowest numerical order sequence. These priority numbers are separated from the remainder of the configuration number by a hyphen. The remaining portion of the configuration number is derived by viewing the structure from the highest-priority ligating atom on the highest-order axis, or from the axial ligating atom located

above the preferred plane, and by citing the priority number of the ligating atom with the highest priority in the plane adjacent to that atom. The configuration number is then completed by continuing to cite the priority numbers of the ligating atoms in sequence as they are encountered, either clockwise or anticlockwise around the projection of the model structure, alternating between planes where necessary, when viewing from the highest priority atom. For those model structures with eclipsed pairs of ligating atoms, the priority numbers are given in pairs with the priority number for the preferred atom in the first plane followed by that for the eclipsed atom. The remaining priority numbers are given as they are encountered, either clockwise or anticlockwise around the projection of the model structure as viewed from the preferred end of the highest-order axis. For compounds in which clockwise and anticlockwise citations of the configuration number give two different configuration numbers (generally chiral compounds), the correct one is the lower numerical sequence as determined at the first point of difference. The remaining five model structures, *CU-8*, *SA-8*, *DD-8*, *TPS-8*, and *TPS-9*, do not have a ligating atom on the highest-order axis and thus do not have a distinct portion of the configuration number set off by a hyphen. These model structures are viewed from a point on the highest-order symmetry axis above the preferred terminal plane as defined previously. The configuration number is derived by first citing the priority number of the preferred ligating atom in the preferred end plane and then citing the priority number of the ligating atom it eclipses, if one exists. In the next step, one proceeds clockwise or anticlockwise around the projection of the model structure, giving the priority numbers of the ligating atoms as they are encountered, alternating between planes when necessary. Again, the clockwise or anticlockwise direction is chosen to give the lowest-order numerical sequence for the configuration number as determined at the first point of difference.

When there are two or more equivalent bidentate or tridentate ligands and the same priority numbers thus occur in equivalent ligands, the ties are broken by identically priming all the CIP priority numbers of the ligating atoms within a ligand to determine both the configuration number and the chirality symbol. In those complexes with symmetrical polydentate ligands, tetradentate, hexadentate (including symmetrical macrocyclic) ligands, etc., ties between equivalent ligating atoms are broken by priming the ligating atom priority numbers in chelating groups or pairs, thereby reducing the polydentate ligand to groupings of equivalent bidentate or tridentate ligands. When two or more nonequivalent tie-breaking choices exist for the coordination polyhedra of coordination numbers 7, 8, and 9, the tie is resolved by (a) assigning the lowest priming to the preferred symmetry axis or plane, and (b) assigning the lowest priming to give the lowest numerical value to the configuration number at the point of difference. Primes are restricted to the configuration number for octahedral complexes containing two identical tridentate ligands and trigonal-prismatic complexes containing two or more identical polydentate ligands and for all 7, 8 and 9 coordinate complexes. The use of primes is exemplified by the first example below, which is explained in some detail.

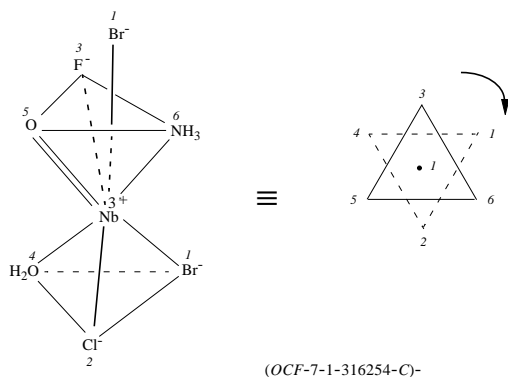
Examples:

Pentagonal bipyramidal (PB-7)

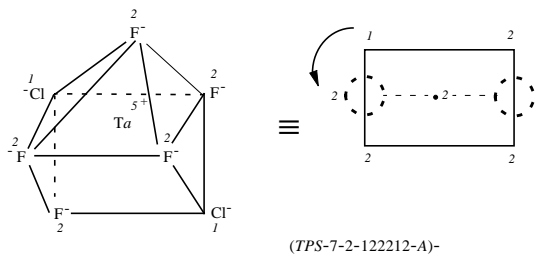


The ligands of highest atomic number (chlorine) are numbered 1. An exploration table (not shown) may be needed to establish the order of priorities (2,3, and 4) of the nitrogen ligands.⁷ No chirality symbol (C or A) is needed.

Octahedral faced monocapped (OCF-7)

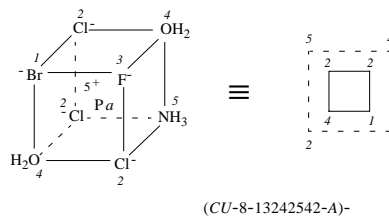


Trigonal prismatic square faced monocapped (TPS-7)



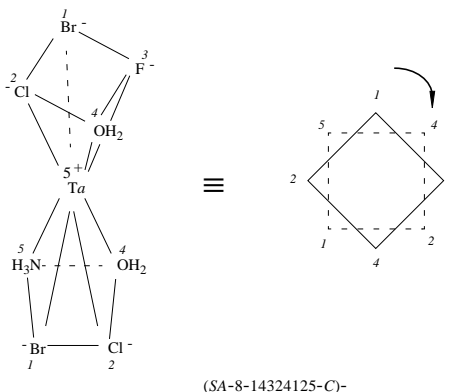
(The direction must be selected so as to cite the priority number of the atom in the next lower plane.)

Cubic (CU-8)



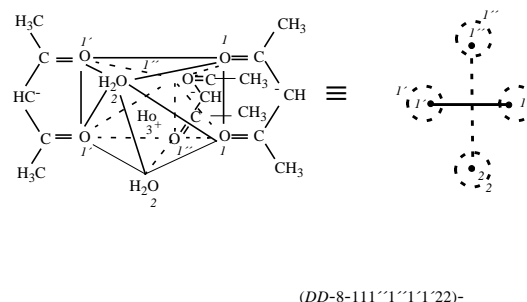
(Each face must be tested to determine the preferred terminal plane. As drawn in this example, the preferred face (terminal plane) is on the left side of the cube. Consequently the cube must be re-oriented before assigning the descriptor.)

Square antiprismatic (SA-8)



(The preferred orientation must be determined before the descriptor assigned.)

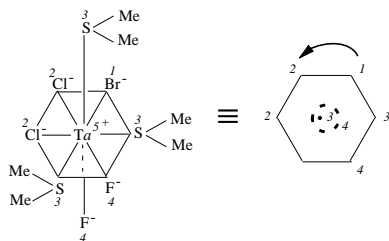
Dodecahedral (DD-8)



(The preferred orientation must be determined before the descriptor is assigned; also, the pathway is selected to pass through the atom of highest priority (lowest numerical value) in the next lower plane.)

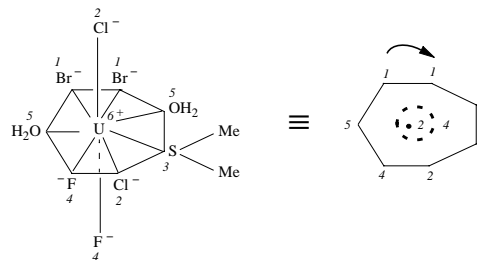
⁷R. S. Cahn, C. K. Ingold, and V. Prelog, *Angew. Chem. Int. Ed. Engl.* **1966**, *5*, 391-395.

Hexagonal bipyramidal (HB-8)



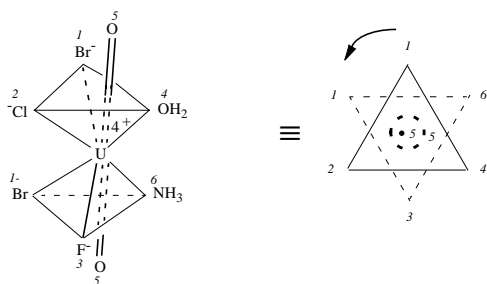
(HB-8-34-122343-A)-

Heptagonal bipyramidal (HB-9)



(HB-9-24-1153245-C)-

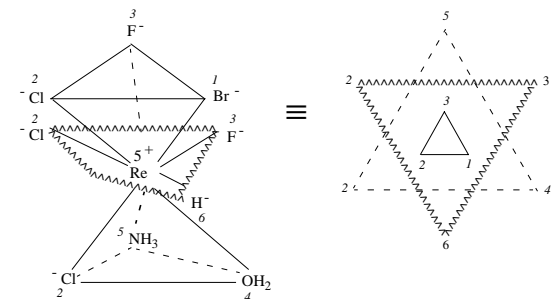
Octahedral trans-bicapped (OCT-8)



(OCT-8-55-112346-A)-

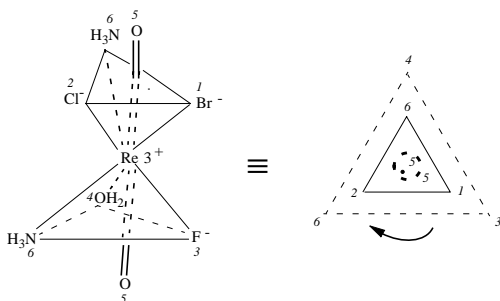
(The preferred orientation must be determined before the descriptor is assigned.)

Trigonal prismatic square faced tricapped (TPS-9)



(TPS-9-143352226-A)-

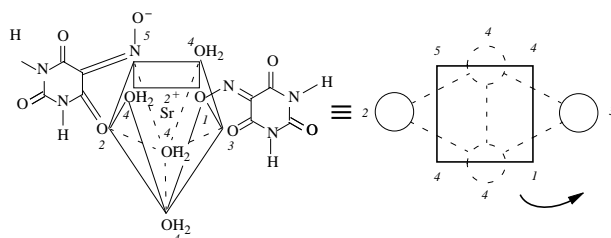
Trigonal prismatic triangular faced bicapped (TPT-8)



(TPT-8-55-132664-C)-

(The preferred orientation must be determined before the descriptor is assigned.)

Trigonal prismatic square faced bicapped (TPS-8)



(TPS-8-13445244-A)-

(The pathway is selected to pass through the atom of highest priority (lowest numerical value) in the next lower plane.)

Mononuclear coordination complexes containing ligands which require the use of η do not follow the stereochemical rules for other mononuclear coordination complexes. When the author indicates stereochemistry for the total complex, the term "stereoisomer" is used. Ligand stereochemistry in π -complexes is described using the rules for systematic organic stereochemistry (see ¶ 203 I). No ligand stereochemical descriptor is cited unless all ligand stereochemistry can be described. However, ligand stereochemical descriptors are cited even if the geometry about the metal is unknown. When more than one ligand is stereogenic, the stereochemistry for the complex is cited as if all ligand stereochemistry is in one organic ligand. An exception is made for metallocenes.

Metallocenes, when asymmetrically disubstituted, are not superimposable on their mirror images; they can therefore exist as enantiomers. The absolute configuration of the chiral center of highest priority is determined by the Sequence Rule and cited as *R* or *S* when specific information is stated in the original document. (The configuration of the other four centers is then fixed.)

Metallocenes which have stereochemistry only in the substituents have that indicated as described by the rules in I above.

Partial stereochemistry is not cited for coordination compounds.

204. Alkaloids are divided into classes largely in accordance with their stereochemical complexity. Class A alkaloids include substances containing only one chiral center, or none at all, or whose stereochemistry, typically restricted to a single ring system, is easily defined. Alkaloids of this class are indexed systematically; cross-references are found at the alkaloid names.

Example:

Tropine

See 8-Azabicyclo[3.2.1]octan-3-ol, 8-methyl-, (3-endo)-

Class B alkaloids possess more complex stereochemistry. They have been organized as derivatives of a single stereoparent of known absolute configuration common to several alkaloids. (Class C alkaloids are those which have not yet been organized in this way, but whose absolute configuration is known.) Class B stereoparents are illustrated in the *Chemical Substance Index* when justified by current entries. The following is a partial list of those currently employed for alkaloids:

Aconitane	Hasubanan
Ajmalan	Hetisan
Aspidospermidine	Ibogamine
Cevane	Morphinan
Cinchonan	Oxayohimban
Curan	Sarpagan
Eburnamenine	Solanidane
Ergoline	Strychnidine
Ergotaman	Veatchane
Erythrinan	Yohimban
6,14-Ethenomorphinan	

Deviations in stereochemistry for specific derivatives of Class B alkaloids are indicated in the modification (¶ 203 II). The prefixes, suffixes, conjunctive names, etc., of regular substitutive nomenclature are employed in naming derivatives. Radicals, e.g., aconitanyl, are formed from the stereoparent names in the usual way. Ring modifications as expressed by prefixes such as *cyclo*, *homo*, *nor*, and *seco*, on the heading parent, are not permitted and systematic nomenclature is used. Carboxylic acids are formed from Class B stereoparents by oxidation of an existing carbon to form an “-oic acid” or by addition of a carboxyl group to form a “-carboxylic acid”; the latter type of name is preferred if a choice is presented. Removal of hydrogen is indicated by “dehydro” terms in the inverted part of the heading.

Class C alkaloids are indexed at stereoparent names supplied in the literature, the numbering system is that most commonly adopted in original documents, and the numbering is extended, if necessary, to include all positions except acyclic hetero atoms. The latter are denoted by italic element symbols, with superscripts, if necessary, derived from the lowest numbered atom to which the hetero atom is attached, e.g., *N*⁶, *O*². Illustrative diagrams in the *Chemical Substance Index* at Class C alkaloid names, currently **Cephalotaxine** and **Vincalokoblastine**, indicate the stereochemistry and numbering systems. Derivatives of Class C alkaloids are named, when sufficient information is presented, by modifying the stereoparent name. Suffixes are not used except for “-oic acid,” to denote oxidation of a methyl group or removal of an ester group. “Hydro” terms are employed to indicate saturation of positions; “de” terms, e.g., “dehydro,” “deoxy,” “deepoxy,” “deoxo,” “demethyl,” “de(methoxycarbonyl),” denote removal of atoms or groups, which may be replaced by other groups; e.g., **Vincalokoblastine, 3-de(methoxycarbonyl)-3-(hydroxymethyl)**-. Higher functions attached to Class C stereoparents are indexed as substituents. When an alkaloid derivative can be named at two or more Class C stereoparents, the decision depends in descending order of preference on (a) removal of the fewest different substituents; (b) removal of substituents of lowest molecular weight; (c) retention of the stereoparent of highest molecular weight; (d) addition of prefixes related to the lowest number of smallest substituents; (e) the least stereochemical change; (f) the lowest locants for substituents; (g) the earliest index positions of the index name.

Derivatives of Class C alkaloids that meet the criteria for Class A alkaloids are named systematically by substitutive nomenclature. When a Class C stereoparent structure contains an oxo group, derivatives of the group, e.g., oximes or hydrazones, are expressed in the modification; otherwise they are expressed as substituents, e.g., as (hydroxyimino) or hydrazinylidene radicals. Esters are named analogously in the modification or by (acyloxy) or [(alkyloxy)carbonyl] substituents. Stereochemical deviations of Class C alkaloid derivatives are expressed as the final term in the modification in the usual way.

Quaternary alkaloids are either (a) alkaloids that contain a cationic nitrogen atom, or (b) alkaloids that have been quaternized, e.g., by methylation of a tertiary nitrogen group. Names of (a) are completed by citing the anion (if known) in the modification, e.g., “chloride”; (b) are usually named by adding “ium” to the neutral alkaloid name, and indicating the quaternizing substituents as in regular substitutive nomenclature; e.g., **Morphinanium, 17,17-dimethyl-**, iodide (1:1) by quaternization of **Morphinan**. When the location of the quaternary center is unknown, the “ium” ending is omitted and the quaternary compound is named as alkaloid compd. with iodomethane (1:1). Nonquaternary derivatives of the alkaloids described in (a), above, are named by subtractive prefixes, e.g., demethyl, or by “dihydro” terms.

Removal of a methyl group from the carbon skeleton of an alkaloid is indicated by “nor” with the locant of the carbon atom lost, but removal of a methyl group from a hetero atom is expressed by “demethyl.”

Ring contraction and enlargement in alkaloids is not permitted, and revert to systematic nomenclature.

Ring closure may be effected by insertion of heteroatoms (other than nitrogen) as bridges while maintaining stereoparent nomenclature, e.g., **Aspidospermidine, 19,21-epoxy**-. Such a bridge may also include one carbon atom, e.g., **6,14-Ethenomorphinan, 7,5-(methyleneoxy)**-. Replacement of one carbon atom by a heteroatom or insertion of additional nitrogen or replacement of existing nitrogen is not permitted.

Seco alkaloids are formed by ring cleavage and addition of hydrogen at the resulting terminal groups. Such compounds are given systematic names.

Ring-fused derivatives of alkaloid stereoparents are named systematically.

Degradation products of alkaloids in which ring cleavage and removal of large portions of the molecule still leave intact some rings and the original stereochemical relationships are named, when possible, as derivatives of a smaller alkaloid stereoparent. When this is impossible and the structure is known, degradation products of Class C alkaloids are named systematically, but for those of unknown structure, only the author's names are employed.

For steroidal alkaloids, see ¶ 211.

205. Amino acids. The following biologically significant amino acids are

stereoparents:

Alanine	Isoleucine
β-Alanine	Isovaline
Alloisoleucine	Leucine
Allothreonine	Lysine
Arginine	Methionine
Asparagine	Norleucine
Aspartic acid	Norvaline
Cysteine	Ornithine
Cystine	Phenylalanine
Glutamic acid	Proline
Glutamine	Serine
Glycine	Threonine
Histidine	Tyrosine
Homocysteine	Tryptophan
Homoserine	Valine

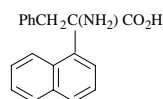
The following amino carboxylic, amino sulfonic, and amino arsonic acids, indexed prior to 1972 at their trivial names, are now named either systematically or as derivatives of an amino acid listed above:

Trivial name	CA Index Name
Allocystathionine	Homocysteine, S-(2-amino-2-carboxyethyl)-
Anthranilic acid	Benzoic acid, 2-amino-
Arsanilic acid (3 isomers)	Arsonic acid, As-(aminophenyl)-
Carnosine	Histidine, β-alanyl-
Creatine	Glycine, N-(aminoiminomethyl)-N-methyl-
Cystathionine	Homocysteine, S-(2-amino-2-carboxyethyl)-
Ethionine	Homocysteine, S-ethyl-
Hippuric acid	Glycine, N-benzoyl-
Lanthionine	Cysteine, S-(2-amino-2-carboxyethyl)-
Metanilic acid	Benzenesulfonic acid, 3-amino-
Panthothenic acid	β-Alanine, N-(2,4-dihydroxy-3,3-dimethyl-1-oxobutyl)- (see ¶ 224)
Sarcosine	Glycine, N-methyl-
Sulfanilic acid	Benzenesulfonic acid, 4-amino-
Taurine	Ethanesulfonic acid, 2-amino-
Thyronine	Tyrosine, O-(4-hydroxyphenyl)-
Thyroxine	Tyrosine, O-(4-hydroxy-3,5-diiodophenyl)-3,5-diiodo-

The configurational descriptors D- and L- are placed before the stereoparent names; no descriptor is cited for the optically inactive mixture or racemic form; thus, L-Leucine; D-Valine; Phenylalanine. In the absence of contrary evidence, the L-isomer is assumed for amino acid stereoparents, except **Glycine** and **β-Alanine**, which possess no asymmetric center, and **Alloisoleucine** and **Allothreonine** (see below). When the original document clearly indicates that an amino acid is synthetic, it is indexed as the racemic form. The same assumptions are made for their radicals, which are employed in peptide nomenclature, and for derivatives such as esters, salts, and *N*-, *O*-, and *S*-derivatives indexed at the stereoparent. No assumptions are made for carbon-substituted derivatives or for derivatives named systematically. Systematically named amino acids of known stereochemistry are assigned the absolute descriptors *R* and *S* in the modification. Of the diastereoisomeric pairs, assumptions in favor of **Isoleucine** over **Alloisoleucine** and of **Threonine** over **Allothreonine** are made. The absolute descriptors *R* and *S* (with locants) are cited in the modifications of diastereoisomeric derivatives of amino acid stereoparents to define the second asymmetric center, e.g., L-**Aspartic acid, 3-hydroxy-**, (3*R*)- and L-**Proline, 4-methyl-**, (4*S*)-

Phenylalanine is a stereoparent employed for Alanine, 3-phenyl-. It is treated in substitutive nomenclature as though it were the conjunctive name Benzenealanine. The naturally occurring isomer is L-**Phenylalanine**, which affords the radical L-phenylalanyl. Derivatives containing higher functions or more preferred ring systems are named systematically according to the regular rules.

Example:



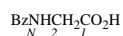
1-Naphthaleneacetic acid, α-amino-α-(phenylmethyl)-

Radicals derived from the names of amino acid stereoparents, e.g., glycyL, L-alanyl, L-phenylalanyl, are employed only in naming peptides (¶ 206). In other situations, systematically named radicals are used; e.g., (2-aminoacetyl) instead of glycyL. The phenylalanyl radical is considered to be a specially named one-part radical; no parentheses are placed around it when it is unsubstituted. Stereoparent radical names are derived by replacing the final “-ine” by “-yl” (an exception is **Cysteine**, which affords cysteinyl); **Tryptophan** gives tryptophyl; **Aspartic acid** and **Glutamic acid** radicals are as follows:

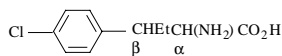
-COCH ₂ CH(NH ₂)CO-	aspartoyl
HO ₂ CCH ₂ CH(NH ₂)CO-	α-aspartyl
-COCH ₂ CH(NH ₂)CO ₂ H	β-aspartyl
-CO(CH ₂) ₂ CH(NH ₂)CO-	glutamoyl
HO ₂ C(CH ₂) ₂ CH(NH ₂)CO-	α-glutamyl
-CO(CH ₂) ₂ CH(NH ₂)CO ₂ H	γ-glutamyl

Amino acids are given less preference for special treatment than other stereoparents. They are ranked just above the unsubstituted parent acids; thus, **Alanine** (2-aminopropanoic acid) is ranked above **Propanoic acid** but below **Butanoic acid**. All carbon-substituted derivatives of **Glycine** and **β-Alanine** are indexed at systematic names, but the carbon-substituted *radicals* are permitted in peptide nomenclature.

Examples:



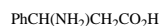
Glycine, N-benzoyl-



L-Phenylalanine, 4-chloro-β-ethyl-
(β*R*)- (not L-Norvaline, 3-(4-chlorophenyl)-, (3*R*)-)



Octanoic acid, 2-amino-2-methyl-
(not Alanine, α-hexyl-)

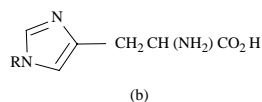
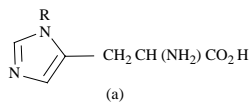


Benzenepropanoic acid, β-amino-
(β*R*)- (not β-Alanine, 3-phenyl-, (3*R*)-)

O-Substituted derivatives of the hydroxy amino acids (**Allothreonine**, **Homoserine**, **Serine**, **Threonine**, and **Tyrosine**) and *S*-derivatives of the mercapto amino acids (**Cysteine** and **Homocysteine**) are named at those stereoparents, e.g., **Serine, O-methyl-** and **L-Cysteine, S-acetyl-**. The stereoparent **Methionine**, CH₃SCH₂CH₂CH(NH₂)COOH, is the *S*-methyl derivative of **Homocysteine**. Derivatives in which this methyl group is substituted are indexed as **Homocysteine** derivatives. *S*-Oxide derivatives of **Cysteine** and **Homocysteine** are indexed as sulfinyl and sulfonyl derivatives of simpler parents; however, *S*-oxides of *S*-substituted derivatives (including Methionine) are named as such.

Conjunctive names are not formed from amino acid stereoparents attached to ring systems; instead, such a combination is usually indexed at a systematic conjunctive name with an "α-amino" substituent. Derivatives of **Arginine**, H₂NC(:NH)NH(CH₂)₃CH(NH₂)COOH, substituted in the guanidino group are indexed as derivatives of **Ornithine**, H₂N(CH₂)₃CH(NH₂)COOH.

Histidine (R = H) is capable of existing in the following tautomeric forms:



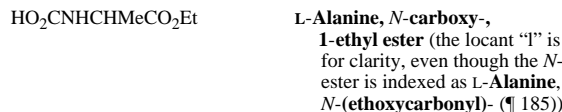
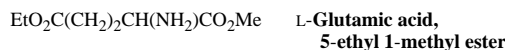
When the tautomers are stabilized by substitution on a nitrogen atom of the ring, two isomers result. The side chain has been arbitrarily assigned to the 4-position of the ring and, if R = ethyl, the structures shown above are indexed:

- (a) **L-Histidine, 3-ethyl-**
(b) **L-Histidine, 1-ethyl-**

It should be noted that while (b) conforms to the correct treatment for **1*H*-Imidazole**, the numbering of (a) violates the rules (**3*H*-Imidazole** is not used as a heading parent) and is adopted only for these special cases. A 1-substituent is assumed in indexing indefinite 1- or 3-derivatives of **Histidine**.

Esters of amino acid stereoparents with nonstereoparents are indexed at the amino acid names; e.g., **L-Alanine, 4-carboxyphenyl ester**. Esters with other stereoparents are indexed at the parent which represents the greatest number of highest functions. Usually only one index entry is made for an ester. Locants are used with ester terms when necessary.

Examples:

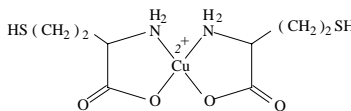


Amides of amino acids are indexed at systematic names, e.g., **Acetamide**, **2-amino-** (not **Glycinamide**), but peptide amides (¶ 206) are indexed at C-terminal amino acid names, e.g., **Glycinamide**, **L-alanyl-**.

Anhydrides of amino acids are indexed at the amino acid name with "anhydride" or "anhydride with" terms in the modification. Cyclic anhydrides and lactones are indexed as heterocycles. Hydrazides are indexed at acid leadings with "hydrazide" terms in the modifications. Molecular addition compounds of nonstereoparents with amino acids named as stereoparents receive preferred index names at the latter, but *Formula Index* entries will be found also at the other component(s). The preferred name of an addition compound of two or more stereoparents is chosen on the basis of the maximum number of highest functions in the stereoparent.

Beryllium, magnesium, aluminum, gallium, indium, thallium, and transition-metal salts of amino acids are indexed as coordination compounds (¶ 215) if sufficient information is presented, and the special stereochemical descriptors (¶ 203 III) for such compounds are then adopted. Other salts are indexed at such names as **Glycine**, sodium salt (1:1); **L-Phenylalanine**, methyl ester, hydrochloride (1:1).

Example:

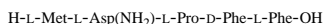


Copper, bis(L-homocysteinato-κ*N*, κ*O*)-, (T-4)-

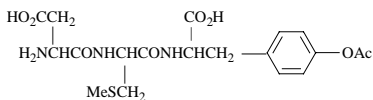
206. Peptides are generally named by use of amino acid stereoparents (¶ 205) and stereoparent radicals; the L-isomers are assumed for indexing purposes in the absence of contrary information. Trivial names of some peptides and all proteins are employed, and special "Cyclo" names are used for tri- and higher cyclic peptides.

Linear peptides without trivial names are indexed at "amino acid sequence names." The heading parent is the C-terminal amino acid. Enclosing marks and locants for points of attachment of the amino acid radicals are omitted; however, Greek-letter locants are cited for aspartyl and glutamyl radicals, and "N⁶." and "N⁵." are used with **Lysine** and **Ornithine**, respectively, and their radicals, when the attachment is not on the α-amino group (*N*²-position). *N*-Derivatives of the radicals are expressed as substituents. Esters of carboxy groups of aspartic and glutamic acid residues are cited in the modification; *O*- and *S*-acyl derivatives of seryl, cysteinyl, etc., radicals are named as, e.g., *O*-acetyl-L-seryl, etc., radicals and even when a hydroxyl- or mercapto-group-containing amino acid is the heading parent, the *O*- or *S*-acyl group is treated as a substituent.

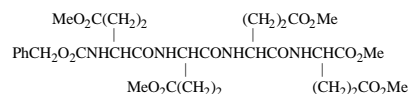
Examples:



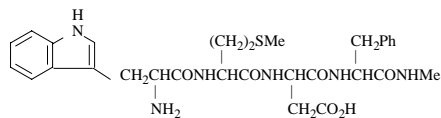
L-Phenylalanine, L-methionyl-L-asparaginyl-L-prolyl-D-phenylalanyl-



L-Tyrosine, L-α-aspartyl-S-methyl-L-cysteinyl-O-acetyl-



L-Glutamic acid, N-[(phenylmethoxy)carbonyl]-L-α-glutamyl-L-α-glutamyl-L-α-glutamyl-, 1,2,3,4,5-pentamethyl ester



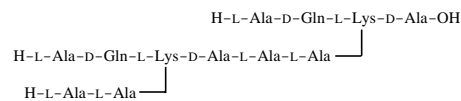
L-Phenylalaninamide, L-tryptophyl-L-methionyl-L-α-aspartyl-N-methyl-

To be named as such, a linear peptide must have at least two standard amino acids. In peptide nomenclature, standard amino acids are defined as amino acid stereoparents (¶ 205), plus α -Asparagine, $\text{H}_2\text{NCOCH}(\text{NH}_2)\text{CH}_2\text{COOH}$, and α -Glutamine, $\text{H}_2\text{NCOCH}(\text{NH}_2)(\text{CH}_2)_2\text{COOH}$. Peptides that do not meet this requirement are named systematically; e.g., **Butanoic acid, 4-amino-2-[(2-aminoacetyl)amino]-, (2S)-**.

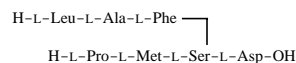
When the above requirement is met, nonstandard α -amino acids are allowed as residues in terminal or nonterminal positions. Nonstandard amino acids in which the amino group is not α to the carbonyl are allowed provided they are nonterminal. All nonstandard amino acids are assigned systematic acid or acyl names. Absolute stereochemistry is described by the use of *R/S* terms preceded by locants; e.g., **L-Alanine, 5-oxo-L-prolyl-(α S)- α -amino-4-chlorobenzenebutanoyl-**; **1H-Indole-2-carboxylic acid, L-seryl-L-methionylactahydro-, (2S,3aR,7aR)-**; **L-Proline, L-histidyl-(3R)-3-(methylamino)hexanoylglycyl-L- α -aspartyl-**.

Branched-chain peptides may comprise N^5 - or N^6 -isopeptide derivatives of **Ornithine** or **Lysine**, respectively, or *O*- or *S*-derivatives of hydroxy or mercapto amino acids (heterodetic homomeric peptides). Both types are named as substituted derivatives of the parent linear peptides.

Examples:



D-Alanine, L-alanyl-D-glutamyl-N⁶-[L-alanyl-D-glutamyl-N⁶-(L-alanyl-L-alanyl)-L-lysyl-D-alanyl-L-alanyl-L-alanyl]-L-lysyl-

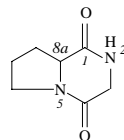


L-Aspartic acid, L-prolyl-L-methionyl-O-(L-leucyl-L-alanyl-L-phenylalanyl)-L-seryl-

Higher functions in peptides are expressed as substituents. When the C-terminal residue is not an amino acid or amino acid amide, but an acid-related compound such as an alcohol, aldehyde, or nitrile, the adjacent amino acid amide residue is adopted as the heading parent, and the terminal group is expressed as an *N*-(cyanomethyl), *N*-(2-oxoethyl), etc., substituent.

Cyclic dipeptides are indexed at systematic heterocycle names, with cross-references at "Cyclo" names (see below).

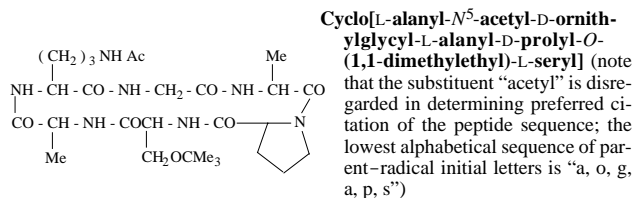
Example:



Pyrrolo[1,2-a]pyrazine-1,4-dione, hexahydro-

Tripeptides and longer peptides containing two or more standard amino

acids are assigned "Cyclo" names formed by citing the amino acid radicals (with substituents) as for an amino acid sequence name, placing them in enclosing marks, and prefixing the term "Cyclo". The order of citation is by lowest alphabetical order of *parent* amino acid residues (substituents are disregarded) when the residue is standard, but when it is nonstandard (e.g., 2-aminobutanoyl), substituents are included in determining the order of citation.



Cyclo[L-alanyl-N⁵-acetyl-D-ornithylglycyl-L-alanyl-D-prolyl-O-(1,1-dimethylethyl)-L-seryl] (note that the substituent "acetyl" is disregarded in determining preferred citation of the peptide sequence; the lowest alphabetical sequence of parent-radical initial letters is "a, o, g, a, p, s")

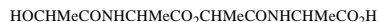
When ring formation has taken place by way of a side-chain peptide linkage, the acyclic peptide is named and the linkage expressed in the modification by a phrase of the type "(10→4)-lactam" in which the lactam linkage is denoted by amino acid residue locants (numbered from the N-terminus) with the acid end of the linkage cited first.

Peptide lactones not assigned desipeptide names (see below) are expressed by modification terms such as "(3→1)-lactone." Peptides containing disulfide linkages are indexed at the reduced (cysteinyll-group-containing) form with terms such as "(2→2')-disulfide," "cyclic (1→6)-disulfide" and "(5→3)-disulfide with ..." in the modification.

N-(Peptidyloxy) derivatives of nitrogenous heterocycles are indexed at the peptide names, with the rings cited as ester terms.

Desipeptides contain ester linkages with hydroxy acids as well as amide (peptide) linkages with amino acids. Those with three or more acid residues, of which at least two are standard amino acid residues, are indexed by "desipeptide nomenclature"; otherwise a systematic name is employed. A desipeptide name is based on the C-terminal amino acid and indexed by methods analogous to those for amino acid sequence names. Trivially named hydroxyacyl radicals (lactoyl, glycoloyl, etc.) are given systematic acyl radical names when nonterminal, but treated as substituents or ester terms when terminal.

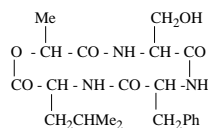
Example:



L-Alanine, N-[(2R)-2-hydroxy-1-oxopropyl]-L-alanyl-(2R)-2-hydroxypropanoyl-

Cyclic dipeptides are indexed as heterocycles. Cyclic tri- and higher desipeptides are indexed at "Cyclo..." names analogous to those for cyclic peptides. Cyclic desipeptides with one hydroxy acid are named as such, not as lactones.

Example:

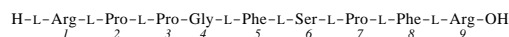


Cyclo(2S)-2-hydroxypropanoyl-L-seryl-L-phenylalanyl-L-leucyl] (the hydroxy acyl radical is alphabetized at "h," not "p")

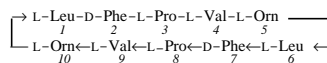
The Greek letter ψ , shorthand for "pseudo," is used to convey the fact that a peptide bond has been replaced by a pseudopeptide bond. If the structure contains the moiety $\dots\text{NH-CHR-X-X'-CHR'-CO}\dots$, where R and R' are amino acid side-chain groups and X and X' are the groups that replace the peptide bond, then the format of the ψ term is $\dots\text{A-}\psi(\text{X-X}')\text{-B}\dots$, where A is the amino acid whose carbonyl group has been modified to X (or remains unmodified) and B the amino acid whose α -amino group has been modified to X' (or remains unmodified). X and X' are shown as strings of element symbols, separated by a bond; e.g., **L-Leucine, L-alanyl-L-valyl- ψ (CH₂-CH₂)-L-isoleucyl-L-alanyl-**.

Naturally occurring biologically active peptides with five or fewer amino acid residues are indexed as described above. The more common natural peptides with six to fifty residues are assigned the trivial names commonly used in the literature. For cysteine-containing natural peptides, only the reduced form is illustrated (**Oxytocin** and **Vasopressin**, below, are exceptions).

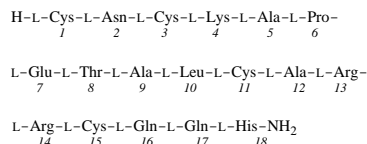
Examples:



Bradykinin



Gramicidin S



Apamin (reduced)

Species variations are dealt with by citing the name of the species as a homograph definition after the heading. Each species variant is an independent stereoparent; e.g., **Calcitonin (salmon reduced)**; **Calcitonin (human reduced)**.

Replacement of one amino acid residue by another is indicated at a trivially named peptide heading by citing the names of the new amino acids in numerical (not alphabetical) order as substituents; e.g., **Glucagon (swine), 4-L-serine-10-L-alanine**. In addition, the chain of the reference compound can be extended at either end, either by substitution of the N-terminal α -amino group or by citing additional terms with locants derived from the highest present by addition of "a," "b," etc. In a similar manner, *insertion* of amino acid units between existing ones is indicated by "endo" terms with "a" locants derived from the lower of the two neighboring units (e.g., "3a" indicates insertion between "3" and "4"). Removal of a unit is indicated by a "de" term such as "4-desulfo" to indicate removal of only a modifying group in a unit, or "6-de-L-glutamic acid" to express removal of an entire unit.

Examples:

Kallidin, N²-L-alanyl- (N-terminal extension)

Glucagon (swine), N-acetyl- (N-terminal extension)

Bradykinin, 9a-L-valine-9b-L-lysine- (C-terminal extension)

Fibrinopeptide A (human), 16a-D-serinamide- (C-terminal extension)

Bradykinin, 6a-endo-L-alanine- (insertion)

Caerulein, 4-desulfo- (removal of modifying group)

Caerulein, 4-de(O-sulfo-L-tyrosine)- (removal of unit)

Combinations of various types of structural modifiers are indicated by citing them in numerical order. When the modifying operations total at least one-half the number of units in the original parent, a regular peptide name is employed.

The Greek letter ψ (see above) is used in derivative names to indicate a modified peptide bond. The format of the ψ term is ...-Aⁿ ψ ⁿ⁺¹(X-X')-B-..., where n is the residue number of the amino acid A whose carbonyl group has been modified to X (or remains unmodified) and n+1 the residue number of the amino acid B whose α -amino group has been modified to X' (or remains unmodified). A and B are cited in the name only if they are otherwise modified; e.g., **Bradykinin, ψ^8 (CH=CH,E)-8-L-tyrosine-**. The formatting of the stereochemical data for X-X' follows standard literature practice.

In **Angiotensin I** and **Angiotensin II**, the amino acid in the 5-position, if known, is cited in the inverted part of the heading, e.g., **Angiotensin I, 5-L-isoleucine-**.

Oxytocin and **Vasopressin** derivatives in the disulfide form are named at these headings with replacement, etc., terms as usual, but reduced analogs are indexed at amino acid sequence names, not at **Oxytocin (reduced)** and **Vasopressin (reduced)**. The amino acid at position 8 of Vasopressin is always specified if known.

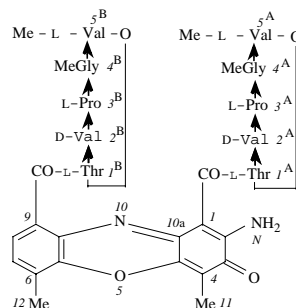
In α^{1-39} -**Corticotropin (swine)** "a" indicates that this was the first principle isolated; the superscripts give the range of amino acid units. Fragments containing more than twelve sequential units receive names such as α^{1-24} -**Corticotropin** and α^{11-39} -**Corticotropin**. An amino acid sequence name is employed for fragments of fewer than twelve units.

Insulin contains two peptide chains, an A-chain of 21 amino acid units and a B-chain of 30 units, connected at two points by disulfide bridges. Replacement names that retain the disulfide bridges and have fewer than 11 and 15 residue changes in the A- and B-chains, respectively, are formed in the usual way. Locants have superscript letters to indicate to which chain they belong; e.g., **In-**

sulin (cattle), 30^B-L-methionine-. The reduced forms of the individual insulin chains are also stereoparents; internal disulfide bonds are expressed in the modification.

Actinomycins are a class of natural products that contain peptide chains attached to non-peptide moieties. **Actinomycin D** (sometimes called C₁) is one member of the actinomycin family.

Example:



Actinomycin D

The "Me-L-Val" symbol denotes N-methyl-L-valine and "Me-Gly" denotes N-methylglycine (sarcosine). Substitution in the phenoxazine ring is expressed before amino-acid replacement, etc., in the peptide moiety.

Examples:

Actinomycin D, 8-bromo-7-chloro-

Actinomycin D, 2-deamino-2-hydroxy-3^A-D-proline-4^A-D-norleucine-

Homopolymers of amino acids are indexed by polymer procedures (¶ 122); e.g., **L-Alanine**, homopolymer. The structural repeating unit is indexed at **Poly[imino[(1S)1-methyl-2-oxo-1,2-ethanediyl]]**. The stereochemical assumptions are the same as for the monomeric amino acids. Peptides of indefinite molecular weight with repeating peptide sequences are named as homopolymers at the peptide monomer names and at structural repeating unit names.

207. Proteins. Proteins are arbitrarily defined for indexing purposes as peptides containing more than 50 amino acids. Proteins whose complete amino acid sequences are known are indexed as chemical substances from all patents and journals covered by CAS. The protein sequence is entered into the CAS sequence database, and is searchable and displayable on STN. Partial protein sequences are also indexed from selected journals.

Each protein sequence is given a unique name based on controlled vocabulary, as well as author terminology, the species of origin, and additional information which may include strain/clone, gene, and subunit/isoform, etc., as applicable.

Protein fragments may be prefixed with two numbers, relating to the range of amino acids represented; e.g., 1-124-Somatotropin (cattle). Replacement names, as for peptides, are used for analogs. If the range of amino acids cannot be based on a complete protein, fragment is included in the name.

208. Carbohydrates. Carbohydrate stereoparents are defined for indexing purposes as polyhydroxy acids, aldehydes, ketones, alkanes, and their derivatives, with a skeleton of five or more carbon atoms, more than half of which must be attached to oxygen (or another chalcogen) or nitrogen, and at least one of the chalcogen attachments must be by a single bond to a nonterminal carbon atom. At least half of the nonterminal carbon atoms must be asymmetric. Anomeric carbon atoms, whether terminal or non-terminal, are not counted in determining the number of asymmetric carbon atoms. Except for uronic and ulosuronic acids, the open chain is numbered to give the highest function the lowest possible locant. Illustrative structural diagrams related to current index entries will be found in the *Chemical Substance Index* for open-chain forms and common cyclic forms of carbohydrate stereoparents. Stereoparents representing the following carbohydrates and their derivatives are employed as heading parents:

Pentoses:
Hexoses:

2-Hexuloses:
Acids:

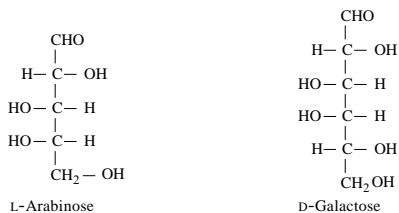
Arabinose, Lyxose, Ribose, Xylose.
Allose, Altrose, Galactose, Glucose,
Gulose, Idose, Mannose, Talose.
Fructose, Psicose, Sorbose, Tagatose.
Ascorbic acid (¶ 224), Muramic acid,
Neuraminic acid.

Monosaccharides that exist in the open form are indexed at the stereoparents. Higher functions are expressed as substituents or in the modification. Derivatives of the cyclic forms are indexed at the highest function if a glycosyl radical can be used to express the sugar, which is ranked as a polyhydric alcohol unless a higher function, e.g., a nonglycosidic ketone or aldehyde, is expressed as a suffix.

When a second stereoparent is represented in a structure, the parent of higher functionality is chosen in indexing.

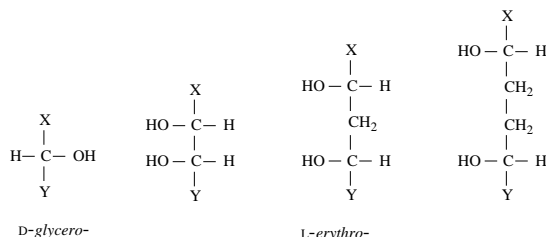
Configurational descriptors, D and L, are placed before stereoparent names, including monosaccharide semisystematic names (see below). Examples are **D-Glucose** and **L-arabino-Hexose, 2-deoxy-**. In the Fischer projections of the open forms, the carbon skeleton is displayed vertically, with locant "1" at the top. The D-series can then be recognized by the hydroxyl group to the *right* of the bottom nonterminal asymmetric carbon atom.

Examples:



Configurational prefixes, derived from trivial aldose names, are used in semisystematic carbohydrate nomenclature; for one asymmetric carbon atom, e.g., >CHOH, >CHOCH₃, >CHNH₂, *glycero* is the prefix used (with D or L as described above); with two, *erythro* and *threo*; with three, *arabino*, *lyxo*, *ribo*, and *xylo*; with four, *allo*, *altro*, *galacto*, *gluco*, *gulo*, *ido*, *manno*, and *talo*. (The centers need not be on neighboring carbon atoms.) For more than four consecutive centers, combinations of these terms are used.

Examples ("X" is the group with the lowest-numbered carbon atom):



In choosing a monosaccharide stereoparent name (when such a choice is necessary), (a) the oxo (or higher) function is numbered low (except the carboxyl group in uronic and ulosuronic acids); (b) the name appearing earliest alphabetically is chosen; (c) "D" is preferred to "L"; (d) the anomeric prefix "α" is preferred to "β"; (e) lowest locants for substituents are employed; (f) the lowest locant is used for the first-cited substituent.

Systematic carbohydrate names, employed for monosaccharides other than those with trivial names, are based on stem names which express the size and function; the stem names for open-chain aldoses of five or more carbon atoms are **Pentose, Hexose, Heptose, Octose, Nonose**, etc.; corresponding ketose stems are **Pentulose, Hexulose**, etc. (Additional terms are used to indicate ring size if necessary; see below.) The stem names are preceded by stereochemical descriptors. 2-Hexuloses have trivial names (see above); other ketoses are named systematically, e.g., **L-erythro-2-Pentulose**. For meso-forms, the D- and L- configurational symbols are not needed; e.g., **erythro-3-Pentulose**. Diketoses have names of the type **D-threo-2,4-Hexodiolose**; ketoaldoses have "osulose" names such as **D-ribo-Hexos-3-ulose**; dialdoses have names such as **D-gluco-Hexodialdose**; chalcogen analogs are indexed by use of thio, etc., prefixes, e.g., **D-Glucose, 1-thio-**; replacement of hydroxyl by hydrogen is denoted by "deoxy" terms.

Substitution on carbon with prior removal of a hydroxyl group requires citation of "deoxy" and the substituent prefix in alphabetic order, e.g., **D-Glucose, 2-(acetylamino)-2-deoxy-**. When the existing hydrogen is substituted on a carbon atom already carrying an oxygen (or other chalcogen) or nitrogen group in the open or cyclic forms, the italic capital letter *C* is employed, e.g., **D-Ribose, 3-C-(nitromethyl)-**. When both the hydrogen and hydroxyl are replaced by nonchalcogen, nonnitrogen substituents, the stereochemistry is expressed by a Sequence Rule descriptor at the systematic saccharide name, e.g., **D-ribo-Hexose, 3-bromo-3-chloro-3-deoxy-**, (3*S*).

Substitution of hydrogen on a hydroxyl group of a carbohydrate is denoted by "O" locants (or by "S", etc., if chalcogen replacement has also taken place). Examples:

D-Mannose, 2,3,4,5,6-penta-O-methyl-

D-Glucose, 2-S-ethyl-2-thio-

D-Glucitol, 1-O-ethyl-1-C-(phenylamino)-

Cyclic acetals employ bivalent radicals with "O" terms, e.g., **D-Ribose, 2,3:4,5-bis-O-(1-methylethylidene)-**.

Oximes and hydrazones are expressed in the modification, osazones similarly as dihydrazones of osuloses. Hydrates, acetals, hemiacetals and esters

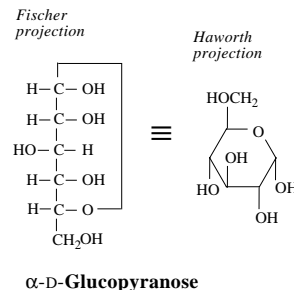
are also named in the modification.

Examples:

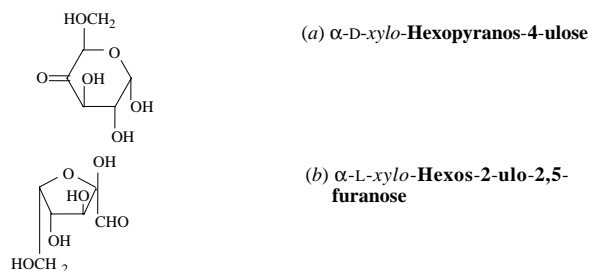
D-Xylose
diethyl dithioacetal

D-Xylose
2,3-diacetate 4,5-dibenzoate

Cyclic hemiacetal forms of monosaccharides are indexed by inclusion in the name of a term indicating the ring size, if known; five, six, and seven-membered rings, are denoted by "furanose," "pyranose," and "septanose" suffixes. Two anomers, named "α" and "β," result on ring formation, and these Greek letters are employed as anomeric prefixes, which are placed ahead of the configurational descriptors (D or L) in the name.



The following examples show the derivation of names for ketoaldoses when the ring closure involves (a) the aldehyde, and (b) the keto function.

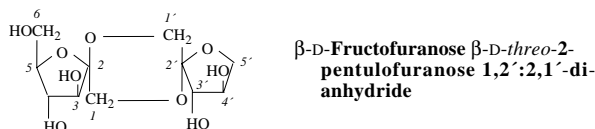


More complicated cases, e.g., cyclic forms of dialdoses and higher ketoses, are named in accordance with rules (lowest locants for the keto group, alphabetically preferred configurational prefixes, etc.) already described. Locants, e.g., "-6,10-" are inserted before the ring-size descriptor in the name, and "α" or "β" is also cited if the anomeric carbon is numbered lower than the reference carbon atom in the ring being formed, otherwise *R* or *S* is used.

Nitrogen analogs of cyclic sugars are named systematically.

Intramolecular *anhydrides* are denoted by terms such as "1,5-anhydro" in which the locants define the pair of hydroxyl groups involved. The sulfur analogs are named with "dideoxy-epithio" terms. Intermolecular anhydrides are polysaccharides (below); intermolecular dianhydrides are named by citing the word "dianhydride" after the name(s) of the parent monosaccharides (an aldose precedes a ketose); two pairs of locants define the positions of the anhydride linkages.

Example:

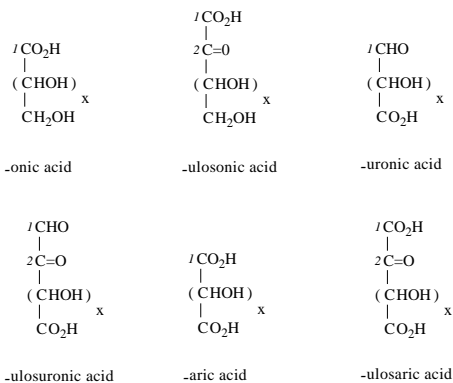


Carbohydrate *acids* are named by characteristic suffixes, as follows:

The stems of aldaric, aldonic and uronic acid names are derived from trivial (common) aldose names whenever possible. Acids containing a keto function are named from the systematic stem names. Acid halide, amide, and nitrile names are derived as usual. Esters, hydrazides, salts, and lactones are expressed in the modification. Lactams are named systematically (§171).

Examples:

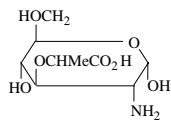
D-Gluconoyl chloride



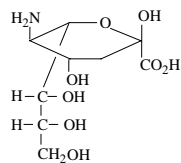
L-Ribonic acid γ -lactone

The trivial names **Muramic acid** and **Neuraminic acid** are used for the structures shown below; the acyl radicals muramoyl and neuraminoyl, and the glycosyl radicals muramosyl and neuraminosyl, are also employed in indexing. (**Isomuramic acid** is treated similarly; it is the muramic acid (*S*)-epimer about the carbon atom bearing the carboxyl group.)

Examples:



α -Muramic acid
(the *R*-epimer)



β -Neuraminic acid

Glycosyl radicals derived from trivially and systematically named saccharides by removal of the anomeric (hemiacetal) hydroxyl group have the suffix “-osyl,” e.g., β -D-mannopyranosyl (if the ring size is known), D-mannosyl, α -D-arabino-hexopyranos-2-ulos-1-yl. Uronic acid radicals are derived by replacing the “-ic acid” by “-osyl,” e.g., β -D-glucopyranuronosyl; acid derivatives, e.g., uronamides, yield “-uronamidosyl” radicals, etc.

The following stereochemical and ring size assumptions are made when an author does not completely define a glycosyl radical:

<u>FOR</u>	<u>ASSUME</u>
galactosyl	D-galactopyranosyl
glucosyl	D-glucopyranosyl
mannosyl	D-mannopyranosyl
xylosyl	D-xylopyranosyl
L-fucosyl	6-deoxy-L-galactopyranosyl
D-fucosyl	6-deoxy-D-galactopyranosyl
rhamnosyl	6-deoxy-L-mannopyranosyl
fructosyl	D-fructofuranosyl
apiosyl	D-apio- β -D-furanosyl

Note that no assumption is made for fucosyl when the absolute stereo is not indicated.

Glycosyl halides, isocyanates, etc., without functions higher than a polyol in the unsubstituted saccharide have names containing the “-osyl” radical; otherwise the heading parent expresses the higher function.

Examples:

α -D-Mannopyranosyl bromide

β -D-Glucopyranuronic acid, 1-chloro-1-deoxy-

Glycosylamines are named by similar principles.

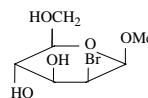
Examples:

α -D-Glucopyranosylamine

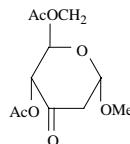
α -D-Glucopyranuronamide, 1,1'-iminobis[1-deoxy-

Glycosides are mixed acetals derived by replacement of the hydrogen atom on the anomeric hydroxyl group of a saccharide by a group derived from an alcohol or phenol. Glycoside heading parents, e.g., α -D-Ribofuranoside, are employed. In the inverted part of the heading, the radical derived from the alcoholic or phenolic aglycon is cited, followed by a space. Then any substituents of the saccharide are expressed in the usual way. When functions higher than the saccharide (which is normally a polyol) are present in the aglycon, a heading parent which expresses the greatest number of highest functions is chosen, provided that an appropriate glycosyl radical name can be employed to express the saccharide as a substituent. When the functionality is equal in the two portions of the molecule, the stereoisomer is preferred. Glycoside parents are also derived from uronic acids and ulosonic acids, e.g., α -D-Mannopyranosiduronic acid; α -D-arabino-2-Hexulofuranosidonic acid.

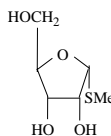
Examples:



β -D-Mannopyranoside, methyl 2-bromo-2-deoxy-



α -D-erythro-Hexopyranosid-3-ulose, methyl 2-deoxy-4,6-diacetate



α -D-Ribofuranoside, methyl 1-thio-

Glycosides of ring systems are indexed at the saccharide headings unless the aglycon contains a higher function or the glycosyl attachment is at a nitrogen atom. C-Glycosides (glycosyl derivatives with carbon-carbon bonds) of ring systems are indexed at the higher function.

Examples:

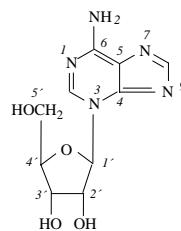
D-Glucitol, 1,5-anhydro-1-C-phenyl-(1*R*)-

4*H*-1-Benzopyran-4-one, 8- β -D-glucopyranosyl-2-phenyl-

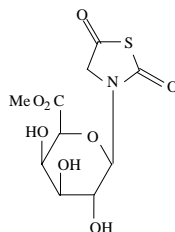
A naturally occurring glycoside is indexed at the systematic (or stereoparent) name if the structure, including the ring-size of the saccharide, is known, whether or not the stereochemistry has been elucidated. (A “glucoside” is assumed to be the β -D-glucopyranoside, a “rhamnoside” the 6-deoxy- α -L-mannopyranoside.)

N-Glycosyl derivatives of heterocycles are usually indexed at the heterocycle names (see also Nucleosides and Nucleotides, ¶ 210), but a saccharide containing an expressed aldehyde or higher functional suffix is preferred.

Examples:



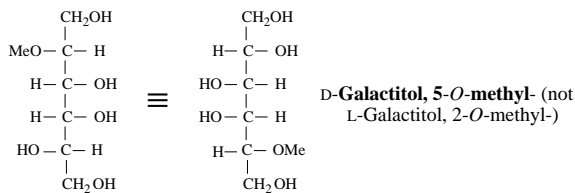
3*H*-Purin-6-amine, 3- β -D-ribofuranosyl-



β -D-Galactopyranuronic acid, 1-deoxy-1-(2,5-dioxo-3-thiazolidinyl)-, methyl ester

Alditols are polyhydric alcohols derived mainly by reduction of aldehydes. They are named by changing the suffix “-ose” to “-itol.” Since the end groups are alike, they are more symmetrical than saccharides; the preferred heading parent is the one in which the trivial name (or the configurational prefix (*erythro*, etc.) of a semisystematic name) and then the configurational descriptors (D and L) expresses the lowest alphabetic order. Hence Gulitol is cross-referred to **Glucitol**, and *D-glycero-L-gulo* is preferred over *D-glycero-D-ido*. Lowest locants for substituents are considered only after the heading parent has been determined.

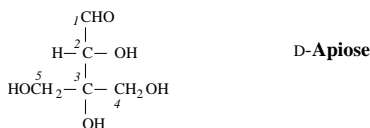
Example:



The *meso* alditols (**Ribitol**, **Xylitol**, **Allitol**, and **Galactitol**) do not require D or L unless they are substituted unsymmetrically, in which case the D-form is chosen. Higher chemical functions than the alditol are expressed as substituents of the alditol parent.

Branched-chain monosaccharides are generally named as derivatives of the linear saccharides, selecting first the highest function and then the longest chain, but the trivial name **Apiose** is used.

Example:



Olefinic monosaccharides are expressed by “en” in the stereoparent. Destruction of the anomeric center leads to an anhydro unsaturated alditol with the multiple bond assigned the lowest possible locant after the alphabetic choice (D before L, α before β) has been made. Geometrical isomerism about a double bond, when known, is indicated by *E* and *Z* descriptors.

Examples:

D-threo-Hex-2-enose, 2-(acetyl-amino)-2,3-dideoxy-
(2*Z*)-

9H-Purin-6-amine, 9-(2,3-dideoxy- β -D-erythro-hex-2-enopyranosyl)-

D-xyllo-Hex-1-enofuranosylamine, 2-deoxy-N-phenyl-

Oligosaccharides of known structure are given carbohydrate names which express the monosaccharide content. The open-chain form is used in naming reducing oligosaccharides in the absence of anomeric prefixes or contrary derivative information.

Trisaccharides and higher members are named by use of “arrow” nomenclature, in which arrows and locants indicate the direction and position of linkages from anomeric carbon atoms to hydroxylic carbon atoms. The reducing monosaccharide unit is named as the stereoparent. Other substituents of the parent are named last.

Examples:

<p>Lactose. Sucrose. Cellotriose. Stachyose.</p>	<p>See <i>D-Glucose, 4-O-β-D-galactopyranosyl-</i> See α-<i>D-Glucopyranoside, β-D-fructofuranosyl</i> See <i>D-Glucose, O-β-D-glucopyranosyl-(1\rightarrow4)-</i> <i>4-O-β-D-glucopyranosyl-(1\rightarrow4)-</i> See α-<i>D-Glucopyranoside, β-D-fructofuranosyl</i> <i>O-α-D-galactopyranosyl-(1\rightarrow6)-O-α-D-</i> <i>galactopyranosyl-(1\rightarrow6)-</i></p>
--	--

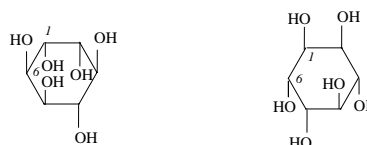
Polysaccharides are often indexed at common names, e.g., **Agar**, **Amylopectin**, **Cellulose**, **Starch**. Homoglycans (polysaccharides derived from one type of sugar residue) are named by converting the “-ose” suffix of an aldose or ketose, or the “-ic acid” of a glycuronic acid, to “-an,” e.g., β -**D-Mannan**, (1 \rightarrow 4)-; L-**Arabinan**; D-**Glucuronan**. Heteroglycans contain more than one kind of saccharide; the name, e.g., **Glucuronarabinoxylan**, expresses the saccharide with the higher chemical function first; if the functions are alike, longer chain and then alphabetic order decide. Esters and most other derivatives are cited in the modification. Synthetic homopolymers and copolymers are indexed by polymer nomenclature, e.g., L-**Arabinose**, homopolymer.

209. Cyclitols are cycloalkanes in which a hydroxyl group is attached to each of three or more ring atoms. Cyclitols of the cyclohexane series constitute the *inositols*; those that contain at least five asymmetric centers in the ring, of which at least three are directly bonded to oxygen (or another chalcogen) or nitrogen, are given **Inositol** stereoparent names; the others are named systematically as cyclohexanepolyols. Relative stereochemistry is expressed by special italicized configurational prefixes. The eight **Inositol** stereoparents, arranged according to the number and position of hydroxyl groups on the same side of the cyclohexane ring (as indicated by the numerical locants, which are not used in indexing) are:

<i>cis</i> - Inositol	(1,2,3,4,5,6)
<i>epi</i> - Inositol	(1,2,3,4,5)
<i>allo</i> - Inositol	(1,2,3,4)
<i>myo</i> - Inositol	(1,2,3,5)
<i>muco</i> - Inositol	(1,2,4,5)
<i>neo</i> - Inositol	(1,2,3)
<i>chiro</i> - Inositol	(1,2,4)
<i>scyllo</i> - Inositol	(1,3,5)

Choice of a preferred index name for an inositol derivative depends on (a) the alphabetically preferred configurational prefix in the order: *allo*, *chiro*, *cis*, *epi*, *muco*, *myo*, *neo*, *scyllo*; (b) the preferred configurational descriptor (D over L); (c) the lowest set of locants for substituent prefixes (¶ 137). The configurational descriptor D or L may be determined by numbering the hydroxyl groups (or replacement groups) which lie on *one side* of the ring beginning at each possible “position 1.” If the groups, e.g., the 1,2,4-groups in *chiro*-**Inositol**, are up when numbering clockwise, or down when numbering counterclockwise, the descriptor is L; if the groups are up in numbering counterclockwise or down in numbering clockwise, the descriptor is D. The D-stereoparent is chosen regardless of high locants for substituent prefixes. The D and L descriptors are used only when optical activity is present and can be determined from the original document.

Example:



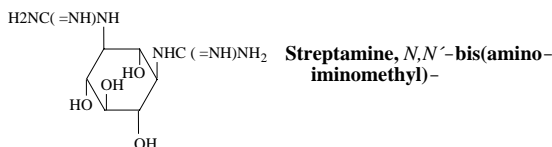
D-*chiro*-Inositol

L-*chiro*-Inositol

Ethers are named as *O*-derivatives; chalcogen analogs are expressed by “thio,” etc., in the inverted part of the heading. Esters are expressed by modification terms, e.g., “hexaacetate.” Glycosides are indexed at the **Inositol** stereoparent with *O*-glycosyl substituent prefixes. 1,2,3,4,5-Cyclohexanepentols (quercitols) are indexed at the alphabetically preferred **Inositol** parent by use of a “deoxy” prefix, and D or L determined as described above, e.g., *D-chiro*-**Inositol, 2-deoxy-** (not *D-chiro*-Inositol, 5-deoxy; not *D-muco*-Inositol, 2-deoxy; not *L-muco*-Inositol, 1-deoxy-). Replacement of one, two, or three hydroxyl groups, with retention of configuration, is expressed by “deoxy” terms and appropriate radicals. The capital italic letter *C* is used to denote replacement of hydrogen on a carbon atom to which a hydroxyl group is also attached, e.g., *scyllo*-**Inositol, 1-C-methyl-**.

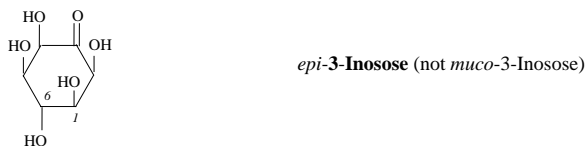
Inosamines and their *N*-acyl (including carboxy) derivatives are usually indexed at such names as *neo*-**Inositol, 2-amino-2-deoxy-**, but **Streptamine** is the stereoparent for 1,3-diamino-1,3-dideoxy-*scyllo*-inositol and derivatives.

Example:



Inosose is the stereoparent for 2,3,4,5,6-pentahydroxycyclohexanone stereoisomers.

Example:



210. Nucleosides and Nucleotides are hydrolytic products of nucleic acids; chemically, nucleosides are *N*-glycosyl derivatives of heterocyclic bases, principally purine and pyrimidine, and nucleotides are esters of nucleosides with phosphoric acid and polyphosphoric acids.

The bases are named systematically, with the tautomerism resolved for indexing purposes in favor of highest expressed function, etc. (¶ 122).

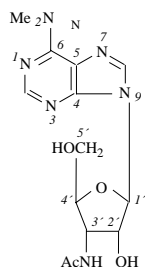
Trivial Name	Index Name
Adenine	9<i>H</i>-Purin-6-amine
Cytosine	2(1<i>H</i>)-Pyrimidinone, 4-amino-
Guanine	6<i>H</i>-Purin-6-one, 2-amino-1,7-dihydro-
Hypoxanthine	6<i>H</i>-Purin-6-one, 1,7-dihydro-
Thymine	2,4(1<i>H</i>,3<i>H</i>)-Pyrimidinedione, 5-methyl-
Uracil	2,4(1<i>H</i>,3<i>H</i>)-Pyrimidinedione
Xanthine	1<i>H</i>-Purine-2,6-dione, 3,7-dihydro-

Trivial names for seven common nucleosides and the related nucleotides are employed as stereoparents; these nucleosides are:

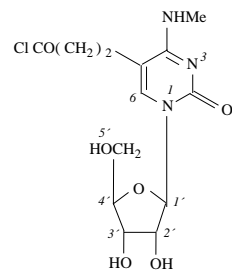
Purine derivatives	Pyrimidine derivatives
Adenosine	Cytidine
Guanosine	Thymidine
Inosine	Uridine
Xanthosine	

The seven stereoparents (above) are heading parents for derivatives, including *N*-acyl and *N*-carboxy derivatives, e.g., **Adenosine, *N*-acetyl-**; **Cytidine, *N*-(ethoxycarbonyl)-**. When a chemical function higher than carboxamide (¶ 106), except *N*-carboxy, is present, an index parent which expresses it is chosen, unless lack of a suitable radical precludes expression of the nucleoside residue as a substituent prefix (this occurs when the higher function is attached to the saccharide at any position other than "1"). Replacement of oxygen in the saccharide moiety or on the heterocycle by sulfur is expressed by a "thio" prefix, and the regular methods of carbohydrate nomenclature (¶ 208) are employed for other saccharide modifications, including ester formation other than phosphates.

Examples:



Adenosine, 3'-(acetylamino)-3'-deoxy-*N,N*-dimethyl-

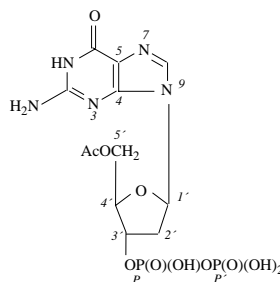


5-Pyrimidinepropanoyl chloride, 1,2-dihydro-4-(methylamino)-2-oxo-1-β-D-ribofuranosyl- (not Cytidine, 5-(3-chloro-3-oxopropyl)-*N*-methyl-)

Nucleotides are indexed at stereoparents descriptive of the type and position of the phosphate residue on the sugar moiety. Esters with phosphoric acid, H₃PO₄, are "ylic acid" stereoparents. Each isomer has its own heading, e.g., **5'-Adenylic acid** for the 5'-(dihydrogen phosphate) of **Adenosine**. When more than one such acid residue is present, the lowest locant is chosen for the stereoparent, e.g., **3'-Adenylic acid**, 5'-(dihydrogen phosphate). Cyclic phosphates are expressed in the modification at the nucleoside name by such phrases as "cyclic 3',5'-(hydrogen phosphate)."

Nucleoside esters with unsubstituted linear polyphosphoric acids are indexed at stereoparents which express the complete ester name, e.g., **Guanosine 3'-(trihydrogen diphosphate)**. An unspecified isomer is assumed to be the 5'-isomer. Di- and triesters with the same acid are indexed at the lowest numbered isomer heading. Substituted derivatives and esters with nonphosphorus acids are named like those of the nucleotides.

Example:



Guanosine 3'-(trihydrogen diphosphate), 2'-deoxy-5'-acetate

Coenzyme A is employed as a stereoparent for adenosine 5'-(trihydrogen diphosphate) 3'-(dihydrogen phosphate) *P'*-(3*R*)-hydroxy-4-[[3-[(2-mercaptoethyl)amino]-3-oxopropyl]amino]-2,2-dimethyl-4-oxobutyl ester; functional derivatives, notably esters such as "S-acetate," are also indexed at this stereoparent.

Esters and molecular addition compounds of nucleoside and nucleotide stereoparents, including "ylic acids," with nonstereoparents are indexed at the stereoparents regardless of functionality.

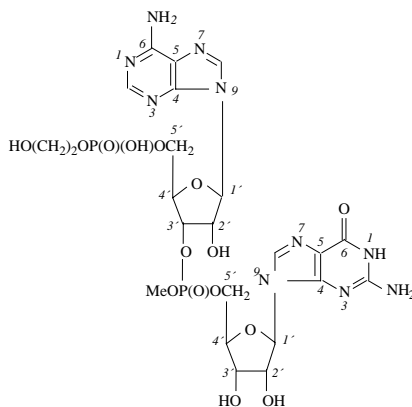
Example:

Inosine 5'-(trihydrogen diphosphate) 2'-(dihydrogen phosphate), *P'* → 5'-ester with 3-(aminocarbonyl)-1-β-D-ribofuranosylpyridinium, inner salt

Oligonucleotides contain not more than eight nucleotide units connected by phosphoric acid residues. Higher-molecular-weight compounds are indexed as polynucleotides (see Polymers ¶ 222) or at the headings **DNA** or **RNA**. Phosphate links attached to the preferred stereoparent of an oligonucleotide form parts of "yl" radical substituents.

The heading parent is attached to the rest of the nucleotide chain at its 5' position. Arrows are employed with locants, as in oligosaccharide nomenclature (¶ 208), to indicate progression and points of attachment on saccharide residues beginning at the end of the chain furthest from the preferred stereoparent. Esters and substituents of "yl" radicals are named as substituents without regard to higher functions. Nonnucleotidyl esters of the stereoparent are expressed in the modification. When a cyclic ester is part of the polynucleotide linkage, the locants for the ester are separated by a hyphen, and the arrow to the point of attachment follows in the usual way, e.g., **Adenylic acid, adenylyl-(2'-3'→5')**.

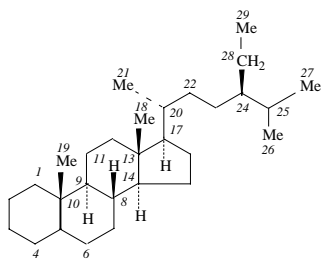
Example:



Guanosine, 5'-0-[hydroxy(2-hydroxyethoxy)phosphinyl]-*P*-methyladenylyl-(3'→5')

Intermolecular cyclic nucleotides are named like the linear compounds, but with the term "cyclic nucleotide" in the modification.

211. Steroids are cyclopenta[*a*]phenanthrene derivatives that are indexed as stereoparents (¶ 202) at trivial names that imply stereochemistry. The following steroid numbering system is employed:



When two methyl groups are present at the 4-position, as well as one at the 14-position, along with a 1,5-dimethylhexyl substituent at position 17, the compound is indexed as a terpene stereoparent (¶ 212); otherwise the steroid or terpene stereoparent is employed that requires least modification.

The hydrogenated ring system without substituents is **Gonane**; **Estrane** has a methyl group only at the 13-position; the compound with only a 10-methyl group is named as **18-Norandrostane**. The following stereoparents are derivatives of **Androstane** (hexadecahydro-10,13-dimethyl-1*H*-cyclopenta[*a*]phenanthrene) with various side chains at the 17-position:

-CH ₂ Me	Pregnane
-CHMePr	Cholane
-CHMe(CH ₂) ₃ CHMe ₂	Cholestane
-CHMe(CH ₂) ₂ CHMeCHMe ₂	Ergostane
-CHMe(CH ₂) ₂ CHEtCHMe ₂	Stigmastane

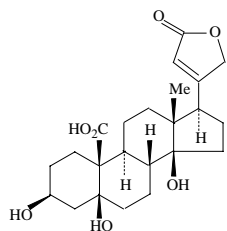
The implied configurations in all cases are 8 β ,9 α ,10 β ,13 β ,14 α . The configuration at the 5-position, when known, is cited as added stereochemistry in the modification. **Pregnane** is 17 β ; **Cholane** and **Cholestane** are 17 β ,20*R*; **Ergostane** is 17 β ,20*R*,24*S*; **Stigmastane** is 17 β ,20*R*,24*R*.

Unsaturation in steroids is expressed by "en" and "yn" infixes, e.g., **Estra-1,3,5(10)-triene**; **Androst-1-en-16-ol**, (5 α)-. The first example requires two locants for the last cited double bond; this situation is avoided where possible, with steroids containing benzenoid rings, by rearrangement of bonds; e.g., **Gona-5,7,9-triene** (not Gona-5(10),6,8-triene).

Cyclosteroids contain an additional ring formed by a valence bond between two existing ring positions or between a ring position and an angular methyl group or side-chain atom. They are indexed at such stereoparents as **3,5-Cyclopregnane** and **9,19-Cycloandrostane**.

Bufanolide and **Cardanolide** are stereoparents with a δ -lactone and a γ -lactone ring, respectively, attached to the 17-position of **Androstane**. The configurations are as for **Cholane** except for 14 β instead of 14 α . When a carboxylic acid or higher function is present the lactone ring is opened and named in the modification.

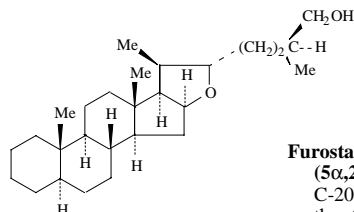
Example:



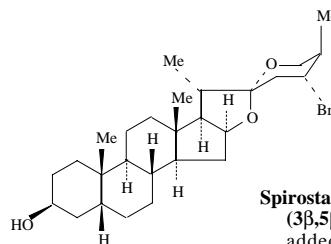
24-Norchol-20(22)-ene-19,23-dioic acid, 3,5,14,21-tetrahydroxy- γ -lactone, (3 β ,5 β ,14 β)-

Furostan is a stereoparent which represents 16 β ,22-epoxycholestane; this has a furan ring fused to the steroid system in the 16,17-position. **Spirostan** is a 16,22:22,26-diepoxycholestane derivative. Configurations at the 5-, 22-, and 25-positions of furostan and at the 5- and 25-positions of spirostans are expressed in the modifications if known.

Examples:



Furostan-26-ol (5 α ,20 β ,22 α ,25*S*)-(configuration at C-20 is reversed from that shown in the stereoparent diagram)



Spirostan-3-ol, 24-bromo-(3 β ,5 β ,24*R*,25*R*)-(configurations for added stereochemistry at C-3 and C-24 are indicated; there is no modified stereochemistry)

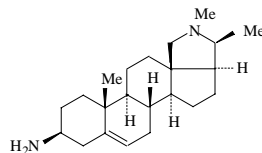
Elimination of an acyclic carbon atom (or methyl group) from a steroid is expressed by the prefix "nor" with the locant for the carbon removed; (but 21-Norpregnane is indexed at **Androstane, 17-methyl-**). Elimination of one or two carbon atoms from the C-17 side chain of C₂₇ and larger steroids may be expressed by "nor" and "dinor," unless a smaller stereoparent is thereby obtained; e.g., **21,27-Dinorcholestan-26-oic acid**; **26,27-Dinorcholestane**; but **Cholane-24-carboxylic acid** (not 26,27-Dinorcholestan-25-oic acid). Removal of C-18 and C-19 by "nor" terms is independent of treatment of the C-17 side chain; hence **18,19-Dinorpregnane** (not Gonane, 17-ethyl-).

Ring modification expressed by "nor", "homo" and "seco" are no longer permitted. Such substances are named systematically.

Replacement ("a") nomenclature (¶ 127) is no longer used for heterosteroids, e.g., **2-thiaandrostane**, and **3-aza-A-homoandrostane**, are now given systematic names.

Steroidal alkaloids containing exocyclic nitrogen are indexed at steroid stereoparents. Thus Irehine is cross-referred to **Pregn-5-en-3-ol, 20-(dimethylamino)-**, (3 β ,20*S*)-. Kurchi alkaloids are named as derivatives of the stereoparent **Conanine**; implied configurations are the same as for **Pregnane**, with the addition of 20 β .

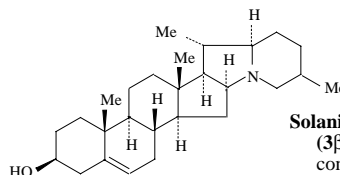
Example:



Con-5-enin-3-amine (3 β)-

The solasodine-tomatidine and solanidine groups of *Solanum* alkaloids are indexed at **Spirosolane** and **Solanidane** stereoparents, respectively.

Example:



Solanid-5-en-3-ol (3 β)-(When C-5 is asymmetric, its configuration, when known, is cited.)

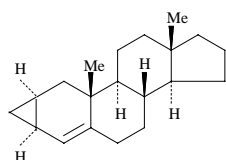
Veratrum alkaloids are indexed, according to type, at the stereoparents **Veratraman** and **Cevane**. Buxus alkaloids are indexed at such headings as **9,19-Cyclopregnane**.

Radicals derived from steroid stereoparents are employed when the highest function is present in a nonsteroid part of the molecule (except the esters, semicarbazones and additional compounds are always indexed at the stereoparents (¶ 202)). Radical names are formed in the usual way, and the free valency can be at an acyclic atom; e.g., *estra-1,3,5(10)-triene-17-yl*, *cholest-4-en-26-yl*. No radical names are formed from cardanolides or bufanolides. Configurations are cited ahead of the entire substituted radical; e.g., [(3 β ,5 α)-3-hydroxyandrost-5-yl]-. For acetals of steroids, see ¶ 202.

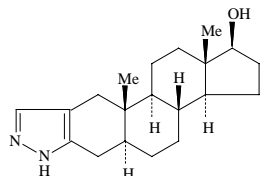
Steroids with -O- and -OO- bridges are indexed by use of "epoxy" and "epidioxy" substituents at the stereoparents. Steroid stereoparents may be adopted as components of spiro systems (¶ 156), e.g., **Spiro[androst-4-en-2,1'-cyclopropan]-3-one**.

Fused steroid names are used on a restricted basis. The steroid component is named first when fusion is to a heterocycle; the reverse order occurs with less preferred carbocycles. Each system retains its own numbering and the nonsteroid is given primed locants. When saturation is expressed at positions common to both components, steroid locants are cited if possible.

Examples:

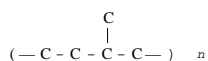


3'H-Cyclopropa[2,3]androsta-2,4-diene, 2,3-dihydro-, (2 α ,3 α)-



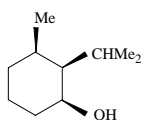
2'H-Androst-2-eno[3,2-c]pyrazol-17-ol, (5 α ,17 β)-

212. Terpenes contain repeating isopentane units:

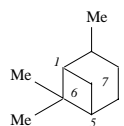


Mono-, sesqui-, di-, sester-, tri-, and tetraterpenes contain two, three, four, five, six, and eight such units; tetraterpenes are usually called carotenes (see below). Most mono-, sesqui-, and diterpenes are indexed by the principles of systematic substitutive nomenclature; stereoparents are employed for terpenes that contain four or more rings, or possess three or more elements of stereochemistry, at least one of which is associated with a bridged or side-chain center, or a center in a ring of twelve or more members.

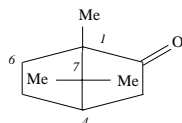
Examples:



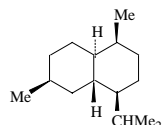
Cyclohexanol, 3-methyl-2-(1-methylethyl)-, (1S,2R,3R)- (o-Neoisomenthol)



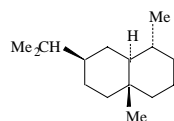
Bicyclo[3.1.1]heptane, 2,6,6-trimethyl- (Pinane)



Bicyclo[2.2.1]heptan-2-one, 1,7,7-trimethyl- (Camphor)



Naphthalene, decahydro-1,6-dimethyl-4-(1-methylethyl)-, (1S,4S,4aS,6S,8aS)- (Cadinane)



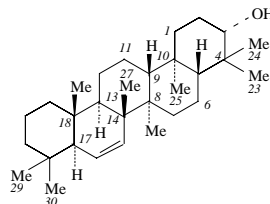
Naphthalene, decahydro-1,4a-dimethyl-7-(1-methylethyl)-, (1R,4aR,7R,8aS)- (Eudesmane)

The stereoparent **Trichothecane**, a sesquiterpene "epoxide," is used in indexing, and other derivatives of sesquiterpenes and diterpenes may be used as stereoparents when they meet the criteria. **Gibbane** is a partially stereospecific stereoparent employed in naming gibberellic acid derivatives. Two tetracyclic diterpene stereoparents are **Kaurane** and **Atisane**. Cyclic triterpenes include **Gammacerane**, **Lanostane**, **Lupane**, **Oleanane**, and **Ursane**.

Abnormal configurations are expressed by " α " or " β " at angular carbon atoms in ring systems, and by "*R*" and "*S*" when there is inversion on a bridge or side-chain. Additional stereochemistry produced by substitution is expressed similarly. All terms cited with a stereoparent are considered to be absolute, not relative. The geminate methyl groups of triterpenes have no implied configuration associated with the locants; " α " or " β " is cited when substitution in the methyl groups makes this necessary.

Because lowest locants are assigned to principal groups, in accordance with general systematic nomenclature, the author's numbering may be changed in indexing, especially with a symmetrical stereoparent such as **Gammacerane**.

Example:

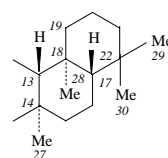


Gammacer-15-en-3-ol, (3 β)- (not Gammacer-6-en-21-ol, (21 α)-)

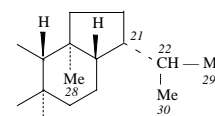
"Friedo," preceded by *D*, has been used to indicate *D:A*, *D:B*, or *D:C* as prefixed to pentacyclic triterpene stereoparents that angular methyl groups have shifted from their normal positions. These names are no longer used, and these substances are named as derivatives of other triterpenes.

The prefix "neo-" preceded by an italicized capital *A* indicates that ring *A* has undergone a rearrangement. These names are no longer used.

In the gammacerane skeleton, *A*'-Neo- is used.



Normal arrangement



A'-Neo-

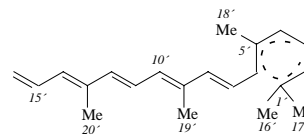
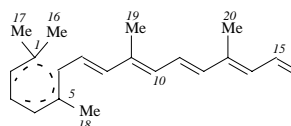
The prefix "cyclo" indicates a valence bond forming an extra ring, e.g., in **9,19-Cyclanostane** a "fused" cyclopropane ring is formed.

Principal groups are expressed as "-oic acid," "-al," "-one," "-ol," etc., by the procedures of general substitutive nomenclature. Terpene radicals are formed in the usual way. Configurational terms are placed ahead of the complete radical (cf. Steroids, ¶ 211).

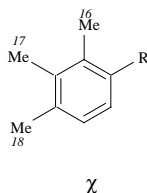
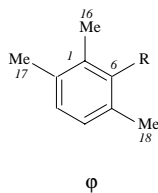
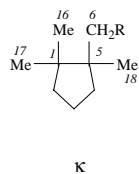
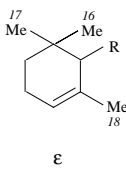
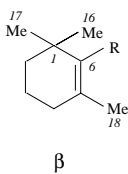
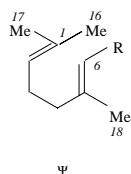
Lactones of triterpene acids are indexed at the acid names; cyclic acetals are likewise expressed in the modification at stereoparent headings.

Carotenoids comprise carotenes (hydrocarbons) and xanthophylls (their oxygenated derivatives) in which eight isoprene units are joined in such a manner that the arrangement is reversed at the center of the molecule, whereby the two central substituent methyl groups are in 1,6-relationship and the remaining methyl groups in 1,5-relationship. The class also includes some rearranged and degraded compounds, but excludes Retinol and related C_{20} -compounds (see below).

General entries are found at **Carotenoids** in the *General Subject Index*. Specific substances are indexed at **Carotene**:



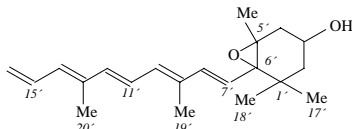
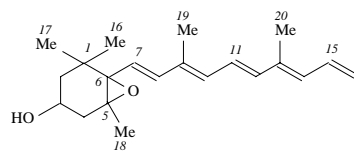
Each dotted curved line represents two double bonds or their equivalent; thus, individual compounds may have acyclic end groups with two double bonds, or terminal cyclohexenyl groups, or one of each. By extension, **Carotene** is used as the stereoparent representing dihydro and tetrahydro derivatives which possess cyclopentyl and phenyl end-groups. Two Greek letter prefixes on the **Carotene** stereoparent, cited in (Greek) alphabetical order, are employed to express the terminal structures of specific compounds:



α-Carotene is indexed at β,ε-**Carotene**; β-carotene is β,β-**Carotene**; γ-carotene is β,ψ-**Carotene**; and lycopene is ψ,ψ-**Carotene**. The plain (unprimed) locants are assigned to the end of the molecule related to the first-cited Greek letter.

“Hydro” and “dehydro” express addition and subtraction of hydrogen; oxygen functions are expressed by “-oic acid,” “-al,” “-one,” “-ol,” etc., in the usual way. Oxygen bridges are indicated by “epoxy,” it being understood that the oxygen replaces one hydrogen atom at each bridgehead; thus, an “epoxide” is an epoxy-dihydro derivative.

Example:



β,β-Carotene-3,3'-diol, 5,6:5',6'-di-epoxy-5,5',6,6'-tetrahydro-

Addition of water (H, OH) or methanol (H, OCH₃) to a double bond is expressed by “dihydro-hydroxy” and “dihydro-methoxy.” When the “-ol” suffix can be used only for *some* of the hydroxy groups, the “dihydro-hydroxy” method is employed for all.

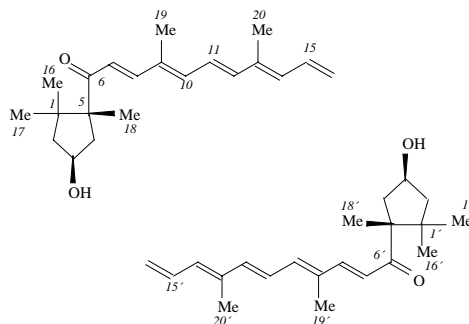
Carotenoids with diosphenol end-groups are indexed as the keto tautomers; e.g., β,β-**Carotene-3,3',4,4'-tetrone**. For carotenoids with identical end groups, lowest locants are assigned to the principal groups, if present, and then to prefixes; e.g., ε,ε-**Carotene-2,3'-dione, 2'-methoxy-** (not ε,ε-Carotene-2',3-dione, 2-methoxy-).

“Retro” carotenes have undergone a shift of the alternating single-double bond system by one position. A prefix such as “4,7'-retro-” is applied to the stereoparent; to express this situation; the first cited locant shows where a proton has been gained, the second, where a proton has been lost.

“Apo” carotenes names are no longer used. Oxidative degradation products of carotenes are named as retinol, retinoic acid, etc., or systematically.

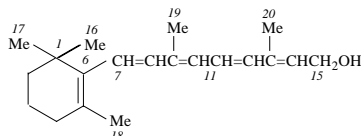
Stereochemistry of carotenoids is of two types. The geometrical configuration around double bonds is implied by the stereoparent stem **Carotene** to be *all-trans*. Abnormal configuration at one or more positions is indicated in the modification by terms such as “15-*cis*.” Absolute configuration at chiral centers is expressed by “*R*” or “*S*.”

Example:



κ,κ-Carotene-6,6'-dione, 3,3'-di-hydroxy-, (3*S*,3'*S*,5*R*,5'*R*)-

Retinol and its relatives are indexed at stereoparent headings.



Retinol (stereoparent)

Illustrative diagrams for **Retinol** and **Retinoic acid** appear in the *Chemical Substance Index*. Vitamin A₁ is indexed at **Retinol**; Vitamin A₂ at **Retinol, 3,4-didehydro-**. The hydrocarbon “Retin” is used as a stereoparent, as well. The *all-trans* configuration is assumed; if abnormal stereochemistry is reported, it is expressed in the modification by terms such as “13-*cis*”.

F. SPECIALIZED SUBSTANCES

Introduction	¶ 213	Inorganic compounds	¶ 219
Alloys	214	Isotopes	220
Coordination compounds	215	Mixtures	221
Dyes	216	Polymers	222
Elementary particles	217	Porphyryns and Bile pigments	223
Enzymes	218	Vitamins	224

213. Introduction. The special classes of chemical substances discussed in this section exclude those natural products and their derivatives, largely indexed at stereoparents, which were the subject of the previous section. The topics covered here fall into three groups: inorganic (alloys, coordination compounds, elementary particles, and general inorganic compounds); biological (enzymes, porphyrins and bile pigments, and vitamins); and special subjects not chemically related to any particular class (dyes, isotopes, mixtures, and polymers). The arrangement is alphabetic.

214. Alloys, including those with nonmetallic and gaseous components, are indexed and registered by CAS as specific chemical substances. The percentage composition is expressed in the modification in descending order of abundance of metals, either as individual round numbers or as ranges. Components present in amounts below 0.1% are generally ignored. The metal in greatest amount is indexed at an "element alloy base" heading parent.

Example (an alloy of 69.93% copper, 17.45% nickel, 10.29% aluminum, 1.50% cobalt, 0.83% iron):

Copper alloy, base
Cu 70, Ni 17, Al 10, Co 1.5, Fe 0.8

Binary alloys of 50-50% composition are indexed at the base heading for the metal with the earliest alphabetical element *symbol*.

If ranges, rather than specific compositions, are supplied in the original document for all or some components, they are cited thus: Cu 68-73, Ni 16-18, Al 9-10, Co 1-2, Fe 0.7-1. Alloys of unknown percentage composition are entered only at nonbase headings, unless the base component is known.

Example (An alloy of iron and thulium, base component unknown):

Iron alloy, nonbase
Fe, Tm

The symbols are cited in alphabetical order, except that the base element is placed first if known; e.g., Al, Co, Fe, Ni or (for a cobalt base alloy) Co, Al, Fe, Ni.

Alloys with trade names or code designations (other than standards) sometimes vary in reported composition; therefore, the numerical values are omitted from the entries. The base metal symbol is placed first and the others in alphabetical order; finally, the trade name or code designation is cited in parentheses. If only the base metal is known, the parenthetical expression alone is cited in the modification.

Examples:

Copper alloy, base
Cu, Fe, Ni (Cumifer I)

Nickel alloy, base
(Permalloy)

Numerical values are included in entries for trade-named alloys of fixed composition and for those identified by the following U.S. standards: AA, Al-Si, AMS, ASTM, AWS, CDA, SAE, and UNS. The international standards of ISO and the standards of most other countries are also recognized for the purpose of CA indexing of alloys.

Cermets are alloys containing nonmetals. They are indexed at metal alloy headings or at nonmetal headings with "alloy" in the modification depending on the composition.

Example (a cermet containing tungsten carbide (WC) 94%, cobalt 6%):

Tungsten carbide (WC)
alloy, WC 94, Co 6

Alloys containing gases (0.1% or more) are indexed similarly.

Example:

Nickel alloy, base
Ni 99, H 1

Steel is a heading parent for iron-carbon alloys so described and either containing a minimum of 97% iron or having no disclosed compositions. The steel composition or a designation (such as AISI 1017) which implies the composition is cited in the modification.

Examples:

Steel
(AISI 1017)

Steel
Fe 98, Mn 1.5, Si 0.5, C 0.1

Isotopically labeled alloys are distinguished by the mass number on the element symbol.

Example:

Aluminum alloy, base
Al 95, ²³⁵U 5

215. Coordination compounds are molecules or ions in which a central atom (in polynuclear compounds, more than one) has atoms or groups of atoms, called ligands, attached to it to the extent of its coordination valency. The central atom may be of any element, but it is usually a metal atom. The metals comprise all elements except the following: Ar, As, At, B, Br, C, Cl, F, He, H, I, Kr, Ne, N, O, P, Rn, Se, Si, S, Te, Xe. (Prior to CA Volume 95 (see ¶ 101), antimony was also indexed as a nonmetal.) Compounds of nonmetals are generally not indexed as coordination compounds, but there are several exceptions, e.g., tetra- and hexavalent sulfur compounds (¶ 200), and borates containing ligands other than oxo and hydroxy. Hydride derivatives of antimony, bismuth, germanium, tin, and lead are not named as coordination compounds, but rather as covalent derivatives of the hydride heading parents, e.g., **Stibine, Germane** (¶¶ 181, 199).

A *ligand* is any atom or group of atoms, charged or neutral, that is attached to the central atom of a coordination complex. The atoms of a ligand that are attached to the central atom are called coordinating atoms regardless of the type of bonding involved. A ligand with more than one coordinating site is described as multidentate; when more than one such site is engaged with a single central atom, it is a chelate ligand; when it is coordinated with two or more central atoms it is a bridging ligand.

Neutral compounds with monoatomic ligands (except hydride) and mono-nuclear carbonyls and nitrosyls are given binary salt names. Common oligomeric salts are named in the monomeric form, e.g., **Aluminum chloride (AlCl₃)**, but studies of the dimers, etc., are indexed at the oligomeric names, e.g., **Aluminum, di-μ-chlorotetrachlorodi-**.

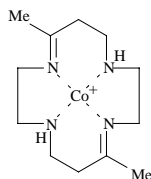
Coordination compounds may be anionic, neutral, or cationic, in accordance with the oxidation state of the central atom and the number and nature of the ligands; when the latter are derived from the molecular skeletons of substitutive nomenclature, including nonmetal hydrides, by loss of hydrogen, they are considered negative in computing the total charge of the complexes containing them. This charge is expressed by an Ewens-Bassett number, e.g., (3+) or (2-), placed after the heading parent derived from the name of the central element; thus, **Copper(1+), Borate(2-)**. Absence of an Ewens-Bassett number indicates that the complex expressed by the *complete boldface heading* is neutral. Ligands are cited in alphabetical order and their ligating atoms are identified by a modification of the Kappa system¹. The periodic table symbol of the ligated atom is stated as an italic capital-letter locant preceded by the greek letter kappa, e. g. κN, κO¹, κS¹. These letter locants are placed at the portion of the name corresponding to their attachment on the coordination center. Letter locants are not cited with (a) regular substituent prefixes, e.g., methoxy, phenyl, 2-pyridinyl; (b) other sigma-bonded ligands in which hetero atoms are either absent or uninvolved in the coordination; (c) monoatomic ligands, e.g., hydro, iodo; (d) ligands with unspecified bonding; (e) neutral and monoanionic organic ligands derived from cyclic or acyclic compounds containing only one hetero atom capable of coordination, e.g., triethyl phosphine, pyridine, *N,N*-dimethylmethanamine, *N*-methylmethanaminato, provided that the hetero atom is coordinated but no carbon atom is also bonded; (f) the following simple polyatomic inorganic ligands: amido, ammine, aqua, selenyl, telluryl, hydroxy, imido, mercapto, phosphino, and (except sometimes when present as bridges) azido, carbonyl, dinitrogen, dioxygen, nitrosyl, peroxy, and carbonothioyl.

¹IUPAC, *Nomenclature of Inorganic Chemistry, Recommendations 1990*, Blackwell Scientific Publications, Oxford (England), 1990.

The preferred *Chemical Substance* and *Formula Index* entries for coordination compounds are made at the central element names (or the derived “-ate” names) as discussed above.

Example:

Cobalt(1+), (5,12-dimethyl-1,4,8,11-tetraazacyclotetradeca-4,11-diene-κN¹,κN⁴,κN⁸,κN¹¹)-, (SP-4-1)-, [131154-44-4]



Cationic complexes are highest in order of precedence (¶ 106) among coordination compounds. (A positive element heading, e.g., **Phosphorus(1+)**, is ranked just above the corresponding “-onium” heading, e.g., **Phosphonium**.) Neutral complexes are lower in the order of precedence, followed by anionic coordination compounds. For mixed polynuclear complexes, the preferred element (or derived “-ate”) heading is that appearing earliest in the following list: Rn, Xe, Kr, Ar, Ne, He, Fr, Cs, Rb, K, Na, Li, H, Ra, Ba, Sr, Ca, Mg, Be, (Lr to Ac), (Lu to La), Y, Sc, Hf, Zr, Ti, Ta, Nb, V, W, Mo, Cr, Re, Tc, Mn, Os, Ru, Fe, Ir, Rh, Co, Pt, Pd, Ni, Au, Ag, Cu, Hg, Cd, Zn, Tl, In, Ga, Al, B, Pb, Sn, Ge, Si, C, Bi, Sb, As, P, N, Po, Te, Se, S, O, At, I, Br, Cl, F.

Many ligand names correspond to those of the substituent prefixes of general nomenclature. They include hydro, chloro (etc.), oxo, thioxo, hydroxy, mercapto, peroxy, diazenyl, and sulfo. Among ligand names which differ are the following: superoxido (O₂⁻), amido (H₂N⁻), imido (HN=), chloramido (ClHN⁻), nitrido (N≡), phosphido (P≡), arsenido (As≡).

“Ato” ligand names are employed to express loss of hydrogen from inorganic “oxo” acids named as “-ic acids” and their chalcogen analogs. Those named as “-ous acids” correspondingly afford “-ito” ligands. Loss of one, two, etc., protons from polybasic acids is expressed by Ewens-Bassett numbers (loss of one hydrogen atom from most other classes of compounds is denoted simply by omission of a Ewens-Bassett number). Letter locants (see above) are sometimes employed. “Ato” and “ito” ligand names are always placed in enclosing marks.

Examples:

$^-O-PF(O)-O^-$	[phosphorofluoridato(2-)]
O_3ClO^-	(perchlorato)
$^-OSO_2O^-$	[sulfato(2-)]
$^-OS(O)O^-$	[sulfito(2-)]
$^-O_2N^-$	(nitrito-κN) (not nitro)
$^-O=NO^-$	(nitrito-κO) (not nitrito)
$^-O=N=N-O^-$	[hyponitrito(2-)]
$OP(O^-)_3$	[phosphato(3-)]


The following cyanato radicals are employed:

$^-OCN^-$	(cyanato-κN) (not isocyanato)
$^-NCO^-$	(cyanato-κO) (not cyanato)

and similarly for thiocyanato, etc. Oxo acids which require synonym line formulas at their own heading parents are given more specific names when converted into ligands, e.g., [monothiosulfato(2-)], [trimetaborato(3-)].

Anionic carbon-attached ligands containing no anionic hetero atom attachments to the metal, and acyl ligands containing no anionic hetero atom attachments except for the acyl portion, are given names identical with those of normal substituent prefixes, e.g., ethyl, 2-pyridinyl, 1*H*-imidazol-2-yl, (phenylsulfonyl). Phosphino, phosphinyl, and (2-phenyldiazenyl) radicals are also used. Anionic ligands derived from heterocycles by loss of a proton only from a hetero atom in the ring, and containing no additional hetero atoms in the ring or substituents, are also named by substituent prefixes, e.g., 1-piperidinyl. All other anionic heterocyclic ligands are given “ato” names; they include porphines, phthalocyanines, corrins, other heterocycles containing rings of more than ten members, and heterocyclic ligands containing more than one hetero atom (including substituents). Unsubstituted phenoxy and methoxy through (dodecyloxy) radicals are used to express these ligands, but the chalcogen analogs and the substituted oxy radicals are named (1-chloromethanolato), (2-propanolato) (not (1-methylethoxy)), (ethanethiolato), etc. Organic “-ic acids” and organophosphorus acids afford ligand names in which “-ic acid” or “-ous acid” is replaced by “-ato” or “-ito”, respectively. Ligands from esters are named in uninverted form. The “ato” suffix denotes loss of one proton in all cases unless a Ewens-Bassett number, e.g., “(2-),” is cited.



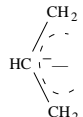
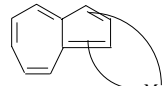
Examples (letter locants are added to many of these names in particular coordination names; e.g., (acetato-κO,κO⁻):

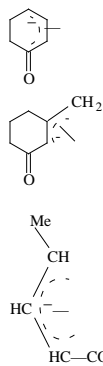
$^-O_2C^-$	(carboxylato) (this is an exception: not [carboxylato(2-)])
AcO^-	(acetato)
$^-CH_2CO_2^-$	[acetato(2-)]
$Ph_2(O)P^-$	(diphenylphosphinyl)
$Ph_2P(O)O^-$	(diphenylphosphinito)
	[1,2-benzenediolato(2-)]
$^-O_2C(CH_2)_3CO_2^-$	[pentanedioato(2-)]
$AcO(CH_2)_2O^-$	(2-hydroxyethyl acetato) (an ester is named in its uninverted form)
$MeO-S(O)_2O^-$	(monomethyl sulfato) (derived from methyl hydrogen sulfate)
$H_2N-CH_2CO_2Me$	(methyl glycinate) (derived from glycine methyl ester)

Metal radical names (¶ 194) such as aluminio, aurio, and sodio, are used in the presence of higher compound classes or more preferred metals when the metal replaces a single hydrogen, but not to “place” a metal directly on another metal (see polynuclear complexes, below); e.g., **Ethyl, 2-sodio-** (a free-radical name); **Potassium, (5-lithio-1-naphthalenyl)-**. Because metal radicals carry no implication of valency, hydrogen and other attached atoms and groups must be expressed, e.g., dihydroaluminio for H₂Al⁻.

π-bonded ligands, and ligands attached to metal atoms by both π and σ bonds, are named by prefixing the Greek letter η (eta) or by using a combination of η and κ treatments. (Delocalized bonds are “fixed” for the purpose of naming the ligand so that lowest locants are given first to the point of attachment, then for unsaturation, etc.) Locants (if available) for atoms contributing to the ligand-metal bonding are cited ahead of “η” and the entire descriptor so formed is enclosed in parentheses; alternatively, if all the skeletal atoms of an unsubstituted conjugated acyclic or cyclic molecule or radical are involved, a superscript denoting the number of such atoms is cited immediately after “η” and the locants are omitted. Ligands with negative charges on adjacent hetero atoms are named instead as the neutral unsaturated compounds. σ-bonded ligands are named as regular radicals, e.g., 2,4-cyclopentadien-1-yl. (The name cyclopentadienyl is used without locants in the absence of further information.)

Examples:

	[(1,2,3-η)-2,4-cyclopentadien-1-yl]
	(η ⁵ -2,4-cyclopentadien-1-yl)
	(η ³ -2-propen-1-yl)
	[(1,2,3,3a-η)-azulene]



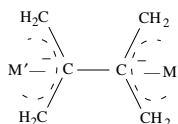
[(1,2,3-η)-4-oxo-2-cyclohexen-1-yl]-

(η³-2-methylene-6-oxocyclohexyl)
(The choice is based on the preferred parent radical; the locants "α,1,2-" cannot be used because "α-" does not relate to the parent radical.)

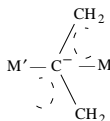
[(1,2,3-η)-4-ethoxy-1-methyl-4-oxo-2-buten-1-yl]

In polynuclear compounds (see below) a colon partitions the locants into sets to indicate bonding to different metal atoms.

Examples:



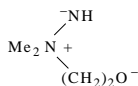
[μ-[(η³:η³)-2,3-bis(methylene)-1,4-butanediyl]]



[μ-[(1,2-η:2,3-η)-1,2-propadiene]]

Cationic molecules (¶ 184) are named in the unchanged (but uninverted) form when present as ligands, except that a Ewens-Bassett number denotes the charge when necessary; e.g., oxonium, [hydrazinium(1+)], [hydrazinium(2+)], (1-methyl-4-aza-1-azoniabicyclo[2.2.2]octane). When protons have been lost from hetero atoms of such ligands, "ato" names are used.

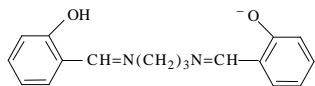
Example:



[1-(2-hydroxyethyl)-1,1-dimethyl-hydraziniumato(2-)]

Enclosing marks are used with all "ato" ligand names and with ligands, like (cyano-κC), that have letter locants; "bis," etc., (rather than "di," etc.) are used to indicate two or more, e.g., bis(benzoato). When a Ewens-Bassett number is also present, the "ato" name is bracketed, e.g., [tetrahydroborato(1-)]. When such a ligand name includes a multiplicative radical (¶ 125), it is closed off and followed by the Ewens-Bassett number, which in this case may be (1-), and the total name bracketed.

Example:



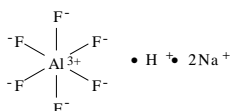
[[2,2'-[1,3-propanediylbis(nitrilo-methylidyne)]bis[phenolato]](1-)]

Ligands from dioximes, trihydrazones, etc., are expressed by enclosing the name and then citing the Ewens-Bassett number (which may be (1-)) in this case also) to indicate the number of protons lost; e.g., [(2,3-butanedione dioximato)(1-)].

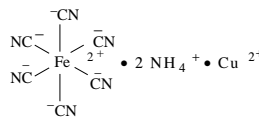
Neutral ligands are enclosed by parentheses or brackets (as required), except for ammine, aqua, carbonyl, and nitrosyl, e.g., (dinitrogen), (phosphine), (benzene); they are multiplied by "bis," "tris," etc.

Anionic mononuclear complexes are indexed at "ate" headings derived from the name of the central element, e.g., **Borate**, **Cuprate**. The total charge of the complex anion is cited by a Ewens-Bassett number, and in the inverted part of the name the ligands are cited in alphabetical order. All cations are named in the modification in alphabetical order, except that hydrogen is placed last. Ratios are employed for all univalent and multivalent cations. For metals of variable valency, Ewens-Bassett numbers are cited after their names.

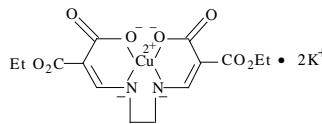
Examples:



Aluminate(3-), hexafluoro-, sodium hydrogen (1:2:1), (OC-6-11)-
(For the significance of the final term, see ¶ 203III.)



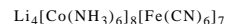
Ferrate(4-), hexakis(cyano-κC)-, ammonium copper(2+) (1:2:1), (OC-6-11)- (Note that the ratio is expressed in the same order as the index name, i.e., first the heading, then the modification terms.)



Cuprate(2-), [[1,1'-diethyl 2,2'-[1,2-ethanediylbis(imino-κN)methylidyne]]bis[propanedioato-κO³]](4-)-, potassium (1:2) (Note that ring systems formed entirely by coordination are not recognized as such in index names.)

Anionic mononuclear complexes which contain simple anions as well as simple cations are named at the complex anion heading, as shown above. The cations are named in the modification, followed by the simple anions. Thus **Borate(1-), tetrahydro-, europium(2+) bromide (1:1:1)**. When a complex or organic cation is present, this receives the preferred entry.

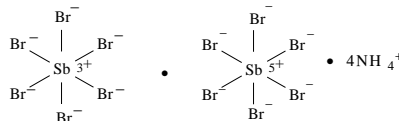
Example:



Cobalt(3+), hexaammine-, (OC-6-11)-, lithium (OC-6-11)-hexakis(cyano-κC)ferrate(4-) (8:4:7)

When more than one complex anion is present, the choice is determined first by the preferred central element (see above); then by the highest numerical value, e.g., **Antimonate(3-)** is preferred over **Antimonate(1-)**; finally, by the earliest index position of the entire entry.

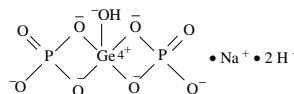
Example:



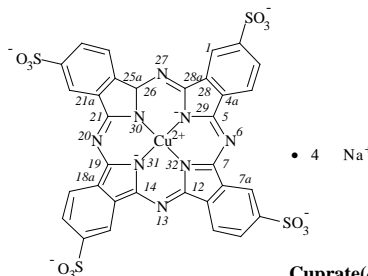
Antimonate(3-), hexabromo-, (OC-6-11)-, ammonium (OC-6-11)-hexabromoantimonate(1-) (1:4:1)

Complexes that contain ligands with *uncoordinated acid functions*, e.g., carboxylic acids or inorganic oxo acids, are named as though all acidic protons were dissociated from the uncoordinated groups; the cations and acid hydrogens are then cited in the modification.

Examples:



Germanate(3-), hydroxybis[phosphato(3-)-κO, κO']-, sodium hydrogen (1:1:2)

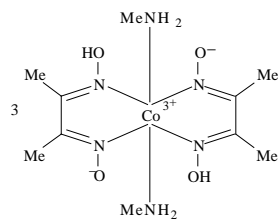


Cuprate(4-), [29H,31H-phthalocyanine-2,9,16,23-tetrasulfonato(6-)-κN²⁹,κN³⁰,κN³¹,κN³²]-, sodium (1:4), (SP-4-1)- (not Copper, [29H,31H-phthalocyanine-2,9,16,23-tetrasulfonato(2-)-κN²⁹,κN³⁰,κN³¹,κN³²]-, tetrasodium salt)

Cationic mononuclear complexes are indexed at the central element names with a Ewens-Bassett number to indicate the total charge on the cation. The ligands are cited in the inverted part of the heading in alphabetical order, the associated anions (if any) in the modification; ion terms, e.g., "ion(1+)," are not cited. Ratios are used with all anions (both univalent and multivalent) and with mixtures of anions and cations, the first numeral relating to the heading cation, the others to the modification terms in sequence. The *Formula Index* headings

exclude the atoms expressed by modification terms.

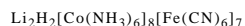
Example:



Cobalt(1+), bis[(2,3-butanedione di(oximate-κN))(1-)]bis(methanamine)-, (OC-6-11)-, (OC-6-11)-hexakis(cyano-κC)ferrate(3-) (3:1)

Cationic complexes containing both complex mononuclear cations and simple cations are indexed at the names of the former; associated complex anions are also indexed as usual.

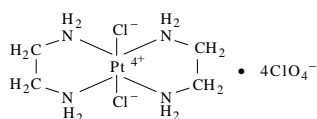
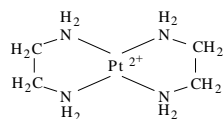
Example:



Cobalt(3+), hexaammine-, (OC-6-11)-, lithium hydrogen (OC-6-11)-hexakis(cyano-κC)ferrate(4-) (8:2:2:7)

When more than one complex cation is present in a compound, the choice of preferred index entry is based on the nature of the central atom (see above for precedence list of elements), e.g., the heading parent **Platinum(2+)** is preferred over **Palladium(3+)**. If the elements are alike, the complex with the higher positive charge is preferred.

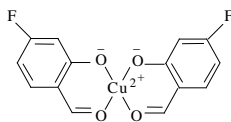
Example:



Platinum(2+), bis(1,2-ethanediamine-κN¹,κN²)-, (SP-4-1)-, dichlorobis(1,2-ethanediamine-κN¹,κN²)platinum(2+) perchlorate (1:1:4)

Neutral mononuclear coordination complexes are indexed at the central element names without a Ewens-Bassett number.

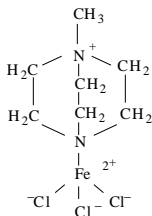
Example:



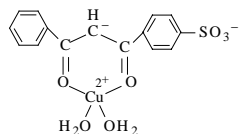
Copper, bis[4-fluoro-2-(hydroxy-κO)benzaldehydato-κO]-

Neutral complexes with internal charge compensation, e.g., with ligands which are inner salts, etc., are named according to structures provided in the original documents.

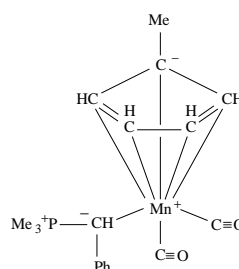
Example:



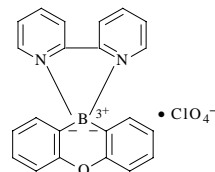
Iron, trichloro(1-methyl-4-aza-1-azoniabicyclo[2.2.2]octane-κN⁴)-



Copper, diaqua[4-[1,3-di(oxo-κO)3-phenylpropyl]benzenesulfonato(2-)]-



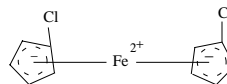
Manganese, dicarbonyl[(1,2,3,4,5-η)-1-methyl-2,4-cyclopentadien-1-yl][phenyl(trimethylphosphonio)methyl]-



Boron(1+), (2,2'-bipyridine-κN¹,κN^{1'}) (oxydi-2,1-phenylene)-, (T-4)-, perchlorate (1:1)

Metallocenes (dicyclopentadienyl metal complexes in which all carbon atoms of the cyclopentadiene rings contribute to the metal-ligand bondings) are indexed at the parents **Ferrocene**, **Nickelocene**, **Cobaltocene**, **Osmocene**, **Ruthenocene**, etc.

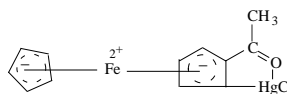
Example:



Ferrocene, 1,1'-dichloro-

When additional ligands or ring systems more complex than cyclopentadiene are present, the compounds are indexed at the names of the central metals. All positions of each cyclopentadiene ring are considered equivalent, and substituents are assigned lowest locants without regard to attachment of the metal. In order of precedence, metallocenes are ranked with the neutral coordination complexes (¶ 106). **Ferrocene**, for example, being placed just below **Iron** as an index parent. Radical names, e.g., ferrocenyl, 1,1'-ferrocenediyl, can be formed.

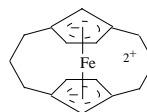
Example:



Mercury, [2-(acetyl-κO)ferrocenyl-κC]chloro-

Suffixes are not attached to metallocene heading parents, and conjunctive names are not derived from them; thus, **Ferrocene, carboxy-** (not Ferrocene-carboxylic acid); **Ferrocene, 1,1'-bis(carboxymethyl)-** (not 1,1'-Ferrocenediacetic acid). Bridged derivatives are named by use of bivalent substituent prefixes.

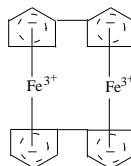
Example:



Ferrocene, 1,1':3,3'-bis(1,3-propanediyl)-

The cationic analog of **Ferrocene** is named **Ferrocenium**.

Example:



1,1'':1,1'''-Biferrocenium(2+)

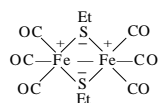
Polynuclear coordination complexes may have (a) direct linkages between the central metal atoms; (b) bridging ligands connecting them; (c) both kinds of linkages. A bridging ligand is designated by the Greek letter μ (mu); when it binds more than two central atoms, a subscript is cited with it, e.g., μ₃. When the ligand name itself requires enclosing marks, an extra set is employed for the μ-ligand, otherwise none are used; e.g., μ-chloro, [μ-(acetato-κO:κO')]. A μ-ligand is cited just ahead of the same ligand without the prefix, disregarding

in the ordering process any accompanying letter locants, e.g., [μ -(acetato- κO : $\kappa O'$)] (acetato- κO). Colons within letter-locant sets indicate the distribution of bonds from a bridging ligand to individual metal atoms.

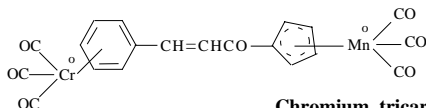
Bridging ligands are not treated as multiplying radicals; i.e., the total of nonbridging ligands on all nuclear atoms is indicated directly. The number of nuclear atoms is indicated, after citation of all ligands, by "di," "tri," etc. Letter-locant sets are partitioned by colons. The cyclic structure of an oligomeric complex is indicated by "cyclo" as the first term in the modification. Direct linkages between like or unlike metals are always indicated, if known, by such terms as "(Fe-Fe)" or "(Co-Re)," whether or not bridging ligands are present. (In more complicated cases the total number of various bondings is expressed in terms such as "(3Co-Co)(3Co-Fe).") For "cluster" compounds, in which three or more central atoms form a core, the geometrical descriptors *triangulo*, *tetrahedro*, or *octahedro* are assigned if the information is available. The term *cluster* is used for 13 or more direct metal linkages.

The entry is made at the name (or derived "-ate" term) of the preferred metal, e.g., **Cobalt**, **Cobalt(2+)**, **Cobaltate(1-)**; other metals with their associated ligands are named as complex ligands of the preferred atom(s). These complex ligands are placed in a single alphabetical sequence with bridging and nonbridging ligands bonded to the preferred metal. (Metal radicals, e.g., cobaltio, mercurio, are not used in naming polynuclear complexes.)

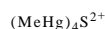
Examples:



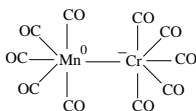
Iron, hexacarbonylbis[μ -(ethane-1-thiolato)]di-, (Fe-Fe)



Chromium, tricarbonyl[μ -(1,2,3,4,5- η)-1-[1-oxo-3-(η^6 -phenyl)-2-propen-1-yl]-2,4-cyclopentadien-1-yl]](tricarbonylmanganese)-

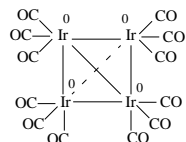


Mercury(2+), tetramethyl- μ_4 -thioxotetra-

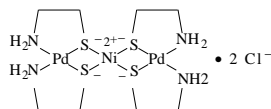


Chromate(1-), pentacarbonyl-(pentacarbonylmanganate)-, (Cr-Mn)

(Note: The "-ate" ending is used in all central atoms names in *anionic* complexes)



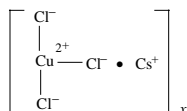
Iridium, dodecacarbonyltetra-, tetrahedro



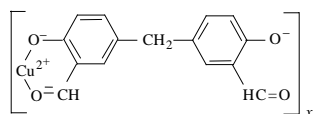
Palladium(2+), tetrakis[μ -[2-(amino- κN)ethanethiolato- κS : κS]](nickel)di-, chloride (1:2)

Polynuclear complexes with *extended structures* caused by bridging ligands are indexed at monomer headings, with a modification term such as "homopolymer." Bridging ligands within the monomeric unit are named as usual, but those which bind the units to one another are not named by use of the " μ " prefix.

Examples:



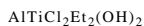
Cuprate(1-), trichloro-, cesium (1:1), homopolymer



Copper, [5-[(3-formyl-4-hydroxyphenyl)methyl]-2-(hydroxy- κO)-benzaldehydato(2-)- κO]-, homopolymer

A polynuclear coordination complex of known formula but unknown structure is indexed at the heading parent for the most preferred central element (or its "-ate" term). The ligands are cited in the inverted part of the heading in alphabetical order, followed by the less preferred metals (or their "-ate" terms) in descending order of precedence.

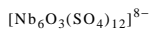
Examples:



Titanium, dichlorodiethyl-di-hydroxy(aluminum)-



Aurate(2-), hexachloroargentate-



Niobate(8-), trioxododecakis[sulfato(2-)]hexa-

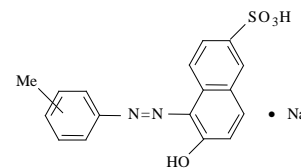


Copper(3+), pentahydroxy-tetrakis[2,2',2''-nitrilotris[ethanol]]tetra-

216. Dyes of established structure are indexed at their systematic names by the regular rules of substitutive nomenclature. The *Colour Index*² is employed as the chief reference source for the chemical constitution of trade-named dyes.

A dye of unknown structure is indexed at the C.I. name if this is available, otherwise only at a trade name or other designation used in the original document. When the *Colour Index* shows an indefinite structure, the systematic name is still used if this can be done by omission of one or more locants or by use of alternative locants, e.g., "5(or 6)-chloro-"

Example:



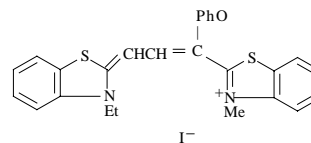
2-Naphthalenesulfonic acid, 6-hydroxy-5-[2-(methylphenyl)diazonyl]-sodium salt (1:1) (cross-reference at C.I. Acid Orange 16)

Deliberate mixtures (¶ 221) of dyes with known structures are indexed at each component with a "mixt. with" modification. Reaction products are not considered to be deliberate mixtures.

When an author supplies a structure for a trade-named dye which has been assigned a C.I. name but no constitution in the *Colour Index*, an entry will be found at the systematic name for the author's structures, and a separate entry, in the *Chemical Substance Index* only, at the C.I. name. The cross-reference continues to be based on *Colour Index* information; i.e., it runs from the trade name to the C.I. name as usual. If a trade name (or common name) is not listed in the *Colour Index*, the author's information (a C.I. number or name, or a structure) is used to make the index entry, cross-references and synonym.

Cyanine dyes (methines) are indexed systematically. Because the location of the charge may be shown differently in different documents, the preferred ring system (¶ 138) is selected as the site of the quaternized center in every case and, if further criteria are needed, the structure named is chosen to conform to the principles of maximum number of substituents, lowest locants, and earliest index position.

Example (name in original document: 3'-ethyl-3-methyl-8-phenoxythiacarbocyanine iodide):

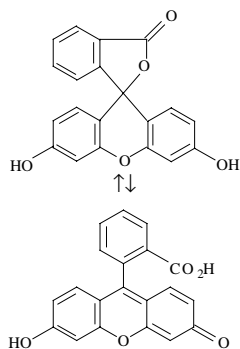


Benzothiazolium, 2-[3-(3-ethyl-2-(3H)-benzothiazolylidene)-1-phenoxy-1-propen-1-yl]-3-methyl-, iodide (1:1)

²*Colour Index*, Society of Dyers and Colourists, Bradford, Yorkshire; and American Society of Textile Chemists and Colorists, Research Triangle Park, N.C., 3rd ed., 5 vols., 1971; vol. 6 (supplement to vols. 1-4), 1975; vol. 7 (supplement to vols. 1-4 and 6); 1982; vol. 5 (3rd revision) and vol. 8 (supplement to vols. 1-4, 6, and 7), 1987.

Fluoresceins, phthaleins, and sulfonephthaleins have tautomeric structures in which a heterocyclic ring may be considered closed or opened, with generation of a carboxyl or sulfo group.

Example (fluorescein):



Spiro[isobenzofuran-1(3H),9'-(9H)xanthen]-3-one, 3',6'-dihydroxy-

Benzoic acid, 2-(6-hydroxy-3-oxo-3H-xanthen-9-yl)-

These compounds and their derivatives, including metal salts, are named in the closed forms unless a covalently bound derivative of the acid group, e.g., an ester or amide, is present. The preferred (closed) forms are indexed as shown by the following cross-references:

Fluorescein.	See <i>Spiro[isobenzofuran-1(3H),9'-(9H)-xanthen]-3-one, 3',6'-dihydroxy-</i>
Phenolphthalein.	See <i>1(3H)-Isobenzofuranone, 3,3-bis(4-hydroxyphenyl)-</i>
Sulfonefluorescein.	See <i>Spiro[3H-2,1-benzoxathiole-3, 9'-(9H)-xanthen]-3',6'-diol, 1,1-dioxide</i>
Phenolsulfonephthalein.	See <i>Phenol, 4,4'-(1,1-dioxido-3H-2,1-benzoxathiole-3-ylidene)bis-</i>

Azo dyes from pyrazolines and from acetoacetanilide derivatives are indexed as the keto rather than the enol forms.

Cationic resonance-stabilized diamino derivatives of phenazine, phenoxazine, phenothiazine, xanthen, etc., are generally indexed as possessing the cation within the ring.

Lakes are pigments which comprise insoluble salts of soluble dyes. They are indexed at the systematic names, e.g., as calcium or barium salts at the acid heading parent, if the constitution is known. The structure of a transition-metal lake is usually not precisely defined; when it is, a coordination name (¶ 215) is used; otherwise it is indexed at a C.I. name (if such a name has been assigned to the lake itself) or at trade names.

New dyes, as reported in patent specifications, are indexed at systematic names, including coordination names (for metal complexes of precisely stated structure).

Zinc chloride double salts cause an indexing problem, both because the same dye can be used in the zinc-containing and zinc-free forms, and because the toxicity of soluble zinc salts renders misindexing a serious matter. The presence of zinc is never assumed; it is excluded from cross-references at C.I. names and included in index entries for a specific trade-named dye only when it is listed in the *Colour Index* as a zinc salt, or when its presence is indicated by an original document. When a ratio is known, the appropriate entry is made at the cationic heading, e.g., **Benzenediazonium**. Otherwise it is indexed as a molecular addition compound (¶ 192) of the “-ium” chloride and **Zinc chloride (ZnCl₂)** with an indefinite ratio.

Sulfur dyes seldom have a known constitution. The preferred entry is a C.I. name, if available; otherwise the trade name is indexed, or, as a last resource, the starting material, e.g., **Phenol, 4-amino-**, sulfur dyes from.

217. Elementary particles and their atomic and molecular states are indexed as chemical substances. Elementary particle names follow a systematic scheme.³ In this scheme, a given letter (Roman or Greek, upper or lower case) is used in the context of a given set of quantum numbers. This scheme replaces the haphazard assignment of letters used previously. These particles may be subdivided as follows:

(a) Particle classes; e.g., **Bosons, Fermions, Leptons, Hadrons, Baryons, Mesons, Hyperons, Nucleons, Tachyons, Quarks**. These terms are employed as *General Subject Index* headings.

(b) Particles with symbols but no reported mass; e.g., Σ -Hyperon, π -Meson, Muon, Alpha particle, Beta particle, Neutron, Proton, Neutrino, Deuteron, Tau particle. The index headings have the form **Meson, π** , in which the particle symbol appears in the heading after the name.

(c) Particles with unique symbols and masses; e.g., Hyperon $\Lambda(2100)$, Positive Muon, π^+ -Meson(140). The index entries are of the form **Muon, μ^+ (106)** and **Meson, π^+ (140)**.

(d) Particle resonances without reported masses; e.g., Meson resonance $K^+ \pi$, Nucleon resonance Δ , Nucleon resonance N^* . The index entry corresponds to the information available, e.g., **Nucleon, resonance; Nucleon, resonance Δ** . For multiple resonances, more than one *Chemical Substance Index* entry appears; e.g., **Meson, K, resonance $K\pi\pi$** ; **Meson, π , resonance $K\pi\pi$** .

(e) Particle resonances with reported masses.
Examples of index entries:

**Nucleon
resonance $N^*(2040)$**

**Meson, K
resonance $K^+K^+(1280)$**

**Meson, K
resonance $KN(1780)$ (preferred entry)**

**Nucleon
resonance $KN(1780)$ (additional entry)**

(f) Particles composed of nuclei of elements of less than 98% natural abundance; e.g., lithium-6, boron-10, are indexed in the modification at the element headings. Specific particles from isotopes of hydrogen and helium-3 and -4 are indexed at **Proton, Deuteron, Triton, Tau particle, and Alpha particle**, respectively. The zero-charge nucleon is indexed at **Neutron**.

Examples of index entries (Notation in the original document: $^{115}\text{In}(\text{}^7\text{Li},3n)^{119m}\text{Te}$):

**Lithium, reactions
isotope of mass 7, indium-115 bombardment by**

**Indium, reactions
isotope of mass 115, bombardment of, by lithium-7**

**Tellurium, properties
isotope of mass 119, nuclear energy levels of, metastable, from lithium-7 bombardment of indium-115**

**Neutron
from lithium-7 bombardment, of indium-115**

In particle-particle and particle-nuclei interactions, all new particles and nuclei are indexed, otherwise, interactions of known particles and nuclei are indexed according to the author's emphasis.

(g) Particles of nuclei of elements of at least 98% natural abundance. Such particles are not named at the beginning of the modification at the element name.

Examples of index entries (Notation in the original document: $^{63}\text{Cu}(\text{}^{12}\text{C},\alpha p)$):

**Carbon, reactions
ions of carbon-12, copper-63 bombardment by**

**Copper, reactions
isotope of mass 63, bombardment of, by carbon-12**

**Proton
from carbon-12 bombardment, of copper 63**

**Alpha particle
from carbon-12 bombardment, of copper 63**

(h) Antielements and antiparticles are indexed at the element and particle names with “Anti-” as a prefix; the symbol (the usual one with a vinculum added) is cited in the heading after a comma, and the isotope number of the antielement is given in the modification; e.g., **Antihelium, He, isotope of mass 4; Antiproton, p**. The antielectron is indexed at **Positron**, and the negative muon and positive pion antiparticles are named as the particles of opposite charge, e.g., **Meson, π^+** ; **Muon, $\mu^-(106)$** .

³“Review of Particle Properties” published by the Particle Data Group is recognized as an authority in this field. It appears in alternate years in *Physics Letters B* and *Review of Modern Physics* (for example, see *Physics Letters B*, 1990, 239, 1.6-1.11).

(i) Atomic and molecular states of elementary particles. General studies are indexed at such headings as **Mesonic atom**, **K-Mesonic atom**, and **Muonic molecule**. Specific atomic and molecular states are indexed at the element name ("compounds" category) or particle name.

Examples of index entries:

1. The original document describes the *K*Be mesonic atom:

Meson, K
mesonic atom with beryllium (KBe)

2. The original document describes the exotic combination of muonium with chlorine:

Muon, μ
leptonic mol. with chlorine ($\mu^+e^-Cl^0$)

The atomic and molecular states of elementary particles are assigned the preferred entry at the particle name, with an additional entry for the atom or molecule.

(j) **Muonium** and **positronium** are used for the bound states (μ^+e^-) and (e^+e^-).

(k) Hypernuclei from hyperon interaction with atomic nuclei, and quark nuclei from quark binding in atomic nuclei are indexed in the *Chemical Substance Index* at the element name.

Examples:

Helium
hypernucleus of helium-5

Helium
quark nucleus $q(2 - \frac{1}{3})\text{He} \frac{1}{3}^+$

218. Enzymes are indexed by *CA* at the names recommended by the Nomenclature Committee of the International Union of Biochemistry (IUB)⁴ and Supplements as far as is compatible with *CA* nomenclature and indexing practices. Each specific enzyme is assigned a CAS Registry Number which is cited after the preferred index name in the *Chemical Substance Index*, where entries are to be found.

Names for enzymes may comprise (a) a trivial substrate name combined with an action term, e.g., Lactate dehydrogenase, which is indexed at **Dehydrogenase, lactate** (this is E.C. 1.1.1.27, at which designation a cross-reference can be found); (b) a substrate name and the suffix "-ase," e.g., Adenosine triphosphatase, which is indexed at **Phosphatase, adenosine tri-**; (c) a name, similar to those in (b), but from which a heading parent expressing the enzyme action cannot be readily separated, e.g., **Asparaginase**, which is indexed at this name; and (d) other single terms which may describe the source, e.g., **Papain**, or the action, e.g., **Lysozyme** or **Chymotrypsin**; such enzymes (mainly proteinases) are indexed at these names.

Qualifying phrases, which form part of the total enzyme name, appear in parentheses in the boldface heading after the main part of the name and express coenzyme specificity, secondary enzyme activity, secondary product formed, etc. Sometimes more than one type of information is expressed in this way.

Examples:

Dehydrogenase, malate (decarboxylating)

Synthetase, acyl coenzyme A (guanosine diphosphate-forming)

Dehydrogenase, glyceraldehyde phosphate (nicotinamide adenine dinucleotide phosphate) (phosphorylating)

General studies of enzymes, and new enzymes, will be found at **Enzymes** in the *General Subject Index*. When complete primary structural information (amino acid sequence) is reported for an enzyme, an entry with as much source specificity as possible is made, e.g., **Pepsin A (human pancreas)**, and a separate CAS registration linked to the structural information is prepared.

219. Inorganic compounds are indexed at names based on United States usage and the recommendations of the International Union of Pure and Applied Chemistry. For elements 104-110, CAS follows the recommendations of the ACS Committee on Nomenclature: 104 - Rutherfordium (Rf); 105 - Dubnium (Db); 106 - Seaborgium (Sg); 107 - Bohrium (Bh); 108 - Hassium (Hs); 109 -

Meitnerium (Mt); and 110 - Darmstadtium (Ds). For isotopically labeled inorganic compounds, see ¶ 220.

Elements of atomic number higher than 110, prior to 1982, were indexed at such headings as **Element 114**. They are now named by a combination of three syllables derived from the atomic number, the numerals 0-9 corresponding to the syllables nil, un, bi, tri, quad, pent, hex, sept, oct, and enn. The final "n" of enn is elided before nil, and the "i" of bi and tri before ium, which is the invariant suffix.

Example:

Ununquadium (formerly Element 114)

The initial letters of the first three syllables of the names provide the symbols from which synonym line formulas are derived for binary compounds of these superheavy elements.

Example:

Ununquadium fluoride (UuqF₄) (formerly Element 114 fluoride (1:4))

These index headings are not subdivided into categories as is done for elements with established names (i.e., 1 through 110).

Elements reported or discussed without specific reference to atomic number are indexed at **Elements** in the *General Subject Index*. Class headings in the same index, e.g., **Group IVA elements**, **Alkaline earth metals**, **Halogens**, **Helium-group gases**, **Platinum metals**, **Transition metals**, are employed for general studies of varying specificity.

Molecular forms of the elements are indicated in the modification, except that hydrogen and its isotopes, and nitrogen, oxygen, and the halogens are assumed to be diatomic (unless the term "atomic" is cited). Examples: **Sulfur**, mol. (S₈); **Oxygen**; **Hydrogen**, atomic.

Uninverted salt-type heading parents are used to index binary compounds, double salts, mixed salts, and certain other ionic and simple covalent compounds. The electropositive (cationic) constituents are named first in alphabetical order, followed by electronegative (anionic) constituents in alphabetical order. In the case of binary compounds between nonmetals, that constituent is placed first which appears earlier in the following sequence: Rn, Xe, Kr, Ar, Ne, He, B, Si, C, As, P, N, H, Te, Se, S, At, I, CN, SCN, Br, Cl, O, O₂²⁻, F, N₃¹⁻, OCN. (Elements not listed here are treated as metals; prior to the Tenth Collective Index (1977-1981) antimony was included among the nonmetals.) For monoatomic anions, the ending "-ide" is cited. When a binary compound contains only nonmetals, the same sequence determines the order of the total name, e.g., Silicon carbide (SiC).

A synonym line formula follows the name of each uninverted salt-type heading parent. (Prior to the Tenth Collective Index (1977-1981), line formulas did not appear with unambiguous names, e.g., **Sodium chloride**, **Zinc sulfide**.) Beginning with the Twelfth Collective Period (1987-1991), line formulas may be expressed with decimals or numerical ranges as well as integers.

Example:

Sodium tungsten oxide (Na_{0.37}WO₃)

Hydrides of the metals antimony, bismuth, germanium, tin, and lead are indexed at hydride names such as **Germane** (¶ 199). Halides are indexed as derivatives at these headings, e.g., **Stannane**, **tetrachloro-** (not Tin chloride (SnCl₄)); **Plumbane**, **diiodo-**. Hydrides, halides, etc., of most other elements are indexed at headings such as **Sodium hydride (NaH)**; **Thorium hydride iodide (ThHI₃)**. The hydrides of nitrogen have trivial names: **Ammonia**, for NH₃; **Amidogen**, for NH₂; **Hydrazine**, for N₂H₄; and **Hydrazoic acid**, for HN₃. Some derivatives of ammonia also have trivial names: **Chloramine**, for NH₂Cl; **Fluorimide**, for NHF₂; **Hydroxylamine**, for HONH₂; **Sulfamide**, for SO₂(NH₂)₂; **Sulfimide**, for SO₂NH. The cyclic trimer of sulfimide is indexed at the heterocyclic name: **1,3,5,2,4,6-Trithiatriazine, 1,1,3,3,5,5-hexaoxide**.

Chalcogen hydride names include **Water**, for H₂O; **Hydrogen peroxide (H₂O₂)**; **Hydrogen trioxide**, for H₂O₃; **Hydroxyl**, for HO; **Hydroperoxo**, for HO₂; **Hydrotrioxo**, for HO₃; **Selenyl**, for HSe; and **Hydrogen sulfide (H₂S)**.

Salts of hydric cations such as **Ammonium**, **Phosphonium**, **Nitric acidium**, are indexed at uninverted salt names with the "-ium" term cited first, or at "oxo" acid headings with "-ium salt" terms in the modification.

Examples:

Ammonium chloride ((NH₄)Cl)

Phosphonium cyanide ((PH₄)CN)

Oxonium chloride ((OH₃)Cl)

Perchloric acid, compounds

ammonium salt (1:1) (named like a metal salt of the same acid, see below)

Salts of **Hydrazine** and **Hydroxylamine** are named as molecular addition compounds (¶ 192), e.g., **Hydrazine, sulfate (2:1)**.

Binary oxides are indexed at headings such as **Sodium oxide (Na₂O)**, **Iron oxide** (with a synonym line formula, if known), **Chlorine oxide (ClO₂)**. Uninverted peroxide, superoxide, and ozonide headings are also employed, e.g.,

⁴*Enzyme Nomenclature, 1992*. Academic Press, Orlando, Florida, 1992, 862 pp. Supplements 1-3, *Eur. J. Biochem.* 1994, 223, 1-5; 1995, 232, 1-6; 1996, 237, 1-5.

Sodium peroxide (Na_2O_2). The oxides CO , CO_2 , SO_2 , SO_3 , and SiO_2 are indexed at **Carbon monoxide**, **Carbon dioxide**, **Sulfur dioxide**, **Sulfur trioxide**, and **Silica**, respectively.

Mixed-metal oxides containing only the oxide (O^{2-}) anion are indexed at oxide headings, with the metals cited in alphabetic order, e.g., **Iron zinc oxide** (Fe_2ZnO_4). Hydroxides of one or more metals are indexed at metal hydroxide headings, e.g., **Chromium hydroxide** ($\text{Cr}(\text{OH})_3$). Mixed-metal oxides, hydroxides, and oxide-hydroxides that also contain a Group IA and/or Group IIA metal are named at oxy-anion headings with cation terms in the modification, e.g., **Stannate** ($\text{Sn}(\text{OH})_6^{2-}$), **potassium (1:2)**, (*OC-6-11*); **Tantalate** ($\text{Ta}_6(\text{OH})_{18}^{7-}$), **potassium (1:7)**; **Molybdate**($2-$), **tetra- μ -oxotetraoxoferrate**-, **sodium (1:2)**. Hydroxide-oxides that contain no Group IA or IIA metals are indexed at such headings as **Manganese hydroxide oxide** ($\text{Mn}(\text{OH})\text{O}$). The index heading parents **Chromic acid** (H_2CrO_4), **Chromic acid** ($\text{H}_2\text{Cr}_2\text{O}_7$), **Manganic acid** (H_2MnO_4) and **Permanganic acid** (HMnO_4) are retained. Hydroperoxides are indexed at peroxide headings with synonym line formulas, e.g., **Sodium peroxide** ($\text{Na}(\text{HO}_2)$), for $\text{Na}(\text{OOH})$. Mixed peroxide, hydroperoxide, ozonide, and superoxide headings are also employed. Sulfides, selenides, and tellurides are named like the oxides. The compounds CS_2 and COS are indexed at **Carbon disulfide** and **Carbon oxide sulfide** (COS), respectively.

Uninverted salt-type headings are used for halides, amides, arsenides, azides, borides, carbides, cyanides, hydrazides, hydroxylamides, imides, nitrides, phosphides, and silicides. Synonym line formulas are used to differentiate the hydrazides ($\text{H}_3\text{N}_2^{1-}$) and ($\text{H}_2\text{N}_2^{2-}$); for special cases such as iodide (I_3^{1-}), chloride (HCl_2^{1-}), and fluoride (HF_2^{1-}); and for arsine, phosphine, and stibine which have lost one or two protons, e.g., **Arsenide** (HAs^{2-}). Otherwise it is understood the anions are monoatomic and have lost all protons, e.g., As^{3-} , P^{3-} , Si^{4-} . Examples: **Sodium chloride** (NaCl), **Potassium iodide** (KI), **Potassium iodide** (KI_3), **Calcium niobium fluoride** [formula unknown], **Sodium phosphide** ($\text{Na}(\text{H}_2\text{P})$), **Cyanogen chloride** ($(\text{CN})\text{Cl}$).

In these compounds, and the oxides, sulfides, etc., discussed earlier, all metals are considered to be cationic. Nonmetals are placed in cationic or anionic sequence to balance the charges. If this violates the electronegativity sequence described earlier, all metals are named as cations and all nonmetals as “-ide” anion terms.

Examples:

Aluminum gallium arsenide ($(\text{Al,Ga})\text{As}$)

Cadmium silicon phosphide (CdSiP_2) (not Cadmium phosphide silicide)

Thallium phosphide selenide (TlPSe) (not Thallium selenium phosphide)

Mercury iodide phosphide ($\text{Hg}_3\text{I}_4\text{P}_2$)

Solid solutions are normally indexed as mixed salts (oxides, etc.). Decimal fractions, which can include ranges of composition, are used as subscripts in the accompanying formulas to specify stoichiometric relationships when applicable. As a result of nonstoichiometry, decimal fractions may not add to whole numbers. The omission of such numerical designations indicates incomplete information on the proportions in the original document.

Examples:

Aluminum gallium arsenide ($\text{Al}_{0.5}\text{Ga}_{0.5}\text{As}$)

Cadmium mercury telluride ($(\text{Cd,Hg})\text{Te}$)

Copper platinum sulfide ($\text{Cu}_{1.7-1.8}\text{Pt}_{3-3.2}\text{S}_6$)

Iron manganese zinc oxide ($\text{Fe}_{2.3}\text{Mn}_{0.5}\text{Zn}_{0.2}\text{O}_{3.9}$)

Solid solutions that involve classes of substances, or are otherwise incompletely defined as to elemental constituents, are identified in the index modification by a phrase such as “solid solns. with ...”

Example:

Iron oxide (Fe_3O_4)
solid solns. with ferrites

Salts of interhalogen anions are indexed as coordination compounds (¶ 215), e.g., **Iodate**($1-$), **dichloro-**, **sodium**, for $\text{Na}[\text{ICl}_2]$. Acetylides are indexed at names such as **Sodium acetylide** ($\text{Na}(\text{C}_2\text{H})$). The common name **Calcium carbide** ($\text{Ca}(\text{C}_2)$) is the single exception. Metal derivatives of *substituted Ethyne* and of other alkynes are indexed by organometallic nomenclature (¶ 194).

Examples:

$\text{BrC}\equiv\text{CAg}$ **Silver, (2-bromoethynyl)-**

$\text{EtC}\equiv\text{CNa}$ **Sodium, 1-butyne-1-yl-**

Graphite compounds are indexed as molecular addition compounds. Prior to CA Volume 95 (see ¶ 101), binary headings such as **Graphitic acid**, **Graphite nitrate**, etc., were employed.

Example:

$\text{C} \cdot 1/10 \text{HNO}_3$ **Nitric acid, compd. with graphite (1:10)**

The following metal-oxide radical names are sometimes used: americyl ($\text{O}_2\text{Am}-$ and $\text{O}_2\text{Am}=\text{}$), chromyl ($\text{O}_2\text{Cr}=\text{}$), neptunyl ($\text{O}_2\text{Np}-$ and $\text{O}_2\text{Np}=\text{}$), permanganyl ($\text{O}_3\text{Mn}-$), perrhenyl ($\text{O}_3\text{Re}-$), pertechnetyl ($\text{O}_3\text{Tc}-$), plutonyl ($\text{O}_2\text{Pu}-$ and $\text{O}_2\text{Pu}=\text{}$), titanyl ($\text{O}_2\text{Ti}=\text{}$), uranyl ($\text{O}_2\text{U}-$ and $\text{O}_2\text{U}=\text{}$), vanadyl ($\text{OV}-$, $\text{OV}=\text{}$, and $\text{OV}\equiv\text{}$), and zirconyl ($\text{OZr}=\text{}$). These names, and those for the thio, seleno, and telluro analogs, are used for the ions, e.g., **Vanadyl ion**($2+$), and to complete the salt names at coordination anion headings (¶ 215). They are not used for their compounds with simple inorganic salts, nonmetal oxo acids, or organic acids.

Examples:

UO_2Cl_2 **Uranium, dichlorodioxo-**
 $\text{K}_2\text{UO}_2(\text{SO}_4)_2$ **Uranate**($2-$), **dioxobis[sulfato-**
($2-$)- κO]-, potassium (1:2)

The following nonmetal oxide radicals and their chalcogen analogs are employed: nitrosyl ($\text{ON}-$), nitryl ($\text{O}_2\text{N}-$), sulfinyl ($\text{OS}=\text{}$) (thionyl is limited to halides and halogenides), sulfonyl ($\text{O}_2\text{S}=\text{}$) (sulfuryl is limited to halides and halogenides), thiothiazyl (N_3S_4-), diphosphoryl (O_3P_2-), disulfonyl (O_5S_2-), chlorosyl ($\text{OCl}-$), chloryl ($\text{O}_2\text{Cl}-$), perchloryl ($\text{O}_3\text{Cl}-$) (and similarly for other halogen radicals). For other phosphorus and sulfur radicals see ¶ 197, 200, 276, and the Illustrative List of Substituent Prefixes (Section H, ¶ 294).

Examples:

$\text{Cl}-\text{S}(\text{O}_2)-\text{S}(\text{O}_2)-\text{Cl}$ **Disulfonyl chloride**
 $(\text{SO})\text{Br}_2$ **Thionyl bromide**
 $\text{NOH}(\text{S}_2\text{O}_7)$ **Nitrosyl (disulfate) ((NO)H(S₂O₇))**
 $(\text{SeO}_2)\text{Cl}_2$ **Selenonyl chloride**

Compounds of the nonmetal radicals with “organic” acids (i.e., those named as principal groups on molecular skeletons, such as carboxylic and sulfonic acids, ¶ 165) are indexed as anhydrides (¶ 179). For carbonyl compounds, e.g., **Carbonic dihydrazide**, **Imidodicarbonic diamide**, **Urea**, see ¶ 183.

Metal carbonyls and nitrosyls are indexed at binary headings when they are either mononuclear or of unknown polynuclear structure, e.g., **Chromium carbonyl** ($\text{Cr}(\text{CO})_6$), (*OC-6-11*)-. Polynuclear carbonyls and nitrosyls of known structures are named as coordination complexes. (Simple metal nitrosyl dimers may be hyponitrites, e.g., $\text{Na}_2\text{N}_2\text{O}_2$, **Hyponitrous acid**, sodium salt (1:2).) Polynuclear carbonyls and nitrosyls of known composition are indexed as coordination compounds (¶ 215).

Helium-group compounds are indexed like the analogous metal compounds, except that salts with acids are named at their own headings.

Examples:

KrF_2 **Krypton fluoride (KrF₂)**
 XeO_4 **Xenon oxide (XeO₄)**
 $\text{K}_2[\text{XeF}_8]$ **Xenonate**($2-$), **octafluoro-**
potassium (1:2)
 $\text{Xe}(\text{ClO}_4)_2$ **Xenon perchlorate (Xe(ClO₄)₂)**
(not Perchloric acid, xenon($2+$) salt)

Oligomeric inorganic compounds, except clusters, are reduced to their empirical formulas when the structures are unknown. When the actual structure of the oligomer is defined in the source document or known from references, an entry is made at the empirical formula. Clusters with unspecified oligomeric bonding are not reduced to their empirical formulas.

Examples:

Al_2Cl_6 **Aluminum, di- μ -chlorotetra-**
chlorodi-
 Be_3Cl_6 **Beryllium, hexa- μ -chlorotri-**
triangulo

Metal-containing inorganic clusters receive standard nomenclature for inorganic compounds, e.g., **Sodium fluoride** (Na_7F_7), **Lithium potassium chloride** ($\text{Li}_6\text{K}_4\text{Cl}_{10}$). Nonmetallic inorganic clusters receive oligomeric names when the monomeric form does not receive a line formula. All other nonmetallic inorganic clusters receive regular inorganic names with a line formula denoting the oligomeric formula.

Examples:

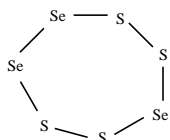
(HF) ₃	Hydrofluoric acid, trimer
(SF ₆) ₇	Sulfur fluoride (S₇F₄₂)

Complex, mixed, and multiple salts are indexed at their own headings or (if complex cations or anions are present) as coordination compounds (¶ 215). Mixed salts of a single oxo acid are indexed at the acid heading.

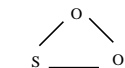
Examples:

	Cobaltate(2-), tetrachloro-, cesium chloride (1:3:1), (T-4)
UOCl ₂	Uranium chloride oxide (UCl₂O)
Co ₅ (NO ₃) ₂ (SO ₄) ₄	Cobalt nitrate sulfate (Co₅(NO₃)₂(SO₄)₄)
H ₂ O ₃ S•1/2Fe•NH ₃ •3H ₂ O	Sulfuric acid, ammonium iron(2+) salt, hydrate (2:2:1:6)
2NaCl•Na ₂ SO ₄	Sodium chloride sulfate (Na₄Cl₂(SO₄))
B ₂ O ₃ •P ₂ O ₅	Boron phosphate (B(PO₄))

Cyclic inorganic substances composed of two or more elements and containing no metals of Groups 1-13 are named as ring systems.

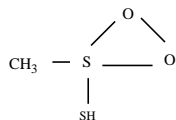


1,2,4,5,3,6,7-Tetrathiatriselenepane



Dioxathirane

Organic derivatives of these substances may also be named as rings when there is no coordinate bonding.



Dioxathirane, 3,3-dihydro-3-mercapto-3-methyl-

Ammoniates are expressed in the modification at salt names, unless the ammonia is coordinated, in which cases "ammine" coordination names (¶ 215) are employed.

Hydrates of simple metal salts are named by modification phrases and as coordination compounds if water is the only coordinating ligand. When other ligands are present, "aqua" coordination names (¶ 215) are used. Uncoordinated water is expressed as "hydrate" in the modification.

Examples:

[Ni(OH ₂) ₆] ²⁺ •2Cl ⁻	Nickel(2+), hexaaqua-, chloride (1:2), (OC-6-11)-
NiCl ₂ •6H ₂ O	Nickel chloride (NiCl₂), hydrate (1:6)
Ca ₃ (PO ₄) ₂ •3/2H ₂ O	Phosphoric acid, calcium salt, hydrate (4:6:3)

Binary and pseudobinary inorganic acids are restricted to **Hydrofluoric, Hydrochloric, Hydrobromic, Hydriodic, Hydrocyanic, Hydrazoic** (HN₃), **Fulminic** (HONC), **Cyanic**, and **Thiocyanic acid**, together with **Hydrogen triiodide** (HI₃) and oligomers such as **Hydrochloric acid, dimer**. (For isocyanic and isothiocyanic acids, see ¶ 183.)

Inorganic oxo acids. Protonic acids of anions containing only oxo or hydroxy ligands are given names terminating in "-ic acid" or "-ous acid." Acids ending in "-ous acid" are limited to the lower valent compounds of the elements F, Cl, Br, I, S, Se, N, P, and As. The prefix "per-" is used to designate one oxo acid of manganese (see below), peroxy acids of boron, and oxo acids of the halogens in the 7+ oxidation state. Inorganic oxo "-ic" and "-ous" acid names are in general limited to hydroxy and oxo-hydroxy compounds of the nonmetals As, At, B, Br, Cl, F, I, N, P, S, Se, Si, and Te, in any oxidation state. Prior to the Tenth Collective Index (1977-1981), metal acid headings were employed;

now, acids of metals (including antimony) are generally indexed at metal oxide and hydroxide headings, e.g., **Antimony hydroxide** (Sb(OH)₃); however, the metal acid names **Chromic acid** (H₂CrO₄), **Chromic acid** (H₂Cr₂O₇), **Manganic acid** (H₂MnO₄), and **Permanganic acid** (HMnO₄) are retained as index heading parents. Chalcogen and peroxy analogs of these metal and nonmetal acids are named by prefixing the "-ic" or "-ous" acid name by seleno-, thio-, telluro-, or peroxy-. The number of substituting atoms or groups is indicated in the synonym line formula in the heading.

For **Carbonic, Carbonothioic, and Carbonoperoxy acids**, see ¶ 183. Other peroxy acid names include **Peroxychromic acid** (H₂CrO₂(O₂)₂), etc. The two mononuclear **Boric acid** headings are differentiated by the synonym line formulas HBO₂ and H₃BO₃. Cyclic metaborates of the general formula H_nB_nO_{2n}, in which *n* is equal to or greater than 3, are also indexed at this heading. Thio-, etc., acids are named at such headings as **Thioboric acid** (H₃BS₃). Isopoly acids can be considered to arise formally by condensation of a mononuclear acid, thus, 2H₃BO₃ → H₄B₂O₅ + H₂O. The names used in indexing isopoly acids are the same as those of the mononuclear precursors, e.g., **Boric acid** (H₄B₂O₅). The synonym line formulas are usually empirical, but molecular formulas are shown for cyclic "meta" acids. Thus, **Boric acid** (H₃B₃O₃). For the former Hypoboric acid ((HO)₂BB(OH)₂) and its derivatives, see ¶ 182.

Examples of peroxy and chalcogen analogs of isopoly acids are **Peroxydicarbonic acid** (see ¶ 183), **Thioboric acid** (H₂B₂S₄), **Thiosilicic acid** (H₄Si₃O₄S₃), **Selenotellurodiarsenous acid** (H₄As₂Se₃Te₂).

The single name **Telluric acid** is used in association with the following synonym line formulas: H₂TeO₃, H₂TeO₄, H₂Te₂O₅, H₂Te₂O₇, H₆TeO₆, H₈Te₂O₁₀.

Selenious and Selenic acid analogs in which one hydroxyl has been replaced by a univalent group are indexed at acid headings with nondetachable prefixes, e.g., **Fluoroselenious acid** (HSeFO₂), **Amidoselenic acid** (Se(NH₂)(OH)O₂). Replacement of both groups leads to a nonacid heading, e.g., **Selenic diamide** (Se(NH₂)₂O₂), **Amidoselenonyl fluoride** ((SeO₂)(NH₂)F) (acid halides rank higher than amides (¶ 106)). An example of a polyselenic acid derivative is **Imidodiselenic diamide** (NH[Se(NH₂)O₂]₂).

Sulfur oxo acids are functional parent compounds. Analogs in which sulfur is directly attached to a molecular skeleton, e.g., **Benzene, Hydrazine, or Germane**, are named as sulfonic, sulfinic, and sulfenic acids (¶ 165). For thionic acids, see ¶ 200. For **Hydroxylamine-O-sulfonic acid**, see ¶ 193. (Selenium oxo acids are named similarly, except that selenium analogs of **Sulfoxylic acid** and **Hydroxylamine-O-sulfonic acid** and those thionic acids in which the sulfur has been totally replaced are not recognized in indexing.) The mononuclear sulfur acids are:

(HO) ₂ S	Sulfoxylic acid
(HO) ₂ SO	Sulfurous acid (the selenium analog is Selenious acid .)
(HO) ₂ SO ₂	Sulfuric acid (the selenium analog is Selenic acid .)

Analogs and derivatives of these acids are named by use of nondetachable prefixes such as amido, imido, chloro, azido, thio, seleno, and peroxy, with replacement of the acid class name by the preferred suffix or class term if all hydroxyl groups have been removed. Compounds containing only sulfur (or selenium) and halogen are indexed at binary names, e.g., **Sulfur chloride** (SCl₂). Monohydrazides are indexed at hydrazine headings, e.g., **Hydrazinesulfonyl chloride** for H₂NNHSO₂Cl. Some trivial names are employed. For **Sulfur diimide**, see ¶ 200.

Examples:

H ₂ N(HO)S	Amidosulfoxylic acid
H ₂ NSCl	Amidosulfonyl chloride
HO(NC)SO	Cyanosulfurous acid
Cl(NC)SO	Thionyl chloride cyanide
(HO) ₂ S(S) (or HO(HS)S(O))	Thiosulfurous acid (H₂S₂O₂)
Cl(H ₂ N)S=NH	Amidoimidodisulfurous chloride
HO(N ₃)SO ₂	Azidosulfuric acid
Cl(HO)SO ₂	Chlorosulfuric acid
HO(H ₂ N)SO ₂	Sulfamic acid
Cl ₂ SO ₂	Sulfuryl chloride
F(ON)SO ₂	Nitrososulfonyl fluoride
HO(H ₂ N)S(O)=NH	Imidosulfamic acid
F ₂ N(H ₂ N)SO ₂	Sulfamide, N,N-difluoro-
Cl(HO)S(O)=NH	Chloroimidodisulfuric acid
Cl ₂ S(O)S	Thiosulfuryl chloride ((S₂O)Cl₂)
(H ₂ N) ₂ S(O)=NH	Imidosulfamide

HOO(HO)SO ₂	Peroxymonosulfuric acid
HO(HSS)SO ₂	Thioperoxymonosulfuric acid (HO)(HSS)SO ₂

Polynuclear sulfur and selenium acids have such names as **Disulfuric acid** for (HO)S(O₂)O(O₂)S(OH), **Diselenious acid** for (HO)Se(O)O(O)Se(OH), **Trisulfuric acid**, etc. Analogs are named by use of nondetachable prefixes and replacement of the acid term (if all hydroxyl groups are absent).

Examples:

(N ₃)SO ₂ OSO ₃ H	Azidodisulfuric acid
HO(SO ₂ NH) ₂ SO ₃ H	Diimidotrisulfuric acid
H ₂ NSO ₂ NHSO ₃ H	Amidoimidodisulfuric acid
HO ₃ SOOSO ₃ H	Peroxydisulfuric acid ((HO)S(O) ₂) ₂ (O) ₂
ClSO ₂ OSO ₂ OSO ₂ Cl	Trisulfuryl chloride
H ₂ NSO ₂ OSO ₂ NH ₂	Disulfamide
(ClSO ₂) ₂ NNH ₂	1,1-Hydrazinedisulfonyl dichloride

Phosphorus and arsenic acids. For mononuclear phosphorus and arsenic acids, both nonsubstitutive, e.g., **Phosphoric acid**, **Arsenous acid**, and substitutive, e.g., **Phosphonic acid**, see ¶ 197. There are no official rules for naming polynuclear phosphorus and arsenic acids; they are indexed by *CA* at names traditionally used in the literature. Pyrophosphoric acid and its analogs and derivatives are indexed at **Diphosphoric acid** names, and similarly for Pyrophosphorous acid. Specific esters of **Metaphosphoric acid** (H₃P₃O₉) are indexed at the heterocyclic parent **1,3,5,2,4,6-Trioxatrisphosphorinane** (¶ 197), and other meta acids are treated similarly. Mixed polynuclear phosphoric-phosphorous acids are indexed at headings which include Stock numbers (parenthetical Roman numerals) to indicate the sequence of trivalent and pentavalent phosphorus atoms. When all hydroxyl groups have been replaced, the acid term gives way to acid halide, amide, etc., suffixes. Amides of polyphosphorous acids are indexed by replacing the word "acid" by "amide" preceded by a multiplicative prefix; amides of polyphosphoric acids have names in which "ic acid" is simply replaced by "-amide," e.g., **Diphosphorous tetraamide**, for [(H₂N)₂P]₂O, and **Peroxydiphosphoramidate**, for [(H₂N)₂P(O)]₂O₂. P, P', etc., locants are used to designate the position of replacement amido and imino, bridging imido, etc., groups.

Arsenic analogs are named analogously to the phosphorus examples below, except that "Hypo-" and "Isohypo-" names and headings in which mixed valencies are denoted by "III" and "V" terms are not employed.

Examples:

(HO) ₂ P(O)OP(O)(OH) ₂	Diphosphoric acid
(HO) ₂ P(O)OP(O)(OH)OP(O)(OH) ₂	Triphosphoric acid
(HO) ₂ P(O)P(O)(OH) ₂	Hypophosphoric acid
(HO)HP(O)P(O)(OH) ₂	Isohypophosphoric acid
(HO) ₂ POP(OH) ₂	Diphosphorous acid
(HO) ₂ POP(O)(OH) ₂	Diphosphoric(III,V) acid
(HO) ₂ POP(O)(OH)OP(O)(OH)OP(O)(OH) ₂	Tetraphosphoric(III,V,III,V) acid
(HO) ₂ P(O)NHP(O)(OH) ₂	Imidodiphosphoric acid
[(HO) ₂ P(O)OP(O)(OH)] ₂ NH	P'-Imidotetraphosphoric acid
Cl ₂ P(O)OP(O)(OH)Cl	Trichlorodiphosphoric acid
H ₂ N(HO)P(O)OP(O)(OH) ₂	Amidodiphosphoric acid
(HO) ₂ POP(O)(OH)NH ₂	P'-Amidodiphosphoric(III,V) acid
HO(HS)P(O)SP(O)(OH)SH	Thiodiphosphoric acid ((HO)(HS)P(O)) ₂ S
(HO) ₂ P(S)SSP(S)(OH) ₂	Thioperoxydiphosphoric acid ((HO) ₂ P(S)) ₂ S ₂
H ₂ N(HO)POP(S)(OH) ₂	P-Amido-P'-thiodiphosphoric(III,V) acid
Cl(H ₂ N)P(O)OP(O)Cl ₂	Amidodiphosphoryl chloride
Cl ₂ P(O)OP(O)(Cl)F	Diphosphoryl chloride fluoride (Cl ₂ P(O)OP(O)Cl)F
[(HO) ₂ P(O)] ₃ N	Nitridotriphosphoric acid
[(H ₂ N) ₂ P(O)NH] ₂ P(=NH)NH ₂	P'-Iminodiimidotriphosphoramidate

For further examples, see ¶ 197.

Nitrogen oxo acids are indexed at the following headings:

HONO	Nitrous acid
HONO ₂	Nitric acid
HON=NOH	Hyponitrous acid
HON=N(O)OH	Hyponitric acid

Halide and halogenoid derivatives are indexed at nityl and nitrosyl names, e.g., **Nitrosyl chloride ((NO)Cl)**. The amides of nitric and nitrous acid are **Nitramide** and **Nitrosamide**, respectively; organic derivatives are named as *N*-nitro and *N*-nitroso amines.

Halogen oxo acids include:

HOCl	Hypochlorous acid
HOBrO	Bromous acid
HOClO ₂	Chloric acid
HOIO ₂	Iodic acid (HIO₃)
(HO) ₂ IO ₂	Iodic acid (H₂IO₄)
HOClO ₃	Perchloric acid
HOIO ₃	Periodic acid (HIO₄)
(HO) ₃ IO	Periodic acid (H₃IO₆)

Mixed halides are indexed at such names as **Chloryl fluoride ((ClO₂)F)**.

Silicon oxo acids in *CA* indexing are named as **Silicic acid** with one of the following synonym line formulas: **H₂SiO₃**, **H₄SiO₄**, **H₂Si₂O₅**, **H₆Si₂O₇**. The same index heading is employed for cyclic acids of the general formulas H_{2n}Si_nO_{3n} and H_{2n}Si_{2n}O_{5n} in which n is equal to or greater than 3. The compound (HO)₃SiSi(OH)₃ is named **Disilanehexol**. (See also ¶ 199.)

Anhydrides of inorganic oxo acids with carboxylic, sulfonic, etc., acids are indexed at the organic acid heading (¶ 179); mixed inorganic anhydrides which contain neither free nor esterified hydroxyl groups are given uninverted salt names.

Examples:

ClONO ₂	Chlorine nitrate (Cl(NO₃))
B(OPO ₂) ₃	Boron metaphosphate (B(PO₃)₃)

When free (or esterified) hydroxyl groups are present, the index entry is made at the preferred acid heading with an "anhydride with" phrase is the index modification.

Examples:

EtOSO ₂ OCIO ₃	Perchloric acid, anhydride with ethyl hydrogen sulfate
HOSO ₂ OSi(OH) ₂ OSO ₂ OH	Sulfuric acid, anhydride with silicic acid (H₄SiO₄) (2:1)

Mixed anhydrides of inorganic peroxy and thio (etc.) acids are indexed similarly, with use of "anhydrosulfide with" terms when appropriate, but anhydrides with a peroxy, dithio, etc., linkage are indexed at **Peroxide**, **Disulfide**, etc.

Example:

HO ₃ SSSP(O)(OH) ₂	Disulfide, phosphono sulfo
--	-----------------------------------

Metal (and helium-group element) *salts* of inorganic oxo acids and their analogs are indexed at the oxo heading if only one anion is present (otherwise the salt is indexed at its own heading, e.g., **Potassium phosphate sulfate (K₂H₃(PO₄)(SO₄))**). A Ewens-Bassett number is cited with a metal of variable valence, and the stoichiometry of the salt is indicated by "mono," multiplicative prefixes, or ratios, when necessary.

Examples:

3 HClO ₃ • Al	Chloric acid, aluminum salt (3:1)
3 HNO ₃ • Ag	Nitric acid, silver(1+) salt (3:1)
H ₂ SO ₄ • Ca	Sulfuric acid, calcium salt (1:1)
HOSO ₂ OSO ₂ OH • Na	Disulfuric acid, sodium salt (1:1)
2 H ₂ NSO ₂ OH • Sn	Sulfamic acid, tin(2+) salt (2:1)
HN(SO ₂ F) ₂ • Ag	Imidodisulfonyl fluoride, silver(1+) salt (1:1)
H ₃ PO ₄ • NH ₃ • Mg	Phosphoric acid, ammonium magnesium salt (1:1:1)
2 HClO ₄ • Xe	Xenon perchlorate (Xe(ClO₄)₂)

Alums, chrome alums, etc., are indexed (*a*) at oxo acid names, e.g., **Sulfuric acid, compounds, aluminum potassium salt, hydrate (2:1:1:12)**, (*b*) at "ium" headings, e.g., **Methanaminium, N,N,N-trimethyl-, aluminum sulfate (1:1:2)** or (*c*) (if they contain conjugate acids of nitrogen bases) at names of acids and bases, e.g., **Sulfuric acid, aluminum salt, compd. with guanidine (1:1:1)**.

Anions are indexed at names usually identical with those employed in binary cation-anion headings (see above), e.g., **Hydride**, for H^{1-} ; **Carbide**, for C^{4-} ; **Carbide (C_2^{2-})**; **Hydrazide ($H_2N_2^{2-}$)**. Anions from inorganic oxo acids are indexed at "ate" and "ite" headings with the retained hydrogen atoms or derivatives expressed in the modification; an ion term is expressed for esters and salts. Oxo anions of metals have synonym line formulas; other polyatomic anions are assigned coordination anion names.

Examples:

$H_2PO_4^-$	Phosphate, hydrogen (1:2)
$EtSO_4^-$	Sulfuric acid, monoethyl ester, ion(1-)
AlO_2^-	Aluminate (AlO_2^{1-})
NO_3^{2-}	Nitrate(2-), trioxo-

Anions of elements without "ide" names are indexed at the element names, with "ion" modification terms followed by a symbol to show the charge and composition, e.g., ion (Re^{1-}), ion (Hg_2^{2-}), ion (S_8^{1-}).

Cations. The cation of hydrogen in the gas phase is indexed at **Proton** (¶ 217). Examples of other cation names are **Sulfonium**, for SH_3^{1+} ; **Chloronium**, for ClH_2^{1+} ; **Ammonium**, for NH_4^{1+} ; **Ammoniumyl**, for NH_3^{1+} ; **Hydrazinium(1+)**, for $N_2H_5^{1+}$; **Diphosphinium(2+)**, for $P_2H_6^{2+}$; **Thiosulfuric acidium(1+)** ($H_3S_2O_3^{1+}$); **Plutonyl ion(1+)**, for PuO_2^{1+} ; **Nitryl ion**, for NO_2^{1+} ; **Magnesium(1+)**, **diiodo-**, for MgI_2^{1+} ; **Helium(1+)**, **hydro-**, for HeH^{1+} . Cations of elements are indexed at element headings with the ion specified in the modification, e.g., **Carbon**, ion (C_2^{1+}).

Minerals are indexed at traditional and new mineral names as correlated by the Commission on New Minerals and Mineral Names of the International Mineralogical Association and reported in *The American Mineralogist*. Other references used to standardize the spelling and transliteration of mineral and rock names, as well as to standardize mineral formulas in the *CA* indexes are:

- American Geological Institute, *Glossary of Geology*, Washington, D.C., 1972, 857 pp.
- E. S. Dana, *A Textbook of Mineralogy*, 4th ed., revised and enlarged by W. E. Ford, John Wiley and Sons, New York, 1958, 851 pp.
- J. D. Dana and E. S. Dana, *System of Mineralogy*, 7th ed., entirely rewritten and enlarged by C. Palache, H. Berman, and C. Frondel, John Wiley and Sons, New York, Vol. I, 1944; Vol. II, 1951; Vol. III, 1962.
- R. W. Fairbridge, *The Encyclopedia of Geochemistry and Environmental Sciences* (Volume IVA of *The Encyclopedia of Earth Sciences* series), Van Nostrand Reinhold Co., New York, 1972, 1321 pp.
- M. Fleischer, *Glossary of Mineral Species*, Mineralogical Record, Tucson, Arizona, 1980, 192 pp.
- M. H. Hey, *An Index of Mineral Species and Varieties*, 2nd rev. ed., Trustees of the British Museum (Natural History), London, 1955, 728 pp. Appendixes, 1963, 135 pp; 1974, 168 pp.
- C. Hintze, *Handbuch der Mineralogie*, Supplement 2, *Neue Mineralien und Neue Mineralnamen*, Walter de Gruyter, Berlin, 1960, 958 pp.
- C. M. Rice, *Dictionary of Geological Terms*, Edwards Brothers, Ann Arbor, Mich., 1961, 465 pp.
- H. Strunz, *Mineralogische Tabellen*, 4th rev. ed., Akademische Verlagsgesellschaft Geest und Portig K.-G., Leipzig, 1966, 560 pp.
- P. W. Thrush, *A Dictionary of Mining, Mineral, and Related Terms*, U.S. Department of the Interior, 1968, 1269 pp.

Minerals of definite composition have a synonym line formula cited after the name, e.g., **Chromatite ($Ca(CrO_4)$)**. When no mineral formula is given in the original document, the assumed formula is that given in reference (*e*), above. New minerals are indexed at names and formulas supplied in original documents and collected in each issue of the *General Subject Index* at **New minerals**.

When one or more elements have replaced the whole or part of the original element in a mineral, and no new mineral name has been coined, the replacing element is named in the modification at the original heading.

Examples:

$BaSi_2O_5$	Sanbornite ($Ba(Si_2O_5)$)
$Li_2Si_2O_5$	Sanbornite lithium ($Li_2(Si_2O_5)$)
$LiNaSi_2O_5$	Sanbornite lithium sodium ($LiNa(Si_2O_5)$)
Zn_2SiO_4	Willemite ($Zn_2(SiO_4)$)
$ZnMgSiO_4$	Willemite magnesium ($ZnMg(SiO_4)$)

When partial replacement has occurred but stoichiometric information is lacking, or when unusual elements are present, adjectival terms for these elements are cited in the modification in the *Chemical Substance Index*. The ad-

jectival terms all end in "-an," and are derived from the English or Latin names of the elements, e.g., aluminian, beryllian, hydrogenian, aurian (from gold), sodian, zincian. The forms "-oan" and "-ian" are used for the lower and higher oxidation states of arsenic, copper (cuproan and cuprian), iron (ferroan and ferrian), lead (plumboan and plumbian), manganese, mercury, and uranium.

Example:

$(Ba,Li)Si_2O_5$	Sanbornite, lithian
------------------	----------------------------

Intermetallic compounds are indexed like molecular addition compounds (¶ 192). Only one index entry is made at the name of metal that is alphabetically preferred.

Example:

Sb_2Fe	Antimony, compd. with iron (2:1)
----------	---

220. Isotopes. The isotopes of hydrogen of atomic masses two and three are indexed at **Deuterium** and **Tritium**, respectively. Isotopes of other elements with a natural abundance less than 98% are indexed at the usual element names with a phrase in the modification: "isotope of mass..." When the isotope is metastable, this word appears in the descriptive part of the modification, e.g., "formation of metastable." Anions of nonmetals are named in the index headings, metal anions and all cations in the modification.

Examples:

$^{38}Cl^{1-}$	Chloride ($^{38}Cl^{1-}$)
(not Deuteride)	Hydride-d
$^{120}Sn^{1-}$	Tin, isotope of mass 120 ($^{120}Sn^{1-}$)
$^{37}Cl^{1+}$	Chlorine, isotope of mass 37 ($^{37}Cl^{1+}$)

Molecular forms of isotopic elements are named in the index heading or indexed with "mol." or "ion" terms in the modification; "mol. with" phrases are employed for mixed hydrogen isotopes.

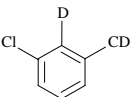
Examples:

$^{131}I_3^{1-}$	Iodide ($^{131}I_3^{1-}$)
$N^{15}N$	Nitrogen mol. ($N^{15}N$) (a labeled atom is cited <i>after</i> an unlabeled atom of the same element)
3He_2	Helium mol. (3He_2)
D_2^{1+}	Deuterium ion (D_2^{1+})
HT	Tritium mol. with hydrogen (HT)

Isotopically labeled organic compounds are indexed by the Boughton system by placing the symbol for the isotope (with a subscript numeral to indicate the number of isotopic atoms) after the name or after the relevant portion of the name. When the isotopic labeling is part of the heading parent, locants are cited unless the labeled atom is one of the following: (a) one or more labeled atoms attached to or replacing the central atom of a mononuclear molecular skeleton; (b) one or more labeled atoms included in a single functional suffix; (c) a single labeled atom included in a homogeneous parent with two skeletal atoms and no functional suffix; (d) a single labeled atom included in a homogeneous monocyclic ring with no functional or conjunctive suffix; (e) a labeled heteroatom included in a ring that has only one heteroatom of that kind; or (f) a labeled atom whose locant duplicates the element symbol. The locants (except Greek letters) and symbols are in italics, and hyphens are used to separate them from one another and from the remainder of the names. (In the following examples "d" has been used, but the tritium-labeled compounds are named quite analogously by citation of "t." When both "d" and "t" are cited, they are separated by a hyphen, e.g., **Ethane-1-d-2-t**.)

In labeled heading parents with single-word names and no hydrogen-containing principal group, the *d* is placed after the parent.

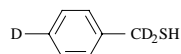
Examples:

MeD	Methane-d
CD_4	Methane-d₄
F_3CCH_2D	Ethane-d, 2,2,2-trifluoro- (not Ethane-2-d, 1,1,1-trifluoro-)
	Benzene-d, 2-chloro-6-(methyl-d₃-) (not Benzene-2-d, 1-chloro-3-(methyl-d ₃ -))
$MePD_2$	Phosphine-d₂, methyl-
$(D_2N)_2CO$	Urea-N,N,N',N'-d₄

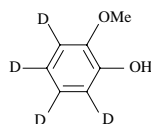
Deuterated alcohols, amines, or imines are indexed similarly. The “*d*” symbol is placed after the appropriate part(s) of the name.

Examples:

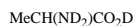
DOND ₂	Hydroxyl-<i>d</i>-amine-<i>d</i>₂
D ₃ CCD ₂ OD	Ethan-2,2,3,3,3-<i>ol-d</i>
(D ₃ C) ₂ NH	Methan-<i>d</i>₃-amine, <i>N</i>-(methyl-<i>d</i>₃)-
H ₃ SiND ₂	Silanamine-<i>d</i>₂
DNHOD	Hydroxyl-<i>d</i>-amine-<i>d</i>
D(CH ₂) ₂ NH ₂	Ethan-2-<i>d</i>-amine
MeOD	Methanol-<i>d</i>
MeSO ₃ CH ₂ D	Methan-<i>d</i>-<i>ol</i>, 1-methanesulfonate (isotopically labeled “Class I” alcohols (¶ 185) belong to “Class II”)



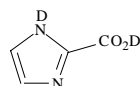
Benzene-4-*d*-methane- α , α -*d*₂-thiol



Phen-2,3,4,5-*d*₄-*ol*, 6-methoxy- (not Phen-3,4,5,6-*d*₄-*ol*, 2-methoxy-)



Alanine-*N,N*,1-*d*₃



1*H*-Imidazole-1-*d*-2-carboxylic acid-*d*

When a heading parent contains locants the labeling of each part is expressed separately and locants for the labeling are cited.

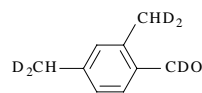
Example:

DOCD ₂ CD ₂ OD	1,2-Ethane-1,1,2,2-<i>d</i>₄-diol-1,2-<i>d</i>₂
--------------------------------------	--

The “*d*” symbol is placed after the appropriate word in multiword headings for classes not yet discussed, e.g., **Acetic-2,2,2-*d*₃ acid-*d***; **Acetyl-2,2,2-*d*₃ chloride**. In most other cases the “*d*” is cited after the complete heading parent, and conventional locants or italicized words are often necessary to denote the labeled position.

Examples:

DCH ₂ CDO	Acetaldehyde-1,2-<i>d</i>₂
D(CH ₂) ₂ CONHD	Propanamide-<i>N</i>,3-<i>d</i>₂

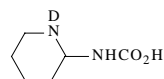


Benzaldehyde-formyl-*d*, 2,4-di-(methyl-*d*₂)- (not “bis(methyl-*d*₂)”; the labeled and unlabeled compound names are kept as similar as possible)

Enclosing marks are used with a labeled radical if it is preceded by a locant which expresses its attachment to a heading parent or parent radical, but not if such a locant belongs to the radical itself.

Examples:

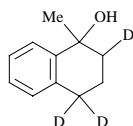
D ₃ C--CH ₂ CD ₃	Benzene, 1-(ethyl-2,2,2-<i>d</i>₃)-4-(methyl-<i>d</i>₃)-
---	---



Carbamic acid, *N*-(2-piperidinyl-1-*d*)-

Addition of deuterium, alone or with hydrogen, to a ring system is indicated by hydro “substituents” and the “*d*” symbol. Where there is a choice, deuterium is expressed in the heading parent.

Example:



1-Naphthalen-2,4-*d*₂-*ol*, 1,2,3,4-tetrahydro-4-*d*-1-methyl-

Labeled protonated species (¶ 184) are expressed in index modifications by terms such as “conjugate acid-*d* (1:1)” and “monoprotonated-*d*”.

When locants are expressed in a heading parent or parent radical for unsaturation, hetero atoms, indicated hydrogen, spiro or ring-assembly junctions, bridges (in fused ring systems), suffixes, or points of attachment (in radicals), locants are cited for the labeled positions, whether or not their use would otherwise be necessary.

Example:

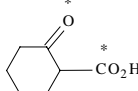
(D ₃ C) ₂ CO	2-Propanone-1,1,1,3,3,3-<i>d</i>₆
------------------------------------	---

Exceptions are “*d*” and “*r*” terms placed after the word “acid” and after the suffixes of amines, imines, alcohols, etc. (see above), for which locants are seldom employed.

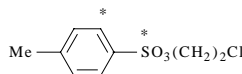
The examples above have dealt with organic compounds labeled with deuterium (tritium-labeling is handled similarly). Isotopes of elements other than hydrogen in organic compounds are expressed by the appropriate symbols. Nomenclature is similar, except that the instances in which the isotopic symbol appears within the name are restricted to (*a*) names comprising more than one word, (*b*) acids and acid derivatives with “carboxylic”, “sulfonic,” etc., names, and (*c*) conjunctive names.

Examples (labeled atoms are indicated by asterisks):

MeC(O)OH	Acetic-¹⁷O₂ acid
PhC(O)OMe	Benzoic-¹⁸O acid ¹⁶O-methyl ester
PhCH ₂ CO ₂ H	Benzeneacetic-carboxy, α-¹⁴C₂ acid
MeCOF	Acetyl-¹⁷O fluoride
O=C=O	Carbon dioxide-¹⁸O₂
H ₃ GeCN	Germane-⁷⁴Ge-carbonitrile-¹⁵N



**Cyclohexanecarboxylic-¹⁴C acid,
2-(oxo-¹⁷O)-**



**Benzene-2-¹⁴C-sulfonic-³⁵S acid
2-chloroethyl ester** (labeled “Class I” acids (¶ 185) belong to “Class II”)

In general, for all other compounds isotopic labeling of a heading parent is expressed after the name, although, as in the first example below, a combination of these policies with those for “*d*” (or “*r*”) is sometimes necessary. Symbols for different isotopic elements which fall together are cited in alphabetical order and separated by hyphens. Labeling of radicals is expressed after the individual simple radical names.

Examples:

DCH ₂ CH ₂ OH	Ethan-2-<i>d</i>-<i>ol</i>-1-¹⁴C
MeCONH ₂	Acetamide-1-¹³C-¹⁵N
MeCONDCH ₂ CHDMe	Acetamide-<i>N-d</i>-¹⁵N, <i>N</i>-(propyl-2-<i>d</i>)-
H ₂ C=CHCH ₂ O--CO ₂ H	Benzoic acid, 4-(2-propen-1-yl-3-¹⁴C-<i>oxy</i>)-

Apart from isotopes of “hydro” (see above), a multiplicity of substituents that are identical except for labeling are named separately. Multiplicative nomenclature is not employed with unsymmetrically labeled parents; instead, that heading parent is chosen which contains (*a*) the maximum number of isotopic atoms, (*b*) the alphabetically earliest isotope symbol.

Examples:

(H ₃ C) ₂ SiMe ₂	Silane, dimethyldi(methyl-¹³C)-
Cl ₂ C:	Methylene, chloro-³⁵Cl-chloro-³⁷Cl-
Me ₂ CHNHCDMe ₂	2-Propanamine-2-¹⁴C, <i>N</i>-(1-methylethyl-1-<i>d</i>)- (not 2-Propan-2- <i>d</i> -amine, <i>N</i> -(1-methylethyl-1- ¹⁴ C)-)

For derivatives named in modifications, labeling is expressed by such terms as "oxime-¹⁵N," "calcium-⁴⁴Ca salt," "hydrate-*d*₂ (1:2)." Ammonium-*d*₄ salts are treated like the analogous metal salts.

A name containing isotopic symbols is always employed for a labeled compound, regardless of how little of the labeled species is present so long as its nature is known. When the number of labeled atoms is unknown, the heading for the unlabeled compound is indexed and the modification contains a phrase such as "labeled with deuterium" or "labeled with chlorine-37."

Examples:

Acetamide, labeled with carbon-14

1-Propene, 1,1,2,2,3,3,3-hexachloro-, labeled with chlorine-36

When only the positions of the isotopic atoms are unknown, the labeling is indicated, if possible, in the appropriate part of the name without citation of locants. Otherwise a "labeled with..." modification is used.

Examples:

1-Propene-¹⁴C₂, 2-methoxy-

Benzoic acid, 4-(ethyl-¹⁴C)-

Benzoic acid, 4-ethyl-, labeled with carbon-14

Isotopically labeled *inorganic compounds* are named by procedures similar to those above when the unlabeled compounds have unambiguous names.

Examples:

DNHT	Ammonia-<i>d</i>-<i>t</i>
P(SiD ₃) ₃	Phosphine, tri(silyl-<i>d</i>₃)-
DP(O)(O ⁻) ₂	Phosphonic-<i>d</i> acid ion(2-)
H ₃ ³² PO ₄	Phosphoric-³²P acid
H ₃ PO ₄ • 3 ²² Na	Phosphoric acid, sodium-²²Na salt (1:3)
HDSO ₄	Sulfuric acid-<i>d</i>
³⁵ ClT	Hydrochloric-³⁵Cl acid-<i>t</i>
¹⁸ OSO	Sulfur dioxide-¹⁸O
D ₂ ¹⁸ O	Water-<i>d</i>₂-¹⁸O

In other cases labeled inorganic compounds are differentiated by synonym line formulas which contain isotope symbols. Isotopic atoms are cited after unlabeled atoms of the same element.

Examples:

Hydrogen sulfide (D₂S)
Cobalt iron oxide (CoFe₂O₃¹⁸O)
Molybdenum carbonyl (Mo(CO)₄(¹³CO)₂)
Nitrogen fluoride (N¹⁵NF₂)
Sodium chloride (²⁴NaCl)
Sodium sulfide (Na₂³⁵S)
Uranium chloride (²¹³UCl₃)

Salts of inorganic oxo acids with labeled *cations* are named in the modification by such terms as "strontium-⁹⁰Sr salt (1:1)" and "ammonium-*d*₄ salt (1:2)," but synonym line formulas are needed to indicate unsymmetrical labeling of cations or anions.

Examples:

Phosphoric acid calcium salt (Ca₂⁴⁴Ca(PO₄)₂)
Phosphoric-³²P acid calcium salt (Ca₃(PO₄)₃(³²PO₄))

Compounds with indefinite labeled structures are indexed at the unlabeled headings with "labeled with" modification phrases.

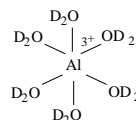
Labeled *alloys* are indexed like the unlabeled counterparts but with isotope symbols included in the elemental composition at each heading, e.g., **Aluminum alloy, base, Al 95, ²³³U 5**. For intermetallic compounds, synonym line

formulas are cited in the modification instead of a ratio, e.g., **Iron, compound with uranium (Fe₂²³⁵U)**.

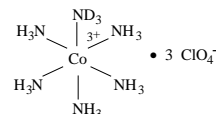
Labeled *minerals* are indexed at the systematic and mineral names, as well as at the name of the unlabeled mineral if it is studied. Labeling is indicated at the mineral name by synonym line formulas which contain isotope symbols or by modification phrases such as "labeled with boron-10" or "deuterated hydrate."

Coordination compounds (¶ 215) containing isotopic nuclear atoms are indexed at the labeled element or "ate" term, e.g., **Copper-⁶⁴Cu, Borate(1-)-¹⁰B**. Labeled ligands have the isotopic symbols appended; the ligand names are enclosed in parentheses if multiplicative prefixes are needed.

Examples:



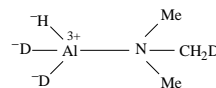
Aluminum(3+), hexa(aqua-*d*₅)-, (OC-6-11)- (see also ¶ 203 III)



Cobalt(3+), pentaammineamine-*d*₃-, (OC-6-22)-, perchlorate (1:3)

Isotopes of hydro ligands, like those of hydro "substituent" prefixes for labeled organic compounds, are expressed by "*d*" or "*t*" terms placed after citation of the hydro set.

Example:



Aluminum, (N,N-dimethylmethan-*d*-amine) trihydro-*d*₂-, (T-4)-

221. Mixtures. Certain mixtures are indexed like individual chemical substances and are assigned CAS Registry Numbers. These are compositions that are intentionally admixed prior to the intended uses, and remain discrete within the medium of the identified mixtures. Included are commercial products with trade or trivial names, as well as mixtures reported by authors to have particular properties or uses.

Such mixtures are indexed at the name of the preferred component, with all other such components expressed in the modification of the main entry. Solvents, fillers, binders, antioxidants, stabilizers, emulsifiers, plasticizers, and flavoring and coloring agents are disregarded if not specified as "active" in terms of the intended or implied uses of the formulations. Inactive trace materials are also omitted.

The percentage composition is not expressed in the index entry; thus, in the modification term "mixt. with copper(2+) sulfate (1:1)," the ratio refers to the copper sulfate, not to the mixture. Cross-references appear at trade and trivial names encountered in original documents.

The preferred index entry is made at a stereoparent (¶ 202) if possible, e.g., **D-Glucose** or **Pregn-4-ene-3,20-dione**. Choices among stereoparents and non-stereoparents depend on functionality, as for molecular addition compounds (¶ 192) and polymers (¶ 222). Components are cited in the modification in alphabetical order, esters and salts being expressed in their uninverted format. The "compounds" functional subdivision is used for components that have subdivided headings.

Example:

Glycine, compounds mixt. with egg white and sodium chloride (NaCl)
(*Chemical Substance Index* entry; cross-reference at Yumol)

Mixtures with ten or more indexable components are indexed and registered as the individual components only with the phrase "mixt. contg." as derivative information in the index entry. Mixtures of ten or more indexable components with trade or trivial names are indexed at the commercial name only.

A mixture of salts of a single parent is indexed only once.

Example:

Carrageenan, hydrogen sulfate, calcium salt, mixt. with potassium and sodium salts

Mixed reactants and impure reaction products are not indexed in this way, nor are unresolved natural products, mixed stereoisomers (other than pure racemates), commercially available mixtures of structural isomers, column fractions from distillations or chromatography, catalyst systems, welding fluxes, polymer blends, composites, or mixtures involved in physicochemical studies (as of phase systems) without emphasis on intended use. In these cases, separate entries are made at the headings for each significant component, with information on other components included in the index modifications (¶ 10A).

Certain specific substances that are mixtures, but not regarded as sufficiently well defined to be classified as chemical substances of unique composition, are identified by headings in the *General Subject Index*. Examples are **Air**, **Copper ores**, **Gasoline**, **Granite**, **Peanut oil**, **Petroleum**.

222. Polymers. Classes of polymers, natural and synthetic, are indexed in the *General Subject Index*.

Specific polymers are named on the basis of the monomers from which they are formed and/or on the basis of their structure, as represented by a structural repeating unit (SRU). Since original documents do not always provide sufficient structural information to allow generation of the SRU name, the method most frequently used for describing polymeric substances is by citation of the component monomers. A few commercial polymers, each of which accounts for a large number of index entries, are indexed only at the SRU-based systematic polymer name. Systematic nomenclature is discussed first in the following paragraphs, followed by monomer-based polymer nomenclature.

Systematic (SRU) nomenclature for polymers has been adapted from the system developed by the Committee on Nomenclature of the Division of Polymer Chemistry of the American Chemical Society⁵. Names derived by this system, in addition to monomer-based entries, are cited for polymers whose structural repeating units are well-documented or can confidently be assumed. "Expected," "idealized," or "drawn-for-convenience" SRUs are not given systematic polymer names. Occasionally, when there is no information on the component monomers in the original document, an entry derived from the SRU name is the only index entry available.

The SRU is named by citation of one or more multivalent radicals of regular substitutive nomenclature. Many of these radical names will be found in the Illustrative List of Substituent Prefixes (Section H, ¶ 294); others are supplied in the various sections dealing with classes of compounds from which the radicals are derived. The SRU name is enclosed in parentheses or brackets, and prefixed by the term "Poly". Each multivalent radical retains its own numbering and is oriented, if possible, so that the point of attachment written at the left end of the repeating unit is assigned the lowest possible number. This permits the naming of the SRU in a directional manner, reading from left to right. The largest possible multivalent radicals are chosen as all or part of the name, and naming proceeds from left to right, starting with the most preferred multivalent radical. (See the following sections for the choice of most preferred radical.) Unsaturation and substituents are indicated by appropriate locants. Functional derivatives, such as esters and hydrazones and oxides of hetero atoms which are an integral part of the repeating unit are expressed by prefixes rather than by modification terms, and are numbered as low as possible while preserving the preferred names of the parent radicals. Salts of acids and anions of quaternary "onium" compounds, and oxides of hetero atoms which are an integral part of the repeating unit are cited following the name of the SRU. The number of free valencies between units is minimized; i.e., unsaturated radicals are preferred.

Polymers of unspecified length and chains of reported "average" length, are named by the methods described above. The prefix "oligo-" is not used to differentiate polymers of relatively low molecular weight from high polymers. When, however, the number of structural repeating units is exactly specified, the oligomer is usually named according to the principles of substitutive nomenclature.

Examples:

$(-\text{CH}_2-)_n$	Poly(methylene)
$(-\text{CHMeCH}_2-)_n$	Poly(1-methyl-1,2-ethanediyl)
$(-\text{CH}=\text{CH}-)_n$ (not $(=\text{CHCH}=\text{CH}-)_n$)	Poly(1,2-ethenediyl) (not Poly(1,2-ethanediylidene))
$[-(\text{CO})_2(\text{CH}_2)_2-]_n$	Poly(1,2-dioxo-1,4-butanediyl) (not Poly(1,4-dioxo-1,4-butanediyl))
$(-\text{CH}=\text{CHCHMeCH}_2-)_n$	Poly(3-methyl-1-butene-1,4-diyl)

For more complex examples, further criteria for arranging the components of an SRU are required. The descending order of priority of citation (and of structuring of the SRU) is (a) heterocyclic rings, (b) acyclic hetero atoms in the order: O, S, Se, Te, N, P, As, Sb, Bi, Si, Ge, Sn, Pb, B, Hg, (c) carbocyclic rings, (d) acyclic carbon chains. If substituents are present, otherwise identical parent radicals in the SRU are chosen by the principles, in turn, of maximum number, lowest locants, and earliest alphabetical order of substituents. The shortest path (smallest number of atoms) is taken from the most preferred multivalent radical to another occurrence of the same radical (if present) within the SRU, then to the next most preferred radical, and so on.

Examples:

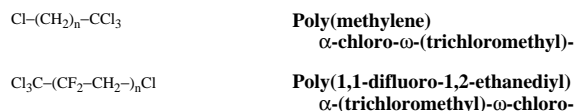
	Poly(oxy-1,4-phenylene-1-propene-1,3-diyl)
$[-\text{NHCO}(\text{CH}_2)_2-]_n$	Poly[imino(1-oxo-1,3-propanediyl)]
$[-(\text{SO}_2)(\text{CH}_2)_2-]_n$	Poly(disulfonyl-1,2-ethanediyl)
	Poly[oxy-carbonyloxy(methyl-1,2-ethanediyl)] (The position of the methyl group is not assumed in this polyester from carbonic acid and 1,2-propanediol.)
	Poly[oxy-1,4-phenylenesulfonyl-1,4-phenyleneoxy-1,4-phenylene(1-methylethyldene)-1,4-phenylene] (With equal numbers of atoms between the oxygen atoms in two possible arrangements, the preferred path includes the other hetero atom, sulfur, as early as possible.)
$[-\text{OCH}_2\text{SNH}(\text{CH}_2)_2\text{OCH}_2\text{SCH}_2\text{NHCH}_2-]_n$	Poly(oxymethylenethioimino-1,2-ethanediyl-oxymethylenethio-methyleneimino-methylene) (With equal distances between the two oxygen atoms and between the oxygen and sulfur atoms, the direction is determined by the shortest distance between the oxygen atom and the hetero atom of third preference (nitrogen).)
	Poly(iminocarbonyl-1,4-phenylene-iminocarbonyl-1,3-phenylene-carbonylimino-1,4-phenylene-carbonylimino-1,6-hexanediyl) (The citation proceeds in the increasing order of distances between the nitrogen atoms: 5, 5, 5, and 6 intervening carbon atoms.)
	Poly([2,2'-bithiazole]-4,4'-diyl-1,4-phenylene-1,2-diazenediyl-1,4-phenylene)
$[-\text{NHCOCH}(\text{CO}_2\text{Pr})-]_n$	Poly[imino[1-oxo-2-(propoxycarbonyl)-1,2-ethanediyl]] (not Poly[imino(1-carboxy-2-oxo-1,2-ethanediyl)], propyl ester)
	Poly[(dimethylimino)-1,2-ethanediyl bromide (1:1)] (the ionic derivative term is included in the SRU)

⁵"A Structure-based Nomenclature for Linear Polymers", *Macromolecules* **1968**, 1(3), 193-198. The IUPAC recommendations (*Pure Appl. Chem.* **1976**, 48, 373-385; **1993**, 65 (7), 1561-1580) are in full agreement with CAS practice. The IUPAC term "constitutional repeating unit" (CRU) corresponds to CA's SRU.

When SRUs are bridged only by metals, systematic polymer nomenclature is not used; instead, the substance is indexed either at the monomeric salt name or by coordination nomenclature (¶ 215), with a modification phrase, in either case, such as "homopolymer" or "polymer with" (see below).

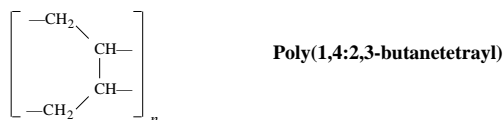
End groups, when known, are specified by means of appropriate radical names, together with Greek letters "α-" and "ω-" expressed as substituents. The α-end group is the group attached to the left end of the SRU when the structure is ordered by the specified rules; it is cited first, regardless of alphabetical order.

Examples:



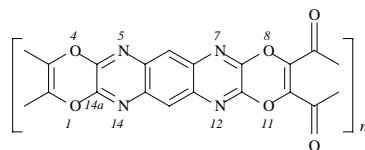
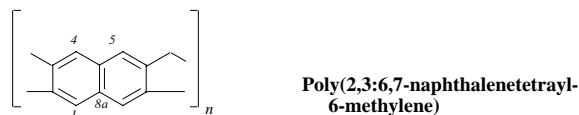
Linear double-strand ("ladder" and "spiro") polymers may sometimes be named as a chain of quadrivalent radicals. Two pairs of locants, separated by a colon, indicate the distribution of bonds.

Example:

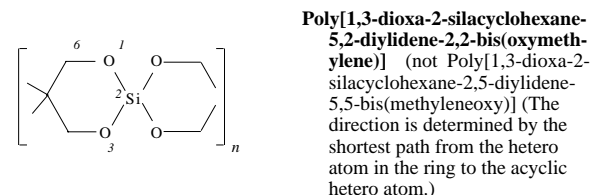


When a ladder polymer must be named as an SRU of one or more quadrivalent radicals linked through one or more bivalent radicals (here, these terms are extended to mean radicals attached to four or two different atoms, not only to radicals with four or two free valence bonds) the direction of citation is from the most favored quadrivalent radical by the shortest path to the next most favored quadrivalent radical, and so on; then toward the most favored bivalent radical. Rings are broken (*a*) to minimize the number of free valencies of the total "mer," (*b*) to maximize the number of most preferred hetero atoms in the ring system, (*c*) to maintain intact the most preferred ring system (¶ 138). End groups, when known, are identified by α and α' (at the left terminus as the structure is drawn) and by ω and ω' (at the right terminus) as locants for substituent prefixes, e.g., α,α'-dihydroxy-ω,ω'-dihydro-

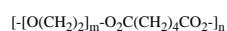
Examples:



Poly([1,4]dioxino[2,3-b]-1,4-dioxino[2',3':5,6]pyrazino[2,3-g]quinoxaline-2,3:9,10-tetrayl-9,10-dicarbonyl) (The same number of free valences can be expressed by breaking the oxygen ring or the partially saturated hydrocarbon ring; the latter course keeps intact the maximum number of heterocyclic rings.)



Linear polymers composed of SRUs within SRUs, e.g.,



are not assigned systematic names; they are indexed at the monomer names only.

The previous paragraphs described a systematic nomenclature for polymers of well characterized structure, and for polymers whose structural repeating unit (SRU) can be confidently assumed. The latter are restricted to (*a*) polyamides from a dibasic acid (or derivative) and a diamine, or from an amino acid or lactam; (*b*) polyesters from a dibasic acid (or derivative) and a dihydric alcohol, or from a hydroxy acid or lactone; (*c*) polyurethanes from a diisocyanate and a dihydric alcohol; and (*d*) polycarbonates from carbonic acid (or an ester or halide) and a dihydric alcohol.

Polymers manufactured from known monomers are generally indexed at the monomer names whether or not systematic (SRU) entries are also made. An exception is the treatment of a few very common industrial polymers, e.g., nylon 6, nylon 66, terephthalic acid polymer with ethylene glycol, which, to preclude inordinate repetition of a large number of index entries at various names assigned SRU names.

Example:

Terephthalic acid

See *1,4-Benzenedicarboxylic acid*

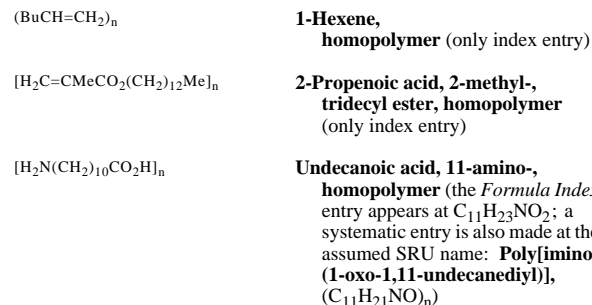
1,4-Benzenedicarboxylic acid, polymers

polymer with 1,2-ethanediol—see *Poly(oxy-1,2-ethanediolyloxy-carbonyl-1,4-phenylenecarbonyl)*

A cross-reference appears also at **1,4-Benzenedicarboxylic acid, esters, 1,4-dimethyl ester, polymer with 1,2-ethanediol**; and two corresponding cross-references at **1,2-Ethanediol, polymers**.

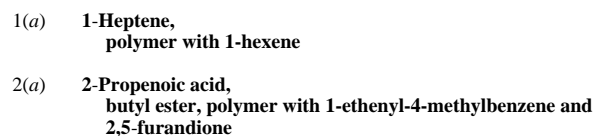
Polymers from a single monomer are indexed at the monomer name with the term "homopolymer" cited in the modification. (The terms "peptides," "polyamides," and "polyesters" are not used for specific homopolymers at monomer headings.)

Examples:



Polymers formed from two or more monomers are indexed at the preferred monomer name with the modification term "polymer with" followed by the other monomer names in alphabetical order. No attempt is made to indicate the percentage composition of copolymers. Ratios typically refer to specific monomer salts. The preferred index name is determined by the usual rules for selection of a heading parent (¶ 138) but a stereoparent is preferred over a non-stereoparent, e.g., **D-Glucose**, polymer with butanedioic acid. For identical heading parents, the choice is determined by (*a*) maximum number of substituents, (*b*) lowest locants of substituents, (*c*) maximum number of occurrences of the index heading parent (in a multiplicative name), (*d*) earliest index position of the index heading. When the choice is dependent on modification terms, it is determined as follows: (*a*) underivatized heading preferred over derivatives cited in the modification; thus, a free acid is preferred over an ester; (changes in format caused by elevation of modification terms into the heading for purposes of subdivision are ignored in applying this rule; thus **Acetic acid** is preferred over **Acetic acid ethenyl ester**); (*b*) class of derivative in the descending order: anhydride, ester, hydrazide, hydrazone, oxime; (*c*) largest number of (most preferred) derivative; thus, monoester preferred over dioxime preferred over monooxime; (*d*) lowest expressed locants of derivative terms; thus, for **1,2,4-Benzenetricarboxylic acid**, a 1,2-diester is preferred over a 1,4-diester; (*e*) the earliest alphabetical order; thus, "ethyl ester" preferred over "propyl ester."

Examples:



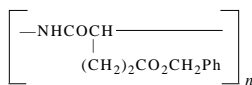
Peptides of established structure are indexed at systematic peptide names such as **Glycine, glycyglycyl-** (see ¶ 206). Peptides of unknown structure are indexed as polymers.

Example:



L-Glutamic acid,
5-(phenylmethyl) ester, homo-
polymer

and the assumed structural repeating unit:



Poly[imino(2*S*)-1-oxo-2-[3-oxo-3-(phenylmethoxy)propyl]-1,2-ethanediy]]

When more than one amino acid is present and the sequence is unknown, a copolymer is indexed, and named at the preferred amino acid monomer.

Alternating, block, and graft polymers are distinguished from random polymers by indexing as copolymers at the monomer names. The term “alternating”, “block”, or “graft” (or a combination thereof) is cited in a special modification after all other structural information but before descriptive phrases relating to properties, uses, etc. The more specific block terms, diblock, triblock, tetrablock, and pentablock are also used. Differentiation between the polymeric substrate and the applied monomer is not made; e.g., whether 1-hexene is grafted on 1-heptene homopolymer or vice versa, the index entry is at **1-Heptene**, polymer with 1-hexene, graft. The term “random” is not employed by CA in indexing specific polymers.

Siloxanes prepared by hydrolytic polymerization of chlorosilanes are indexed at the monomer names with the term “hydrolytic” cited in the modification to indicate the essential role of water in forming a polymer chain of -Si-O-units. The term “hydrolytic” is used in addition to the term “homopolymer” or “polymer with”.

Example:

Benzene, 1,1'-(dichlorosilylene)bis-, polymer with dichlorodimethylsilane, hydrolytic

Polymers of specific compounds with classes of compounds are indexed at the specific monomers in the *Chemical Substance Index* and at the class name, e.g., **Aldehydes** or **Nitriles**, in the *General Subject Index*.

Example:

1-Hexene, 5-methyl-, polymer with unsat. nitriles
Nitriles

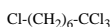
unsat.; polymers with 5-methyl-1-hexene

Formaldehyde homopolymers containing only oxymethylene repeating units are indexed only at the heading **Poly(oxymethylene)** in the *Chemical Substance Index*. Commercial and impure polyformaldehydes are indexed at **Polyoxymethylenes** (a plural class heading in the *General Subject Index*) unless author emphasis is centered on **Paraformaldehyde**. Formaldehyde copolymers are indexed as polymers formed from two or more monomers (except **Formaldehyde** copolymers with **Phenol**, **Urea**, or **1,3,5-Triazine-2,4,6-triamine**).

Oligomers of definite structure are indexed as specific compounds by the regular principles of index nomenclature. When the precise structure is not known but the number of units is specific, “dimer,” “trimer,” etc., is expressed in the modification at the name of the monomer. The term “oligomeric” may be cited after “homopolymer” or “polymer with . . .” if this aspect is stressed in the original document.

Telomers with a definite structure are named systematically.

Examples:



Heptane, 1,1,1,7-tetrachloro-



Poly(1,1-difluoro-1,2-ethanediy), α -chloro- ω -(dichloromethyl)-

Telomers of unknown structure are indexed as copolymers with the term “telomer with . . .” cited in the modification.

Example:

1-Hexene, telomer with tetrachloromethane

Post-treated polymers are described by modification terms after the polymer has been described.

Examples:

2-Propenoic acid, homopolymer, sodium salt
(No ratios are used for polymer salts unless specific stoichiometry is possible and is specified.)

Benzenamine, 4-ethenyl-, polymer with ethenylbenzene, hydrochloride
(No ratios are used for polymer salts unless specific stoichiometry is possible and is specified.)

1,4-Dioxane-2,5-dione, 3,6-dimethyl-, homopolymer, copper(2+) salt (2:1)
(The polymer chain has only one carboxy group and one hydroxy group a specific salt ratio is possible.)

2-Propenoic acid, 2-methyl-, homopolymer, 9-anthracenylmethyl ester

2-Propenoic acid, 2-methyl-, decyl ester, homopolymer, hydrolyzed

Poly[1-(4-sulfophenyl)-1,2-ethanediy], propyl ester

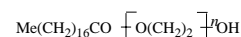
Ethanol (vinyl alcohol) polymers that are indexed at that heading are exceptions (they are prepared by hydrolysis of ethenol ester polymers). Acetals of ethenol homopolymer and ethenol polymers with ethenyl acetate are indexed at the homopolymer or copolymer with the term “cyclic acetal” followed by the specific aldehyde name in the modification. Additional entries appear in the *General Subject Index* at the trivially named class terms, **Polyvinyl acetals** and **Polyvinyl butyrals**. Acetals of other ethenol polymers and acetals with unspecified aldehydes are indexed at the underivatized polymer and at the class term with a modification term, e.g., chlorinated benzals, to indicate the type of acetal when appropriate.

Molecular addition compounds of polymers are indexed in the usual way (¶ 192), e.g., **Ethenesulfonic acid**, homopolymer, compd. with 4-ethenylpyridine homopolymer. The preferred name is cited at each molecular formula in the *Formula Index*. (See ¶ 198)

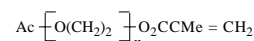
Polyethylene and polypropylene glycols are indexed as specific compounds when the precise structure is reported and not more than ten repeating units are present, e.g., **3,6,9,12,15-Pentaoxaheptadecane-1,17-diol, hexamethyl-**. The position of methyl substituents is not assumed; if it is reported, locants are cited. Glycol polymers of eleven units or more are indexed at **Poly(oxy-1,2-ethanediy), α -hydro- ω -hydroxy-**, and **Poly(oxy(methyl-1,2-ethanediy), α -hydro- ω -hydroxy-**. The class term **Polyoxyalkylenes** in the *General Subject Index* is used as an additional entry for all specific polyalkylene glycols except when the alkanediyl group is ethanediy or propanediyl and for cases where the nature of the alkanediyl group is unknown. When it is known, the SRU can be named specifically; thus, **Poly[oxy(2-phenyl-1,3-propanediyl)], α -hydro- ω -hydroxy-**. Polyethylene-polypropylene glycols are named as copolymers: **Oxirane, 2-methyl-**, polymer with oxirane.

Esters and ethers of polyalkylene glycols containing not more than ten repeating units are indexed by the regular principles of substitutive nomenclature. For larger polymers, the ester or ether is expressed as a substituent at the SRU-based heading. Mono derivatives are cited in the α -position, with ω -hydroxy at the other terminus. Dissimilar diesters or diethers are expressed in alphabetical order. Ester-ethers have the acyl group or the inorganic-type ester, including borono, phospho, sulfo, substituted sulfonyl groups, etc., assigned to the α -position, and the ether at the ω -end. When appropriate information is lacking, an ester or ether term is cited without locant. When multiplying radicals must be employed, they are given α -locants.

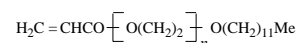
Examples:



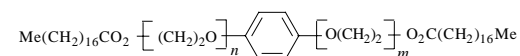
Poly(oxy-1,2-ethanediy), α -(1-oxooctadecyl)- ω -hydroxy-



Poly[oxy-1,2-ethanediy], α -acetyl- ω -[(2-methyl-1-oxo-2-propen-1-yl)oxy]-



Poly(oxy-1,2-ethanediy), α -(1-oxo-2-propen-1-yl)- ω -(dodecyloxy)-



Poly(oxy-1,2-ethanediy), α, α' -1,4-phenylenebis[ω -[(1-oxooctadecyl)oxy]-

Polynucleotides (cf. Nucleotides, ¶ 210) are indexed as “homopolymer” or “polymer with . . .” at the “-ylic acid” monomers (5'-isomers).

Examples:

5'-Adenylic acid, homopolymer

Cytidine, 5'-O-phosphoadenylyl-(3'→5')-, homopolymer

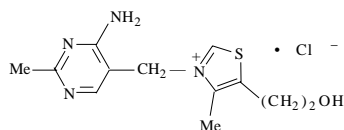
5'-Guanylic acid, polymer with 5'-adenylic acid and 5'-cytidylic acid

224. Vitamins, being structurally diverse, are indexed by more than one method. The headings **Vitamin B**, **Vitamin K**, etc., are used to index groups of compounds having similar physiological activities, especially for biological studies. Such headings as **Vitamin B₄**, **Vitamin B₆**, **Vitamin F**, may each refer to one or more specific compounds or to nothing more than an ill-defined vitamin activity. They are used in indexing when employed in original documents, and CAS Registry Numbers are assigned to them.

Vitamin A is a heading parent employed for the group of A vitamins and for vitamin A activity in general. Vitamin A₁ is indexed at the carotenoid heading **Retinol** (§ 212); Vitamin A₂ is indexed at **Retinol, 3,4-didehydro-**. Related trivially named heading parents are **Retinoic acid** and **Retinal**. In all these cases, an *all-trans*-configuration about the double bonds is implied by the names. Abnormal stereochemistry is specifically cited in the modification.

Vitamin B is a heading parent employed for the B-complex and vitamin B activity in general. **Vitamin B₁** and related compounds are indexed at the systematic names. (The trivial name Thiamine, not used as a CA index heading, implies presence of a chloride anion.)

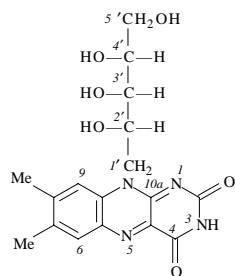
Example:



Thiazolium, 3-[(4-amino-2-methyl-5-pyrimidinyl)methyl]-5-(2-hydroxyethyl)-4-methylchloride (1:1)

The diphosphoric (pyrophosphoric) acid ester of Vitamin B₁ (cocarboxylase) is indexed by expressing the ester as an "a"-named substituent; i.e., the 5-(2-hydroxyethyl) group becomes 5-(4,6,6-trihydroxy-4,6-dioxido-3,5-dioxo-4,6-diphosphahex-1-yl)-. Vitamin B₂ contains a ribitol residue and is indexed at the stereoparent

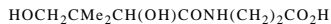
Riboflavin:



Riboflavin

Plain locants are employed for ring substituents, primed locants for the ribitol moiety. Binary headings analogous to those for nucleotides (§ 210) are used for phosphates, diphosphates (pyrophosphates), etc., e.g., **Riboflavin 5'-(dihydrogen phosphate)**. Functional derivatives of **Riboflavin** are expressed in the modification, e.g., 2',3',4'-triacetate, other derivatives as substituents. Analogs in which ribitol is replaced by other alditols are indexed at the alditol stereoparent names, e.g., **D-Galactitol, 1-deoxy-1-(3,4-dihydro-7,8-dimethyl-2,4-dioxobenzo[*g*]pteridin-10(2*H*)-yl)-**.

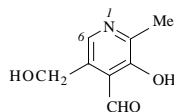
Vitamin B₃ is indexed at **3-Pyridinecarboxamide**; Vitamin B₅ is a little-used term for Pantothenic acid, which is indexed at **β-Alanine**:



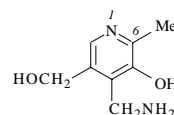
β-Alanine, N-[(2*R*)-2,4-dihydroxy-3,3-dimethyl-1-oxobutyl]-

Vitamin B₆ is a heading parent employed for studies in which the precise compound is not further specified. The individual compounds and their derivatives are indexed systematically at pyridine headings.

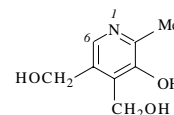
Examples:



4-Pyridinecarboxaldehyde, 3-hydroxy-5-(hydroxymethyl)-2-methyl-

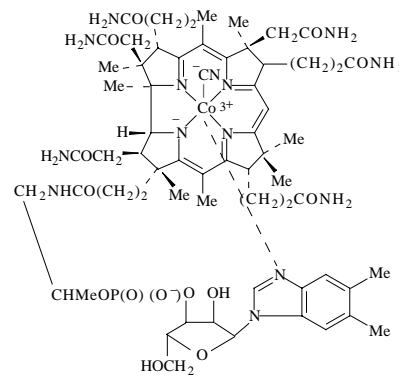


3-Pyridinemethanol, 4-(amino-methyl)-5-hydroxy-6-methyl-



3,4-Pyridinedimethanol, 5-hydroxy-6-methyl-

Vitamin B₁₂ is an index heading used for the vitamin itself:

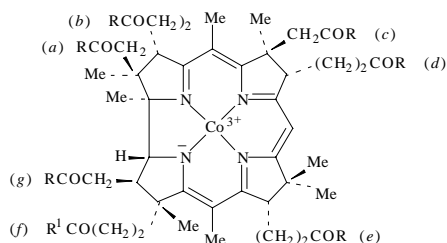


Vitamin B₁₂

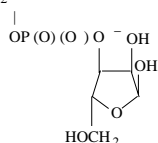
The terms Cyanocobalamin and Cobalamin are not used in index names. Derivatives, other than functional derivatives, of Vitamin B₁₂ are indexed largely in accordance with rules of the International Union of Pure and Applied Chemistry,⁶ which should be consulted for details.

The fundamental ring system is Corrin, which is numbered like Porphyrin, the locant "20" being omitted to facilitate analogous treatment of derivatives; the methene bridges which remain are numbered "5," "10," and "15." The index heading (in the *General Subject Index*) for this class of compounds is Corrinoids, and specific compounds are generally indexed at the largest appropriate heading parent chosen from the following: **Cobyric acid**, **Cobinic acid**, **Cobamic acid**, or the corresponding amides.

⁶IUPAC, "Nomenclature of Corrinoids (Rules approved 1975)", *Pure Appl. Chem.* **1976**, 48, 495-502; *Biochemistry* **1974**, 13, 1555-60.



R = R ¹ = OH	Cobyirinic acid
R = R ¹ = NH ₂	Cobyriamide acid
R = OH; R ¹ = NHCH ₂ CHMeOH	Cobinic acid (in Cabinamide, R = NH ₂)
R = OH; R ¹ = NHCH ₂ CHMe	Cobamic acid (in Cobamide, R = NH ₂)

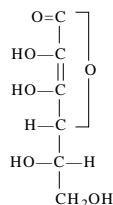


In **Cobamic acid** and **Cobamide**, the structures (above) have been shown as inner salts; the cobalt(3+) nucleus is also coordinated with the nitrogen atoms with loss of one proton overall. The compound therefore still possesses a 1+ charge. Similarly, **Cobyirinic** and **Cobinic acids** (and their amides), which lack the phosphate group, have a 2+ charge, and can form dihydroxides, cyanide hydroxides, etc. Partial amides of **Cobyirinic acid** are designated by use of the small italic locants shown in the diagram above; e.g., **Cobyirinic acid-abcdeg-hexamide**, dicyanide. Substitution on amide groups is indicated by *N* with a superscript, e.g., *N*¹-(carboxymethyl)-. In modifications at corrinoid headings, the various types of derivatives are cited in the following order: (a) groups linked to the cobalt atom, e.g., *Co*-amine, *Co*-methyl deriv., *Co*-(pyridine); followed by anions, e.g., cyanide, acetate (salt); and then "hydrate" if present; (b) lactones and lactams formed between acetic or propanoic residues and existing or added hydroxyl and amino groups; (c) esters of the corrin moiety, e.g., dihydrogen phosphate (ester); (d) "inner salt" (for zwitterionic structures); (e) further ester terms for a polybasic acid residue such as phosphoric acid, e.g., "3-ester with . . ."

When the cobalt is in a 2+ rather than a 3+ oxidation state, Ewens-Basset numbers (¶ 215) or Stock numbers are cited in the heading; e.g., **Cobinamide-Co(I+)**, **Co-ethyl deriv., hydrate (1:1)** (the "1+" designation belongs to the entire cobinamide parent, and results from coordination of the Co(2+) atom with loss of a proton from corrin; the modification term renders the total compound neutral); **Cobamide-Co(II)** (the Stock number is employed because no charge remains; a proton has been lost from corrin and another from the phosphoric acid group by inner salt formation).

Analogs of **Cobyirinic acid**, etc., in which cobalt is replaced by another metal are named by substituting a suitable term for "Co-" in the original name. Thus, the iron(2+) and nickel(3+) analogs of cobyirinic acid are named **Ferrocobyirinic acid** and **Nickelcobyirinic acid**, respectively. The hydrogen analog is **Hydrogenobyirinic acid**.

Vitamin C is indexed at **L-Ascorbic acid**:

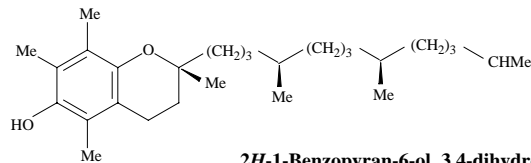


L-Ascorbic acid

Derivatives are named in accordance with the rules for carbohydrates (¶ 208), e.g., **L-Ascorbic acid, 5,6-O-(1-methylethylidene)-**; **L-threo-2,3-Hexodiulosonic acid**, γ -lactone (cross-reference from L-Dehydroascorbic acid). **Vitamin D** is an index heading used for vitamin D activity in general. Vitamin D₁ is a molecular addition compound of Vitamin D₂ and (3 β ,9 β ,10 α)-ergosta-5,7,22-trien-3-ol (lumisterol). Vitamins D₂ and D₃ are given systematic names.

Vitamin E is used as a heading for Vitamin E activity in general. Individual compounds, notably α -tocopherol, exhibiting this activity are indexed systematically.

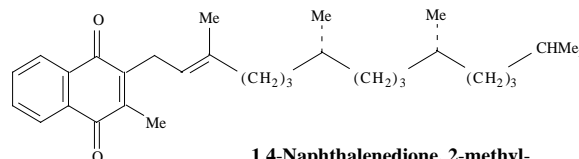
Example:



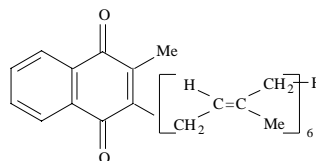
2H-1-Benzopyran-6-ol, 3,4-dihydro-2,5,7,8-tetramethyl-[(4R,8R)-4,8,12-trimethyltridecyl]-, (2R-)

Vitamin K is used as a group heading; the specific compounds are named systematically.

Examples:



1,4-Naphthalenedione, 2-methyl-3-[(2E,7R,11R)-3,7,11,15-tetramethyl-2-hexadecen-1-yl]-



1,4-Naphthalenedione, 2-[(2E,6E,10E,14E,18E)-3,7,11,15,19,23-hexamethyl-2,6,10,14,18,22-tetracosahexaen-1-yl]-3-methyl-

G. CHEMICAL SUBSTANCE NAMES FOR RETROSPECTIVE SEARCHES

Introduction	¶ 225	Ketene	¶ 261
Acetals	226	Ketones	262
Acid halides	227	Locants	263
Acids	228	Metallocenes	264
Additive Nomenclature	228A	Mixtures	265
Alcohols and Phenols	229	Molecular addition compounds	265A
Aldehydes	230	Multiplicative prefixes	266
Alkaloids	231	Nitriles	267
Alloys	232	Nitrone	268
Amides	233	Nucleosides and Nucleotides	269
Amidines	234	Onium compounds	270
Amines	235	Order of precedence of compound classes	271
Amino acids	236	Organometallic compounds	272
Anhydrides	237	“Oxo” acids	273
Azo and azoxy compounds	238	Peptides	274
Boron compounds	239	Peroxides	275
Carbohydrates	240	Phosphorus compounds	276
Carbonic acid and relatives	241	Polymers	277
Coordination compounds	242	Porphyrins and Bile pigments	278
Diazo compounds	243	Replacement (“a”) nomenclature	279
Dyes	244	Replacement nomenclature for functions	280
Elementary particles	245	Ring systems	281
Enzymes	246	Salts	281A
Esters	247	Silicon compounds	282
Ethers	248	Spelling	283
Formazan	249	Stereochemistry	284
Functional derivatives	250	Stereoparents	285
Guanidine and relatives	251	Steroids	286
Hydrazine	252	Substituent prefixes (radicals)	287
Hydroxylamine	253	Sulfur compounds	288
Imines	254	Sulfones and Sulfoxides	289
Index name selection	255	Tautomers	289A
Indicated hydrogen	256	Terpenes	290
Inorganic compounds	257	Thiols	291
Inositols	258	Urea	292
Iodine compounds	259	Vitamins	293
Isocyanides	260	Zwitterionic compounds	293A

225. Introduction. The current name-selection policies for chemical substances described in Sections A through F above were introduced in 1972. These policies, which are now well-established, enable the index user to derive preferred *CA* names for substances of specific molecular structure and thereby to find information about them in current and recent indexes. However, in carrying searches back beyond 1972, difficulties can arise. The current *CA* name of our compound has been determined; but where will we find this same substance in older *CA* indexes? Cross-references in these indexes are helpful, but of course none exist that lead from current names to those in Eighth (and earlier) Collective Indexes. As a last resource, the Formula Indexes can be consulted. But a simpler method, especially in searching for *groups* of compounds, is to read the appropriate paragraphs of this section. Although published originally (in the Volume 76 *Index Guide* under the title “Ninth Collective Index Changes”) to alert index users to prospective changes, it will now be found most serviceable to remind retrospective searchers of the main nomenclature changes occurring in 1972. For example, ¶ 228 (below) indicates that peroxo acids, in Volume 75 and earlier indexes, will be found at Peroxy headings, that aldehydic, anilic, and hydroxamic acid headings were also employed, and that many acids were indexed at trivial names; ¶ 270 explains that cationic compounds currently indexed at aminium headings were formerly entered at **Ammonium**; and ¶ 281 gives examples of current and former names for cyclic epoxides.

The changes in name selection policies described in this section are 1972 changes unless otherwise specified. The very few revisions found necessary in the Tenth (1977-1981) and Eleventh (1982-1986) Collective Index periods mainly affect inorganic compounds and are described in ¶¶ 239, 257, and 273. Changes in name-selection policies for the Twelfth (1987-1991) and Thirteenth (1992-1996) Collective Index periods affect alloys, carbohydrates (lactams), coordination compounds, formazans, index name-selection (multiplicative names), inorganic compounds (line formulas of clusters, intermetallic compounds), molecular addition compounds (common components; hydrates), nitrilimines, onium compounds (free radicals), peptides, phosphonium ylides, phosphoryl-halides and halogenoids, polymers (block, graft, and hydrolytic), ring systems (list of common systems), salts (list of common anions), stereochemistry (sign of optical rotation), and zwitterions (inner salts, syndones). These are described in this section at their respective paragraphs listed above.

The changes for the Fourteenth (1997-2001) Collective Index periods affect coordination nomenclature, stereochemical practices, and stereoparents and are described in ¶¶ 242, 284, and 285.

The arrangement of subjects is alphabetic, and references are supplied in each case to the paragraphs in Sections A through F where a complete account of current policies will be found. The index (Section M) may also be consulted.

Headings found in current indexes are shown in boldface within the following paragraphs.

226. Acetals are indexed like ethers (¶ 196); thus, Acetone, diethyl acetal became **Propane, 2,2-diethoxy-**. Cyclic acetals, except those of stereoparents

(¶ 202), are indexed at the ring names. Epoxides are likewise indexed at the names of the appropriate ring systems, e.g., **Oxirane**.

227. Acid halide names (¶ 170) were affected by the discontinuance of most trivial acid names. Isocyanates, isothiocyanates, and isocyanides are now named like the halides. In the following examples, names prior to 1972 are shown in parentheses.

Benzenepropanoyl chloride	(Hydrocinnamoyl chloride)
Butanethiyl fluoride	(Butyryl fluoride, thio-)
Benzenesulfonyl isocyanate	(Benzenesulfonic acid, anhydride with isocyanic acid)

228. Acids. Carbonic acid and related compounds including **Formic acid** (¶ 183) are now relegated to a position below “organic” acids and above inorganic “oxo” acids (¶ 106).

Among carboxylic acids, the only trivial names retained were **Acetic acid** and **Benzoic acid**. (When oxygen in the functional group of these two acids is replaced, systematic functional replacement names, e.g., **Ethanimidic acid**, **Benzenecarbothioic acid**, are employed.) All other organic acids (carboxylic, sulfonic, sulfinic, etc.) are named systematically (¶ 165); e.g., **Propanoic acid** (formerly Propionic acid); **Benzoic acid, 2-hydroxy-** (Salicylic acid); **2-Butenedioic acid (2E)-** (Fumaric acid); **Benzenesulfonic acid, 4-amino-** (Sulfanilic acid).

Use of replacement affixes (¶ 129) for modified carboxylic, sulfonic, etc., groups was extended for Volume 76. In the following examples, the names formerly used are shown in parentheses:

Ethanimidothioic acid	(Acetimidic acid, thio-)
3-Pyridinecarbohydrazonic acid, methyl ester	(Nicotinic acid, methyl ester, hydrazone)
Butanediperoxoic acid	(Peroxysuccinic acid)
2-Propanesulfo(thioperoxoic) acid	(Peroxy-2-propanesulfenic acid, thio-)

Aldehydic, amic, anilic, hydroxamic, hydroximic, nitrolic, and nitrosolic acids are now named as derivatives of carboxylic acids, amides, etc.

Examples:

1-Naphthalenecarboxylic acid, 8-formyl-	(Naphthalaldehydic acid)
Propanoic acid, 3-amino-3-oxo-	(Malonamic acid)
Butanoic acid, 4-oxo-4-(phenylamino)-	(Succinanic acid)
Acetamide, N-hydroxy-	(Acetohydroxamic acid)
Ethanone, 1-nitro-, oxime	(Acetonitrolic acid)

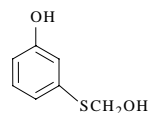
See also **Oxo acids** (¶ 273).

228A. Additive Nomenclature. The terms oxide, sulfide, selenide, and telluride are used as part of the modification to describe the presence of a chalcogen atom attached to trivalent antimony, arsenic, bismuth, nitrogen or phosphorus, or to divalent sulfur, selenium, or tellurium (¶ 123). However, acceptable unambiguous locants are often lacking to describe the exact location when multiple possibilities are present and the result is a name which is less specific than the structure.

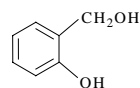
Effective with Volume 124, oxides, etc. attached to the parent portion of the name continue to be cited as oxide, sulfide, etc., with an appropriate locant in the modification portion of the name, however, if the attachment is not to the parent, terms such as oxido, sulfido, selenido, or tellurido will be cited with locants in the substituent or modification, as appropriate.

229. Alcohols and Phenols (¶ 175) are treated as of equal seniority in the order of chemical functions; previously, alcohols (in which the hydroxyl group is formally attached to a saturated carbon atom) were placed just ahead of phenols. Now, the preference of cyclic over acyclic hydrocarbons (¶ 138) often causes a change of nomenclature unless a conjunctive name can be used.

Examples:



Phenol, 3-[(hydroxymethyl)thio]-
(formerly Methanol, [(*m*-hydroxy-phenyl)thio]-)



Benzenemethanol, 2-hydroxy-
(formerly Benzyl alcohol, *o*-hydroxy-) (the preferred heading parent is larger than Phenol)

Radicofunctional names previously used for unsubstituted Ethyl through Dodecyl alcohol were replaced by **Ethanol, 1-Propanol**, etc. *iso*-, *sec*- and *tert*-names are no longer used, except to index "isooctanol," etc., when no further information is provided. Isopropyl alcohol is now indexed at **2-Propanol**; *sec*-Butyl alcohol at **2-Butanol**; and *tert*-Butyl alcohol at **2-Propanol, 2-methyl-**. Phenol was retained as a heading parent, but all other trivially named phenols, including polyhydroxy benzene derivatives, are named systematically at such names as **Phenol, 2-methyl-** (formerly *o*-Cresol) and **1,3,5-Benzenetriol, Naphthalenol** (formerly Naphthol) and **Anthracenol** (formerly Anthrol) are now spelled out.

230. Aldehydes (¶ 173) are named systematically by use of the suffixes "-al" and "-carboxaldehyde," except for the three trivial names **Acetaldehyde, Formaldehyde, and Benzaldehyde**. Chalcogen analogs are all named systematically. Examples (previous index names are on the right):

Propanal	(Propionaldehyde)
Benzaldehyde,	(2,3-Cresotaldehyde)
2-hydroxy-3-methyl-	
Benzenecarbothioaldehyde	(Benzaldehyde, thio-)
Butanedithial	(Succinaldehyde, dithio-)

231. Alkaloids (¶ 204). Many alkaloids indexed prior to 1972 at trivial names are now indexed systematically. The remaining trivial headings (stereoparents) are limited to alkaloids exhibiting stereochemical complexity. Class A alkaloids (named systematically) therefore comprise a much larger group than previously, when it was restricted to compounds containing no asymmetric center. Classes B and C are largely unchanged, except that the number of Class B alkaloid stereoparents ("systematic" alkaloid names) has been greatly increased with a consequent reduction in the number of Class C alkaloid stereoparents (trivial names for alkaloids of known constitution, including all stereochemistry). Class D alkaloids (those not fully elucidated) are indexed at systematic names without stereodescriptors if sufficient information is available, otherwise at author names or as Class B stereoparents with partial stereochemical information.

232. Alloys (¶ 214) are now indexed and registered as specific chemical substances. The components, if known, are cited as symbols in the modification with their percentage compositions (when present to the extent of 0.1% or more). Cross-references from trade names and some code designations have been provided (without percentage compositions); e.g., **Alnico V**. See *Iron alloy, base, Fe,Al,Co,Cu,Ni,Si,Ti (Alnico V)*. Beginning in 1992 "nonbase" headings, e.g., **Cobalt alloy, nonbase**, for the other component elements are no longer made. For alloys of unknown percentage composition, only the "nonbase" headings for the components are employed.

233. Amides (¶ 171) are named systematically by use of the suffixes "-amide" and "-carboxamide." The three remaining exceptions are **Formamide, Acetamide, and Benzamide**, but their chalcogen and imidic analogs are now named systematically; for example, Acetamide, thio- is named as **Ethanthioamide**. Anilides are now indexed as *N*-phenyl amides. Secondary and tertiary amides are named at the preferred primary amide name. This analogs of sulfonamides are named as sulfonylthioamides and sulfonyldithioamides. See also **Urea** (¶ 292).

234. Amidines (¶ 171) are indexed systematically as imidamides, i.e., as amides of imidic acids; thus, Formamidine in Volume 76 became **Methanimidamide**. Amidoximes are named as *N*-hydroxy imidamides.

235. Amines (¶ 176) are all named systematically; Aniline is indexed at **Benzenamine**; Methylamine became **Methanamine**. Derivation of amine names for amino derivatives of nitrogen heterocycles is now permitted; Pyridine, 2-amino- (pre-1972 name), is now **2-Pyridinamine**; and Piperidine, 4-(2-aminopropyl)-, became **4-Piperidineethanamine, α -methyl-**. Secondary and tertiary amines are named as derivatives of the preferred primary amines, e.g.,

Ethanamine, *N*-ethyl- (formerly Diethylamine). Amino derivatives of the hydrides **Borane, Phosphorane, and Stannane** are now indexed at **Boranamine, Stannanediamine**, etc.

236. Amino acids (¶ 205) which are biologically significant are usually indexed at the trivial (or "common") names which are now classed as stereoparents. A few trivial names of α -amino carboxylic acids (Allocystathionine, Carnosine, Creatine, Cystathionine, Ethionine, Hippuric acid, Lanthionine, Pantothenic acid, Sarcosine, Thyronine, Thyroxine) and all trivial names of amino sulfonic acids were discontinued. The configurational descriptor is now placed in the heading as a prefix, thus: **L-Leucine**. The new stereoparent **Phenylalanine** is now employed, instead of Alanine, phenyl-, for $C_6H_5CH_2CH(NH_2)COOH$. Amino acid radicals are now employed only in naming peptides. *O*- and *S*-Derivatives of hydroxyl- and mercapto-group-containing amino acids, e.g., **Serine** and **Cysteine**, are now indexed at those heading parents. Esters of stereoparent amino acids with systematically named hydroxy compounds are indexed at the stereoparents. An ester with another stereoparent is indexed at the component possessing the higher function. Normally, only one entry is now made for each ester (¶ 247).

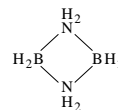
Beginning in 1992, primed locants are assigned to the side-chain methyl group of isoleucine, alloisoleucine, leucine, valine, and isovaline. Such branched-chained derivatives of these acids are no longer named as derivatives of the linear acid (Butanoic acid or Norvaline).

237. Anhydrides (¶ 179) of unsubstituted monobasic organic acids prior to Volume 76 (1972) were named in the heading, e.g., Acetic anhydride; now they are cited in the modification at the acid heading. Anhydrides of organic acids with inorganic monobasic oxo acids are named at the organic acid heading with an "anhydride with..." phrase in the modification, not at such former headings as Acetyl nitrate, but anhydrides of organic acids with isocyanic and isothiocyanic acids are treated like the corresponding acid halides. The term "bimol. monoanhydride" is employed when appropriate, with locants before the second word if necessary, at polybasic organic acid headings.

Cyclic anhydrides are now indexed as diones at the oxygen heterocycle names. Heading parents such as **Dicarbonic, Dicarbonimidic, and Tricarbonic acid** are used for carbonic acid anhydrides and their analogs (¶ 183). Anhydrides of phosphonic, phosphorous, arsenic, and arsonous acids are now treated like phosphoric acid anhydrides, e.g., **Diphosphonic acid**. "A" names are used for anhydrides when the requirements (¶ 127) are met.

238. Azo and azoxy compounds (¶ 193) in the absence of higher functions (e.g., nitrogen heterocycles, or functions expressible by a suffix) are indexed at **Diazene**, HN=NH (formerly Diimide). Azobenzene thus became **Diazene, diphenyl-**, and Naphthalene-2-*NNO*-azoxymethane became **Diazene, methyl-2-naphthalenyl-, 1-oxide**. Prior to 1992, formazans were of higher functionality than azo and azoxy compounds, but now have no special rank (¶ 249).

239. Boron compounds (¶¶ 159, 182). Cyclic compounds in which ligands bridge two boron atoms are named as coordination compounds; for example, Diazoniadiboratacyclobutane



is now indexed at **Diborane(6), di- μ -amino-**. Derivatives of polyboranes are given low numbers for substituents regardless of the direction of numbering. Boronic acid is treated as an independent index heading parent; thus, Benzeneboronic acid was renamed **Boronic acid, phenyl-** in 1972.

Since the Tenth Collective Index period (1977-81), most molecular addition compounds of boron have been indexed as coordination compounds. From the same date, Hypoboric acid, $((HO)_2BB(OH)_2)$, has been indexed at **Diborane(4), tetrahydroxy-**.

240. Carbohydrates (¶ 208). Glycosides of known constitution are now indexed at the systematic names; they are ranked as polyhydroxy alcohols, not as aldehydes or ketones, and when attached to a carbon atom of an aglycone containing a higher chemical function are indexed at a name which expresses that function. *N*-Glycosyl derivatives of heterocycles have continued to be indexed at the heterocyclic parents.

Radical (substituent prefix) names are no longer formed from aldolts.

Oligosaccharides indexed prior to Volume 76 at common names, e.g., Sucrose, are now named by systematic carbohydrate nomenclature.

The names Erythrose and Threose were discontinued except in the naming of polysaccharides. "Arrow" nomenclature was extended to all tri- and higher oligosaccharides, including those indexed at "-oside" heading parents.

Configurational descriptors (D-, L-, and DL-) are now always placed ahead of the heading parent; e.g., **D-Glucopyranoside**.

The index parent Cellulose acetate was discontinued; entries since 1972 have been made instead at **Cellulose, esters**, with modifications such as "monoacetate," "diacetate," and (for the indefinite ester) "acetate."

The naming of intramolecular amides of carbohydrate acids as lactams was discontinued for the Twelfth Collective Index. Such amides are named systematically as heterocyclic derivatives (¶ 171).

241. Carbonic acid and relatives (¶ 183) underwent name changes in several respects. **Carbonic acid** itself was retained but is now classed below all "organic" acids, including carboxylic and sulfonic acids, and above inorganic oxo acids (¶ 106). It is the parent of numerous acids, amides, acid halides, etc., derived from it by the use of affixes and suffixes. Thus, Carbonic acid, thio-, became **Carbonothioic acid**; Imidocarbonic acid, HN=C(OH)₂, became **Carbonimidic acid**; Formic acid, chlorothio-, hydrazone, H₂NN:C(Cl)SH, became **Carbonochloridohydrazone-thioic acid**. **Cyanic acid, Thiocyanic**

Benzenedicarboximidamide but below **Benzamide**.

Biguanide and Triguanide are now named systematically as **Imidodicarboximidic diamide** and **Diimidotricarboximidic diamide**, respectively.

252. Hydrazine (¶ 193) was retained as a trivial name for Diazane, and functional suffixes may be appended to it; thus, **Hydrazinecarboxylic acid**, H_2NNHCO_2H (formerly Carbazic acid), ranks above monocarboxylic acids derived from carbon skeletons.

Hydrazides (¶ 189) and hydrazones (¶ 190) of principal chemical functions expressed in the heading parent are cited in the modification as before, but these derivatives of functions expressed as substituents are now "named through" as in the case of esters (¶¶ 247, 250), by use of hydrazinyl and hydrazinylidene radicals.

Diacyl hydrazines are now indexed not at **Hydrazine** but as acyl hydrazides of the preferred acid (¶ 189). Semicarbazones of nonstereoparents are no longer indexed as such but as derivatives of **Hydrazinecarboxamide**, either as an index heading parent or as an appropriate substituent. Semioxamazines are treated as alkylidene hydrazides of **Acetic acid, 2-amino-2-oxo-**, $RCH:NNHC(O):C(O)NH_2$. The heading parent **Carbonic dihydrazide** (¶ 183) was introduced for $H_2NNHC(O)NHNH_2$ (formerly Carbohydrazide) and its derivatives, including compounds previously indexed as carbohydrazones of oxo parents.

253. Hydroxylamine (¶ 193) was retained as a heading parent; it ranks low among nonfunctional nitrogen parents between **Hydrazine**, H_2NNH_2 , and **Thiohydroxylamine**, H_2NSH (formerly Hydrosulfamine). *N*-Acyl derivatives of **Hydroxylamine** are now indexed at amide headings; *N*-alkyl derivatives at amine names. In the absence of *N*-substituents, *O*-derivatives are usually indexed at **Hydroxylamine**. Alkylidene derivatives are indexed as oximes of the corresponding carbonyl compounds unless higher functions are present, in which case a (hydroxyimino) substituent prefix is employed (see ¶ 195).

254. Imines (¶ 177) are indexed by means of the suffix "imine" appended to the molecular skeleton, which may now be a nitrogen heterocycle; e.g., **4(1*H*)-Pyridinimine** (formerly Pyridine, 1,4-dihydro-4-imino-). Cyclic imines are indexed at the ring names; e.g., **Aziridine** (formerly Ethylenimine). Imines rank below amines and all other compounds expressed by functional suffixes. 1-Iminoalkyl radicals are so named, not as imidoalkyl radicals; hence, formimidoyl has become (iminomethyl), and propionimidoyl is indexed as (1-imino-propyl).

255. Index name selection policies for chemical substances (¶ 138) were revised for Volume 76 and subsequent volumes as follows:

- "Like treatment of like things" was abandoned.
- The principle of "complexity" (a measure of the number of parentheses and brackets in a name) is no longer employed.
- The principle of "lowest locants" of substituents on an index heading parent (¶¶ 137, 138) was introduced on a regular basis.
- The principle of "centrality" is now applied when a compound contains a sequence of three or more occurrences of the same heading parent.
- Conjunctive nomenclature (¶ 124) was extended for the first time to benzene with a *single* acyclic functional substituent, as in **Benzenemethanol** (names such as **Benzenediactic acid** were used previously). It was discontinued for compounds in which ring attachment is by a double bond, and for **Carbamic** and **Sulfamic acids**, unsaturated acyclic functional compounds, and acyclic difunctional compounds.
- Multiplicative nomenclature (¶ 125) based on hydrocarbons is now permitted, as in **Ethane, 1,1'-oxybis-**, and **Benzene, 1,1'-[1,2-ethanediyl-bis(thio)]bis-**. The terms "bis," "tris," etc., not "di-," "tri-," etc., are always employed in multiplying a parent. The use of two-part unsymmetrical multiplying radicals prior to 1972 meant that names such as (ethylidenesilylene) could be misconstrued to be either $CH_3CH=Si=$ or $-CH(CH_2)-SiH_2-$. Thus, in 1972 the use of "ylidene" radicals in combination with other bivalent radicals in forming names of multiplying radicals was forbidden. Now, stringent symmetry is required of compounds for which multiplicative names may be used, and thus, beginning in 1994 such combinations in forming multiplying radicals are no longer prohibited (¶ 125). (Ethylidenesilylene) can only represent $CH_3CH=Si=$ in a multiplicative CA index name.

Beginning with Volume 119, the principle of selection of a parent based on preferred atomic content (¶ 138(b)) is also applied to a choice between two acyclic skeletons named by organic replacement nomenclature ("a" names).

256. Indicated hydrogen (¶ 135) is always cited, never implied; thus, Indene became **1*H*-Indene**, and Fluorene is now named **9*H*-Fluorene**. Hydrogen not required for formation of a ring system, but "added" at the same time as a functional (or radical) suffix is now described as "added hydrogen" (¶ 136). In tautomeric systems (¶ 122), lowest locants for indicated hydrogen are normally preferred; thus **1*H*-Purine**, not **7*H*-Purine**, is indexed in the absence of information to the contrary.

257. Inorganic compounds (¶ 219) are largely indexed at names previously used. Binary names for derivatives of elements possessing hydride names were changed to derivatives of the hydrides; e.g., **Silane, tetrachloro-** (formerly Silicon chloride ($SiCl_4$)); **Borane, trifluoro-** (formerly Boron trifluoride). When the compound is the halide of a recognized acid, it is so named; e.g., **Phosphorous trichloride** (formerly Phosphorus chloride (PCl_3)). Pyrophosphoric acid, $(HO)_2P(O)OP(O)(OH)_2$, was renamed **Diphosphoric acid**, and analogous compounds are named similarly; for example, **Diphosphoryl chloride**, $Cl_2P(O)OP(O)Cl_2$; **P,P'-Diamidodiphosphoryl fluoride**, $(H_2N)FP(O)OP(O)F(NH_2)$; **P'-Amidodiphosphoric(III,V) acid**, $(HO)_2POP(O)(OH)(NH_2)$.

Since the Tenth Collective Index period (1977-81), antimony has been classed as a metal, and synonym line formulas have been cited in index headings with *all* binary salt-type names, e.g., **Sodium chloride (NaCl)**. See also ¶¶ 239, 273. Graphite derivatives have been indexed as molecular addition compounds instead of at the pre-1977 headings **Graphitic acid**, **Graphite**

nitrate, etc.

Beginning in 1982, elements of atomic number 104 and above have been indexed at names derived from these numbers, e.g., **Unnilquadium** (formerly Element 104).

Starting with Volume 122, for elements 104-109, CAS follows the recommendations of the ACS Committee on Nomenclature: 104 - Rutherfordium (Rf); 105 - Dubnium (Db); 106 - Seaborgium (Sg); 107 - Bohrium (Bh); 108 - Hassium (Hs); and 109 - Meitnerium (Mt). Likewise, starting with Volume 139, element 110 is called Darmstadtium (Ds).

Starting in 1987 inorganic line formulas may be expressed with decimals or numerical ranges as well as integers, e.g. **Aluminum gallium arsenide** ($Al_{0.15}Ga_{0.85}As$).

For intermetallic compounds, beginning in 1992, additional entries for the metals with the less alphabetically preferred names are discontinued.

258. Inositols (¶ 209) are now indexed at the separate stereoparents derived by combining individual configurational prefixes with the name Inositol, e.g., *myo*-**Inositol**; *scyllo*-**Inositol**. These names in turn are preceded by the configurational descriptors *D*- and *L*-. When a choice must be made for derivatives, the earliest alphabetic prefix is preferred; then the prefix *D*- is selected, rather than *L*-; finally, lowest locants are assigned to substituent prefixes. **Inosose** and **Streptamine** are retained as stereoparents.

259. Iodine compounds (¶ 188) with abnormal valencies are indexed by coordination nomenclature (¶ 215); e.g., **Iodine, dichlorophenyl-** (formerly Benzene, (dichloroiodo)-).

260. Isocyanides (¶ 188). Alkyl isocyanides, RNC, are now indexed systematically; acyl isocyanides are treated like acid halides. For example, Isopropyl isocyanide became **Propane, 2-isocyno-**; **2-Naphthalenecarbonyl isocyanide** was formerly indexed at 2-Naphthoic acid, anhydride with hydroisocyanic acid.

261. Ketene (¶ 174) is now indexed systematically at **Ethenone**; Ketene, thio- at **Ethenethione**. Cyclic ketenes are named as cycloalkylidene (etc.) derivatives of the new heading parent **Methanone**, H_2CO . Unsubstituted H_2CO is still indexed at **Formaldehyde**, but unsubstituted CH_2S is named **Methanethial**. In the presence of chemical functions higher than ketone, the $=CO$ radical is named carbonyl (if the carbon atom does not form part of an acyclic chain) or as (oxoalkyl). The isolated $=CS$ radical is named carbonothioyl if both free valencies are attached to a single atom, or if it is used in a multiplying prefix; otherwise as (thioxomethyl).

262. Ketones (¶ 174). All trivial names (including Acetone, Chalcone, Benzil, Benzoin, and all flavone, quinone, phenone and naphthone headings) were abandoned. The heading parent Ketone was discontinued. **Methanone**, $H_2C=O$, is used to index ketones having two ring systems directly attached. The analogous headings **Methanethione**, $H_2C=S$, etc., were introduced. Acetone was changed to **2-Propanone**, Acetophenone to **Ethanone, 1-phenyl-**, Acetophenone, thio- to **Ethanethione, 1-phenyl-**, Anthraquinone to **9,10-Anthracenedione**, Benzil to **Ethanedione, diphenyl-**, Flavone to **4*H*-1-Benzopyran-4-one, 2-phenyl-**, and Uracil to **2,4(1*H*,3*H*)-Pyrimidinedione**. For a discussion of this last name, see ¶ 289A.

The ketone function is no longer overstepped; hence **Ethanone, 1,1'-(1,5-naphthalenediyl)bis-** (formerly Naphthalene, 1,5-diacetyl-).

263. Locants (¶¶ 114, 137). The locants *o*-, *m*-, and *p*- were replaced by Arabic numerals in all cases; *as*-, *s*-, and *v*- were likewise replaced, except in *as*- and *s*-**Indacenes** and their fused derivatives. Locants for unsaturation are now always cited for molecular skeletons of three or more atoms except for monocyclic hydrocarbons containing one multiple bond. Polyvalent radicals with free valencies located at two or more positions now have all locants cited; thus, ethylene became 1,2-ethanediyl. In ring assemblies, locants for positions of attachment are always cited except for two-component assemblies of cycloalkenes, cycloalkadienes, etc. Thus, 4-Biphenylamine became **[1,1'-Biphenyl]-4-amine**.

In multiplicative names, locants are always cited to indicate the position of attachment of the multiplying radical to the heading parent.

Special rules whereby locants for *fully halogenated compounds* and radicals were sometimes omitted are now discontinued.

Urea is now assigned the locants *N*- and *N'*- in place of 1- and 3- (¶ 183).

When locants are required for derivatives, e.g., esters, cited in modifications, *all* such locants are used (¶ 119).

Letter locants are now employed with ligand names in coordination nomenclature to define the ligating atoms (¶ 215).

264. Metallocenes (¶ 215), including **Ferrocene** and its derivatives, are now considered to be neutral coordination complexes. Suffix-type names and conjunctive names are no longer used; hence Ferrocenecarboxylic acid is now indexed at **Ferrocene, carboxy-**; and 1,1'-Ferrocenediacetic acid at **Ferrocene, 1,1'-bis(carboxymethyl)-**.

265. Mixtures (¶ 221) are now indexed and registered as individual chemical substances if they are considered significant in their own right, e.g., pharmaceutical and pesticide mixtures which possess trade names, or mixtures which are emphasized in an original document as possessing special properties. Ingredients which are considered to be inactive within the intended use of a mixture are disregarded, e.g., solvents, fillers, and inactive trace components. Ratios of components are not cited. Cross-references from trade names, etc., are provided; e.g., **Terracoat**. See **1,2,4-Thiadiazole, 5-ethoxy-3-(trichloromethyl)-**, mixt. with pentachloronitrobenzene.

265A. Molecular addition compounds (¶ 192). Ten additions were made to the list of common components for the Twelfth Collective Index. The new additions are Acetic acid, trifluoro-; Acetonitrile; Benzene; Benzene, methyl-; Benzenesulfonic acid; Benzoic acid; Borate(1-), tetrafluoro-, hydrogen; Ethanimine, *N,N*-diethyl-; Methane, dichloro-; and Pyridine.

The prefixes hemi- and sesqui- were replaced by the ratios (2:1) and (2:3), respectively in names of hydrates and ammoniates for the Twelfth Collective Index.

Beginning with the Thirteenth Collective Index period, restriction of the expression of the number of molecules of solvation to fifteen (pentadeca) is abandoned. Fractional coefficients are limited to two digits in both the numerator and the denominator.

Beginning with the Fifteenth Collective period, molecular addition compounds are indexed at the preferred name only. The preferred name appears in the *Formula Index* at the formula of each of the components. See ¶ 192 for the components for which no name is printed in the *Formula Index*.

Beginning with the Sixteenth Collective period, ratios are used for all molecular addition compounds for which stoichiometry is expressed. Because polymers are nonstoichiometric compounds, ratios are rarely used for molecular addition compounds of polymers.

266. Multiplicative prefixes (¶ 110). Bis-, tris-, etc., are used in multiplicative names instead of di-, tri-, etc., even when the heading parent is not otherwise substituted. Bis-, tris-, etc., are used with methylene in every circumstance in general index nomenclature (but "di-*O*-methylene" is used with sugar names), and with oxy and thio, etc., to denote a multiplicity of single chalcogen atoms; thus, [methylenebis(oxy)] denotes $-O-CH_2-O-$, while (methyldioxy)- denotes CH_3-O-O- . Bi-, etc., names for ring assemblies were discontinued for assemblies of rings joined by double bonds. All ring-assembly names are enclosed in brackets when followed by a suffix; derived radicals are treated similarly. Binaphthyl and Bianthryl become **Binaphthalene** and **Bianthracene** (see ¶ 281). Bi-, etc., names derived from acyclic compounds, e.g., Bicarbamic acid, Triguamide, are discontinued.

267. Nitriles (¶ 172). Only the trivial names **Acetonitrile** and **Benzonitrile** are retained; otherwise, changes in nitrile names are almost entirely parallel to those for the carboxylic acids (¶ 165) from which they and their names are derived. Thus, Hydrocinnamonitrile became **Benzenepropanenitrile**. **Cyanamide** was retained for H_2NCN , but conjunctive "carbamonitrile" names were discontinued.

The zwitterionic nitrilimines ($RC=N-N^+-R^-$) are named as substituted hydrazinium hydroxide inner salts (¶ 201) beginning in the Twelfth Collective period.

268. Nitron, $H_2C=NH=O$, was renamed **Methanimine**, *N*-oxide (¶ 177); *N*-alkyl nitrones are indexed as oxides at amine index heading parents; *N*-acyl nitrones at amide headings.

269. Nucleosides and Nucleotides (¶ 210) have continued to be indexed at trivial names, e.g., **Adenosine**, **Cytidine**, although the purine and pyrimidine bases from which they are derived are now named systematically; e.g., Cytosine is indexed at **2(1*H*)-Pyrimidinone**, **4-amino-** (¶ 122). *N*-Acyl derivatives of nucleosides are indexed at the nucleoside parents instead of at amide names, but higher functions have continued to be indexed at the parents which express them.

Substituents are now expressed at nucleotide headings, e.g., **5'-Uridylic acid**, **2-amino-2'-deoxy-3'-thio-**. Mixed phosphate esters are indexed at the preferred phosphate heading rather than at the plain nucleoside name; e.g., **Inosine 5'-(trihydrogen diphosphate)**, **2'-(dihydrogen phosphate)**. Nucleosides and nucleotides are considered to be stereoparents (¶ 203), and their esters with systematically named substances are therefore indexed at nucleoside or nucleotide index heading parents.

270. Onium compounds (¶ 184). Ammonium compounds are named from the corresponding preferred amines by use of "aminium" as a suffix and expression of the remaining groups as *N*-substituents; e.g., **Ethanaminium**, ***N*-ethyl-*N,N*-dimethyl-, iodide (1:1)** (formerly Ammonium, diethyl-dimethyl-, iodide). Naming of cyclic quaternary nitrogen compounds and other cationic species, e.g., sulfonium compounds, is largely unchanged.

Localized cationic free radicals centered on hetero atoms (¶ 184) were named as derivatives of the index heading parents **Ammoniumyl**, **Oxoniumyl**, **Sulfoniumyl**, etc. prior to the Thirteenth Collective period.

271. Order of precedence of compound classes (¶ 106) has continued to play an important role in the selection of a preferred index name. Changes include the following:

(a) The heading parent Silane now ranks below cyclic carbon parents and above acyclic carbon parents. This change does not apply to any other silicon parents.

(b) More emphasis is placed on the presence of a principal chemical functional group (expressed as a suffix attached to a molecular skeleton). Thus **Ethanamine** (a functional compound) is ranked above **Quinoline** (a nonfunctional molecular skeleton).

(c) **Ferrocene** and other metallocenes are ranked with neutral coordination complexes.

(d) Peroxy acids expressed as principal groups are ranked, as a class, higher than all other acids. Previously, each such acid was placed just above the corresponding parent acid. Carbonic acid and related compounds are placed below those acids, e.g., carboxylic and sulfonic, expressed as functional suffixes, and above inorganic "oxo" acids. Derivatives of **Arsonic** and **Boronic acids** are named like those of other inorganic "oxo" acids with replaceable nuclear hydrogen atoms; thus, Benzene-*arsonic* acid has become **Arsonic acid**, **phenyl-**. Derivatives of isocyanic acid and its chalcogen analogs are named substitutively by use of the prefixes isocyanato, isothiocyanato, etc.

(e) Alcohols and phenols now rank as equal in precedence.

(f) Ether, Sulfide, Selenide, and Telluride are no longer employed as heading parents and are therefore not listed in the Order of Precedence. Single chalcogen atoms are named substitutively (by use of oxy, thio, etc., radicals) or

at organic replacement ("a") names.

(g) Phosphorus compounds without functional suffixes are ranked together (following nitrogen compounds). Formerly, phosphine oxide was placed above amines with phosphine and phosphorane following them. The same policy is adopted in descending order for nonfunctional heading parents derived from arsenic, antimony, bismuth, boron, silicon, germanium, tin, and lead. Then follow nonfunctional oxygen parents in the order: oxygen heterocycles, acyclic polyoxides (**Trioxide**, **Peroxide**), acyclic "oxa" names. Other chalcogens are ranked below oxygen in the order: sulfur, selenium, tellurium. Lowest in order of precedence are nonfunctional carbon skeletons.

(h) In each class of nonfunctional compounds, ranked in the order of the most preferred heteroatom it contains, cyclic compounds are preferred over acyclic, and acyclic parents named by "a" nomenclature are less preferred than other acyclic parents of that hetero atom class. Among carbon compounds, similarly, carbocycles are preferred to acyclic carbon chains, regardless of length. Unsaturated skeletons are preferred to saturated skeletons with the same number and type of skeletal atoms; thus, **Benzene** is preferred to **Cyclohexane** (no policy change), and **Pyridine** is preferred to **Piperidine** (reversal of policy).

272. Organometallic compounds (¶ 194). Binary compounds of element hydrides, e.g., **Arsorane**, AsH_3 , **Plumbane**, PbH_4 , **Germane**, GeH_4 , are indexed at those headings. Thus, Lead chloride ($PbCl_4$) became **Plumbane**, **tetrachloro-**. (In the carbon series, Carbon tetrachloride became **Methane**, **tetrachloro-**.) Amino derivatives of hydrides are now assigned "amine" names, e.g., **Germanediamine**, and other functional suffixes are also employed, e.g., **Bismuthinecarboxylic acid**, but "ol" to express a hetero-atom-attached hydroxyl is used only with carbon and silicon. "A" names must (as usual) be employed when appropriate.

273. Oxo acids (¶ 219). Some changes (¶ 185) were made in 1972 to the content of the "Class I" list for esters of inorganic "oxo" acids. Pyrophosphoric acid, $(HO)_2P(O)OP(O)(OH)_2$, was renamed **Diphosphoric acid**. The new heading parent **Diphosphonic acid** was previously indexed at Phosphonic acid, anhydride. Since 1972, arsenic mononuclear acids have been treated analogously to phosphorus acids.

Examples:

Arsonic acid (H_3AsO_4)	$(HO)_3AsO$
Arsonic acid	$(HO)_2HASO$
Arsinic acid	$(HO)H_2AsO$
Arsenic acid	$HOAsO_2$

Cyclic esters of arsenic and phosphorus acids are indexed at the ring names.

Since the Tenth Collective Index period (1977-81), metal oxo acids (including oxo acids of antimony) and their salts have been indexed as coordination compounds or as mixed salts. The only exceptions are **Chromic acid** (H_2CrO_4), **Chromic acid** ($H_2Cr_2O_7$), **Manganic acid** (H_2MnO_4) and **Permanganic acid** ($HMnO_4$), which were retained as index heading parents. A few little-used nonmetallic oxo acid names, e.g., **Mesosulfuric acid**, were also discontinued.

274. Peptides (¶ 206), other than biologically active peptides with trivial names, containing two through twelve amino-acid residues are now indexed at the name of the C-terminal unit in every case; peptide amides are treated analogously. No change was made in the treatment of larger peptides. Some trivial acyl names were changed starting in the Twelfth Collective period (1987-1991). Thus α -aminobutyryl became 2-aminobutanoyl and lactoyl became 2-hydroxypropanoyl. Cyclic peptides of two or three units are indexed at systematic ring-system names, larger compounds at "Cyclo" names such as **Cyclo[*L*-alanyl-*N*³-acetyl-D-ornithylglycyl-*L*-alanyl-D-propyl-*O*-(1,1-dimethylethyl)-*L*-seryl]** in which the units are cited in the order of occurrence, with preference given to the lowest alphabetic arrangement of *parent* amino-acid radicals. Prior to 1987 the term "Cyclic" was used instead of "Cyclo". Additional entries are made at ring-system names. Peptides with fewer than four units and which contain disulfide linkages are now indexed, like larger peptides, at cysteine rather than cystine names.

Linear desipeptides are now usually indexed at the C-terminal *amino*-acid names; terminal hydroxy acids are expressed as carboxyalkyl esters. Cyclic desipeptides are indexed at ring names or "Cyclo" names in analogy with peptides.

Effective with Volume 129, the rules for naming peptides have been revised as follows: (1) In desipeptide nomenclature, the chalcogen in a nonterminal hydroxy, mercapto, selenyl, or telluryl acid residue need no longer be α to the carbonyl. Any position is acceptable. (2) In ψ nomenclature (adopted in Volume 126 for certain pseudopeptides), glycine may now serve as one of the ψ residues—the amino acids cited before and after the ψ term—provided the other ψ residue is a standard chiral amino acid. In addition, a ψ residue may now be N-terminal, provided its CO is not replaced, or C-terminal, provided its NH is not replaced.

Naturally-occurring biologically active peptides and desipeptides of six to fifty units are indexed at the trivial names; those of five or fewer units are named like other peptides at the C-terminal amino acid or "Cyclo" name; trivially named stereoparents such as **Bradykinin** and **Gramicidin S** have continued to be employed for substances containing six through fifty units. Small species variations in trivially-named peptides are now interrelated by using one form as the reference compound; e.g., **Fibrinopeptide B** (**orang-utan**). See

Fibrinopeptide B (human), 10-L-leucine-12-glycine-; similar cross-references are now made between trivial names of closely-related peptides and corticotropin sequences; e.g., **Kallidin**. See *Bradykinin*, N²-L-lysyl-; $\alpha^{1,39}$ -**Corticotropin (human)**. See $\alpha^{1,39}$ -*Corticotropin (pig)*, 31-L-serine-.

Esters of hydroxy and mercapto groups in amino-acid radicals of peptides are now expressed as substituents; e.g., *O*-acetyl-L-seryl. Functional derivatives of carboxy substituents are expressed by radicals which include the carboxyl group; e.g., *N*-[(phenylmethoxy)carbonyl].

Such former headings as Angiotensins were made singular in Volume 76. The indexing of *Oxytocins* and *Vasopressins* was further refined. Bovine insulin is now the reference compound for insulins, with the name **Insulin (ox)**. **Actinomycin D** is the reference stereoisomer to which other actinomycins are related for indexing purposes.

Proteins (¶ 207) are indexed at trivial names, with accompanying species information.

Synthetic peptides are indexed like polymers; the term "polymer with" is used instead of "peptide with" at amino-acid monomer names.

275. Peroxides (¶ 196). Binary headings were discontinued; Isopropyl peroxide became **Peroxide, bis(1-methylethyl)**. The heading **Peroxide** is a nonfunctional oxygen compound; in the presence of more preferred compound classes, such radicals as (ethyl)dioxy are employed. **Hydroperoxide** is a functional oxygen compound ranking just above amines; such names as Peroxyacetyl hypochlorite are replaced by **Peroxide, acetyl chloro**, etc.

276. Phosphorus compounds (¶ 197, 219). Functional suffixes are now employed with phosphorus hydride names; e.g., **Phosphinecarboxylic acid** (formerly Formic acid, phosphino-) and **Phosphoranamine** (formerly Phosphorane, amino-). The phosphoro radical, -P=P-, was renamed 1,2-diphosphenediyl; phosphino was retained, but diphosphino, H₂P-PH-, was renamed diphosphinyl, and diphosphinetetranyl became 1,2-diphosphinediylidene. **Phosphorothioic** and **Phosphordithioic acids** were added to **Phosphoric** and **Phosphorous acids** in "Class I" (¶ 185) for the indexing of esters. Pyrophosphoric acid was renamed **Diphosphoric acid**. **Diphosphonic acid** became the new name for **Phosphonic acid**, anhydride.

Phosphonium ylides are indexed only as ylide derivatives of **Phosphorane** (¶ 201). Prior to the Twelfth Collective period an additional *Chemical Substance* and *Formula Index* entry appeared for the phosphonium ylide name.

The phosphoryl radical was eliminated for non-acid mononuclear analogs of phosphoric acid in Volume 120; thus phosphoryl chloride (POCl₃) is now phosphoric trichloride.

277. Polymers (¶ 222). Prior to the Fifteenth Collective period, polymers with known component monomers were indexed at the name of each monomer as actually reported in the original document. Polymers are now indexed at the preferred name only. The preferred name appears in the *Formula Index* at the molecular formula of each monomer used in the polymer. Names based on structural repeating units (SRUs) have continued to be used as additional index names for polymers of well characterized or assumed structure. In the cases of very common trade-named industrial polymers of known composition for which cross-references are used, the SRU name is preferred. Thus, **1,4-Benzenedicarboxylic acid, polymers**, polymer with 1,2-ethanediol. See *Poly(oxy-1,2-ethanediyloxycarbonyl-1,4-phenylenecarbonyl)*; **Nylon 6**. See *Poly[imino(1-oxo-1,6-hexane-diy)]*. At monomer names, the terms "polymers," "polyamides," "polyesters," etc., were replaced by "homopolymer" except for general studies; "polymer with" was retained for copolymers named at monomer headings and replaced such terms as "polyamide with," "polyester with," etc.; "copolymers" is an acceptable general term. Block, graft, and alternating copolymers are registered and indexed with their own specific Registry numbers starting in the Twelfth Collective period (1987-1991). The terms "block", "graft" and "alternating" are part of the index name for these kinds of polymers. Starting with Volume 145 (June 2006), diblock, triblock, tetrablock and pentablock polymers are indexed with their own specific Registry numbers. The terms diblock, triblock, tetrablock and pentablock are part of the index names for these polymers.

Siloxanes prepared by hydrolytic polymerization of chlorosilanes are now, starting in 1994, registered and indexed at the monomer names with the term "hydrolytic" cited in the modification, along with the term "homopolymer" or "polymer with".

Cyclic acetals of ethenol homopolymer and ethenyl acetate-ethenol copolymer are indexed with their own specific Registry number starting with the Sixteenth Collective period. (December 2006). The names include the phrase "cyclic acetal with" followed by a specific aldehyde name in the modification.

Phenol condensation products are now indexed at **Phenol polymers**, with "polymer with formaldehyde" or other appropriate term cited in the modification. Urea condensation products are named analogously at **Urea polymers**.

278. Porphyrins and Bile pigments (¶ 223) were affected by the new rule that indicated hydrogen of ring systems is always cited. **21H,23H-Porphine** and **21H,23H-Porphyrine** are the forms preferred for these and related substances unless an original document emphasizes the absence of hydrogen at these positions. The **29H,31H**-form of **Phthalocyanine** is preferred; the heading **21H-Bilene** is employed unless hydrogen is absent from that position, in which case **22H-Bilene** is indexed. (An (*all-Z*) form is now assumed for Bilene.)

Radicals. See Substituent prefixes (¶ 287).

279. Replacement ("a") nomenclature (¶ 127), in which replacement of carbon by heteroatoms is indicated by terms such as "aza," "oxa," and "thia," was unchanged for cyclic skeletons, but was amended for acyclic compounds, primarily to eliminate exceptions for certain classes, including silicon compounds. Now, "a" names are used whenever four or more "hetero units" (isolated hetero atoms, homogeneous hetero chains, or groups for which simple radical names are employed, such as disiloxanediy) are present, so long as the

resulting name, including functional suffixes, does not express a lower functionality than the alternative conventional name. The hetero atoms must not be in an abnormal valency state (unless this valency can be readily expressed), and the "a"-named chain must not be terminated by a nitrogen or chalcogen atom. ("A" names are not used for peptides, polymers or purely inorganic chains.)

280. Replacement nomenclature for functions (¶ 129) was extended to various classes of acids and acid derivatives, as outlined by the following examples (former names are in parentheses):

Ethanethioic acid	(Acetic acid, thio-)
Ethane(dithioic) acid	(Acetic acid, dithio-)
Ethaneperoxoic acid	(Peroxyacetic acid)
Butanebis(thioic) acid	(Succinic acid, 1,4-dithio-)
Carbonothioic acid	(Carbonic acid, thio-)
Carbamodithioic acid	(Carbamic acid, dithio-)
Methanimidamide	(Formamide)
Imidodicarbonic acid	(Imidodicarboxylic acid)
Diimidotricarbonimidic diamide	(Triguanide)
1,3-Benzenedisulfonothioic acid	(<i>m</i> -Benzenedisulfonic acid, 1,3-dithio-)

281. Ring systems (¶ 145-157). Fused oxireno and thiireno derivatives of hydrocarbon rings are now indexed according to the general rule that the base component should be a heterocycle; thus, Naphthalene, 2,3-epoxy- has become **Naphth[2,3-*b*]oxirene**. Adamantane and its replacement derivatives are indexed at **Tricyclo[3.3.1.1^{3,7}]decane, 2-Thiatriacyclo[3.3.1.1^{3,7}]decane**, etc. (¶ 155). The locants *o*-, *m*-, *p*-, and *v*- in ring names were replaced by numerals; *as*- and *ss*- are used only with **Indacene** and its fused derivatives; thus, *m*-Dioxane became **1,3-Dioxane**; *p*-Terphenyl became **1,1':4',1''-Terphenyl**; *s*-Triazine became **1,3,5-Triazine**; and **Benz[*e*]-*as*-indacene** is unchanged. Some trivial names were replaced; thus, Quinuclidine was renamed **1-Azabicyclo[2.2.2]octane**. Radical names from these ring systems were changed correspondingly.

Special names for partially hydrogenated ring systems, e.g., Acridan, Indan, Indoline, Phthalan, Pyrroline, were abandoned; thus Indan became **1H-Indene**, **2,3-dihydro-**. Norbornane, Norcarane, and Norpinane are now indexed at the systematic "Bicyclo-" names.

Ring systems containing metals other than antimony, tin, lead, germanium, or bismuth are now indexed by coordination nomenclature.

In ring-assembly names, points of attachment are now cited, except for two-component assemblies of cycloalkenes. Thus, **1,1'-Biphenyl, 1,2'-Binaphthalene** (formerly 1,2'-Binaphthyl), **Bi-2-cyclohexen-1-yl**. Ring assemblies in which component rings are joined by double bonds are now indexed at a component name, e.g., **Cyclopentane, cyclopentylidene-** (formerly Bicyclopentylidene).

The Hantzsch-Widman system (¶ 146) was extended, beginning in 1987, to partially or fully saturated rings, formerly named by organic replacement nomenclature, e.g. **Stannolane** (formerly Stannacyclopentane). Prior to Volume 121 the rings **1,2,5-Oxadiazole** and **2,1,3-Benzoxadiazole** were named **Furazan** and **Benzofurazan**, respectively.

Non-standard valence states (¶ 158) of certain ring heteroatoms were denoted by the greek letter lambda (λ) starting in 1987, e.g. $1\lambda^4,3\lambda^4,5\lambda^4,7\lambda^4$ -**1,3,5,7,2,4,6,8-Tetrathiatetrazocine** (formerly **1H,3H,5H,7H-1,3,5,7,2,4,6,8-Tetrathiatetrazocine**).

Names for cyclic systems containing ring heteroatoms in non-standard valence states described by the "hydro" prefix (¶ 158) were changed beginning in 1987 to allow the expression of principal suffixes and radicals, e.g. **2H-1,4-Selenazin-2-one, 1,1-dihydro-1,1-dimethyl-**(formerly **2H-1,4-Selenazine, 1,1-dihydro-1,1-dimethyl-2-oxo-**).

281A. Salts (¶ 198). Beginning with the Twelfth Collective Index, salts of substitutive cations no longer have additional index entries at the following common anions: **Acetic acid, 2,2,2-trifluoro-, ion(1-); Borate(1-), tetrafluoro-; Borate(1-), tetraphenyl-; Methanesulfonic acid, 1,1,1-trifluoro-, ion(1-); Phenol, 2,4,6-trinitro-, ion(1-); Phosphate(1-), hexafluoro-; Sulfuric acid, monoethyl ester, ion(1-)**.

282. Silicon compounds (¶ 199). Former binary names for silicon halides are now indexed at **Silane**; for example, Silicon chloride (SiCl₄) is now indexed at **Silane, tetrachloro-**. Functional suffixes are now appended to **Silane, Disilane, Disiloxane**, etc., but conjunctive names are not formed from them. **Silanol** and **Silanediol** now rank above all carbon-skeleton monohydric and dihydric alcohols, respectively, by reason of their hetero atom content (¶ 106). Similarly, **Silanamine** ranks above **Benzenamine**, etc.

Silthianes are now spelled out as silthianes; 1,3-disiloxanediy, 1,5-trisilathianediyl, 1,7-tetrasilazanediy, etc., all rank as single hetero units (¶ 127) in the formation of "a" names. A total of four such units (of any kind) are now necessary for a compound to be named by replacement nomenclature.

Silicic acids now all belong to "Class II" in the naming of esters (¶ 185). Since the Tenth Collective Index period, the **Silicic acid** heading has been generally restricted to mono- and dinuclear oxo acids of silicon.

283. Spelling (¶ 107). Elided forms of radicals were largely discontinued. Nitramino became (nitroamino); acetoxy became (acetyloxy); naphthyl became naphthalenyl. Ethoxy, methoxy, propoxy, butoxy, phenoxy, and thienyl were retained, but branched-chain radicals are now named as derivatives of the straight-chain alkoxy parents; thus, isopropoxy became (1-methyl-ethoxy). Elided forms of heading parents (Pyridol; Pyridone) are now spelled out (**Pyridinol; Pyridinone**). Punctuation in compound names is unchanged.

284. Stereochemistry (¶ 203). Major revisions were made in this area for the Ninth Collective Index Period (1972-76). The concept of stereoparents (¶ 285) was introduced for those substances, mainly natural products, containing complex stereochemistry and not readily indexed at systematic names. For other substances, the stereochemistry is expressed in the name by use of relative and absolute descriptors, including *cis*- and *trans*-; *endo*- and *exo*-; α - and β -; *E*- and *Z*-; *R*- and *S*-; and *R**- and *S**-. The Sequence Rule of Cahn, Ingold, and Prelog is applied in the assignment of these descriptors. A special system was developed for coordination compounds (¶ 203 III).

Beginning with Volume 120, the sign of optical rotation (+), (-), or (\pm) is assigned to substances with visual wavelengths other than the sodium-D line.

Beginning with Volume 126 (1997), in order to provide more accurate descriptions of and improved access to substances whose stereochemistry has not been completely defined, CAS now registers and names substances with partially defined stereochemistry. Previously, partial stereochemistry was generally ignored. The presence of unknown chiral centers is indicated by the addition of their term "[*partial*]" to the end of the normal stereochemical descriptor. When the reference ring or chain has incompletely defined chiral atoms/bonds, the format cites the stereo using *R* and *S* terms with their nomenclature locants for all known centers. If this method is used to describe a substance for which only relative stereochemistry is known, "*rel*" is added to the stereochemical descriptor. Racemic mixtures of substances with single chiral centers are now indexed, registered, and named as non-stereospecific substances. Racemates having more than one chiral center are indexed, registered, and named as having only relative stereochemistry.

Stereochemical descriptors were simplified beginning with Volume 129. The need for a single expression to describe the total stereochemistry of a molecule has been eliminated. Stereochemical terms are now placed within the parts of a chemical name to which the stereochemical information applies. Only the stereochemistry contained in the heading parent is expressed in the name modification following all other structural information. The use of the term "[*partial*]" has been discontinued.

The terms *R* and *S* are employed for chiral elements possessing either absolute or relative stereochemistry. The term *rel* is used in conjunction with *R* and *S* for structures with only relative stereochemistry. *E* and *Z* are used primarily to describe geometrical isomerism about double bonds. The relative terms *cis*, *trans*, *endo*, *exo*, *syn*, *anti*, α , and β are used as alternatives to *R* and *S* in certain limited situations.

285. Stereoparents (¶ 202) are heading parents whose names imply stereochemistry, as indicated by structural diagrams shown at these names in the *Chemical Substance Index*. Synonyms and cross-references for the systematic names are always provided. The stereochemistry implied by the stereoparent, and shown in the diagram, may be augmented or selectively reversed in the name. Stereoparents include biologically significant amino acids, carbohydrates, and cyclic natural products (alkaloids, steroids, terpenes) within certain limitations. Stereoparents are preferred to systematically named substances of higher functionality in the naming of esters, mixtures, molecular addition compounds, and polymers. Derivatives of stereoparents are kept at the stereoparent names as much as practicable, but substituents (¶ 287) are named systematically in accordance with the changes in general index nomenclature.

Beginning with Volume 126 (1997), infrequently used terpene, steroid, alkaloid, and antibiotic stereoparent terms have been replaced by systematic names. For example, Nemuarine and 15-Thialanostane are no longer used in index names. Frequently occurring stereoparents, such as Pregnane, Cholane, Cholestane, 9, 10-Secocholestane, Morphinan, Retinoic acid, and Erythromycin are maintained. Cross-references from the previously used stereoparent names will guide users to the corresponding systematic index names. Amino acid sequence names are now assigned to most systematically named linear peptides. In an amino acid sequence name, the C-terminal residue is the index heading parent, and the other residues are cited in the substituent, beginning with N-terminal residue and continuing from left to right in the sequence; e.g., L-Lysine, D-alanyl-glycyl-L-leucyl-. Psi (ψ) nomenclature is now used to describe certain modifications of the peptide bond. The Greek letter ψ conveys the fact that a peptide bond has been replaced by a pseudopeptide bond. In an amino acid sequence name, the format of the ψ term is ...-A- ψ (X-X')-B-..., where A is the amino acyl radical whose carbonyl group has been modified to X and B the amino acyl radical whose α -amino group has been modified to X'. X and X' are shown as strings of element symbols, separated by a bond; e.g., ...-L-valyl- ψ (CH₂-NH)-L-tyrosyl-.

286. Steroids (¶ 211). Stereochemical descriptors, e.g., "5 α ," which formerly appeared as a prefix at steroid names, were combined in Volume 76 with descriptors required for suffixes and substituent prefixes and are now cited in parentheses in their own field.

Cyclogonanes were discontinued as the names of ring systems. Cyclogonane stereoparents are retained, with stereochemistry defined by illustrative diagrams in the *Chemical Substance Index*.

Trivial names for steroids, including Cholesterol, Ergocalciferol, and Testosterone, were discontinued as heading parents.

Use of "homo" (to denote ring enlargement), "nor" (to denote ring contraction), and "seco" (to denote ring fission), are now further restricted.

Functional derivatives of steroids are indexed at the steroid names, either in the substituents (for derivatives of subsidiary functions) or in the modifications (for derivatives of the principal functions). Acyclic acetals are expressed by alkyloxy or aryloxy substituents (¶ 196); cyclic acetals with formaldehyde by methylenebis(oxy) radicals; other cyclic acetals by a modification phrase such as "cyclic 1,2-ethanediyl acetal" (if a principal group has been acetalized) or by an alkanediylbis(oxy) or alkylidenebis(oxy) substituent. Steroidal lactones

are "opened" to permit the steroid stereoparent to be used; the lactone is then cited in the modification.

287. Substituent prefixes (radicals) (¶¶ 132, 161). Groups always expressed as substituents now include isocyanoyl, isocyanato, isothiocyanato, etc., and groups terminating in oxy, thio, sulfinyl, sulfonyl, and their analogs, such as seleno and telluronyl.

Changes in radical names include iodosyl (instead of iodoso) for -IO; and iodyl (instead of iodoxy) for -IO₂. Morpholino was changed in Volume 76 to 4-morpholinyl; piperidino to 1-piperidinyl; the unsubstituted diazeno radical, HN=N-, to diazenyl; *p*-phenylene, etc., to 1,4-phenylene, etc.; *v*-phenenyl to 1,2,3-benzenetriyl; benzyl to (phenylmethyl); styryl to (2-phenylethenyl); *p*-tolyl to (4-methylphenyl); 2,4-xylyl to (2,4-dimethylphenyl); and similarly for other radicals containing a benzene ring and one or more acyclic chains. Thenyl became (thienylmethyl) and furfuryl became (2-furanylmethyl).

Ring-assembly radicals are now based on the ring assembly names, as, [1,2'-binaphthalen]-8'-yl and [1,1'-biphenyl]-4,4'-diyl (¶ 161).

Acyl radicals in substitutive names were replaced by substituted radicals (exceptions are acetyl, benzoyl, carbonyl, and, when unsubstituted, formyl). Hence propionyl became (1-oxopropyl); acetimidoyl became (1-iminoethyl); succinoyl became (1,4-dioxo-1,4-butanediyl). The three radicals carbonimidoyl, -C(:NH)-; carbonohydrizonoyl, -C(:NNH₂)-, and carbonothioyl, -C(:S)- were introduced for use in multiplicative nomenclature and for cases in which both free valencies are attached to the same atom. In other cases, (iminomethyl) (formerly formimidoyl), (thioxomethyl), etc., are employed.

Replacement ("a") names for acyclic radicals (¶ 128) were introduced under the same restrictions as for heading parents. The free valencies, not the hetero atoms, are preferred for lowest locants, which are always cited; e.g., 4,12-dioxo-7,9-dithiatetradec-1-yl.

Compound and complex radicals are now constructed in accordance with revised rules which reflect the new policies for compounds. The most important changes were emphasis on hetero-atom content of the parent radical, abandonment of "like treatment of like things" and the "complexity" principle, elimination of preference for unsaturated acyclic radicals regardless of size, consistent application of the principle of "lowest locants" for substituents on the parent radical, and adoption of more systematic radical names.

A list of substituent prefixes (radicals) as revised for the Ninth Collective Index Period (1972-1976) constitutes Section H (¶ 294).

288. Sulfur compounds (¶ 200). Sulfide was discontinued as a heading parent in Volume 76, as were such binary headings as Phenyl sulfide. Compounds containing one or more single sulfur atoms are now indexed substitutively by use of thio radicals or at "thia"-named index parents (¶ 127). Thus, Sulfide, ethyl phenyl, became **Benzene, (ethylthio)-**, and Propyl sulfide is now indexed at **Propane, 1,1'-thiobis-**. The retained headings **Disulfide, Trisulfide**, etc., rank as nonfunctional acyclic sulfur parents, below oxygen compounds and above selenium compounds. Within the class, a partial descending order is: heterocyclic sulfur compounds, e.g., **Thiophene**; "a"-named acyclic hetero systems, e.g., **2,6,9,12,13-Pentathiapentadecane**; acyclic trisulfide, disulfone, disulfoxide, disulfide.

1,2-Epissulfides are named as **Thiirane** or **Thiirene** derivatives; 1,3-episulfides as **Thietane** or **Thiete** derivatives. Acyclic mercaptals and mercaptols are now named like sulfides by use of thio radicals.

Selenium and tellurium compounds are treated in strict analogy with sulfur compounds.

289. Sulfones and Sulfoxides (¶ 200). Sulfone was discontinued as a heading parent, as were binary sulfone headings like Isopropyl sulfone, now indexed at **Propane, 2,2'-sulfonylbis-**. Sulfonyl radicals are used for all compounds containing single SO₂ groups, e.g., **Butane, 1-chloro-3-(methylsulfonyl)-** (formerly Sulfone, 3-chloro-1-methylpropyl methyl). **Disulfone, Trisulfone**, etc., are retained. Sulfoxides are indexed in an analogous manner by use of sulfinyl radicals. Acyclic skeletons containing four or more sulfur units may be indexed at "thia"-names with oxide terms in the index modification. Cyclic sulfones and sulfoxides are indexed at ring names; e.g., **Thiirane, 1,1-dioxide** (formerly Ethylene sulfone).

289A. Tautomers (¶ 122). To avoid scattering of information in the index, CA, aided by new machine programs, now indexes certain common tautomeric systems at single preferred index names, regardless of the particular structures presented in original documents. The most common tautomers handled in this way include compounds containing the nitrogenous skeletons N-N-N, N-C-N, N-C-O, and N-C-S, as well as certain phosphorus and sulfur acids and amides. In general, the preferred index name expresses the tautomeric form in which a double bond extends to an oxygen atom, rather than to a sulfur or nitrogen; after this condition has been satisfied, the preferred name usually expresses the maximum number of highest functions.

290. Terpenes (¶ 212) are now named at stereoparent names (¶ 285) only when they contain four or more rings or possess complex stereochemistry. Hence, many trivial names formerly employed as index headings are now cross-referred to systematic names; e.g., **Eudesmane**. See *Naphthalene, decahydro-1,4a-dimethyl-7-(1-methylethyl)-*, (1*R*,4*aR*,7*R*,8*aS*)-.

Illustrative diagrams for terpene stereoparents, e.g., **Gammacerane, Lanostane**, showing the stereochemistry for each, are provided in the *Chemical Substance Index*. New stereoparents, formed by ring enlargement, contraction, scission, or addition, are adopted as they are needed. When ring scission results in a structure which does not qualify for a terpene stereoparent name, systematic nomenclature is used.

Cyclic acetals of terpenes are expressed at stereoparent names, either in the modification or by use of appropriate substituents, in analogy with steroids (¶ 286). Lactones are expressed in the modification at terpene acid headings.

291. Thiols (¶ 175) have been affected only by the general changes in indexing policy (¶ 255), including those for conjunctive names, abandonment of trivial names, and discontinuance of like treatment of like things. Thus, α -Toluenethiol became **Benzenemethanethiol**; *p*-Cymene-2-thiol became **Benzenethiol, 2-methyl-5-(1-methylethyl)-**; and Ethanethiol, 1,2-diphenyl-, became **Benzenethanethiol, α -phenyl-**.

292. Urea (¶ 183) was retained as a heading parent; Urea, thio-, and its derivatives are now indexed at **Thiourea**. In both cases, the locants 1- and 3- were replaced by *N*- and *N'*-. Urea ranks as an amide of **Carbonic acid**, which is now placed below the "organic" acids, including carboxylic and sulfonic acids. Acyclic acyl ureas are therefore indexed at "organic" amide names. Pseudourea was renamed **Carbamimidic acid**. In the following list, former names are shown in parentheses:

Urea, <i>N'</i>-ethyl-<i>N,N</i>-dimethyl-	(Urea, 3-ethyl-1,1-dimethyl-)
Acetamide, <i>N</i>-(amino carbonyl)-	(Urea, acetyl-)
Ethanethioamide, <i>N</i>-(aminocarbonyl)-	(Urea, (thioacetyl)-)
Urea, <i>N</i>-(aminoiminomethyl)-	(Urea, amidino-)
1,2-Hydrazinedicarboxamide	(Biurea)
Imidodicarbonic diamide	(Biuret)
Urea, <i>N,N'</i>-diphenyl-	(Carbanilide)
Diimidotricarbonic diamide	(Triuret)
Carbamimidothioic acid, <i>N</i>-methyl-, ethyl ester	(Pseudourea, 2-ethyl-3-methyl-2-thio-)

293. Vitamins (¶ 224). Index headings such as Vitamin B, Vitamin F, are used for general discussions of vitamin activity and for ill-defined substances named by authors. Otherwise, many specific vitamin names have been cross-referred to more systematic names. The stereoparent **Retinol** is used for Vitamin A₁ (Vitamin A₂ is indexed at **Retinol, 3,4-didehydro-**); **Riboflavine** (**Riboflavin** beginning in Volume 86) for Vitamin B₂; and **L-Ascorbic acid** for Vitamin C. **Vitamin B₁₂** is the only specific vitamin name retained as a heading parent; related compounds have continued to be indexed at names such as **Cobinamide** and **Cobyrinic acid**.

293A. Zwitterionic compounds (¶¶ 201, 224). Prior to Volume 119 the expression "hydroxide, inner salt" was used in the modification of names of zwitterionic compounds at "-ium" headings. "Hydroxide" was used as the salt phrase in the modification. Conceptually, a molecule of water (comprised of the hydroxide anion and a hydrogen atom attached to a hetero atom) was "removed" by the use of the phrase "inner salt". The term "inner salt" now indicates an unspecified compensating anion located in the same molecule as the cation. The assumed "hydroxide" anion is no longer expressed.

Beginning with Volume 121 meso-ionic Sydnone and Sydnone imine derivatives (¶ 201) are structured and named systematically as inner salts of **5-Hydroxy-3-substituted-1,2,3-oxadiazolium** and **5-Amino-3-substituted-1,2,3-oxadiazolium**, respectively. Hydrohalide salts of sydnone imines are structured and named as onium halides.

H. ILLUSTRATIVE LIST OF SUBSTITUENT PREFIXES

294.

(The equals (=) directs the user from the boldface name to the current CA name; absence of the sign indicates that the boldface name is correct.)

abietamido = [[[1,2,3,4,4a,4b,5,6,10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-1-phenathrenyl]carbonyl]amino]
C₁₉H₂₉CONH-

acenaphthenyl = (1,2-dihydroacenaphthylenyl) (C₁₂H₉)-

1,2-acenaphthenylene = (1,2-dihydro-1,2-acenaphthylene) (C₁₂H₈)-

1-acenaphthenylidene = (1,2-dihydro-1,2-acenaphthylene) (C₁₂H₈)-

acetamido = (acetylamino) AcNH-

acetenyl = ethynyl HC≡C-

acetimido = (acetylmino) or (1-iminoethyl) AcN= or MeC(=NH)-

acetimidoyl = (1-iminoethyl) MeC(=NH)-

acetoacetamido = [(1,3-dioxobutyl)amino]
MeCOCH₂CONH-

acetoacetyl = (1,3-dioxobutyl) MeCOCH₂CO-

acetoxydioximoyl = [1-(hydroxyimino)ethyl]
MeC(=NOH)-

acetonyl = (2-oxopropyl) MeCOCH₂-

acetylidenyl = (2-oxopropylidene) MeCOCH=

acetoxy = (acetyloxy) AcO-

acetyl Ac (MeCO-)

acetylene = 1,2-ethanediylidene =CHCH=

acridanyl = (9,10-dihydroacridinyl) (C₁₃H₁₀N)-

acryloyl = (1-oxo-2-propen-1-yl) H₂C=CHCO-

acrylyl = (1-oxo-2-propen-1-yl) H₂C=CHCO-

adamantyl = tricyclo[3.3.1.1^{3,7}]decyl (C₁₀H₁₅)-

adamantylene = tricyclo[3.3.1.1^{3,7}]decenediyl
(C₁₀H₁₄)-

adipaldehydoyl = (1,6-dioxohexyl)
HCO(CH₂)₄CO-

adipamoyl = (6-amino-1,6-dioxohexyl)
H₂NCO(CH₂)₄CO-

adipanyl = [(1,6-dioxo-6-(phenylamino)hexyl)
PhNHCO(CH₂)₄CO-

adipoyl = (1,6-dioxo-1,6-hexanediyl)
-CO(CH₂)₄CO-

adipyl = (1,6-dioxo-1,6-hexanediyl)
-CO(CH₂)₄CO-

alaninamido = [(2-amino-1-oxopropyl)amino]
MeCH(NH₂)CONH-

alanyl¹ = (2-amino-1-oxopropyl)
MeCH(NH₂)CO-

β-alanyl¹ = (3-amino-1-oxopropyl)
H₂N(CH₂)₂CO-

aldo² = oxo O=

alloisoleucyl¹ = (2-amino-3-methyl-1-oxopentyl)
EtCHMeCH(NH₂)CO-

allophanamido = [[[aminocarbonyl]amino]carbonyl]
amino] H₂N(CONH₂)-

allophanoyl = [[[aminocarbonyl]amino]carbonyl]
H₂NCONHCO-

allothreonyl¹ = (2-amino-3-hydroxy-1-oxobutyl)
MeCH(OH)CH(NH₂)CO-

allyl = 2-propen-1-yl H₂C=CHCH₂-

β-allyl = (1-methylethenyl) H₂C=CMe-

π-allyl = (η³-2-propen-1-yl)

[CH₂≡CH≡CH₂]-

allylidene = 2-propen-1-ylidene H₂C=CHCH=

ambrosan-6-yl = [decahydro-3a,8-dimethyl-5-(1-
methylethyl)-4-azulenyl] (C₁₅H₂₇)-

amidino = (aminoiminomethyl) H₂NC(=NH)-

amidoxalyl = (2-amino-2-oxoacetyl) H₂NCOCO-

amino H₂N-

(aminoamidino) = (hydrazinyliminomethyl)
H₂NNH(=NH)-

(aminoiminophosphoranyl) = (P-aminophosphin-
imyl) H₂NPH(=NH)-

ammonio H₃N⁺-

amoxy = (pentyloxy) Me(CH₂)₄O-

amyl = pentyl Me(CH₂)₄-

tert-amyl = (1,1-dimethylpropyl) EtCMe₂-

amylidene = pentyldiene BuCH=

anilino = (phenylamino) PhNH-

anisal = [(methoxyphenyl)methylene]
MeOC₆H₄CH=

anisidino = [(methoxyphenyl)amino]
MeOC₆H₄NH-

anisoyl = (methoxybenzoyl) MeOC₆H₄CO-

anisyl = (methoxyphenyl) or [(methoxyph-
enyl)methyl] MeOC₆H₄- or MeOC₆H₄CH₂-

anisylidene = [(methoxyphenyl)methylene]
MeOC₆H₄CH=

anthranilamido = [(2-aminobenzoyl)amino]
2-H₂NC₆H₄CONH-

anthraniloyl = (2-aminobenzoyl)
2-H₂NC₆H₄CO-

anthranoyl = (2-aminobenzoyl) 2-H₂NC₆H₄CO-

anthraquinonyl = (9,10-dihydro-9,10-dioxoan-
thracenyl) (C₁₄H₇O₂)-

anthraquinonylene = (9,10-dihydro-9,10-
dioxoanthracenediyl) -(C₁₄H₆O₂)-

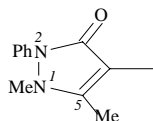
anthroyl = (anthracenylcarbonyl) (C₁₄H₉)CO-

anthryl = anthracenyl (C₁₄H₉)-

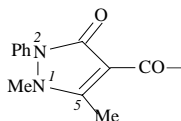
anthrylene = anthracenediyl -(C₁₄H₈)-

antimono = 1,2-distibenediyl -Sb=Sb-

antipyryl (antipyryl) = (2,3-dihydro-1,5-dime-
thyl-3-oxo-2-phenyl-1H-pyrazol-4-yl)



antipyryl = [(2,3-dihydro-1,5-dimethyl-3-oxo-2-
phenyl-1H-pyrazol-4-yl)carbonyl]



apocamphanyl = (7,7-dimethylbicyclo[2.2.1]hep-
t-2-yl) (C₉H₁₅)-

apotrithocanyl = (decahydro-3a,6,8a,8b-tet-
ramethyl-1H-cyclopenta[b]benzofuranyl)
(C₁₅H₂₅O)-

arginyl¹ = [2-amino-5-[(aminoiminome-
thyl)amino]-1-oxopentyl]
H₂NC(=NH)NH(CH₂)₃CH(NH₂)CO-

arseno = 1,2-diarsenediyl -As=As-

arsenoso OAs-

arsinico^{3,4} HOAs(O)=

arsinideno H₂As⁺=

arsinimyl AsH₂(=NH)-

arsino AsH₂-

arsinothioyl AsH₂(S)-

arsinyl AsH₂(O)-

arsinylidene AsH(O)=

arso O₂As-

arsonio H₃As⁺-

arsono⁴ (HO)₂As(O)-

arsononitridyl AsH(=N)-

arsoranyl AsH₄-

arsoranylidene H₃As=

arsoranylidene AsH₃=

arsylene = arsinidene AsH=

arsyldiene = arsinidene As=

asaryl = (2,4,5-trimethoxyphenyl)

2,4,5-(MeO)₃C₆H₂-

asparaginyl¹ = (2,4-diamino-1,4-dioxobutyl)
H₂NCOCH₂CH(NH₂)CO-

α-asparaginyl¹ = (3,4-diamino-1,4-dioxobutyl)
H₂NCOCH(NH₂)CH₂CO-

asparagyl = asparaginyl

aspartoyl¹ = (2-amino-1,4-dioxo-1,4-butanediyl)
-COCH₂CH(NH₂)CO-

aspartyl = aspartoyl or unspecified aspartyl (see
below)

α-aspartyl¹ = (2-amino-3-carboxy-1-oxopropyl)
HO₂CCH₂CH(NH₂)CO-

β-aspartyl¹ = (3-amino-3-carboxy-1-oxopropyl)
HO₂CCH(NH₂)CH₂CO-

astato At-

astatoxy = astatyl O₂At-

atisanyl (from atisane) (C₂₀H₃₃)-

atopoyl = (1-oxo-2-phenyl-2-propen-1-yl)
H₂C=CPhCO-

azelaoyl = (1,9-dioxo-1,9-nonanediyl)

-CO(CH₂)₇CO-

azelaaldehydoyl = (1,9-dioxononyl)
HCO(CH₂)₇CO-

azi² (see also azo) -N=N= 3H-diazirine (compo-
nent ring in a spiro name)

azido N₃-

(azidoformyl) = (azidocarbonyl) N₃CO-

azino =NN= = 1,2-hydrazinediylidene-

azo (see also azi) -N=N= = diazenyl or 1,2-diaz-
enediyl

azoxy -N(O)=N= = (2-oxidodiazene) or
(1-oxido-1,2-diazenediyl)

benzal = (phenylmethylene) PhCH=

benzamido = (benzoylamino) BzNH-

benzenesulfenamido = [(phenylthio)amino]
PhSNH-

benzenesulfonamido = [(phenylsulfonyl)amino]
PhSO₂NH-

benzenetriyl C₆H₃=

benzenyl = (phenylmethylidene) PhC=

benzhydryl = (diphenylmethyl) Ph₂CH-

benzhydrylidene = (diphenylmethylene) Ph₂C=

benzidino = [(4'-amino[1,1'-biphenyl]-4-yl)amino]
4-(4-H₂NC₆H₄)C₆H₄NH-

benzoyl = (2-hydroxy-2,2-diphenylacetyl)
Ph₂C(OH)CO-

benzimidazoliny = (2,3-dihydro-1H-benzimida-
zoly) (C₇H₇N₂)-

2-benzimidazolyl = 1H-benzimidazol-2-yl
(C₇H₅N₂)-

benzimido = (benzoylimino) or (iminophenylme-
thyl) BzN= or PhC(=NH)-

benzimidoyl = (iminophenylmethyl) PhC(=NH)-

benzofuryl = benzofuranyl (C₈H₅O)-

benzohydroximoyl = [(hydroxyimino)phenylme-
thyl] PhC(=NOH)-

o-benzoquinon-3-yl = (5,6-dioxo-1,3-cyclohexa-
dien-1-yl) (C₆H₃O₂)-

p-benzoquinon-2,5-ylene = (3,6-dioxo-1,4-cyclo-
hexadiene-1,4-diyl) -(C₆H₂O₂)-

benzosenophene-yl C₈H₅Se-

benzoxy = (benzoyloxy) BzO-

benzoyl Bz (PhCO-)

(benzoylacetyl) = (1,3-dioxo-3-phenylpropyl)
PhCOCH₂CO-

(benzoylformyl) = (2-oxo-2-phenylacetyl)
PhCOCO-

benzyl = (phenylmethyl) PhCH₂-

benzylidene = (phenylmethylene) PhCH=

benzylidene = (phenylmethylidene) PhC=

(benzyloxy) = (phenylmethoxy) PhCH₂O-

(benzylselenyl) = [(phenylmethyl)seleno]
PhCH₂Se-

bicarbamoyl = (1,2-hydrazinediyl)dicarbonyl)
-CONHNHCO-

bicyclo[1.1.0]butylene = bicyclo[1.1.0]butanediyl
(C₄H₄)-

biphenyl = [1,1'-biphenyl]yl PhC₆H₄-

biphenylene = [1,1'-biphenyl]diyl -(C₁₂H₈)-

biphenylylene = [1,1'-biphenyl]diyl -(C₁₂H₈)-

bismuthino BiH₂-

bismuthylene BiH=

bismuthylidene Bi=

[2,2'-bithiophen]-5-yl C₈H₅S₂-

2-bornyl = (1,7,7-trimethylbicyclo[2.2.1]hept-2-
yl) (C₁₀H₁₇)-

3-bornylidene = (4,7,7-trimethylbicy-
clo[2.2.1]hept-2-ylidene) (C₁₀H₁₆)=

borono⁴ (HO)₂B-

boryl BH₂-

borylene BH=

borylydene B=

bromo Br-

1,3-butadienediylidene = 1,3-butadiene-1,4-
diylidene =C-CHCH=C=

butadienylylene = 1,3-butadiene-1,4-diyl
-C=CC=C-

2-butenylene = 2-butene-1,4-diyl
-CH₂CH=CHCH₂-

butoxy BuO-

sec-butoxy = (1-methylpropoxy) EtCHMeO-

tert-butoxy = (1,1-dimethylethoxy) Me₃CO-

butyl Bu (Me(CH₂)₃-)

butyl^β = (2-methylpropyl) Me₂CHCH₂-

butyl^γ = (1,1-dimethylethyl) Me₂C-

sec-butyl = (1-methylpropyl) EtCHMe-

tert-butyl = (1,1-dimethylethyl) Me₂C-

1,4-butylene = 1,4-butanediyl -(CH₂)₄-

sec-butyliene = (1-methylpropylidene) EtCMe=

(**butyloxy**) = butoxy BuO-

butynediyl = (1,4-dioxo-2-butyne-1,4-diyl)

-COC≡CCO-

butyryl = (1-oxobutyl) PrCO-

cacodyl = (dimethylarsino) Me₂As-

cadinan-1-yl = [octahydro-4,7-dimethyl-1-(1-

methylethyl)-4a(2*H*)-naphthalenyl] (C₁₅H₂₉-)

2-camphanyl = (4,7,7-trimethylbicyclo[2.2.1]hept-

2-yl) (C₁₀H₁₇-)

camphoroyl (from camphoric acid) = [(1,2,2-trimethyl-1,3-cyclopentenediyl)dicarbonyl]

-CO(C₈H₁₄)CO-

5-camphoroyl (from camphor) = (4,7,7-trimethyl-5-

oxobicyclo[2.2.1]hept-2-yl) (C₁₀H₁₅O)-

canavanyl = [O-(aminoinimomethyl)amino]homoseryl¹ or [2-amino-4-[[[aminoimino

methylamino]oxy]-1-oxobutyl]

H₂NC(=NH)NHO(CH₂)₂CH(NH₂)CO-

caprinoyl = (1-oxodecyl) Me(CH₂)₈CO-

caproyl (from caproic acid) = (1-oxohexyl)

Me(CH₂)₄CO-

capryl (from capric acid) = (1-oxododecyl)

Me(CH₂)₈CO-

capryloyl (from caprylic acid) = (1-oxooctyl)

Me(CH₂)₆CO-

caprylyl (from caprylic acid) = (1-oxooctyl)

Me(CH₂)₆CO-

carbamido = [(aminocarbonyl)amino]

H₂NCONH-

carbamoyl = (aminocarbonyl) H₂NCO-

carbamyl = (aminocarbonyl) H₂NCO-

carbanilino = [(phenylamino)carbonyl]

PhNHCO-

carbaniloyl = [(phenylamino)carbonyl] PhNHCO-

carbamidoyl = (hydrazinyliminomethyl)

H₂NNHC(=NH)-

carbazol-9-yl = 9*H*-carbazol-9-yl (C₁₂H₈N)-

carbazoyl = (hydrazinylcarbonyl) H₂NNHCO-

carbethoxy = (ethoxycarbonyl) EtO₂C-

carbobozenyloxy = [(phenylmethoxy)carbonyl]

PhCH₂O₂C-

carbonimidoyl⁷ (see also (iminomethyl))

-C(=NH)-

carbonothioyl⁷ (see also (thioxomethyl)) -CS-

carbonyl -CO-

(**carbonyldioxy**) = [carbonylbis(oxy)] -OCO₂-

(**1-carbonylethyl**) = (1-methyl-2-oxoethenyl)

O=C-CMe-

(**carbonylmethyl**) = (2-oxoethenyl) O=C-CH-

(**carbonylmethylene**) = (1-oxo-1,2-ethanediyyl)

-COCH₂- or (2-oxoethenylidene) O=C=C-

carboxy⁴ HO₂C-

(**carboxyformyl**) = (carboxycarbonyl) HO₂CCO-

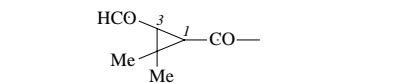
(**5-carboxyvaleryl**) = (5-carboxy-1-oxopentyl)

HO₂C(CH₂)₄CO-

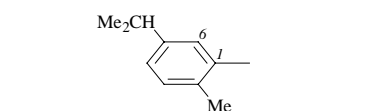
carnosyl = (*N*-β-alanylhistidyl)¹ or [2-[(3-amino-1-oxopropyl)amino]-3-(1*H*-imidazol-4-yl)-1-oxopropyl]



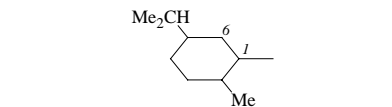
caronaldehydoyl = [(3-formyl-2,2-dimethylpropyl)carbonyl]



carvacryl = [2-methyl-5-(1-methylethyl)phenyl]



carvomenthyl = [2-methyl-5-(1-methylethyl)cyclohexyl]



10-caryl = [(7,7-dimethylbicyclo[4.1.0]hept-3-yl)methyl] (C₉H₁₅)CH₂-

cathyl = [(ethoxycarbonyloxy) EtOCO₂-

cedranyl = (octahydro-3a,6,8,8-tetramethyl-1*H*-

3a,7-methanoazulenyl) (C₁₅H₂₅-)

cetyl = hexadecyl Me(CH₂)₁₅-

chaulmoogroyl (from chaulmoogric acid) = [13-

(2-cyclopenten-1-yl)-1-oxotridecyl]

C₅H₇(CH₂)₁₂CO-

chaulmoogryl (from chaulmoogryl alcohol) = [13-

(2-cyclopenten-1-yl)tridecyl] C₅H₇(CH₂)₁₃-

chloro Cl-

(**chloroformyl**) = (chlorocarbonyl) ClCO-

(**chloroglyoxyloyl**) = (2-chloro-2-oxoacetyl)

CICOCO-

(**chlorooxalyl**) = (2-chloro-2-oxoacetyl) CICOCO-

chlorosyl OCl-

chloryl O₂Cl-

cholesteryl (from cholesterol) = cholest-5-en-3-yl

(from cholestene) (C₂₇H₄₅-)

choloyl (from cholic acid) = (3,7,12-trihydroxy-24-

oxocholan-24-yl) (HO)₃(C₂₃H₃₆)CO-

chromanyl = (3,4-dihydro-2*H*-1-benzopyranyl)

(C₉H₉O)-

cinchoninoyl (from cinchoninic acid) = (4-quinolinylcarbonyl) (4-C₉H₈N)CO-

cinnamal = (3-phenyl-2-propen-1-ylidene)

PhCH=CHCH=

cinnamyl = (2-phenylethenyl) PhCH=CH-

cinnamoyl = (1-oxo-3-phenyl-2-propen-1-yl)

PhCH=CHCO-

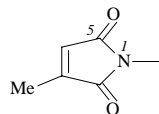
cinnamyl = (3-phenyl-2-propen-1-yl)

PhCH=CHCH₂-

cinnamylidene = (3-phenyl-2-propen-1-ylidene)

PhCH=CHCH=

citraconimido = (2,5-dihydro-3-methyl-2,5-dioxo-1*H*-pyrrol-1-yl)



citraconoyl = (2-methyl-1,4-dioxo-2-buten-1,4-

diyl) -COCMe=CHCO-

conaninyl (from conanine) (C₂₂H₃₆N)-

oresotoyl (from cresotic acid) = (hydroxymethyl-

benzoyl) HO(Me)₂C₆H₃CO-

cresoxy = (methylphenoxy) MeC₆H₄O-

cresyl = (hydroxymethylphenyl) HO(Me)₂C₆H₃- or

(methylphenyl) MeC₆H₄-

cresylene = (methylphenylene) -(MeC₆H₃-)

crotonoyl = (1-oxo-2-buten-1-yl) MeCH=CHCO-

crotonyl = (1-oxo-2-buten-1-yl) MeCH=CHCO-

crotyl = 2-buten-1-yl MeCH=CHCH₂-

cumal = [[4-(1-methylethyl)phenyl]methylene]

4-(Me₂CH)C₆H₄CH=

cumenyl = [(1-methylethyl)phenyl] Me₂CHC₆H₄-

cumidino = [[4-(1-methylethyl)phenyl]amino]

4-(Me₂CH)C₆H₄NH-

cuminal = [[4-(1-methylethyl)phenyl]methylene]

4-(Me₂CH)C₆H₄CH=

cuminyloxy = [[4-(1-methylethyl)phenyl]methyl]

4-(Me₂CH)C₆H₄CH₂-

cuminylidene = [[4-(1-methylethyl)phenyl]meth-

ylene] 4-(Me₂CH)C₆H₄CH=

cumoyl = [4-(1-methylethyl)benzoyl]

4-(Me₂CH)C₆H₄CO-

cumyl⁸ = [(1-methylethyl)phenyl] (Me₂CH)C₆H₄-

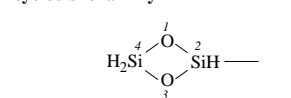
α-cumyl = (1-methyl-1-phenylethyl) -PhCMe₂-

cyanamido = (cyanoamino) NCNH-

cyanato NCO-

cyano NC-

cyclodisiloxan-2-yl



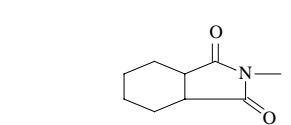
cyclohexadienyne = cyclohexadienediyl -C₆H₆-

cyclohexanecarboxamido = [(cyclohexylcarbo-

nyl)amino] C₆H₁₁CONH-

1,2-cyclohexanedicarboximido = (octahydro-1,3-

dioxo-2*H*-isoindol-2-yl)



cymyl = [methyl(1-methylethyl)phenyl]

Me(Me₂CH)C₆H₃-

cysteinyloxy = (2-amino-3-mercapto-1-oxopropyl)

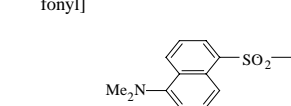
HSCH₂CH(NH₂)CO-

cysteyl = (3-sulfoalanyl)¹ or (2-amino-1-oxo-3-sul-

fopropyl) HO₃SCH₂CH(NH₂)CO-

dansyl = [[5-(dimethylamino)-1-naphthalenyl]sul-

fonyl]



decanedioyl = (1,10-dioxo-1,10-decanediyl)

-CO(CH₂)₈CO-

decanoyl = (1-oxodecyl) CH₃(CH₂)₈CO-

decasiloxanylene = 1,19-decasiloxanediyyl

-SiH₂(OSiH₂)₈OSiH₂-

desyl = (2-oxo-1,2-diphenylethyl) PhCOCHPh-

diarsenyl HAS=As-

diarsinetrayl = 1,2-diarsinediylidene =AsAs=

diarsinyl H₂AsAsH-

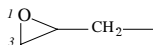
1,2-diazenediyl

(dithiobarbamoyl) = (1,2-hydrazinediyl-dicarbonylthioyl) -CSNHNHCS-
(dithiocarboxy) HS₂C-
(dithiohydroperoxy) = (thiosulfeno)⁴ HSS-
dodecanoyl = (1-oxododecyl) Me(CH₂)₁₀CO-
duryl = (2,3,5,6-tetramethylphenyl) 2,3,5,6-Me₄C₆H-
durylene = (2,3,5,6-tetramethyl-1,4-phenylene) -(2,3,5,6-Me₄C₆)-

enanthoyl = (1-oxoheptyl) Me(CH₂)₅CO-
enanthyl = (1-oxoheptyl) Me(CH₂)₅CO-
epidioxo¹⁰ (see also dioxo) -OO-
epidiseleno¹⁰ (See also diseleno and seleninosele-
 noyl) -SeSe-
epidithio¹⁰ (see also dithio and sulfinothioyl) -SS-
epioxy = epoxy (see also oxy and oxo) -O-
episeleno¹⁰ (see also seleno and selenoxy) -Se-
epithio¹⁰ (see also thio and thioxy) -S-
epoxy¹⁰ (See also oxy and oxo) -O-
(epoxyethyl) = 2-oxiranyl



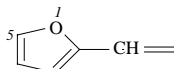
(2,3-epoxypropyl) = (2-oxiranylmethyl)



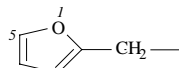
eremophilan-1-yl = [decahydro-4,4a-dimethyl-5-(1-methylethyl)-1-naphthalenyl] (C₁₅H₂₇)-
ethanediyldiene = 1,2-ethanediyldiene =CHCH=
1,2-ethenediyl -CH=CH-
ethinyl = ethynyl HC≡C-
ethoxalyl = (2-ethoxy-2-oxoacetyl) EtO₂CCO-
ethoxy EtO-
(ethoxycarbonyl) EtO₂C-
(1-ethoxyformimidoyl) = (ethoxyiminomethyl) EtOCH(=NH)-
(ethoxyphosphinyl) EtOPH(O)-
ethyl Et (MeCH₂)-
ethylene = 1,2-ethanediyyl -CH₂CH₂-
[ethylenebis(nitrilodimethylene)] = [1,2-ethanediyylbis[nitrilobis(methylene)]] (-CH₂)₂N(CH₂)₂N(CH₂)₂-
(ethylenedioxy) = [1,2-ethanediyylbis(oxy)] -O(CH₂)₂O-
ethylidene CH₃CH=
ethylidene CH₃C≡
1-ethylium-1-ylidene CH₃C⁺=
(ethyloxy) = ethoxy EtO-
(ethylseleny) = (ethylseleno) EtSe-
(ethylthio) EtS-
eudesman-8-yl = [decahydro-5,8a-dimethyl-2-(1-methylethyl)-2-naphthalenyl] (C₁₅H₂₇)-

farnesyl (from farnesol) = (3,7,11-trimethyl-2,6,10-dodecatrien-1-yl) Me₂C=CH(CH₂)₂CMe=CH-(CH₂)₂CMe=CHCH₂-
fenchyl = (1,3,3-trimethylbicyclo[2.2.1]hept-2-yl) (C₁₀H₁₇)-
1,1'-ferrocenediyl -(C₅H₄)Fe(C₅H₄)-
fluoranyl = (3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthenyl]) (C₂₀H₁₁O₃)-
fluoren-9-ylidene = 9H-fluoren-9-ylidene (C₁₃H₈)=
fluoro F-
formamido = (formylamino) HCONH-
1-formazano = [2-(hydrazinylidenemethyl)diazenyl] H₂NN=CHN=N-
5-formazano = [2-(diazinylmethylene)hydrazinyl] HN=NCH=NNH-
formazanyl = (diazinylhydrazinylidenemethyl) HN=N-C(=NNH₂)-
formazyl = [(2-phenyldiazinyl)(2-phenylhydrazinylidene)methyl] PhN=NC(=NNHPh)-
formimidoyl = (iminomethyl) CH(=NH)-
(1-formimidoylformimidoyl) = (1,2-diiminoethyl) HC(=NH)C(=NH)-
(formimidoylformyl) = (2-iminoacetyl) CH(=NH)CO-

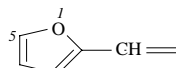
(formimidoylmethyl) = (2-iminoethyl) HC(=NH)CH₂-
formyl⁴ HCO-
fucosyl = (6-deoxygalactosyl) (C₆H₁₁O₄)-
fumaraniyl = [1,4-dioxo-4-(phenylamino)-2-buten-1-yl] PhNHCOC(=CH)CO-
fumaroyl = (1,4-dioxo-2-butene-1,4-diyl) -COCH=CHCO-
furfural = (2-furanylmethylene)



furfuryl = (2-furanylmethyl)

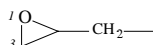


furfurylidene = (2-furanylmethylene)



furoyl = (furanlylcarbonyl) (C₄H₃O)CO-
furyl = furanyl (C₄H₃O)-

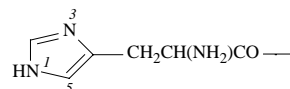
galloyl = (3,4,5-trihydroxybenzoyl) 3,4,5-(HO)₃C₆H₂CO-
gentisoyl = (2,5-dihydroxybenzoyl) 2,5-(HO)₂C₆H₃CO-
geranyl (from geraniol) = (3,7-dimethyl-2,6-octadien-1-yl) Me₂C=CH(CH₂)₂CMe=CHCH₂-
germacran-6-yl = [5,9-dimethyl-2-(1-methylethyl)cyclodecyl] (C₁₅H₂₅)-
germanetetrayl = Ge=
germyl H₃Ge-
germylene H₂Ge=
germyldiyne HGe≡
gibbanyl (from gibbane) (C₁₅H₂₃)-
(glucosyloxy) (C₆H₁₁O₅)O-
glutaminyl¹ = (2,5-diamino-1,5-dioxopentyl) H₂NCO(CH₂)₂CH(NH₂)CO-
α-glutaminyl¹ = (4,5-diamino-1,5-dioxopentyl) H₂NCOCH(NH₂)CH₂CH₂CO-
glutamoyl¹ = (2-amino-1,5-dioxo-1,5-pentanediyyl) -CO(CH₂)₂CH(NH₂)CO-
glutamyl = glutamoyl or unspecified glutamyl (see below)
α-glutamyl¹ = (2-amino-4-carboxy-1-oxobutyl) HO₂C(CH₂)₂CH(NH₂)CO-
γ-glutamyl¹ = (4-amino-4-carboxy-1-oxobutyl) HO₂CCH(NH₂)(CH₂)₂CO-
glutaryl = (1,5-dioxo-1,5-pentanediyyl) -CO(CH₂)₃CO-
glyceroyl = (2,3-dihydroxy-1-oxopropyl) HOCH₂CH(OH)CO-
glyceryl = 1,2,3-propanetriyl -CH(CH₂)₂O-
glycidyl = (2-oxiranylmethyl)



glycinamido = [(2-aminoacetyl)amino] H₂NCH₂CONH-
glycinimidoyl = (2-amino-1-iminoethyl) H₂NCH₂C(=NH)-
glycoloyl = (2-hydroxyacetyl) HOCH₂CO-
glycolyl = (2-hydroxyacetyl) HOCH₂CO-
glycyl¹ = (2-aminoacetyl) H₂NCH₂CO-
glyoxaliny = imidazolyl (C₃H₃N₂)-
glyoxylimidoyl = (1-imino-2-oxoethyl) HCOC(=NH)-
glyoxylyl = (2-oxoacetyl) HCOCO-
(glyoxylylmethyl) = (2,3-dioxopropyl) HCOCOCH₂-
glyoxylyl = (2-oxoacetyl) HCOCO-
guaiacyl = (4-hydroxy-3-methoxyphenyl) 4-OH-3-(CH₃O)C₆H₃- or (2-methoxyphenyl) 2-(MeO)C₆H₄-
guaian-8-yl = [decahydro-1,4-dimethyl-7-(1-meth-

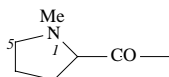
ylethyl)-6-azulenyl] (C₁₅H₂₇)-
guanidino = [(aminoiminomethyl)amino] H₂NC(=NH)NH-
(guanidinoazo) = [3-(aminoiminomethyl)-1-triazen-1-yl] H₂NC(=NH)NHN=N-
guanyl = (aminoiminomethyl) H₂NC(=NH)-
heptadecanoyl = (1-oxoheptadecyl) Me(CH₂)₁₅CO-
heptanamido = [(1-oxoheptyl)amino] Me(CH₂)₅CONH-
heptanedioyl = (1,7-dioxo-1,7-heptanediyyl) -CO(CH₂)₅CO-
heptanoyl = (1-oxoheptyl) Me(CH₂)₅CO-

hexadecanoyl = (1-oxohexadecyl) Me(CH₂)₁₄CO-
2,4-hexadiynylene = 2,4-hexadiene-1,6-diyl -CH₂C≡CC≡CCH₂-
hexamethylene = 1,6-hexanediyyl -(CH₂)₆-
hexanedioyl = (1,6-dioxo-1,6-hexanediyyl) -CO(CH₂)₄CO-
hexanethioyl = (1-thioxohexyl) Me(CH₂)₄CS-
hippuroyl = (N-benzoylglycyl)¹ or [2-(benzoylamino)acetyl] BzNHCH₂CO-
hippuryl = (N-benzoylglycyl)¹ or [2-(benzoylamino)acetyl] BzNHCH₂CO-
histidyl¹ = [2-amino-3-(1H-imidazol-4-yl)-1-oxopropyl]



homocysteinyl¹ = (2-amino-4-mercapto-1-oxobutyl) HS(CH₂)₂CH(NH₂)CO-
homomyrtenyl = [2-(6,6-dimethylbicyclo[3.1.1]hept-2-en-2-yl)ethyl] (C₉H₁₃)CH₂CH₂-
homopiperonyl = [2-(1,3-benzodioxol-5-yl)ethyl] (C₇H₅O₂)CH₂CH₂-
homoseryl¹ = (2-amino-4-hydroxy-1-oxobutyl) HO(CH₂)₂CH(NH₂)CO-
homoveratroyl = [2-(3,4-dimethoxyphenyl)acetyl] 3,4-(MeO)₂C₆H₃CH₂CO-
homoveratryl [2-(3,4-dimethoxyphenyl)ethyl] 3,4-(MeO)₂C₆H₃CH₂CH₂-
hydantoyl = [N-(aminocarbonyl)glycyl]¹ or [2-[(aminocarbonyl)amino]acetyl] H₂NCONHCH₂CO-
hydnocarpoyl (from hydnocarpic acid) = [11-(2-cyclopenten-1-yl)-1-oxoundecyl] (C₅H₇)(CH₂)₁₀CO-
hydnocarpyl (from hydnocarpyl alcohol) = [11-(2-cyclopenten-1-yl)undecyl] (C₅H₇)(CH₂)₁₀CH₂-
hydracryloyl = (3-hydroxy-1-oxopropyl) HO(CH₂)₂CO-
hydratropoyl = (1-oxo-2-phenylpropyl) PhCHMeCO-
hydrazi = diaziridine (component ring in a spiro name) -NHNH-
1,2-hydrazinediyl -NHNH-
1,2-hydrazinediyldiene =NN=
hydrazinyl H₂NNH-
hydrazinylidene H₂NN=
1-hydrazinyl-2-ylidene -NHN=
hydrazo = 1,2-hydrazinediyyl
hydrazono = hydrazinylidene
hydrocinnamoyl = (1-oxo-3-phenylpropyl) Ph(CH₂)₂CO-
hydrocinnamyl = (3-phenylpropyl) Ph(CH₂)₃-
hydroperoxy⁴ HOO-
(hydroperoxyformyl) = (hydroperoxycarbonyl) HOOCO-
hydroxamino = (hydroxyamino) HONH-
hydroximino = (hydroxyimino) HON=
hydroxy⁴ HO-
(hydroxyarsinylidene) = arsenico^{3,4} HOAs(O)=
hydroxyl = hydroxy⁴ HO-
(hydroxyphosphinyl) HOPH(O)-
(hydroxyphosphinylidene) = phosphinico^{3,4} HOP(O)=

hygroyl = (1-methylpropyl)¹ or [(1-methyl-2-pyrrolidinyl)carbonyl]



imidazolidyl = imidazolidinyl (C₃H₇N₂)–

imidazoliny = (dihydro-1*H*-imidazolyl)

(C₃H₅N₂)–

imidocarbonyl = carbonimidoyl⁷ –C(=NH)–

(imidocarbonylamino) = (carbonimidoylamino)

HN=C=N–

imino HN=

iminio H₂N⁺=

(3-iminoacetyl) = (3-imino-2-oxopropyl)

HN=CHCOCH₂–

(iminodisulfonyl) = [iminobis(sulfonyl)]

–SO₂NHSO₂–

(iminomethyl) (see also carbonimidoyl) HN=CH–

(iminonitrilo) = 1-hydrazinyl-2-ylidene –NHN=

(iminophosphoranyl) = phosphinimyl

H₂P(=NH)–

indanyl = (2,3-dihydro-1*H*-indenyl) (C₉H₉)–

indenyl = 1*H*-indenyl (C₉H₇)–

1-indoliny = (2,3-dihydro-1*H*-indol-1-yl)

(C₈H₈N)–

2-indolinyldiene = (1,3-dihydro-2*H*-indol-2-ylidene) (C₈H₇N)=

indyl = 1*H*-indolyl (C₈H₆N)–

iodo I–

iodoso = iodosyl OI–

iodoxy = iodyl O₂I–

isoallyl = 1-propen-1-yl MeCH=CH–

isoamoxy = (3-methylbutoxy) Me₂CH(CH₂)₂O–

isoamyl = (3-methylbutyl) Me₂CH(CH₂)₂–

sec-isoamyl = (1,2-dimethylpropyl)

Me₂CHCHMe–

isoamylidene = (3-methylbutylidene)

Me₂CHCH₂CH=

isobornyl (from isborneol) = (1,7,7-trimethylbicyclo[2.2.1]hept-2-yl) (C₁₀H₁₇)–

isobutenyl = (2-methyl-1-propen-1-yl)

Me₂C=CH–

isobutoxy = (2-methylpropoxy) Me₂CHCH₂O–

isobutyl = (2-methylpropyl) Me₂CHCH₂–

isobutylidene = (2-methylpropylidene)

Me₂CHCH=

isobutyryl = (2-methyl-1-oxopropyl) Me₂CHCO–

isocrotyl = (2-methyl-1-propen-1-yl) Me₂C=CH–

isocyanato OCN–

isociano CN–

isodiazanyl $\bar{N}=\bar{N}$ –

isodiazenyldiene⁶ (see also diazo) N[–]=N⁺=

isohexyl = (4-methylpentyl) Me₂CH(CH₂)₃–

isohexylidene = (4-methylpentylidene)

Me₂CH(CH₂)₂CH=

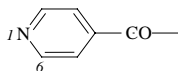
2-isoindoliny = (1,3-dihydro-2*H*-isoindol-2-yl)

(C₈H₈N)–

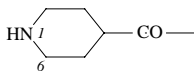
isoleucyl¹ = (2-amino-3-methyl-1-oxopentyl)

EtCHMeCH(NH₂)CO–

isonicotinoyl = (4-pyridinylcarbonyl)



isonipicotoyl = (4-piperidinylcarbonyl)



isonitro = *aci*-nitro HON(O)=

isonitroso = (hydroxyimino) HON=

1-isopentenyl = (3-methyl-1-buten-1-yl)

Me₂CHCH=CH–

isopentyl = (3-methylbutyl) Me₂CH(CH₂)₂–

isopentylidene = (3-methylbutylidene)

Me₂CHCH₂CH=

isophthalal = (1,3-phenylenedimethylidyne)

1,3-C₆H₄(CH=)

isophthalaldehyde = (3-formylbenzoyl)

3-(HCO)C₆H₄CO–

isophthaloyl = (1,3-phenylenedicarbonyl)

1,3-C₆H₄(CO)–₂

isophthalylidene = (1,3-phenylenedimethylidyne)

1,3-C₆H₄(CH=)

isopropenyl = (1-methylethenyl) H₂C=CMe–

isopropoxy = (1-methylethoxy) Me₂CHO–

isopropyl = (1-methylethyl) Me₂CH–

isopropylidene = (1-methylethylidene) Me₂C=

(isopropylidenedioxy) = [(1-methylethylidene)bis(oxy)] –OCMe₂O–

isosemicarbazido = [2-(aminohydroxymethyl-ene)hydrazinyl] H₂NC(OH)=NNH–

isothiocyanato SCN–

isothiocyano = isothiocyanato SCN–

isovaleryl = (3-methyl-1-oxobutyl)

Me₂CHCH₂CO–

isovalyl¹ = (2-amino-2-methyl-1-oxobutyl)

EtCMe(NH₂)CO–

isoviolanthrenylene = (9,18-dihydrodinaphtho[1,2,3-*cd*:1',2',3'-*lm*]perylene)diyl

–(C₃₄H₁₈)–

kauranyl (from kaurane) (C₂₀H₃₃)–

kauranylene = kauranediyl (from kaurane)

–(C₂₀H₃₂)–

kaurenyl (from kaurene) (C₂₀H₃₁)–

keto¹¹ = oxo O=

labdan-15-yl = [5-(decahydro-2,5,5,8a-tetraethyl-1-naphthalenyl)-3-methylpentyl]

(C₂₀H₃₇)–

lactosyl = (4-*O*-β-galactopyranosyl-β-D-glucopyranosyl) (C₆H₁₁O₅)O(C₆H₁₀O₅)–

lactoyl = (2-hydroxypropanoyl)¹ or (2-hydroxy-1-oxopropyl) MeCH(OH)CO–

lanostenylene = lanostenediyl (from lanostane)

–(C₃₀H₅₀)–

lauroyl = (1-oxododecyl) Me(CH₂)₁₀CO–

leucyl¹ = (2-amino-4-methyl-1-oxopentyl)

Me₂CHCH₂CH(NH₂)CO–

levulinoyl = (1,4-dioxopentyl) MeCO(CH₂)₂CO–

linalyl (from linalool) = (1-ethenyl-1,5-dimethyl-4-hexen-1-yl) Me₂C=CH(CH₂)₂CMe(CH=CH₂)–

linolelaidoyl = (1-oxo-9,12-octadecadien-1-yl)

Me(CH₂)₄CH=CHCH₂CH=CH(CH₂)₇CO–

linolenoyl = (1-oxo-9,12,15-octadecatrien-1-yl)

EtCH=CHCH₂CH=CHCH₂CH=CH(CH₂)₇CO–

γ-linolenoyl = (1-oxo-6,9,12-octadecatrien-1-yl)

Me(CH₂)₄CH=CHCH₂CH=CHCH₂CH=CH(CH₂)₄CO–

linoleoyl = (1-oxo-9,12-octadecadien-1-yl)

Me(CH₂)₄CH=CHCH₂CH=CH(CH₂)₇CO–

lupanyl (from lupane) (C₃₀H₅₁)–

lysyl¹ = (2,6-diamino-1-oxohexyl)

H₂N(CH₂)₄CH(NH₂)CO–

maleoyl = (1,4-dioxo-2-butene-1,4-diyl)

–COCH=CHCO–

malonaldehyde = (1,3-dioxopropyl)

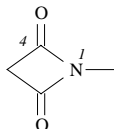
HCOCH₂CO–

malonamoyl = (3-amino-1,3-dioxopropyl)

H₂NCOCH₂CO–

malonaniloyl = [1,3-dioxo-3-(phenylamino)propyl] PhNHCOCH₂CO–

malonimido = (2,4-dioxo-1-azetidiny)



malonyl = (1,3-dioxo-1,3-propanediyl)

–COCH₂CO–

maloyl = (2-hydroxy-1,4-dioxo-1,4-butanediyl)

–COCH(OH)CH₂CO–

maltosyl = (4-*O*-α-D-glucopyranosyl-β-D-glucopyranosyl) (C₆H₁₁O₅)O(C₆H₁₀O₅)–

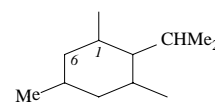
mandeloyl = (2-hydroxy-2-phenylacetyl)

PhCH(OH)CO–

p-menth-2-yl = [2-methyl-5-(1-methylethyl)cyclohexyl] 2,5-Me(Me₂CH)C₆H₉–

p-menth-3,5-yleno = [5-methyl-2-(1-methylethyl)-

1,3-cyclohexanediyl]



mercapto⁴ HS–

mesaconoyl = (2-methyl-1,4-dioxo-2-butene-1,4-diyl) –COCMe=CHCO–

mesidino = [(2,4,6-trimethylphenyl)amino]

2,4,6-Me₃C₆H₂NH–

mesityl = (2,4,6-trimethylphenyl)

2,4,6-Me₃C₆H₂–

α-mesityl = [(3,5-dimethylphenyl)methyl]

3,5-Me₂C₆H₃CH₂–

mesoxaly = (1,2,3-trioxo-1,3-propanediyl)

–COCOCO–

mesyl = (methylsulfonyl) MeSO₂–

metanilamido = [[(3-aminophenyl)sulfonyl]amino]

3-H₂NC₆H₄SO₂NH–

metanilyl = [(3-aminophenyl)sulfonyl]

3-H₂NC₆H₄SO₂–

methacryloyl = (2-methyl-1-oxo-2-propen-1-yl)

H₂C=CMeCO–

methallyl = (2-methyl-2-propen-1-yl)

H₂C=CMeCH₂–

methanetetrayl = C=

methene = methylene H₂C=

methenyl = methylidyne HC≡

methionyl (from methionine) = [methylenebis(sulfonyl)] –SO₂CH₂SO₂–

methionyl¹ (from methionine) = [2-amino-4-(methylthio)-1-oxobutyl]

MeS(CH₂)₂CH(NH₂)CO–

methoxaly = (2-methoxy-2-oxoacetyl)

MeO₂CCO–

methoxy MeO–

(methoxycarbonyl) MeO₂C–

methyl Me (H₃C)–

[(methylthio)sulfonyl] MeSSO₂–

methylene H₂C=

(methylenedioxy) = [methylenebis(oxy)]

–OCH₂O–

[(methylenedioxy)phenyl] = 1,3-benzodioxol-*ar*-yl

(CH₂O)₂C₆H₃–

(methylenedisulfonyl) = [methylenebis(sulfonyl)]

–SO₂CH₂SO₂–

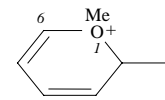
methylidyne HC≡

methylumylidene C⁺H=

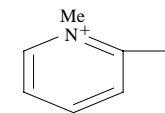
methylol = (hydroxymethyl) HOCH₂–

(methyloxy) = methoxy MeO–

(1-methyl-2*H*-pyranium-2-yl)



(1-methylpyridinium-2-yl)



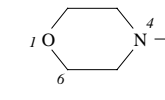
(methylselenyl) = (methylseleno) MeSe–

(methylthio) MeS–

(methyltelluro) MeTe–

(methyltrioxy) MeOOO–

morpholino = 4-morpholinyl



myristoyl = (1-oxotetradecyl) Me(CH₂)₁₂CO–

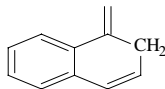
naphthal = (naphthalenyl)methylene (C₁₀H₇)CH=

naphthalimido = (1,3-dioxo-1*H*-benz[*de*]isoquinolin-2(3*H*)-yl) (C₁₂H₆NO₂)–

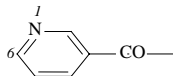
naphthenyl = (naphthalenyl)methylidyne

</

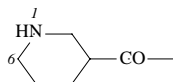
naphthionyl = [(4-amino-1-naphthalenyl)sulfonyl] 4,1-H₃NC₁₀H₆SO₂-
naphthobenzyl = (naphthalenylmethyl) (C₁₀H₇)CH₂-
naphthothiophene-yl = naphthothienyl (C₁₂H₇S)-
naphthoxy = (naphthalenyloxy) (C₁₀H₇)O-
naphthoyl = (naphthalenylcarbonyl) (C₁₀H₇)CO-
naphthyl = naphthalenyl (C₁₀H₇)-
naphthylene = naphthalenediyl -(C₁₀H₆)-
1(2H)-naphthylidene = 1(2H)-naphthalenylidene



(naphthyl)naphthyl = [binaphthalenyl] C₁₀H₇C₁₀H₆-
nazyl = (naphthalenylmethyl) (C₁₀H₇)CH₂-
neopentyl = (2,2-dimethylpropyl) Me₃CCH₂-
neophyl = (2-methyl-2-phenylpropyl) PhCMe₂CH₂-
neryl (from nerol) = (3,7-dimethyl-2,6-octadien-1-yl) -Me₂C=CH(CH₂)₂CMe=CHCH₂-
nicotinimidoyl = (imino-3-pyridinylmethyl) (C₅H₄N)C(=NH)-
nicotinoyl = (3-pyridinylcarbonyl)



nipicotoyl = (3-piperidinylcarbonyl)



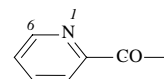
nitramino = (nitroamino) O₂NNH-
aci-nitramino = (aci-nitroamino) HON(O)=N-
nitriilo HN⁺≡
nitriilo N≡
(nitriolphosphoranyl) = phosphononitridyl HP(≡N)-
nitro O₂N-
aci-nitro HON(O)=
nitrosamino = (nitrosoamino) ONNH-
nitrosimino = (nitrosoimino) ONN=
nitroso ON-
(nitrothio) O₂NS-
nonanedioyl = (1,9-dioxo-1,9-nonanediy) -CO(CH₂)₇CO-
nonanoyl = (1-oxononyl) Me(CH₂)₇CO-
norbornyl = bicyclo[2.2.1]heptyl (C₇H₁₁)-
norbornylene = bicyclo[2.2.1]heptanediy -(C₇H₁₀)-
norcamphanlyl = bicyclo[2.2.1]heptyl (C₇H₁₁)-
norcaryl (from norcarane) = bicyclo[4.1.0]heptyl (C₇H₁₁)-
norpinyl (from norpinane) = bicyclo[3.1.1]heptyl (C₇H₁₁)-
norleucyl¹ = (2-amino-1-oxohexyl) Me(CH₂)₃CH(NH₂)CO-
norvalyl¹ = (2-amino-1-oxopentyl) Me(CH₂)₂CH(NH₂)CO-
nosyl = [(4-nitrophenyl)sulfonyl] 4-O₂NC₆H₄SO₂-

octadecanoyl = (1-oxooctadecyl) Me(CH₂)₁₆CO-
octanedioyl = (1,8-dioxo-1,8-octanediy) -CO(CH₂)₆CO-
octanoyl = (1-oxooctyl) Me(CH₂)₆CO-
tert-octyl = (1,1,3,3-tetramethylbutyl) Me₃CCH₂CMe₂-
oentanhyll = (1-oxoheptyl) Me(CH₂)₅CO-
oleananyl (from oleanane) (C₃₀H₅₁)-
oleoyl = (1-oxo-9-octadecen-1-yl) Me(CH₂)₇CH=CH(CH₂)₇CO-
ornithyl¹ = (2,5-diamino-1-oxopentyl) H₂N(CH₂)₃CH(NH₂)CO-
oxalaldehydoyl = (2-oxoacetyl) HCOCO-
oxalyl = (1,2-dioxo-1,2-ethanediy) -COCO-
oxamido = [(2-amino-2-oxoacetyl)amino] H₂NCOCONH-

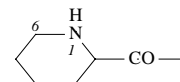
oxamoyl = (2-amino-2-oxoacetyl) H₂NCOCO-
oxamyl = (2-amino-2-oxoacetyl) H₂NCOCO-
oxaniloil = [2-oxo-2-(phenylamino)acetyl] PhNHCOCO-
oxazolinyll = (dihydrooxazolyl) (C₃H₄NO)-
oximido = (hydroxyimino) HON=
oxo² (See also epoxy and oxy) O=
(oxoarsino) = arsenoso OAS-
(oxobornyl) = (trimethylxobicyclo[2.2.1]heptyl) (C₁₀H₁₅O)-
(oxoboryl) OB-
(1-oxoethyl) = acetyl Ac (MeCO)-
(oxoethylene) = (1-oxo-1,2-ethanediy) -COCH₂-
(2-oxo-2-phenylhydrazinyl) = (nitrosophenylamino) PhN(NO)-
(oxophenylmethyl) = benzoyl Bz (PhCO)-
(oxophosphino) = phosphoroso OP-
(oxopyridinylmethyl) = (pyridinylcarbonyl) (C₅H₄N)CO-
(2-oxotrimethylene) = (2-oxo-1,3-propanediy) -CH₂COCH₂-
(2-oxovinyl) = (2-oxoethenyl) OC=CH-
oxy⁹ (see also epoxy and oxo) -O-
[oxybis(methylenecarbonylimino)] = [oxybis[(1-oxo-2,1-ethanediy)imino]] -NHCOCH₂OCH₂CONH-

palmitoyl = (1-oxohexadecyl) Me(CH₂)₁₄CO-
pantothenoil = *N*-(2,4-dihydroxy-3,3-dimethyl-1-oxobutyl)-β-alanyl¹ or [3-[(2,4-dihydroxy-3,3-dimethyl-1-oxobutyl)amino]-1-oxopropyl] HOCH₂CMe₂CH(OH)CONH(CH₂)₂CO-
pelargonoyl = (1-oxononyl) Me(CH₂)₇CO-
pelargonyl = (1-oxononyl) Me(CH₂)₇CO-
pentadecanoyl = (1-oxopentadecyl) Me(CH₂)₁₃CO-
pentamethylene = 1,5-pentanediy -(CH₂)₅-
3-pentanesulfonamido = [(1-ethylpropyl)sulfonyl]amino] Et₂CHSO₂NH-
1,3-pentazadieno = 1,3-pentazadien-1-yl H₂NN=NN=N-
2-pentenediylidene = 2-pentene-1,5-diylidene ≡CCH=CHCH₂C≡
tert-pentyl = (1,1-dimethylpropyl) EtCMe₂-
pentyl Me(CH₂)₄-
pentylidene BuC≡
perchloryl O₃Cl-
perseleno = seleninoselenoyl Se=Se=
perthio = sulfinothioyl S-S=
phenacyl = (2-oxo-2-phenylethyl) PhCOCH₂-
phenacylidene = (2-oxo-2-phenylethylidene) PhCOCH=
phenanthrothiophene-yl = phenanthrothienyl (C₁₆H₉S)-
phenanthryl = phenanthrenyl (C₁₄H₉)-
phenanthrylene = phenanthrenediyl -(C₁₄H₈)-
phenenyl = benzenetriyl C₆H₃≡
phenethyl = (2-phenylethyl) PhCH₂CH₂-
phenethylidene = (2-phenylethylidene) PhCH₂CH=
phenetidino = [(ethoxyphenyl)amino] (EtO)C₆H₄NH-
phenetyl = (ethoxyphenyl) (EtO)C₆H₄-
phenoxy PhO-
phenyl Ph (C₆H₅)-
phenylalanyl¹ (from phenylalanine) = (2-amino-1-oxo-3-phenylpropyl) PhCH₂CH(NH₂)CO-
(phenylarsinico) = (hydroxyphenylarsinyl) PhAs(O)(OH)-
(phenylazo) = (2-phenyldiazetyl) PhN=N-
[(phenylazo)imino] = (3-phenyl-2-triazen-1-ylidene) PhN=NN=
(phenylbenzoyl) = [(1,1'-biphenyl)ylcarbonyl] PhC₆H₄CO
phenylene -(C₆H₄)-
[phenylenebis(azo)] = [phenylenebis(2,1-diazenediyl)] -N=NC₆H₄N=N-
[phenylenebis[2,1-diazenediyl(methylimino)]] = [phenylenebis(1-methyl-2-triazene-3,1-diyl)] -NMeN=NC₆H₄N=NMe-
[phenylenebis(1-oxo-1-ethanyl-2-ylidene)] = [phenylenebis(2-oxo-2-ethanyl-1-ylidene)] =CHCOC₆H₄COCH=
(phenylenedimethylene) = [phenylenebis(methyl-

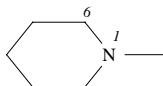
ene)] -CH₂C₆H₄CH₂-
(phenylenedimethylidene) =CHC₆H₄CH=
(phenylenedioxy) = [phenylenebis(oxy)] -OC₆H₄O-
(phenylglyoxyloyl) = (2-oxo-2-phenylacetyl) PhCOCO-
phenylidene = cyclohexadienylidene (C₆H₆)=
(phenylimidocarbonyl) = (phenylcarbonimidoyl)⁷ PhN=C=
(phenylaloxalyl) = (2-oxo-2-phenylacetyl) PhCOCO-
(phenyloxy) = phenoxy PhO-
(phenylphenoxy) = [(1,1'-biphenyl)lyloxy] PhC₆H₄O-
(phenylsulfenyl) = (phenylthio) PhS-
(phenylsulfanyl) PhS(O)-
(S-phenylsulfonimidoyl) PhS(O)(=NH)-
phorbinyll (from phorbine) (C₂₂H₁₇N₄)-
phosphimico^{3,4} HOP(O)=
phosphinidene HP=
phosphinidenio H₂P⁺=
phosphinidene P≡
phosphinimyl H₂P(=NH)-
phosphino H₂P-
phosphinothioyl H₂P(S)-
phosphinothioylidene HP(S)=
phosphinyl H₂P(O)-
phosphinylidene HP(O)=
phosphinylidene P(O)≡
phospho O₂P-
phosphonio H₃P⁺=
phosphono⁴ (HO)₂P(O)-
(phosphonoformyl) = (phosphonocarbonyl) (HO)₂P(O)CO-
phosphononitridyl HP(≡N)-
phosphoranyl H₄P-
phosphoranylidene H₃P=
phosphoranylidene H₃P≡
phosphoro = 1,2-diphosphenediy -P=P-
phosphoroso OP-
phthalal = (1,2-phenylenedimethylidene) 1,2-C₆H₄(CH=)₂
phthalaldehydoyl = (2-formylbenzoyl) 2-(HCO)C₆H₄CO-
phthalamoyl = [2-(aminocarbonyl)benzoyl] 2-(H₂NCO)C₆H₄CO-
phthalanyl = (1,3-dihydroisobenzofuranyl) (C₈H₇O)-
phthalidyl = (1,3-dihydro-3-oxo-1-isobenzofuranyl) (C₈H₅O₂)-
phthalidylidene = (3-oxo-1(3H)-isobenzofuranylidene) (C₈H₄O₂)-
phthalimido = (1,3-dihydro-1,3-dioxo-2H-isindol-2-yl) (C₈H₄NO₂)-
phthalocyaninyl¹ (from phthalocyanine) (C₃₂H₁₇N₃)-
phthaloyl = (1,2-phenylenedicarbonyl) 1,2-C₆H₄(CO)₂-
phthalylidene = (1,2-phenylenedimethylidene) 1,2-C₆H₄(CH=)₂
phylocladanyl = kauranyl (from kaurane) (C₂₉H₅₃)-
phytyl = (3,7,11,15-tetramethyl-2-hexadecen-1-yl) Me[CHMe(CH₂)₃]CMe=CHCH₂-
picolinoyl = (2-pyridinylcarbonyl)



picryl = (2,4,6-trinitrophenyl) 2,4,6-(O₂N)₃C₆H₂-
pimeloyl = (1,7-dioxo-1,7-heptanediy) -CO(CH₂)₅CO-
4-pinanyl (from pinane) = (4,6,6-trimethylbicyclo[3.1.1]hept-2-yl) (C₁₀H₁₇)-
pinanylene = (trimethylbicyclo[3.1.1]heptanediy) -(C₁₀H₁₆)-
pipecoloyl = (2-piperidinylcarbonyl)



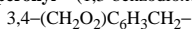
piperidino = 1-piperidinyl



piperidyl = piperidinyl (C₅H₁₀N)-

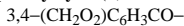
piperidylidene = piperidinylidene (C₅H₉N)=

piperonyl = (1,3-benzodioxol-5-ylmethyl)



piperonylidene = (1,3-benzodioxol-5-ylmethyl-ene) 3,4-(CH₂O)₂C₆H₃CH=

piperonyloyl = (1,3-benzodioxol-5-ylcarbonyl)



pivaloyl = (2,2-dimethyl-1-oxopropyl) Me₃CCO-

pivalyl = (2,2-dimethyl-1-oxopropyl) Me₃CCO-

plumbanetetrayl = Pb=

plumbyl H₃Pb-

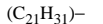
plumbylene H₂Pb=

plumbylidene HPb=

podocarpan-13-yl = (tetradehydro-4b,8,8-trimethyl-2-phenanthrenyl) (C₁₇H₂₉)-

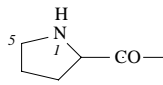
porphyrinyl (from porphine) (C₂₀H₁₃N₄)-

pregna-5,16-dien-21-yl (from pregnadiene)



prenyl = (3-methyl-2-buten-1-yl) Me₂C=CHCH₂-

prolyl¹ = (2-pyrrolidinylcarbonyl)



2-propanesulfonamido = [(1-methylethyl)sulfonyl]amino Me₂CHSO₂NH-

propargyl = 2-propyn-1-yl HC≡CCH₂-

propenyl = 1-propen-1-yl MeCH=CH-

2-propen-1-yl CH₂=CH-CH₂-

propenylene = 1-propene-1,3-diyl -CH=CHCH₂-

propenylidene = 1-propen-1-ylidene MeCH=C=

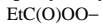
propioloyl = (1-oxo-2-propyn-1-yl) HC≡CCO-

propiolyl = (1-oxo-2-propyn-1-yl) HC≡CCO-

propionamido = [(1-oxopropyl)amino] EtCONH-

propionyl = (1-oxopropyl) EtCO-

(propionylidioxy) = [(1-oxopropyl)dioxy]



propionyloxy = (1-oxopropoxy) EtCO₂-

propoxy PrO-

propyl Pr (CH₂CH₂CH₂-)

sec-propyl = (1-methylethyl) Me₂CH-

propylene = (1-methyl-1,2-ethanediyl)

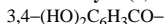


propylidene EtCH=

propylidene EtC=

(propyloxy) = propoxy PrO-

protocatechuyl = (3,4-dihydroxybenzoyl)

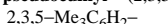


pseudoallyl = (1-methylethenyl) H₂C=CMe-

pseudocumidino = [(2,4,5-trimethylphenyl)amino]



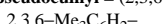
as-pseudocumyl = (2,3,5-trimethylphenyl)



s-pseudocumyl = (2,4,5-trimethylphenyl)



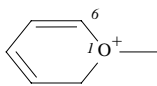
v-pseudocumyl = (2,3,6-trimethylphenyl)



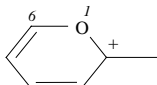
pseudoindolyl = 1*H*-indolyl (C₈H₆N)-

pteroyl = [4-[(2-amino-3,4-dihydro-4-oxo-6-pteridinyl)methyl]amino]benzoyl (C₁₄H₁₁N₆O₂)-

2*H*-pyranio



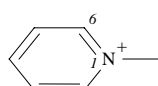
2*H*-pyran-2-ylium-2-yl



pyrazolidyl = pyrazolidinyl (C₃H₇N₂)-

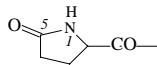
pyrazolinyl = (dihydropyrazolyl) (C₃H₅N₂)-

pyridinio

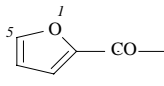


pyridyl = pyridinyl (C₅H₄N)-

pyroglutamoyl = (5-oxopropyl)¹ or [(5-oxo-2-pyrrolidinyl)carbonyl]



pyromucyl = (2-furanylcarbonyl)



pyrrolidyl = pyrrolidinyl (C₄H₈N)-

pyrrolinyl = (dihydropyrrolyl) (C₄H₆N)-

pyrrol-1-yl = 1*H*-pyrrol-1-yl (C₄H₄N)-

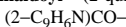
pyrrolyl = (pyrrolylcarbonyl) (C₄H₃N)CO-

pyrryl = pyrrolyl (C₄H₄N)-

pyruvoyl = (1,2-dioxopropyl) MeCOCO-

***p*-quaterphenyl** = [1,1':4',1'':4''-quaterphenyl]yl (C₂₄H₁₇)-

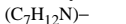
quinaldoyl = (2-quinolinylcarbonyl)



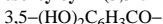
quinolyl = quinolinyl (C₉H₆N)-

quinonyl = (dioxocyclohexadienyl) (C₆H₃O₂)-

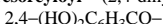
quinuclidinyl = 1-azabicyclo[2.2.2]octyl



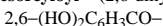
α-resorcyloyl = (3,5-dihydroxybenzoyl)



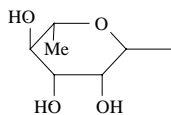
β-resorcyloyl = (2,4-dihydroxybenzoyl)



γ-resorcyloyl = (2,6-dihydroxybenzoyl)



rhamnosyl = (6-deoxymannopyranosyl)

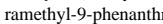


ricinelaidoyl = (12-hydroxy-1-oxo-9-octadecen-1-yl) Me(CH₂)₅CH(OH)CH₂CH=CH(CH₂)₇CO-

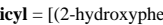
ricinoleoyl = (12-hydroxy-1-oxo-9-octadecen-1-yl) Me(CH₂)₅CH(OH)CH₂CH=CH(CH₂)₇CO-

rosan-6-yl = (2-ethyltetradecahydro-2,4a,8,8-tetramethyl-9-phenanthrenyl) (C₂₀H₃₅)-

salicyl = [(2-hydroxyphenyl)methyl]



salicylidene = [(2-hydroxyphenyl)methylene]

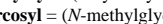


salicyloyl = (2-hydroxybenzoyl) 2-HOC₆H₄CO-

sarcosyl = (*N*-methylglycyl)¹ or [2-(methylamino)acetyl] MeNHCH₂CO-



sebacoyl = (1,10-dioxo-1,10-decanediyl)



λ⁴-selanylidene H₂Se=

λ⁶-selanylidene H₄Se=

seleno⁴ HOSe-

selenino⁴ HOSe(O)-

seleninoselenoyl Se=Se-

seleninyl OSe-

seleno⁹ (see also episeleno and selenoxo) -Se-

selenocyanato NCSe-

selenono⁴ (HO)SeO₂-

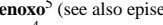
selenonyl O₂Se=

selenophenyl = selenophene-yl (C₄H₃Se)-

selenoxo⁵ (see also episeleno and seleno) Se=

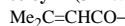
selenyl⁴ HSe-

semicarbazido = [2-(aminocarbonyl)hydrazinyl]



semicarbazono = [2-(aminocarbonyl)hydrazinylidene] H₂NCONHN=

seneciroyl = (3-methyl-1-oxo-2-buten-1-yl)



seryl¹ = (2-amino-3-hydroxy-1-oxopropyl)



siamyl = (1,2-dimethylpropyl) Me₂CHCHMe-

silanetetrayl =Si=

siloxo = (silyloxy) H₃SiO-

silyl H₃Si-

silylene H₂Si=

silylidene HSi=

sorboryl = (1-oxo-2,4-hexadien-1-yl)



spirohex-1-yl (C₆H₉)-

spirostanyl (from spirostane) (C₂₇H₄₃O₂)-

stannanetetrayl =Sn=

stannyl H₃Sn-

stannylene H₂Sn=

stannylidene HSn=

stearoyl = (1-oxooctadecyl) Me(CH₂)₁₆CO-

stibino H₂Sb-

stiboso = (oxostibino) OSb-

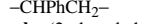
stibyl = stibino H₂Sb-

stibylene HSb=

stibylidene Sb=

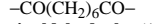
styrene = (1-phenyl-1,2-ethanediyl) -CHPhCH₂-

styrolene = (1-phenyl-1,2-ethanediyl)

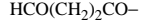


styryl = (2-phenylethenyl) PhCH=CH-

suberoyl = (1,8-dioxo-1,8-octanediyl)



succinaldehydoyl = (1,4-dioxobutyl)



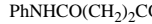
succinamoyl = (4-amino-1,4-dioxobutyl)



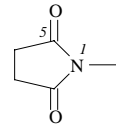
succinamyl = (4-amino-1,4-dioxobutyl)



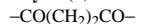
succinaniloyl = [1,4-dioxo-4-(phenylamino)butyl]



succinimido = (2,5-dioxo-1-pyrrolidinyl)



succinyl = (1,4-dioxo-1,4-butanediyl)

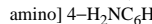


sulfamino = (sulfoamino) HOSO₂NH-

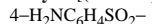
sulfamoyl = (aminosulfonyl) H₂NSO₂-

sulfamyl = (aminosulfonyl) H₂NSO₂-

sulfanilamido = [(4-aminophenyl)sulfonyl]-



sulfanilyl = [(4-aminophenyl)sulfonyl]



λ⁴-sulfanyl H₂S=

λ⁶-sulfanyl H₄S=

sulfeno⁴ HOS-

sulphydryl = mercapto⁴ HS-

sulfimidoyl HN=S=

sulfino⁴ HOS(O)-

sulfinothioyl S=S=

sulfinyl OS=

sulfinylhydrazono = (2-sulfinylhydrazinylidene)



sulfo⁴ HO₂S-

sulfonimidoyl HN=S(O)=

sulfonodiimidoyl (HN=)₂S=

sulfonyl -SO₂-

sulfurtetrayl =λ⁴-sulfanetetrayl =S=

sulfurtriyl =λ⁴-sulfanylidene HS=

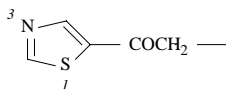
sulfuryl = sulfonyl -SO₂-

tartaroyl = (2,3-dihydroxy-1,4-dioxo-1,4-butanediyl) -COCH(OH)CH(OH)CO-

tartronoyl = (2-hydroxy-1,3-dioxo-1,3-propanediyl) -COCH(OH)CO-

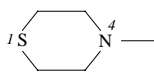
tauryl = [(2-aminoethyl)sulfonyl]

telluryl⁴ HTe-
terephthalal = (1,4-phenylenedimethylidene)
 1,4-C₆H₄(CH=)₂
terephthalaldehydeoyl = (4-formylbenzoyl)
 4-HCOC₆H₄CO-
terephthalamoyl = [4-(aminocarbonyl)benzoyl]
 4-(H₂NCO)C₆H₄CO-
terephthalamoyl = [4-[(phenylamino)carbo-
 nyl]benzoyl] 4-(PhNHCO)C₆H₄CO-
terephthaloyl = (1,4-phenylenedicarbonyl)
 1,4-C₆H₄(CO=)₂
terephthalylidene = (1,4-phenylenedimethyl-
 idene) 1,4-C₆H₄(CH=)₂
m-terphenyl = [1,1':3',1''-terphenyl]yl
 (C₁₈H₁₃)
terphenylidene = [terphenyl]diyl -(C₁₈H₁₂)
tetradecanoyl = (1-oxotetradecyl) Me(CH₂)₁₂CO-
tetramethylene = 1,4-butanediyl -(CH₂)₄-
1,4-tetraphosphinediyl -(PH)₄-
tetrasiloxanylene = 1,7-tetrasiloxanediy
 -SiH₂(OSiH₂)₂OSiH₂-
tetrathio¹³ -SSSS-
tetrazanediyldene = 1,4-tetrazanediyldene
 =N(NH₂)₂N=
tetrazanylene = 1,4-tetrazanediy -(NH)₄-
1-tetrazeno = 1-tetrazen-1-yl H₂NNHN=N-
thenoyl = (thienylcarbonyl) (C₄H₃S)CO-
thenyl = (thienylmethyl) (C₄H₃S)CH₂-
thenylidene = (thienylmethylene) (C₄H₃S)CH=
(thenyloxy) = (thienylmethoxy) (C₄H₃S)CH₂O-
thexyl = 1,1,2-trimethylpropyl Me₂CHCMe₂-
thianaphthenyl = benzo[b]thienyl (C₈H₅S)-
thiazolidyl = thiazolidinyl (C₃H₄NS)-
thiazolinyl = (dihydrothiazolyl) (C₃H₄NS)-
[(5-thiazolylcarbonyl)methyl] = [2-oxo-2-(5-thia-
 zolyl)ethyl]

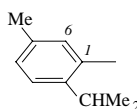


thienyl (C₄H₃S)-
(thienylthienyl) = [bithiophenyl]
 (C₄H₃S)(C₄H₃S)-
thio⁹ (see also epithio and thioxo) -S-
(thioacetyl) = (2-thioxopropylidene)
 MeCSCH=
thioacetyl = (1-thioxoethyl) MeCS-
(thioarseno) = (thioxoarsino) S=As-
(thiobenzoyl) = (phenylthioxomethyl) PhCS-
(thiocarbamoyl) = (aminothioxomethyl) H₂NCS-
thiocarbamyl = (aminothioxomethyl) H₂NCS-
(thiocarbonyl) = carbonothioyl⁷ -CS-
(thiocarboxy)¹⁴ HOSC-
thiocyanato NCS-
thiocyano = thiocyanato NCS-
(thioformyl) = (thioxomethyl) HCS-
(thiohexanoyl) = (1-thioxohexyl) Me(CH₂)₄CS-
thiohydroperoxy = suleno⁴ HOS- or (mercap-
 tooxy)⁴ HSO-
(thiohydroxy) = mercapto⁴ HS-

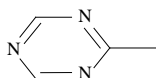
thiomorpholino = 4-thiomorpholinyl



(thionitroso) SN-
thionyl = sulfinyl -SO-
(thiophenacyl) = (2-phenyl-2-thioxoethyl)
 PhCSCH₂-
thiophene-yl = thienyl (C₄H₃S)-
(thiophosphono) = (hydroxymercaptophosphinyl)
 (HO)(HS)P(O)-
(thioseleno)⁴ HSSe-
(thiosulfeno)⁴ HSS-
(thiosulfo)¹⁴ (HO₂S₂)-
thioxo⁵ (see also epithio) S=
(thiooarsino) SAS-
(thioxomethyl) (see also carbonothioyl) S=CH-
thiuram = (aminothioxomethyl) H₂NCS-
threonyl¹ (2-amino-3-hydroxy-1-oxobutyl)
 MeCH(OH)CH(NH₂)CO-
4-thujyl = [2-methyl-5-(1-methylethyl)bicy-
 clo[3.1.0]hex-2-yl] (C₁₀H₁₇)
thymyl (from thymol) = [5-methyl-2-(1-methyl-
 ethyl)phenyl]



thyronyl = [O-(4-hydroxyphenyl)tyrosyl]¹ or [2-
 amino-3-[4-(4-hydroxyphenoxy)phenyl]-1-oxo-
 propyl] [4-(4-HOC₆H₄O)C₆H₄]CH₂CH-
 (NH₂)CO-
toloxy = (methylphenoxy) MeC₆H₄O-
p-toluenesulfonamido = [(4-methylphenyl)sulfo-
 nyl]amino] 4-MeC₆H₄SO₂NH-
toluidino = [(methylphenyl)amino] MeC₆H₄NH-
toluoyl = (methylbenzoyl) MeC₆H₄CO-
toluyl = (methylbenzoyl) MeC₆H₄CO-
tolyl = (methylphenyl) MeC₆H₄-
α-tolyl = (phenylmethyl) PhCH₂-
tolylene = (methylphenylene) -(MeC₆H₃)-
α-tolylene = (phenylmethylene) PhCH=
tosyl = [(4-methylphenyl)sulfonyl]
 4-MeC₆H₄SO₂-
triazano = triazanyl H₂NNHNH-
1-triazeno = 1-triazen-1-yl H₂NN=N-
s-triazin-2-yl = 1,3,5-triazin-2-yl



trichothecanyl (from trichothecane) (C₁₅H₂₅O)-
tridecanoyl = (1-oxotridecyl) Me(CH₂)₁₁CO-
(trimethylammonio) Me₃N⁺-
(trimethylarsonio) Me₃As⁺-
trimethylene = 1,3-propanediyl -(CH₂)₃-
(1,3,3-trimethyl-2-norbornyl) = (1,3,3-trimethyl-
 bicyclo[2.2.1]hept-2-yl) (C₁₀H₁₇)
(trimethylphosphonio) Me₃P⁺-
triseleno¹³ -SeSeSe-
trisilanylene = 1,3-trisilanediy -(SiH₂)₃-

trisiloxane-1,3,5-triyl = 1,3,5-trisiloxanetriyl
 -SiH(OSiH₂)₂-
trithio¹³ -SSS-
trityl = (triphenylmethyl) Ph₃C-
tropanyl = (8-methyl-8-azabicyclo[3.2.1]octyl)
 (C₈H₁₄N)-
tropyl = (3-hydroxy-1-oxo-2-phenylpropyl)
 HOCH₂CHPhCO-
tryptophyl¹ = [2-amino-3-(1H-indol-3-yl)-1-oxo-
 propyl] (C₈H₆N)CH₂CH(NH₂)CO-
tyrosyl¹ = [2-amino-3-(4-hydroxyphenyl)-1-oxo-
 propyl] 4-HOC₆H₄CH₂CH(NH₂)CO-

undecanoyl = (1-oxoundecyl) Me(CH₂)₉CO-
uramino = [(aminocarbonyl)amino] H₂NCONH-
ureido = [(aminocarbonyl)amino] H₂NCONH-
ureylene = (carbonyldiimino) -NHCONH-
(ureylenediureylene) = [carbonylbis(2,1-hydra-
 zinediylcarbonylimino)]
 -NHCONHNHCONHNHCONH-
ursanyl (from ursane) (C₃₀H₅₁)-

valeryl = (1-oxopentyl) BuCO-
valyl¹ = (2-amino-3-methyl-1-oxobutyl)
 Me₂CHCH(NH₂)CO-
vanillal = [(4-hydroxy-3-methoxyphenyl)methyl-
 ene] 4,3-HO(MeO)C₆H₃CH=
vanilloyl = (4-hydroxy-3-methoxybenzoyl)
 4,3-HO(MeO)C₆H₃CO-
vanillyl = [(4-hydroxy-3-methoxyphenyl)methyl]
 4,3-HO(MeO)C₆H₃CH₂-
vanillylidene = [(4-hydroxy-3-methoxyphenyl)-
 methylene] 4,3-HO(MeO)C₆H₃CH=
vanilmandeolyl = [2-hydroxy-2-(4-hydroxy-3-
 methoxyphenyl)acetyl]
 4,3-HO(MeO)C₆H₃CH(OH)CO-
veratral = [(3,4-dimethoxyphenyl)methylene]
 3,4-(MeO)₂C₆H₃CH=
veratroyl = (3,4-dimethoxybenzoyl)
 3,4-(MeO)₂C₆H₃CO-
o-veratroyl = (2,3-dimethoxybenzoyl)
 2,3-(MeO)₂C₆H₃CO-
veratryl = [(3,4-dimethoxyphenyl)methyl]
 3,4-(MeO)₂C₆H₃CH₂-
o-veratryl = [(2,3-dimethoxyphenyl)methyl]
 2,3-(MeO)₂C₆H₃CH₂-
veratrylidene = [(3,4-dimethoxyphenyl)methyl-
 ene] 3,4-(MeO)₂C₆H₃CH=
vinyl = ethenyl H₂C=CH-
vinylene = 1,2-ethenediyl -CH=CH-
vinylidene = ethenylidene H₂C=C=

xanthen-9-yl = 9H-xanthen-9-yl (C₁₃H₉O)-
xanth-9-yl = 9H-xanthen-9-yl (C₁₃H₉O)-
xenyl = [1,1'-biphenyl]-4-yl 4-PhC₆H₄-
xylydino = [(dimethylphenyl)amino]
 Me₂C₆H₃NH-
xyloyl = (dimethylbenzoyl) Me₂C₆H₃CO-
xylyl = (dimethylphenyl) Me₂C₆H₃-
xylylene = [phenylenebis(methylene)]
 -CH₂C₆H₄CH₂-

NOTE: In addition to the following comments it must be understood that stereochemical information is not provided for systematically named natural-product radicals in the list above. For example, the phytlyl radical is named as 3,7,11,15-tetramethyl-2-hexadecenyl. Because the total stereochemistry of a phytlyl compound may be influenced by the presence of other chiral centers, it would be misleading to supply it with the radical name.

¹ This prefix is used in peptide nomenclature.
² This prefix may be used in a generic sense, e.g., aldoxime.
³ This prefix is only used as a multiplying radical and in structural repeating units of polymers.
⁴ This prefix is used only when unsubstituted.
⁵ This prefix is used when both free valencies are attached to the same atom.

⁶ This prefix is used when the free valencies are attached to different atoms which are usually not otherwise connected.
⁷ This prefix is used as a multiplying radical or when both free valencies are attached to the same atom.
⁸ The prefix "cumyl" has been used in the recent literature to mean α-cumyl.
⁹ This prefix is used when the free valencies are attached to different atoms which are not otherwise connected.
¹⁰ This prefix is used when the free valencies are attached to different atoms which are otherwise connected.
¹¹ This prefix may be used in a generic sense, e.g., ketoxime.
¹² This prefix is used only in structural repeating units of polymers.
¹³ This prefix is used to denote a series of chalcogen atoms in a chain or an indefinite structure.
¹⁴ This prefix is not used when the hydrogen atom has been substituted by another atom or group if a definite structure can be determined.

J. SELECTED BIBLIOGRAPHY OF NOMENCLATURE OF CHEMICAL SUBSTANCES

Introduction	¶ 295
IUPAC, IUB, and IUBMB Nomenclature Rules and Recommendations	
Organic chemistry	296
Biochemistry	297
Inorganic chemistry	298
Macromolecular chemistry	299
Miscellaneous	300
American Chemical Society Nomenclature	
Chemical Abstracts Service Index Nomenclature	301

American Chemical Society Committee	¶ 302
History and Development of Chemical Nomenclature	
General	303
Organic chemistry	304
Biochemistry	305
Inorganic chemistry	306
Macromolecular chemistry	307
Stereochemistry	308

295. Introduction. The development of systematic chemical nomenclature is shared by a number of organizations. In the United States the American Chemical Society (ACS) established a Committee on Nomenclature and Notation as early as 1886, followed in 1911 by the ACS Committee on Nomenclature, Spelling, and Pronunciation, now known as the ACS Committee on Nomenclature, Terminology and Symbols. In addition, subject nomenclature committees and subcommittees exist in several ACS divisions.

Internationally, nomenclature commissions of the International Union of Pure and Applied Chemistry (IUPAC) and the International Union of Biochemistry and Molecular Biology (IUBMB)¹ approve and publish detailed recommendations.^{2,3}

Before becoming officially recommended nomenclature policy, a typical path for a proposal originating in the United States has been as follows: an idea (suggested by an author, editor, committee member, etc.) is submitted to a subcommittee of subject specialists, then to an ACS divisional committee, the ACS Committee on Nomenclature, and finally to the appropriate nomenclature commission of the International Union of Pure and Applied Chemistry.

References to current nomenclature rules of IUPAC, IUB, IUBMB, and ACS are listed below. A selection of references to older, superseded rules and to significant proposals of individual authors is also included because of the occasional use of such nomenclature in current chemical literature, and the need in retrospective searching. These older references also provide a historical perspective illustrating the precedents on which modern chemical nomenclature are based.

Additional nomenclature information may be obtained from Chemical Abstracts Service.

IUPAC, IUB, and IUBMB Nomenclature Rules and Recommendations

296. Organic chemistry

1. International Union of Pure and Applied Chemistry. Organic Chemistry Division. Commission on Nomenclature of Organic Chemistry, *A Guide to IUPAC Nomenclature of Organic Compounds, Recommendations 1993*, R. Panico, W. H. Powell, Jean-Claude Richer, eds., Blackwell Scientific Publications, Oxford, UK, 1993, 190 pp. (Includes revisions, both published and hitherto unpublished, to the 1979 edition of *Nomenclature of Organic Chemistry* (see item 2, below). "Corrections to *A Guide to IUPAC Nomenclature of Organic Compounds (IUPAC Recommendations 1993)*", *Pure Appl. Chem.* **1999**, 71, 1327-1330.

2. —, *Nomenclature of Organic Chemistry, Sections A, B, C, D, E, F, and H*, 1979 edition, J. Rigaudy and S. P. Klesney, eds., Pergamon Press, Oxford, UK, 1979, 559 pp. (Section A, Hydrocarbons; Section B, Fundamental Heterocyclic Systems; Section C, Characteristic Groups Containing C, H, O, N, Halogen, S, Se, and/or Te; Section D, Organic Compounds Containing Elements Which Are Not Exclusively C, H, O, N, Halogen, S, Se, and Te (Provisional Recommendations 1978); Section E, Stereochemistry (Recommendations 1974); Section F, General Principles for the Naming of Natural Products and Related Compounds (Provisional Recommendations 1975); Section H, Isotopically Modified Compounds (Approved Recommendations 1978). This edition contains changes from previous editions of various sections. The first edition of Sections A and B, known as the 1957 IUPAC Rules, was published in "Nomenclature of Organic Chemistry, 1957", Butterworths Scientific Pub-

lications, London, 1958, pp 3-70; this edition also appeared with comments in *J. Am. Chem. Soc.* **1960**, 82, 5545-5574. (These sections first appeared as "Tentative Rules for Organic Nomenclature", *C. R. de la Conf. Union Int. Chim.*, Zurich, July 20-28, 1955, pp. 160-184.) A second edition of Sections A and B appeared in "Nomenclature of Organic Chemistry", Butterworths, London, 1966, pp. 3-70. The first edition of Section C was published as "Nomenclature of Organic Chemistry, Section C", Butterworths, London, 1965, 260 pp. and also appeared in *Pure Appl. Chem.* **1965**, 11, 1-260. (Section C first appeared as a paperback edition only as "Tentative Rules for Nomenclature of Organic Chemistry, Section C", Butterworths, London, 1962, 238 pp.). A third edition of Sections A and B and a second edition of Section C were published together as "Nomenclature of Organic Chemistry, Sections A, B, and C", Butterworths, London, 1971, 337 pp. A summary of the changes that were made in Sections A, B, and C for the combined 1971 edition of these sections appears in *J. Chem. Doc.* **1972**, 12, 132-138. An early version of Section D was published in *IUPAC Inf. Bull. Append.* No. 31, August, 1973. The contents of the first edition of Section E appeared in *Pure Appl. Chem.* **1976**, 45, 11-30, previously published as tentative rules in *IUPAC Inf. Bull.* No. 35, June, 1969, pp. 36-80, and in *J. Org. Chem.* **1970**, 35, 2849-2867. Section F appeared earlier in *IUPAC Inf. Bull. Append.* No. 53, December, 1976 and in *Eur. J. Biochem.* **1978**, 86, 1-8. The contents of the first edition of Section H appeared in *Pure Appl. Chem.* **1979**, 51, 353-380, published previously as provisional recommendations in *IUPAC Inf. Bull. Append.* No. 62, July, 1977, and in *Eur. J. Biochem.* **1978**, 86, 9-25.

3. —, "Revision of the Extended Hantzsch-Widman System of Nomenclature for Heteromonocycles (Recommendations 1982)", *Pure Appl. Chem.* **1983**, 55, 409-416. Published previously as provisional recommendations in *Pure Appl. Chem.* **1979**, 51, 1995-2003. For WWW version by G. P. Moss see <http://www.chem.qmw.ac.uk/iupac/iupac.html>

4. —, "Treatment of Variable Valence in Organic Nomenclature (Lambda Convention) (Recommendations 1983)", *Pure Appl. Chem.* **1984**, 56, 769-778. Published previously as provisional recommendations entitled "The Designation of Non-Standard Classical Valence Bonding in Organic Nomenclature" in *Pure Appl. Chem.* **1982**, 54, 217-227. For WWW version by G. P. Moss see <http://www.chem.qmw.ac.uk/iupac/iupac.html>

5. —, "Extension of Rules A-1.1 and A-2.5 Concerning Numerical Terms Used in Organic Chemical Nomenclature (Recommendations 1986)", *Pure Appl. Chem.* **1986**, 58, 1693-1696. Published previously as provisional recommendations in *Pure Appl. Chem.* **1983**, 55, 1463-1466.

6. —, "Nomenclature for Cyclic Organic Compounds with Contiguous Formal Double Bonds (The δ -Convention) (Recommendations 1988)", *Pure Appl. Chem.* **1988**, 60, 1395-1401. For WWW version by G. P. Moss see <http://www.chem.qmw.ac.uk/iupac/iupac.html>

7. —, "Revised Nomenclature for Radicals, Ions, Radical Ions, and Related Species (Recommendations 1993)", *Pure Appl. Chem.* **1993**, 65, 1357-1455. A revision of Subsection C-0.8 of the 1979 edition of *Nomenclature of Organic Chemistry* (See item 2, above).

8. International Union of Pure and Applied Chemistry. Organic Chemistry Division. Commission on Nomenclature of Organic Chemistry. International Union of Pure and Applied Chemistry and International Union of Biochemistry. Commission on Biochemical Nomenclature, "Nomenclature of Carotenoids (Rules Approved 1974)", *Pure Appl. Chem.* **1975**, 41, 405-431 (amendments: *Biochemistry* **1975**, 14, 1803-1804). Published previously as tentative rules in *Biochemistry* **1971**, 10, 4827-4837. (These publications supersede rules in *J. Am. Chem. Soc.* **1960**, 82, 5583-5584.)

9. —, "Rules for Cyclitol Nomenclature (Recommendations 1973)", *Biochem. J.* **1976**, 153, 25-31. Published previously as tentative rules in *J. Biol. Chem.* **1968**, 243, 5809-5819.

10. International Union of Pure and Applied Chemistry. Organic Chemistry Division. Commission on Nomenclature of Organic Chemistry. Commission on Physical Organic Chemistry, "Glossary of Class Names of Organic Compounds and Reactive Intermediates Based on Structure (Recommendations 1995)", *Pure Appl. Chem.* **1995**, 67, 1307-1375. For WWW version by G. P. Moss see <http://www.chem.qmw.ac.uk/iupac/iupac.html>

11. —, "Basic Terminology of Stereochemistry (Recommendations 1996)", *Pure Appl. Chem.* **1996**, 68, 2193-2222. For WWW version by G. P. Moss see <http://www.chem.qmw.ac.uk/iupac/iupac.html>

¹Known as the International Union of Biochemistry (IUB) prior to 1992.

²K L. Loening, "International Cooperation on Scientific Nomenclature", *J. Chem. Doc.* **1970**, 10, 231-236; "Terminology Guidelines and Their Application in the International Union of Pure and Applied Chemistry" in *International Co-operation in Terminology Work*, M. Krommer-Benz and K. G. Saur, eds. Munich, 1986, pp. 92-116 (*Infoterm Series* 8).

³International Union of Pure and Applied Chemistry, "Guidelines for Drafting IUPAC Technical Reports and Recommendations (2002)" in *IUPAC Handbook, 2002-2003*, IUPAC, 2002, pp. 344-353; "Procedure for Publication of IUPAC Technical Reports and Recommendations", *ibid.*, pp. 341-343.

12. International Union of Pure and Applied Chemistry. Organic Chemistry Division. Commission on Physical Organic Chemistry, "Glossary of Terms Used in Physical Organic Chemistry (Recommendations 1994)", *Pure Appl. Chem.* **1994**, 66, 1077-1184. Published previously as Recommendations 1982 in *Pure Appl. Chem.* **1983**, 55, 1281-1371 and as provisional recommendations in *Pure Appl. Chem.* **1979**, 51, 1725-1801. For WWW version by G. P. Moss see <http://www.chem.qmw.ac.uk/iupac/iupac.html>

13. —, "Names for Hydrogen Atoms, Ions, and Groups, and for Reactions Involving Them (Recommendations 1988)", *Pure Appl. Chem.* **1988**, 60, 1115-1116.

14. —, "Nomenclature for Organic Chemical Transformations (Recommendations 1988)", *Pure Appl. Chem.* **1989**, 61, 725-768 (includes provisional recommendations previously published as "Nomenclature for Straightforward Transformations" in *Pure Appl. Chem.* **1981**, 53, 305-321).

15. International Union of Pure and Applied Chemistry. "Nomenclature and Terminology of Fullerenes: A Preliminary Survey", *Pure Appl. Chem.* **1997**, 69, 1411-1434.

16. International Union of Pure and Applied Chemistry. Organic Chemistry Division. Commission on Nomenclature of Organic Chemistry, "Nomenclature of Fused and Bridged Fused Ring Systems (IUPAC Recommendations 1998)", *Pure Appl. Chem.* **1998**, 70, 143-216.

17. —, "Phane Nomenclature. Part I: Parent Phane Names (IUPAC Recommendations 1998)", *Pure Appl. Chem.* **1998**, 70, 1513-1545.

18. —, "Extension and Revision of the von Baeyer System for Naming Polycyclic Compounds (Including Bicyclic Compounds) (IUPAC Recommendations 1999)", *Pure Appl. Chem.* **1999**, 71, 513-529.

19. —, "Extension and Revision of the Nomenclature for Spiro Compounds (IUPAC Recommendations 1999)", *Pure Appl. Chem.* **1999**, 71, 531-558.

20. —, "Revised Section F: Natural Products and Related Compounds (IUPAC Recommendations 1999)", *Pure Appl. Chem.* **1999**, 71, 587-643. Superseded Section F published first in 1976, and then in 1978 (see item 2, above).

21. International Union of Pure and Applied Chemistry. Organic Chemistry Division. Commission on Physical Organic Chemistry, "Glossary of Terms Used in Theoretical Organic Chemistry (IUPAC Recommendations 1999)", *Pure Appl. Chem.* **1999**, 71, 1919-1981.

22. International Union of Pure and Applied Chemistry. Organic and Biomolecular Chemistry Division. Commission on Nomenclature of Organic Chemistry, "Nomenclature for the C₆₀-I_h and C₇₀-D_{5h(6)} Fullerenes (IUPAC Recommendations 2002)", *Pure Appl. Chem.* **2002**, 74, 629-695.

23. —, "Phane Nomenclature. Part II: Modification of the Degree of Hydrogenation and Substitution Derivatives of Phane Parent Hydrides (IUPAC Recommendations 2002)", *Pure Appl. Chem.* **2002**, 74, 809-834.

297. Biochemistry

1. International Union of Biochemistry and Molecular Biology, *Biochemical Nomenclature and Related Documents 1992*, 2nd. ed., Portland Press, Ltd., London, 1993. A compendium of recommendations of IUPAC and IUB produced by the Commission on Biochemical Nomenclature (CBN), the Nomenclature Committee of IUB (NC-IUB), and the IUPAC-IUB Joint Commission on Biochemical Nomenclature (JCBN), prepared by C. Liebecq for the Committee of Editors of Biochemical Journals (CEBJ). The compendium includes Sections E and F of the IUPAC Organic Rules (see ¶ 296, item 2); nomenclature recommendations given in items 8-9, ¶ 296 and items listed below, except for items 20, 22, 23, 24, 29, 38, 39 and 40. It includes only the tentative rules of item 5. Section H of the IUPAC Organic Rules and item 29 appear in the 1979 edition of the compendium published in 1978 by The Biochemical Society, London. Also included in the 1992 compendium are "Isotopically Labeled Compounds: Common Biochemical Practice"; "Isotopically Substituted Compounds"; "Names for Hydrogen Species" (see ¶ 296, item 13); and "Excerpts from Newsletters of the Nomenclature Committees of IUB".

2. International Union of Pure and Applied Chemistry and International Union of Biochemistry. Commission on Biochemical Nomenclature, "Nomenclature of Phosphorus-Containing Compounds of Biochemical Importance (Recommendations 1976)", *Eur. J. Biochem.* **1977**, 79, 1-9.

3. International Union of Pure and Applied Chemistry and International Union of Biochemistry. Joint Commission on Biochemical Nomenclature, "Nomenclature of Tetrapyrroles (Recommendations 1986)", *Pure Appl. Chem.* **1987**, 59, 779-832. Replaces "Recommendations 1978", *Pure Appl. Chem.* **1979**, 51, 2251-2304 of which an amended version appears in *Eur. J. Biochem.* **1980**, 108, 1-30 and an abbreviated version by P. Karlson in *Hoppe-Seyler's Z. Physiol. Chem.* **1981**, 362, vii-xii.

4. —, "Nomenclature of Steroids (Recommendations 1989)", *Pure Appl. Chem.* **1989**, 61, 1783-1822. (corrections: *Eur. J. Biochem.* **1993**, 213, 2). For WWW version by G. P. Moss see <http://www.chem.qmw.ac.uk/iupac/iupac.html>. [Supersedes "Definitive Rules for Nomenclature of Steroids", *Pure Appl. Chem.* **1972**, 31, 283-322 (book form: Butterworths, London, 1972), previously published as tentative rules in *Biochemistry* **1969**, 8, 2227-2242 (amendments. *ibid.* **1971**, 10, 4994), both of which superseded the definitive rules in "Nomenclature of Organic Chemistry, 1957" Butterworths Scientific Publications, London, 1958, pp. 71-82 and *J. Am. Chem. Soc.* **1960**, 82, 5577-5581, and in "Nomenclature of Organic Chemistry" Butterworths, London, 1966, pp. 71-81 (tentative rules for which appeared in *C. R. de la Conf. Union Int. Chim.*, Zurich, July 20-8, 1955, pp. 190-207)].

5. —, "Nomenclature of Lignans and Neolignans (IUPAC Recommendations 2000)", *Pure Appl. Chem.* **2000**, 72, 1493-1523.

Carbohydrates

6. International Union of Pure and Applied Chemistry and International Union of Biochemistry and Molecular Biology. Joint Commission on Biochemical Nomenclature. "Nomenclature of Carbohydrates (Recommendations 1996)", *Pure Appl. Chem.* **1996**, 68(10), 1919-2008. For WWW version by G. P. Moss see <http://www.chem.qmw.ac.uk/iupac/iupac.html> [Supersedes "Tentative Rules for Carbohydrate Nomenclature, Pt. 1", *Biochemistry* **1971**, 10, 3983-4004 (errata: *ibid.* **1971**, 10, 4995)] (see also ¶ 302, item 14).

7. International Union of Pure and Applied Chemistry and International Union of Biochemistry. Joint Commission on Biochemical Nomenclature, "Conformational Nomenclature for Five and Six-Membered Ring Forms of Monosaccharides and their Derivatives (Provisional Recommendations)", *Pure Appl. Chem.* **1981**, 53, 1901-1906. Published as "Recommendations 1980" in *Eur. J. Biochem.* **1980**, 111, 295-298 (A preliminary version was published in *J. Chem. Soc., Chem. Commun.* **1973**, 505-508. See ¶ 302, item 18).

8. —, "Nomenclature of Branched-Chain Monosaccharides (Provisional Recommendations)", *Pure Appl. Chem.* **1982**, 54, 211-215. Published as "Recommendations 1980" in *Eur. J. Biochem.* **1981**, 119, 5-8 (corrections: *ibid.* **1982**, 125, 1).

9. —, "Nomenclature of Unsaturated Monosaccharides (Provisional Recommendations)", *Pure Appl. Chem.* **1982**, 54, 207-210. Published as "Recommendations 1980" in *Eur. J. Biochem.* **1981**, 119, 1-3 (corrections: *ibid.* **1982**, 125, 1).

10. —, "Abbreviated Terminology of Oligosaccharide Chains, Provisional", *Pure Appl. Chem.* **1982**, 54, 1517-1522. Published as "Recommendations 1980" in *J. Biol. Chem.* **1982**, 257, 3347-3351.

11. —, "Polysaccharide Nomenclature (Provisional)", *Pure Appl. Chem.* **1982**, 54, 1523-1526. Published as "Recommendations 1980" in *J. Biol. Chem.* **1982**, 257, 3352-3354.

12. —, "Symbols for Specifying the Conformation of Polysaccharide Chains (Provisional)", *Pure Appl. Chem.* **1983**, 55, 1269-1272 and as "Recommendations 1981", in *Eur. J. Biochem.* **1983**, 131, 5-7.

13. International Union of Biochemistry. Nomenclature Committee, "Numbering of Atoms in myo-Inositol (Recommendations 1988)", *Biochem. J.* **1989**, 258, 1-2.

Amino Acids, Peptides, Proteins, and Nucleic Acids

14. International Union of Pure and Applied Chemistry and International Union of Biochemistry. Commission on Biochemical Nomenclature, "Abbreviated Nomenclature of Synthetic Polypeptides (Polymerized Amino Acids) (Revised Rules)", *Pure Appl. Chem.* **1973**, 33, 437-444. Published previously as revised recommendations in *Biochemistry* **1972**, 11, 942-944.

15. —, "Abbreviations and Symbols for Nucleic Acids, Polynucleotides and their Constituents (Rules Approved 1974)", *Pure Appl. Chem.* **1974**, 40, 277-290. Published previously as revised rules in *Biochemistry* **1970**, 9, 4022-4027.

16. —, "Abbreviations and Symbols for Description of Conformation of Polypeptide Chains (Rules Approved 1974)", *Pure Appl. Chem.* **1974**, 40, 291-308. Published previously as tentative rules in *IUPAC Inf. Bull. Append. No. 10*, February, 1971 and as "Tentative Rules (1969)" in *Eur. J. Biochem.* **1970**, 17, 193-201.

17. —, "Nomenclature of Peptide Hormones (Recommendations 1974)", *Biochemistry* **1975**, 14, 2559-2560.

18. International Union of Pure and Applied Chemistry and International Union of Biochemistry. Joint Commission on Biochemical Nomenclature. "Nomenclature and Symbolism for Amino Acids and Peptides (Recommendations 1983)", *Pure Appl. Chem.* **1984**, 56, 595-624 (corrections: *Eur. J. Biochem.* **1993**, 213, 2). A combination and revision of four previously published recommendations: (a) "Nomenclature of α -Amino Acids (Recommendations 1974)", *Biochemistry* **1975**, 14, 449-462; published previously as provisional recommendations in *IUPAC Inf. Bull. Append. No. 46*, September 1975 (these publications supersede rules published in *J. Am. Chem. Soc.* **1960**, 82, 5575-5577); (b) "Symbols for Amino Acid Derivatives and Peptides (Rules Approved 1974)", *Pure Appl. Chem.* **1974**, 40, 315-331; published previously as recommendations in *Biochemistry* **1972**, 11, 1726-1732; (c) "Naming Synthetic Modifications of Natural Peptides (Definitive Rules)", *Pure Appl. Chem.* **1972**, 31, 647-653; published previously as tentative rules in *Biochemistry* **1967**, 6, 362-364; (d) "A One-Letter Notation for Amino Acid Sequences (Definitive Rules)", *Pure Appl. Chem.* **1972**, 31, 639-645; published previously as tentative rules in *Biochemistry* **1968**, 7, 2703-2715. For WWW version by G. P. Moss see <http://www.chem.qmw.ac.uk/iupac/iupac.html>

19. —, "Abbreviations and Symbols for the Description of Conformations of Polynucleotide Chains (Provisional)", *Pure Appl. Chem.* **1983**, 55, 1273-1280; appeared also as "Recommendations 1982" in *Eur. J. Biochem.* **1983**, 131, 9-15.

20. —, "Nomenclature of Glycoproteins, Glycopeptides, and Peptidoglycans (Recommendations 1985)", *Pure Appl. Chem.* **1988**, 60, 1389-1394 (corrections: *Eur. J. Biochem.* **1989**, 185, 485).

21. International Union of Biochemistry. Nomenclature Committee, "Nomenclature of Iron-Sulfur Proteins (Recommendations 1978)", *Eur. J. Biochem.* **1979**, 93, 427-430 (corrections: *ibid.* **1979**, 95, 369 and **1979**, 102, 315). Published previously as recommendations in *Biochemistry* **1973**, 12, 3582-3583.

22. —, "Nomenclature for Incompletely Specified Bases in Nucleic Acid Sequences (Recommendations 1984)", *Eur. J. Biochem.* **1985**, 150, 1-5 (corrections: *ibid.* **1986**, 157, 1).

23. —, "Nomenclature of Electron-Transfer Proteins (Recommendations 1989)", *Eur. J. Biochem.* **1991**, 200, 599-611 (corrections: *Eur. J. Biochem.* **1993**, 213, 2-3).

24. —, "A Nomenclature of Junctions and Branchpoints in Nucleic Acids", *Eur. J. Biochem.* **1995**, 230, 1-2.

25. International Union of Pure and Applied Chemistry. IUPAC-IUBMB-IUPAB Inter-Union Task Group on the Standardization of Data Bases of Protein and Nucleic Acid Structures by NMR Spectroscopy, "Recommendations for the Presentation of NMR Structures of Proteins and Nucleic Acids (IUPAC Recommendations 1998)", *Pure Appl. Chem.* **1998**, 70, 117-142.

Enzymes

26. International Union of Biochemistry and Molecular Biology Nomenclature Committee, *Enzyme Nomenclature*, 1992, Academic Press, Orlando, Florida, 1992, 862 pp; Supplements 1, 2, 3, 4, and 5. Corrections and Additions, *Eur. J. Biochem.* **1994**, 223, 1-5; **1995**, 232, 1-6; **1996**, 237, 1-5; **1997**, 250, 1-6; **1999**, 264, 610-650. (This edition includes corrections and additions to "Enzyme Nomenclature, 1984", published as three supplements in *Eur. J. Biochem.* **1986**, 157, 1-26; **1989**, 179, 489-533; **1990**, 187, 263-281; the 1984 edition updated the 1978 edition by including corrections and additions published as four supplements in *Eur. J. Biochem.* **1980**, 104, 1-4; **1981**, 116, 423-435; **1982**, 125, 1-13; **1983**, 131, 461-472.)

27. International Union of Pure and Applied Chemistry and International Union of Biochemistry. Commission on Biochemical Nomenclature, "The Nomenclature of Multiple Forms of Enzymes (Recommendations 1976)", *Eur. J. Biochem.* **1978**, 82, 1-3. Published previously as "Rules Approved 1974" in *Pure Appl. Chem.* **1974**, 40, 309-314.

28. International Union of Biochemistry. Nomenclature Committee, "Symbolism and Terminology in Enzyme Kinetics (Recommendations 1981)", *Eur. J. Biochem.* **1982**, 128, 281-291 (corrections: *Eur. J. Biochem.* **1993**, 213, 1).

29. —, "Nomenclature for Multienzymes (Recommendations 1989)", *Eur. J. Biochem.* **1989**, 185, 485-486 (supersedes "Multienzyme Proteins" in *Trends. Biochem. Sci.* **1979**, 4, N275).

Lipids, Vitamins, Coenzymes, and Related Compounds

30. International Union of Pure and Applied Chemistry and International Union of Biochemistry. Commission on Biochemical Nomenclature, "The Nomenclature of Lipids (Recommendations 1976)", *Eur. J. Biochem.* **1977**, 79, 11-21. Previously published as recommendations in *J. Biol. Chem.* **1967**, 242, 4845-4849 (amendments: *ibid.* **1970**, 245, 1511).

31. —, "Trivial Names of Miscellaneous Compounds of Importance in Biochemistry (Tentative Rules)", *J. Biol. Chem.* **1966**, 241, 2987-2988. (Supersedes "Definitive Rules for the Nomenclature of the Vitamins", *J. Am. Chem. Soc.* **1960**, 82, 5581-5583.)

32. —, "Nomenclature of Quinones with Isoprenoid Side Chains (Recommendations 1973)", *Eur. J. Biochem.* **1975**, 53, 15-18. Published previously as tentative rules in *J. Biol. Chem.* **1966**, 241, 2989-2991. (Supersedes Rule V-4 in *J. Am. Chem. Soc.* **1960**, 82, 5581-5583.)

33. —, "Nomenclature and Symbols for Folic Acid and Related Compounds (Recommendations 1986)", *Pure Appl. Chem.* **1987**, 59, 833-836. Published as "Tentative Rules" in *J. Biol. Chem.* **1966**, 241, 2991-2992 which superseded Rule V-13 in *J. Am. Chem. Soc.* **1960**, 82, 5581-5583.

34. —, "Nomenclature of Corrinoids (Rules Approved 1975)", *Pure Appl. Chem.* **1976**, 48, 495-502. Published previously as recommendations in *Biochemistry* **1974**, 13, 1555-1560 and as tentative rules in *J. Biol. Chem.* **1966**, 241, 2992-2994. (Supersedes Rule V-15 in *J. Am. Chem. Soc.* **1960**, 82, 5581-5583; tentative rules for which appeared in "Nomenclature of Organic Chemistry, 1957", Butterworths Scientific Publications, London, 1958, pp. 83-87.)

35. —, "Nomenclature for Vitamins B₆ and Related Compounds (Recommendations 1973)", *Biochemistry* **1974**, 13, 1056-1058. Published previously as tentative rules in *Biochemistry* **1970**, 9, 4019-4021. (Supersedes Section M-7 in *J. Biol. Chem.* **1966**, 241, 2987-2988; see item 29 above.)

36. International Union of Pure and Applied Chemistry and International Union of Biochemistry. Joint Commission on Biochemical Nomenclature, "Nomenclature of Tocopherols and Related Compounds (Recommendations 1981)", *Pure Appl. Chem.* **1982**, 54, 1507-1510 and in *Eur. J. Biochem.* **1982**, 123, 473-475. Published previously as "Recommendations 1973" in *Eur. J. Biochem.* **1974**, 46, 217-219 and as provisional recommendations in *IUPAC Inf. Bull. Append. No. 47*, September, 1975. (Supersedes Section M-3 in *J. Biol. Chem.* **1966**, 241, 2987-2988; see item 29 above.)

37. —, "Nomenclature of Vitamin D (Provisional)", *Pure Appl. Chem.* **1982**, 54, 1511-1516. Published as "Recommendations 1981" in *Eur. J. Biochem.* **1982**, 124, 223-227.

38. —, "Nomenclature of Retinoids (Provisional)", *Pure Appl. Chem.* **1983**, 55, 721-726. Published as "Recommendations 1981" in *Eur. J. Biochem.* **1982**, 129, 1-5.

39. —, "Nomenclature of Prenols (Recommendations 1986)", *Pure Appl. Chem.* **1987**, 59, 683-689.

40. —, "Nomenclature of Glycolipids (IUPAC Recommendations 1997)", *Pure Appl. Chem.* **1997**, 69, 2475-2487; *Carbohydr. Res.* **1998**, 312, 167-175; *Eur. J. Biochem.* **1998**, 257, 293-298; *Glycoconjugate J.* **1999**, 16, 1-6; *J. Mol. Biol.* **1999** 286, 963-970; *Adv. Carbohydr. Chem. Biochem.* **2000**, 55, 311-326. Superseded the glycolipid section in the 1976 Recommendations on lipid nomenclature (see item 30, above).

Miscellaneous

41. International Union of Pure and Applied Chemistry and International Union of Biochemistry. Commission on Biochemical Nomenclature, "Abbreviations and Symbols for Chemical Names of Special Interest in Biological Chemistry (Revised Tentative Rules 1965)", *Biochemistry* **1966**, 5, 1445-1453.

42. —, "Abbreviations and Symbols", *Eur. J. Biochem.* **1977**, 74, 1-5.

43. International Union of Nutritional Sciences. Committee 1/I. Nomenclature, "Generic Descriptors and Trivial Names for Vitamins and Related Compounds (Recommendations 1976)", *Nutrition Abstr. and Revs., Series A: Human and Experimental* **1978**, 48, 831-835.

298. Inorganic chemistry

1. International Union of Pure and Applied Chemistry. Inorganic Chemistry Division. Commission on the Nomenclature of Inorganic Chemistry, *Nomenclature of Inorganic Chemistry Recommendations 1990*, G. J. Leigh, ed., Blackwell Scientific Publications, Oxford, UK, 1990, 289 pp. These recommendations revise and extend the 2nd ed., "Nomenclature of Inorganic Chemistry, 1970", Butterworths, London, 1971, 110 pp., which also appeared in *Pure Appl. Chem.* **1971**, 28, 1-110, and the 1st ed., "Nomenclature of Inorganic Chemistry" (1957 Report of the Commission on the Nomenclature of Inorganic Chemistry), Butterworths Scientific Publications, London, 1958, 93 pp. (in French and English); the latter also appeared with comments in *J. Am. Chem. Soc.* **1960**, 82, 5523-5544. The 1970 edition incorporated "Tentative Proposals for Nomenclature of Absolute Configurations Concerned with Six-Coordinate Complexes Based on the Octahedron", *Inorg. Chem.* **1970**, 9, 1-5; π -Complexes (Tentative), *IUPAC Inf. Bull. No. 35*, June, 1969, pp. 31-35; and Iso- and Heteropolyanions (Rules 5.1 and 5.2, Tentative), *IUPAC Inf. Bull. No. 35*, June, 1969, pp. 22-27.

2. —, "Nomenclature of Inorganic Boron Compounds", *Pure Appl. Chem.* **1972**, 30, 681-710 (see also ¶ 302, item 16).

3. —, *How to Name an Inorganic Substance*. A Guide to the Use of Nomenclature of Inorganic Chemistry: Definitive Rules, 1970, Pergamon Press, New York, 1977, 36 pp.

4. —, "Nomenclature of Inorganic Chemistry: II.2. The Nomenclature of Hydrides of Nitrogen and Derived Cations, Anions, and Ligands (Recommendations 1981)", *Pure Appl. Chem.* **1982**, 54, 2545-2552. Published previously as provisional recommendations in *IUPAC Inf. Bull.* **1978**, (2), 151-160.

5. —, "Recommendations for the Naming of Elements of Atomic Numbers Greater than 100 (Definitive)", *Pure Appl. Chem.* **1979**, 51, 381-384. Previously published as "Recommendations for the Naming of Elements of Atomic Numbers Greater Than 105 (Provisional)" in *IUPAC Inf. Bull. Append. No. 55*, December, 1976.

6. —, "Nomenclature of Inorganic Chemistry: II.1. Isotopically Modified Compounds (Recommendations 1981)", *Pure Appl. Chem.* **1981**, 53, 1887-1900. Previously published as provisional recommendations in *Pure Appl. Chem.* **1979**, 51, 1981-1994.

7. —, "Nomenclature of Polyaniions, Recommendations 1987", *Pure Appl. Chem.* **1987**, 59, 1529-1548.

8. —, "Names and Symbols of Transfermium Elements (IUPAC Recommendations 1997)", *Pure Appl. Chem.* **1997**, 69, 2471-2473. Superseded "Names and Symbols of Transfermium Elements (Recommendations 1994)", *Pure Appl. Chem.* **1994**, 66, 2419-2421 (subsequently reclassified by the IUPAC Bureau as provisional in August, 1995). See K. I. Zamaraev, "IUPAC Recommendations on Names and Symbols of Transfermium Elements", *Chem. Int.* **1996**, 18(1), 34.

9. International Union of Pure and Applied Chemistry. Inorganic Chemistry Division, "New Notations in the Periodic Table", *Pure Appl. Chem.* **1988**, 60, 431-436.

10. International Union of Pure and Applied Chemistry. Inorganic Chemistry Division, Commission on High Temperature and Solid State Chemistry, "Nomenclature and Terminology of Graphite Intercalation Compounds (Recommendations 1994)", *Pure Appl. Chem.* **1994**, 66, 1893-1901.

11. International Union of Pure and Applied Chemistry. Inorganic Chemistry Division. Working Party on IUPAC Glossary of Terms Used in Bioinorganic Chemistry, "Glossary of Terms Used in Bioinorganic Chemistry (IUPAC Recommendations 1997)", *Pure Appl. Chem.* **1997**, 60, 1251-1303.

12. International Union of Pure and Applied Chemistry. Inorganic Chemistry Division. Commission on Nomenclature of Inorganic Chemistry, "Nomenclature of Inorganic Chains and Ring Compounds (IUPAC Recommendations 1997)", *Pure Appl. Chem.* **1997**, 69, 1659-1692.

13. —, "Nomenclature of Organometallic Compounds of the Transition Elements (IUPAC Recommendations 1999)", *Pure Appl. Chem.* **1999**, 71, 1557-1585.

14. International Union of Pure and Applied Chemistry. Inorganic Chemistry Division, Commission on High Temperature Materials and Solid State Chemistry, "Terminology for Compounds in the Si-Al-O-N System (IUPAC Recommendations 1999)", *Pure Appl. Chem.* **1999**, 71, 1765-1769.

15. International Union of Pure and Applied Chemistry. Inorganic Chemistry Division. Commission on Nomenclature of Inorganic Chemistry, "Names for Inorganic Radicals (IUPAC Recommendations 1999)", *Pure Appl. Chem.* **2000**, 72, 437-446.

16. —, "Names for Muonium and Hydrogen Atoms and Their Ions (IUPAC Recommendations 2001)", *Pure Appl. Chem.* **2001**, 73, 377-380.

17. —, *Nomenclature of Inorganic Chemistry II: Recommendations 2000*, J. A. McCleverty and N. G. Connelly, eds., Royal Society of Chemistry, Oxford, UK, 2001, 130 pp.
18. —, "Naming of New Elements (IUPAC Recommendations 2002)", *Pure Appl. Chem.* **2002**, *74*, 787-791.
19. International Union of Pure and Applied Chemistry. Chemistry and Human Health Division. Clinical Chemistry Section. Commission on Toxicology, "'Heavy Metals' - A Meaningless Term? (IUPAC Technical Report)", *Pure Appl. Chem.* **2002**, *74*, 793-807.
20. International Union of Pure and Applied Chemistry. Inorganic Chemistry Division. Commission on Nomenclature of Inorganic Chemistry, "On the Claims for Discovery of Elements 110, 111, 112, 114, 116, and 118 (IUPAC Technical Report)", *Pure Appl. Chem.* **2003**, *75*, 1601-1611.
21. International Union of Pure and Applied Chemistry. Inorganic Chemistry Division, "Name and Symbol of the Element with Atomic Number 110 (IUPAC Recommendations 2003)", *Pure Appl. Chem.* **2003**, *75*, 1613-1615.

299. Macromolecular chemistry

1. International Union of Pure and Applied Chemistry. Physical Chemistry Division. Commission on Macromolecules. Subcommission on Nomenclature, "Report on Nomenclature in the Field of Macromolecules (1951)", *J. Polym. Sci.* **1952**, *8*, 257-277 [modifications and additions (tentative): *J. Polym. Sci., Part B: Polym. Lett.*, **1968**, *6*, 257-260].
2. —, "Report on Nomenclature Dealing with Steric Regularity in High Polymers", *Pure Appl. Chem.* **1966**, *12*, 645-656 (Authors often cited as M. L. Huggins, G. Natta, V. Desreux, and H. Mark); published previously as a preliminary version in *J. Polym. Sci.* **1962**, *56*, 153-161.
3. International Union of Pure and Applied Chemistry. Division of Applied Chemistry. Plastics and High Polymers Section, "Recommendations for Abbreviations of Terms Relating to Plastics and Elastomers", *Pure Appl. Chem.* **1969**, *18*, 583-589.
4. International Union of Pure and Applied Chemistry. Macromolecular Division. Commission on Macromolecular Nomenclature, *Compendium of Macromolecular Nomenclature*, Blackwell Scientific Publications, Oxford, UK, 1991, 171 pp. (a bibliography of the recommendations given as items 5-12 and 18 below). For a bibliography of translations of this compendium prepared by W. V. Metanowski see <http://www.chem.qmw.ac.uk/iupac2/bibliog/purp.html>
5. —, "Nomenclature of Regular Single-Strand Organic Polymers (Rules Approved 1975)", *Pure Appl. Chem.* **1976**, *48*, 373-385. Published previously as provisional recommendations in *Macromolecules* **1973**, *6*, 149-158 and in *IUPAC Inf. Bull. Append.* No. 29, November, 1972 (see also ¶ 302, item 15). Superseded by item 18, below.
6. —, "Glossary of Basic Terms in Polymer Science (Recommendations 1996)", *Pure Appl. Chem.* **1996**, *68*, 2287-2311. Supercedes "Basic Definitions of Terms Relating to Polymers (1974)", *Pure Appl. Chem.* **1974**, *40*, 477-491, and "Basic Definitions Relating to Polymers", *IUPAC Inf. Bull. Append.* No. 13, February 1971.
7. —, "Stereochemical Definitions and Notations Relating to Polymers (Recommendations 1980)", *Pure Appl. Chem.* **1981**, *53*, 733-752. Published previously as provisional recommendations in *Pure Appl. Chem.* **1979**, *51*, 1101-1121.
8. —, "Source-Based Nomenclature for Copolymers (Recommendations 1985)", *Pure Appl. Chem.* **1985**, *57*, 1427-1440.
9. —, "Use of Abbreviations for Names of Polymeric Substances (Recommendations, 1986)", *Pure Appl. Chem.* **1987**, *59*, 691-693. (Supersedes "List of Standard Abbreviations (Symbols) for Synthetic Polymers and Polymer Materials 1974" *Pure Appl. Chem.* **1974**, *40*, 473-476 and "List of Abbreviations for Synthetic Polymers and Polymer Materials", *IUPAC Inf. Bull. Append.* No. 12, February, 1971).
10. —, "A Classification of Linear Single-Strand Polymers (Recommendations 1988)", *Pure Appl. Chem.* **1989**, *61*, 243-254.
11. —, "Definitions of Terms Relating to Individual Macromolecules, Their Assemblies, and Dilute Polymer Solutions (Recommendations 1988)", *Pure Appl. Chem.* **1989**, *61*, 211-241.
12. —, "Definition of Terms Relating to Crystalline Polymers (Recommendations 1988)", *Pure Appl. Chem.* **1989**, *61*, 769-785.
13. —, "Nomenclature of Regular Double-Strand (Ladder or Spiro) Organic Polymers (Recommendations 1993)", *Pure Appl. Chem.* **1993**, *65*, 1561-1580.
14. —, "Graphic Representations (Chemical Formulae) of Macromolecules (Recommendations 1994)", *Pure Appl. Chem.* **1994**, *66*, 2469-2482.
15. —, "Structure-Based Nomenclature for Irregular Single-Strand Organic Polymers (Recommendations 1994)", *Pure Appl. Chem.* **1994**, *66*, 873-889 (Erratum: *Pure Appl. Chem.* **1994**, *66* (9), insert).
16. —, "Source-Based Nomenclature for Non-Linear Macromolecules and Macromolecular Assemblies (IUPAC Recommendations 1997)", *Pure Appl. Chem.* **1997**, *69*, 2511-2521; in *Polymer Networks*, R. F. T. Stepto, ed., Blackie Academic, London, 1998, pp. 316-328.
17. —, "Generic Source-Based Nomenclature for Polymers (IUPAC Recommendations 2001)", *Pure Appl. Chem.* **2001**, *73*, 1511-1519. Errata, *Pure Appl. Chem.* **2002**, *74*, 2002.
18. —, "Nomenclature of Regular Single-Strand Organic Polymers" (IUPAC Recommendations 2002)", *Pure Appl. Chem.* **2002**, *74*, 1921-1956. Superseded item 5, above.
19. International Union of Pure and Applied Chemistry. Macromolecular Division. Commission on Macromolecular Nomenclature and Inorganic Chemistry Division. Commission on Nomenclature of Inorganic Chemistry,

"Nomenclature for Regular Single-Strand and Quasi-Single-Strand Inorganic and Coordination Polymers (Recommendations 1984)", *Pure Appl. Chem.* **1985**, *57*, 149-168. Published previously as provisional recommendations in *Pure Appl. Chem.* **1981**, *53*, 2283-2302.

300. Miscellaneous

1. International Union of Pure and Applied Chemistry. Interdivisional Committee on Nomenclature and Symbols, "Use of Abbreviations in the Chemical Literature (Recommendations 1979)", *Pure Appl. Chem.* **1980**, *52*, 2229-2232. Previously published as provisional recommendations jointly with the Physical Chemistry Division Commission on Molecular Structure and Spectroscopy in *IUPAC Inf. Bull. Append.* No. 58, July, 1977
2. International Union of Pure and Applied Chemistry. Analytical Chemistry Division, *Compendium of Analytical Nomenclature, Definitive Rules 1997*, 3rd ed., Blackwell Science, Oxford, UK, 1998, 840 pp. Superseded *Compendium of Analytical Nomenclature, Definitive Rules 1987*, 2nd ed., Blackwell Scientific Publications, Oxford, UK, 1978, 279 pp. The 1977 Definitive Rules were published by Pergamon Press, Oxford, UK 1978, 223 pp.
3. International Union of Pure and Applied Chemistry. Analytical Chemistry Division. Commission on Analytical Nomenclature, "Guide to Trivial Names, Trade Names, and Synonyms for Substances Used in Analytical Nomenclature", *Pure Appl. Chem.* **1978**, *50*, 339-370. Previously published as provisional recommendations under the title "List of Trivial Names and Synonyms (for Substances Used in Analytical Chemistry)" in *IUPAC Inf. Bull. Append.* No. 45, September, 1975.
4. International Union of Pure and Applied Chemistry. Physical Chemistry Division. Commission on Symbols, Terminology and Units, *Quantities, Units, and Symbols in Physical Chemistry*, 2nd ed., Blackwell Scientific Publications, Oxford, UK, 1993, 166 pp. [An abbreviated list, 4 pp. A4 laminated card, is published by Blackwell Scientific Publications, Oxford, 1993]. This replaces the 1988 edition which in turn replaced "Manual of Symbols and Terminology for Physicochemical Quantities and Units", *Pure Appl. Chem.* **1979**, *51*, 1-41. A 1973 edition was published by Butterworths, London, 1975 and a 1969 edition appeared in *Pure Appl. Chem.* **1970**, *21*, 1-44. (Supersedes rules in *J. Am. Chem. Soc.* **1960**, *82*, 5517-5522.)
5. International Union of Pure and Applied Chemistry. Physical Chemistry Division. Commission on Colloid and Surface Chemistry, "Chemical Nomenclature and Formulation of Compositions of Synthetic and Natural Zeolites (Definitive)", *Pure Appl. Chem.* **1979**, *51*, 1091-1100. Previously published as provisional recommendations jointly with the Inorganic Chemistry Division Commission on Nomenclature of Inorganic Chemistry in *IUPAC Inf. Bull. Append.* No. 41, January, 1975.
6. International Union of Pure and Applied Chemistry; *Compendium of Chemical Terminology (IUPAC Recommendations)*, 2nd ed., A. D. McNaught and A. Wilkinson, compilers, Blackwell Science, Oxford, UK, 1997, 336 pp. Superseded *Compendium of Chemical Technology (IUPAC Recommendations)*, V. Gold, K. L. Loening, A. D. McNaught, and P. Sehmi, compilers, Blackwell Scientific Publications, Oxford, UK, 1987, 456 pp.
7. International Union of Pure and Applied Chemistry and International Union of Pure and Applied Physics. Transfermium Working Group, "Discovery of the Transfermium Elements (criteria that must be satisfied for the discovery of a new chemical element to be recognized)", Part I, *Pure Appl. Chem.* **1991**, *63*, 879-886; Part II: Introduction to Discovery Profiles; Part III: Discovery Profiles of the Transfermium Elements, *Pure Appl. Chem.* **1993**, *65*, 1757-1814. [All three parts have been published together in *Prog. Part. Nucl. Phys.* **1992**, *29*, 453-530.] "Responses to the Report 'Discovery of the Transfermium Elements' Invited by the Transfermium Working Groups from Lawrence Berkeley Laboratory, California, the Joint Institute for Nuclear Research, Dubna, and Gesellschaft für Schwerionenforschung, Darmstadt, and the Reply to the Responses by the Transfermium Working Group", *Pure Appl. Chem.* **1993**, *65*, 1815-1824.
8. International Union of Pure and Applied Chemistry. Inorganic Chemistry Division, Commission on Atomic Weights and Isotopic Abundances, "Atomic Weights of the Elements 2001 (IUPAC Technical Report)", *Pure Appl. Chem.* **2003**, *75*, 1107-1122. Superseded "Atomic Weights of the Elements 1999", *Pure Appl. Chem.* **2001**, *73*, 667-683; "Atomic Weights of the Elements 1997", *Pure Appl. Chem.* **1997**, *71*, 1593-1607; "Atomic Weights of the Elements 1995", *Pure Appl. Chem.* **1996**, *68*, 2339-2359; and "Atomic Weights of the Elements 1993", *Pure Appl. Chem.* **1994**, *66*, 2423-2444.
9. International Union of Pure and Applied Chemistry; Clinical Chemistry Division and the International Federation of Clinical Chemistry (IFCC), *Compendium of Terminology and Nomenclature of Properties in Clinical Laboratory Sciences* (Recommendations 1995), Blackwell Science, Oxford, UK, **1995**, 304 pp.
10. International Union of Pure and Applied Chemistry. Inorganic Chemistry Division. Commission on Atomic Weights and Isotopic Abundances, "History of the Recommended Atomic-Weight Values from 1882 to 1997: A Comparison of Differences from Current Values to the Estimated Uncertainties of Earlier Values", *Pure Appl. Chem.* **1998**, *70*, 237-257.
11. International Union of Pure and Applied Chemistry, *Principles of Chemical Nomenclature. A Guide to IUPAC Recommendations*, G. J. Leigh, H. A. Favre, and W. V. Metanowski, G. J. Leigh, ed., Blackwell Science, Oxford, UK, 1998, 133 pp.
12. International Union of Pure and Applied Chemistry. Inorganic Chemistry Division, Commission on Atomic Weights and Isotopic Abundances, "Atomic Weights of the Elements. Review 2000 (IUPAC Technical Report)", *Pure Appl. Chem.* **2003**, *75*, 683-799.

American Chemical Society Nomenclature

301. Chemical Abstracts Service Index Nomenclature

Introductions to Subject Indexes and Name Selection Manuals

1. American Chemical Society. Chemical Abstracts Service, "The Naming and Indexing of Chemical Compounds from Chemical Abstracts" [a reprint of the Introduction to the *Subject Index* to Volume 56 (January-June, 1962)], Chemical Abstracts Service, Columbus, Ohio, 1962. A previous edition was reprinted from the Introduction to the 1945 *Subject Index* (*Chemical Abstracts* **1945**, 39, 5867-5975) which was combined with revisions introduced in 1957 (*Subject Index* **1957**, 51, 1R-28R).
2. —, "Combined Introductions: Subject, Formula, Ring System, and HAIC Indexes to Volume 66, January-June, 1967", Chemical Abstracts Service, Columbus, Ohio, 1968.
3. —, *Naming and Indexing of Chemical Compounds*, 1969 edition, Chemical Abstracts Service, Columbus, Ohio, 1969.
4. —, "Naming and Indexing of Chemical Substances for *Chemical Abstracts* during the Ninth Collective Period (1972-1976)" [a reprint of Section IV (Selection of Index Names for Chemical Substances) from the Volume 76 *Index Guide*], Chemical Abstracts Service, Columbus, Ohio, 1973.
5. —, *Chemical Substance Name Selection Manual for the Ninth Collective Period (1972-1976)*, Chemical Abstracts Service, Columbus, Ohio, 1973.
6. —, "Selection of Index Names for Chemical Substances" in the Volume 76-85 Cumulative *Index Guide* (1972-1976), Chemical Abstracts Service, Columbus, Ohio, 1977, Appendix IV.
7. —, "Naming and Indexing of Chemical Substances for *Chemical Abstracts*" [a reprint of Appendix IV (Selection of Index Names for Chemical Substances) from the 1977 *Index Guide*], Chemical Abstracts Service, Columbus, Ohio, 1978.
8. —, *Chemical Substance Name Selection Manual*, 1978 edition, Chemical Abstracts Service, Columbus, Ohio, 1978.
9. —, "Selection of Index Names for Chemical Substances" in the 1977-1981 *Index Guide*, Chemical Abstracts Service, Columbus, Ohio, 1982, Appendix IV.
10. —, "Naming and Indexing of Chemical Substances for *Chemical Abstracts*" [a reprint of Appendix IV (Chemical Substance Index Names) from the 1982 *Index Guide*], Chemical Abstracts Service, Columbus, Ohio, 1982.
11. —, *Chemical Substance Name Selection Manual*, 1982 edition, Chemical Abstracts Service, Columbus, Ohio, 1982.
12. —, "Chemical Substance Index Names" in the 1984 *Index Guide*, Chemical Abstracts Service, Columbus, Ohio, 1984, Appendix IV.
13. —, "Naming and Indexing of Chemical Substances for *Chemical Abstracts*" [a reprint of Appendix IV (Chemical Substance Index Names) from the 1985 *Index Guide*], Chemical Abstracts Service, Columbus, Ohio, 1985.
14. —, "Chemical Substance Index Names", in the 1982-1986 *Index Guide*, Chemical Abstracts Service, Columbus, Ohio, 1987, Appendix IV.
15. —, "Naming and Indexing of Chemical Substances for *Chemical Abstracts*" [a reprint of Appendix IV (Chemical Substance Index Names) from the 1987 *Index Guide*], Chemical Abstracts Service, Columbus, Ohio, 1987.
16. —, "Chemical Substance Index Names", Appendix IV in the 1989 *Index Guide*, Chemical Abstracts Service, Columbus, Ohio, 1989.
17. —, "Chemical Substance Index Names", Appendix IV in the 1990 *Index Guide*, Chemical Abstracts Service, Columbus, Ohio, 1990.
18. —, "Chemical Substance Index Names", in the 1987-1991 *Index Guide*, Chemical Abstracts Service, Columbus, Ohio, 1992, Appendix IV (also appears in the "12th Collective Index on CD-ROM, Index Guide Appendixes I-IV [a reprint of Appendixes I-IV from the Index Guide to the 12th Collective Index], Chemical Abstracts Service, Columbus, Ohio, 1993).
19. —, "Naming and Indexing of Chemical Substances for *Chemical Abstracts*" [a reprint of Appendix IV (Chemical Substance Index Names) from the 1992 *Index Guide*], Chemical Abstracts Service, Columbus, Ohio, 1992.
20. —, *Chemical Substance Name Selection Manual*, 1982 edition (Revised, 1989) Chemical Abstracts Service, Columbus, Ohio.
21. —, "Chemical Substance Index Names", Appendix IV in the 1994 *Index Guide*, Chemical Abstracts Service, Columbus, Ohio, 1994.
22. —, "Chemical Substance Index Names" in the 1992-1996 *Index Guide*, Chemical Abstracts Service, Columbus, Ohio, 1997, Appendix IV.
23. —, "Chemical Substance Index Names" in the 1997 *Index Guide*, Chemical Abstracts Service, Columbus, Ohio, 1997, Appendix IV.
24. —, "Naming and Indexing of Chemical Substances for CHEMICAL ABSTRACTS" [A reprint of Appendix IV (Chemical Substance Index Names) from the CHEMICAL ABSTRACTS 1997 *Index Guide*], Chemical Abstracts Service, Columbus, Ohio, 1997.
25. —, "Chemical Substance Index Names" in the 1999 *Index Guide*, Chemical Abstracts Service, Columbus, Ohio, 1999, Appendix IV.
26. —, "Chemical Substance Index Names" in the 1997-2001 *Index Guide*, Chemical Abstracts Service, Columbus, Ohio, 2002, Appendix IV.
27. —, "Chemical Substance Index Names" in the 2002 *Index Guide*, Chemical Abstracts Service, Columbus, Ohio, 2002, Appendix IV.

Ring Nomenclature Handbooks

1. A. M. Patterson and L. T. Capell, *The Ring Index*, Reinhold, New York, 1940, 661 pp.

2. A. M. Patterson, L. T. Capell, and D. F. Walker, *The Ring Index*, 2nd ed., American Chemical Society, Washington, D. C., 1960, 1425 pp.; Supplement 1, 1963, 371 pp.; Supplement 2, 1964, 515 pp.; Supplement 3, 1965, 581 pp.; "New Ring Systems from Chemical Abstracts Volumes 60-63", Chemical Abstracts Service, Columbus, Ohio, 1967, 285 pp.
3. *Parent Compound Handbook*, American Chemical Society, Washington, D. C., 1977 (Annual supplements appeared through 1983).
4. *Ring Systems Handbook*, 1984 edition, Chemical Abstracts Service, Columbus, Ohio, 1984 (Six cumulative supplements were published, the last in November 1987).
5. *Ring Systems Handbook*, 1988 edition, Chemical Abstracts Service, Columbus, Ohio, 1988 (Eight cumulative supplements were published, the last in November, 1992).
6. *Ring Systems Handbook*, 1993 edition, Chemical Abstracts Service, Columbus, Ohio, 1993 (Eight cumulative supplements were published, the last in November 1997).
7. *Ring Systems Handbook*, 1998 edition, Chemical Abstracts Service, Columbus, Ohio, 1998 (Eight cumulative supplements were published, the last in November 2002).
8. *Ring Systems Handbook*, 2003 edition, Chemical Abstracts Service, Columbus, Ohio, 2003.

Nomenclature Publications

1. A. M. Patterson, L. T. Capell, and D. F. Walker, *The Ring Index*, 2nd ed., American Chemical Society, Washington, D.C., 1960. Introduction. pp. ix-xxvi; Suppl. 1, 1963, Introduction, pp. x-xiii.
2. J. E. Blackwood, C. L. Gladys, K. L. Loening, A. E. Petrarca, and J. E. Rush, "Unambiguous Specification of Stereoisomerism about a Double Bond", *J. Am. Chem. Soc.* **1968**, 90, 509-510.
3. J. E. Blackwood, C. L. Gladys, A. E. Petrarca, W. H. Powell, and J. E. Rush, "Unique and Unambiguous Specification of Stereoisomerism about a Double Bond in Nomenclature and Other Notation Systems", *J. Chem. Doc.* **1968**, 8, 30-32.
4. K. L. Loening, W. Metanowski, and W. H. Powell, "Indexing of Polymers in *Chemical Abstracts*", *J. Chem. Doc.* **1969**, 9, 248-251.
5. N. Donaldson, W. H. Powell, R. J. Rowlett, Jr., R. W. White, and K. Yorka, "Chemical Abstracts Index Names for Chemical Substances in the Ninth Collective Period (1972-76)", *J. Chem. Doc.* **1974**, 14, 3-15.
6. R. J. Rowlett, Jr. and F. A. Tate, "A Computer-Based System for Handling Chemical Nomenclature and Structural Representations", *J. Chem. Doc.* **1972**, 12, 125-128.
7. R. J. Rowlett, Jr. and D. W. Weisgerber, "Handling Commercial Product Names at Chemical Abstracts Service", *J. Chem. Doc.* **1974**, 14, 92-95.
8. J. E. Blackwood and P. M. Giles, Jr., "Chemical Abstracts Stereochemical Nomenclature of Organic Substances in the Ninth Collective Period (1972-1976)", *J. Chem. Inf. Comput. Sci.* **1975**, 15, 67-72.
9. M. F. Brown, B. R. Cook, and T. E. Sloan, "Stereochemical Notation in Coordination Chemistry. Mononuclear Complexes", *Inorg. Chem.* **1975**, 14, 1273-1278.
10. M. F. Brown, B. R. Cook, and T. E. Sloan, "Stereochemical Notation in Coordination Chemistry. Mononuclear Complexes of Coordination Numbers Seven, Eight, and Nine", *Inorg. Chem.* **1978**, 17, 1563-1568.
11. A. C. Isenberg, J. T. LeMasters, A. F. Maxwell, and G. G. Vander Stouw, "Procedures for Sorting Chemical Names for Chemical Abstracts' Indexes", *J. Chem. Inf. Comput. Sci.* **1985**, 25(4), 410-412.
12. J. E. Blackwood, P. E. Blower, Jr., S. W. Layten, D. H. Lillie, A. H. Lipkus, J. P. Peer, C. Qian, L. M. Staggengborg, and C. E. Watson, "Chemical Abstracts Service Chemical Registry System. 13. Enhanced Handling of Stereochemistry", *J. Chem. Inf. Comput. Sci.* **1991**, 31, 204-212.
13. C. L. Gladys and A. L. Goodson, "Numbering of Interior Atoms in Fused Ring Systems", *J. Chem. Inf. Comput. Sci.* **1991**, 31, 523-526.
14. P. M. Giles, Jr. and W. V. Metanowski, "The History of Chemical Substance Nomenclature at Chemical Abstracts Service (CAS)" in *Organic Chemistry: Its Language and its State of the Art*, M. Volkan Kisakürek, ed., Verlag Helvetica Chimica Acta, Basel, 1993, pp. 173-196.
15. L. M. Staggengborg, "Stereochemistry in the CAS Registry File", *Spec. Publ. - R. Soc. Chem.* **1993**, 120, 89-112. (Recent Advances in Chemical Information II).
16. A. L. Goodson, C. L. Gladys, and D. E. Worst, "Numbering and Naming of Fullerenes by Chemical Abstracts Service", *J. Chem. Inf. Comput. Sci.* **1995**, 35, 969-978.
17. D. W. Weisgerber, "Chemical Abstracts Service Chemical Substance Index Nomenclature" in *Chemical Nomenclature*, K. J. Thurlow, ed., Kluwer Academic Publishers, Dordrecht, The Netherlands, 1998, pp. 66-102.
18. C. E. Carraher, Jr., "Chemical Abstracts Based Polymer Nomenclature", *J. Polym. Mater.* **2000**, 18, 1-6.
19. S. J. Teague, "Siloxanes and Silicones in the CAS Databases", *Polym. Prepr.* **2001**, 42(1), xviii-xxii.

302. American Chemical Society Committee

1. American Chemical Society, "Recommendations of the Nomenclature Committee of the Organic Division of the ACS to the Nomenclature Committee of the National Society", *J. Am. Chem. Soc. Proc.* **1931**, 40-41.
2. —, "The Pronunciation of Chemical Words", *Ind. Eng. Chem., News Ed.* **1934**, 12, 202-205.

3. —, "Nomenclature of the Hydrogen Isotopes and Their Compounds", *Ind. Eng. Chem., News Ed.* **1935**, 13, 200-201.
4. —, "Report of the Committee for the Revision of the Nomenclature of Pectic Substances", *Chem. Eng. News* **1944**, 22, 105-106.
5. —, "Nomenclature of Carotenoid Pigments", *Chem. Eng. News* **1946**, 24, 1235-1236.
6. —, "The Naming of *cis* and *trans* Isomers of Hydrocarbons Containing Olefin Double Bonds", *Chem. Eng. News* **1949**, 27, 1303.
7. —, "The Designation of 'Extra' Hydrogen in Naming Cyclic Compounds", *Chem. Eng. News* **1949**, 27, 1303.
8. —, "The Naming of Geometric Isomers of Polyalkyl Monocycloalkanes", *Chem. Eng. News* **1950**, 28, 1842-1843.
9. —, "The Report of the ACS Nomenclature, Spelling, and Pronunciation Committee for the First Half of 1952", *Chem. Eng. News* **1952**, 30, 4513-4526.
 - A. "Arene and Arylene", p. 4513.
 - B. "Halogenated Derivatives of Hydrocarbons", pp. 4513-4514.
 - C. "The Use of 'Per' in Naming Halogenated Organic Compounds", pp. 4514-4515.
 - D. "The Use of 'H' to Designate the Positions of Hydrogens in Almost Completely Fluorinated Organic Compounds", p. 4515.
 - E. "Organic Compounds Containing Phosphorus", pp. 4515-4522.
 - F. "Organosilicon Compounds", pp. 4517-4522. (These rules supersede the ACS 1946 rules which appeared in *Chem. Eng. News* **1946**, 24, 1233-1234.)
 - G. "Nomenclature of Natural Amino Acids and Related Substances", pp. 4522-4526. (These rules were reprinted in *J. Am. Chem. Soc.* **1960**, 82, 5575-5577. They replaced the 1947 ACS rules which appeared in *Chem. Eng. News* **1947**, 25, 1364-1367. See also ¶ 297, item 16.)
10. —, "A New General System for the Naming of Stereoisomers", G. E. McCasland, included with the "Report of the Advisory Committee on Configurational Nomenclature", July 14, 1953, H. B. Vickery, Chairman, to the Nomenclature Committee, Division of Organic Chemistry, American Chemical Society, Washington, D.C.
11. —, "Addendum to Definitive Rules for the Nomenclature of Natural Amino Acids and Related Substances", *J. Org. Chem.* **1963**, 28, 291-293. (See also ¶ 297, item 16 and item 9G above).
12. —, "A Proposed System of Nomenclature for Terpene Hydrocarbons", *Chem. Eng. News* **1954**, 32, 1795-1797.
13. —, "Nomenclature for Terpene Hydrocarbons", a report of the Nomenclature Committee of the Division of Organic Chemistry of the American Chemical Society, American Chemical Society, Washington, D.C., 1955, 98 pp. (*Advances in Chemistry Series* No. 14.)
14. —, "Rules of Carbohydrate Nomenclature", *J. Org. Chem.* **1963**, 28, 281-291. (This report was the result of a cooperative effort by the Nomenclature Committee of the Division of Carbohydrate Chemistry of the American Chemical Society and a British Committee on Carbohydrate Nomenclature [a Subcommittee of the Publications Committee of the Chemical Society, London]. They are sometimes referred to as the "Anglo-American Rules" and were accepted by the Council of the American Chemical Society in 1962. They replaced the ACS 1953 rules which appeared in *Chem. Eng. News* **1953**, 31, 1776-1782, which in turn replaced the ACS 1948 Carbohydrate Nomenclature Rules published in *Chem. Eng. News* **1948**, 26, 1623-1629. These rules precede the tentative IUPAC carbohydrate rules, see ¶ 297, item 5.)
15. —, "A Structure-Based Nomenclature for Linear Polymers", *Macromolecules* **1968**, 1, 193-198. These rules precede the IUPAC rules; see ¶ 299, item 5.
16. —, "The Nomenclature of Boron Compounds", *Inorg. Chem.* **1968**, 7, 1945-1964. These rules precede the IUPAC rules; see ¶ 298, item 2.
17. —, "ACS Committee on Nomenclature Recommendations", *J. Chem. Doc.* **1973**, 13, 45 (News and Notes) (On the use of the diagonal, the hyphen, and the dash in chemical names).
18. American Chemical Society. Division of Carbohydrate Chemistry. Nomenclature Committee and the British Carbohydrate Nomenclature Committee, "Rules for Conformational Nomenclature for Five- and Six-Membered Rings in Monosaccharides and Their Derivatives", *J. Chem. Soc., Chem. Commun.* **1973**, 505-508. These rules precede the IUPAC recommendations; see ¶ 297, item 6.
19. American Chemical Society. Division of Polymer Chemistry. Nomenclature Committee, "Abbreviations for Thermoplastics, Thermosets, Fiber, Elastomers, and Additives", *Polym. News* **1983**, 9, 101-110; **1985**, 10, 169-172.
20. J. A. Young, "Revised Nomenclature for Highly Fluorinated Organic Compounds", *J. Chem. Doc.* **1974**, 14, 98-100.
21. W. C. Fernelius and W. H. Powell, "Confusion in the Periodic Table of the Elements", *J. Chem. Educ.* **1982**, 59, 504-508.
22. K. L. Loening, "Recommended Format for the Periodic Table of the Elements", *J. Chem. Educ.* **1984**, 61, 136.
23. K. L. Loening, "Activities in the United States Relating to Chemical Terminology and Nomenclature", *TermNet News* **1987**, (18), 3-6.
24. B. P. Block, W. C. Fernelius, and W. H. Powell, *Inorganic Chemical Nomenclature: Principles and Practice*, American Chemical Society, Washington, D.C., 1990, 210 pp.

History and Development of Chemical Nomenclature

303. General

1. E. J. Crane, "The Standardization of Chemical Nomenclature", *J.*

Chem. Educ. **1931**, 8, 1335-1340. (Contains references.)

2. A. D. Mitchell, *British Chemical Nomenclature*, Edward Arnold & Co., London, 1948, 156 pp.
3. E. J. Crane, "Chemical Nomenclature in the United States" in *Chemical Nomenclature*, American Chemical Society, Washington, D.C., 1953, pp. 55-64. (*Advances in Chemistry Series* No. 8.)
4. R. S. Cahn and A. D. Mitchell, "Chemical Nomenclature in Britain Today" in *Chemical Nomenclature*, American Chemical Society, Washington, D.C., 1953, pp. 49-54. (*Advances in Chemistry Series* No. 8.)
5. K. A. Jensen, "Problems of an International Chemical Nomenclature" in *Chemical Nomenclature*, American Chemical Society, Washington, D.C., 1953, pp. 38-48. (*Advances in Chemistry Series* No. 8.)
6. H. S. Nutting, "Nomenclature in Industry" in *Chemical Nomenclature*, American Chemical Society, Washington, D.C., 1953, pp. 95-98. (*Advances in Chemistry Series* No. 8.)
7. G. M. Dyson, "Development of Chemical Symbols and their Relation to Nomenclature" in *Chemical Nomenclature*, American Chemical Society, Washington, D.C., pp. 99-105. (*Advances in Chemistry Series* No. 8.)
8. J. W. Perry, "The Role of Terminology in Indexing, Classifying, and Coding" in *Chemical Nomenclature*, American Chemical Society, Washington, D.C., 1953, pp. 106-112. (*Advances in Chemistry Series* No. 8.)
9. A. M. Patterson, *Words About Words*, American Chemical Society, Washington, D.C., 1957, 86 pp. (A compilation of the column by A. M. Patterson which appeared in *Chem. Eng. News* 1951-1956.)
10. L. T. Capell, "Effect of Changes in Nomenclature on the Use of Indexes" in *Searching the Chemical Literature*, American Chemical Society, Washington, D.C., 1961, pp. 58-66. (*Advances in Chemistry Series* No. 30.)
11. J. D. Scott and K. L. Loening, "Inorganic-Organic Nomenclature", *J. Chem. Doc.* **1964**, 4, 66-69.
12. O. C. Dermer, G. Gorin, and K. L. Loening, "The Standardization of Chemical Language", *Int. J. Sociol. Lang.* **1976**, 11, 61-83.
13. R. S. Cahn and O. C. Dermer, *Introduction to Chemical Nomenclature*, 5th, ed., Butterworths, London, 1979, 200 pp.
14. K. L. Loening, "Nomenclature" in *Kirk-Othmer Encyclopedia of Chemical Technology*, 3rd ed., John Wiley & Sons, New York, Vol. 16, 1981, pp. 28-46; 2nd ed., Vol. 14, 1967, pp. 1-15.
15. R. Lees and A. F. Smith eds., *Chemical Nomenclature Usage*, Ellis Horwood Ltd., Chichester, UK, 1983, 172 pp.
16. R. Fennell, *History of IUPAC, 1919-1987*, Blackwell Science, Oxford, UK, 1994 354 pp.
17. Council of Biology Editors. Style Manual Committee, *Scientific Style and Format; CBE Manual for Authors, Editors, and Publishers*. E. Huth, ed., 6th ed., Cambridge University Press, Cambridge, UK, 1995. 825 pp.
18. P. A. S. Smith, "Nomenclature" in *Kirk-Othmer Encyclopedia of Chemical Technology*, 4th ed., John Wiley & Sons, New York, Vol. 17, 1996, pp. 238-259.
19. K. J. Thurlow, ed., *Chemical Nomenclature*, Kluwer Academic Publishers, Dordrecht, The Netherlands, 1998, 247 pp.
20. E. D. Godly, "The Need for Good Nomenclature" in *Chemical Nomenclature*, K. J. Thurlow, ed., Kluwer Academic Publishers, Dordrecht, The Netherlands, 1998, pp. 1-26.
21. S. S. Brown, *History of IUPAC 1988-1999. Supplement to History of IUPAC 1919-1987*, IUPAC, 2001, pp. 355-442 (Update of item 16, above).
22. J. Simon, "Authority and Authorship in the Method of Chemical Nomenclature", *Ambix* **2002**, 49, 206-226.

304. Organic chemistry

Geneva Rules

1. A. Pictet, "Le Congres International de Geneve pour la Reforme de la Nomenclature Chimique", *Arch. Sci. Phys. Nat.* **1892**, [3] 27, 485-520.
2. M. Hanriot, "Congres de Nomenclature Chimique, Geneve 1892", *Bull. Soc. Chim. Paris Suppl.* **1892**, s. 3, 7, XIV-XXIV.
3. H. E. Armstrong, "The International Conference on Chemical Nomenclature", *Nature*, **1892**, 46, 56-58.
4. F. Tiemann, "Ueber die Beschlusse des Internationalen, in Genf von 19 bis 22 April 1892, versammelten Congresses zur Regelung der chemischen Nomenklatur", *Ber. Dtsch. Chem. Ges.* **1893**, 26, 1595-1631.

Liege Rules

1. International Union of Chemistry. Commission on the Reform of the Nomenclature of Organic Chemistry, "Definitive Report, Liege Meeting, 1930". (Translation with comments by A. M. Patterson, *J. Am. Chem. Soc.* **1933**, 55, 3905-3925. Appeared also in English, *J. Chem. Soc.* **1931**, 1607-1616.)
2. International Union of Chemistry. Commission on the Reform of the Nomenclature of Organic Chemistry, "Full Text of the New Organic Nomenclature Rules". Reported by A. M. Patterson, *Science* **1938**, 87, 215-216 (Rules 34 and 49 of the Liege Report are given in full).

Amsterdam Rules

1. International Union of Pure and Applied Chemistry. Organic Chemistry Division. Commission on the Nomenclature of Organic Chemistry, "Nomenclature of Organosilicon Compounds", *C. R. de la Quinzieme Conference*, Amsterdam, 1949, 127-132.

2. —, "Changes and Additions to the Definitive Report [of the Liege Meeting]", *C. R. de la Quinzieme Conference*, Amsterdam, 1949, 132-185.

Proposals and Reviews

1. A. Hantzsch and J. H. Weber, *Ber. Dtsch. Chem. Ges.* **1887**, 20, 3118-3132.
2. O. Widman, *J. Prakt. Chem.* **1888**, 38, 185-201.
3. A. Baeyer, "Systematik und Nomenklatur Bicyclischer Kohlenwasserstoffe", *Ber. Dtsch. Chem. Ges.* **1900**, 33, 3771-3775.
4. E. Buchner and W. Weigand, "Bornylen und Diazoessigester [Nebst einer Nomenklatur Tricyclischer Kohlenstoff-Ringsysteme nach Adolf von Baeyer]", *Ber. Dtsch. Chem. Ges.* **1913**, 46, 2108-2117.
5. A. M. Patterson and C. E. Curran, "A System of Organic Nomenclature", *J. Am. Chem. Soc.* **1917**, 39, 1623-1638.
6. A. M. Patterson, "Proposed International Rules for Numbering Organic Ring Systems", *J. Am. Chem. Soc.* **1925**, 47, 543-561.
7. —, "The Nomenclature of Parent Ring Systems", *J. Am. Chem. Soc.* **1928**, 50, 3074-3087.
8. —, "The Nomenclature of Organic Compounds of Complex Function", *Rec. Trav. Chim.* **1929**, 48, 1012-1017.
9. P. E. Verkade, "La revision recente de la nomenclature des combinaisons organiques", *Rec. Trav. Chim.* **1932**, 51, 185-217.
10. A. M. Patterson and L. T. Capell, "The Ring Index", Reinhold, New York, 1940, pp. 20-27.
11. F. Richter, "Basic Features of Nomenclature in Organic Chemistry" in *Chemical Nomenclature*, American Chemical Society, Washington, D.C., 1953, pp. 65-74. (*Advances in Chemistry Series No. 8*.)
12. P. E. Verkade, "Organic Chemical Nomenclature, Past, Present, and Future" in *Chemical Nomenclature*, American Chemical Society, Washington, D.C., 1953, pp. 75-82. (*Advances in Chemistry Series No. 8*.)
13. L. T. Capell and K. L. Loening, "Principles of Organic Nomenclature" in *Treat. Anal. Chem.*, I. M. Kolthoff and P. J. Elving, eds., Interscience, New York, Vol. 11, 1965, Part II, Section B, pp. 1-44.
14. D. R. Eckroth, "Method for Manual Generation of Correct von Baeyer Names of Polycyclic Hydrocarbons", *J. Org. Chem.* **1967**, 32, 3362-3365.
15. A. D. McNaught, "The Nomenclature of Heterocycles" in *Advances in Heterocyclic Chemistry*, A. R. Katritzky and A. J. Boulton, eds., Academic Press, New York, 1976, Vol. 20, pp. 175-247.
16. A. Balaban and P. von Rague Schleyer, "Systematic Classification and Nomenclature of Diamond Hydrocarbons. I. Graph-Theoretical Enumeration of Polymantanes", *Tetrahedron* **1978**, 34, 3599-3609.
17. N. Lozac'h, A. L. Goodson, and W. H. Powell, "Nodal Nomenclature - General Principles", *Angew. Chem.* **1979**, 91, 951-964; *Angew. Chem., Int. Ed. Engl.* **1979**, 18, 887-899.
18. A. L. Goodson, "Graph Based Chemical Nomenclature. 1. Historical Background and Discussion", *J. Chem. Inf. Comput. Sci.* **1980**, 20, 167-172; "2. Incorporation of Graph-Theoretical Principles into Taylor's Nomenclature Proposal", *ibid.* **1980**, 20, 172-176.
19. K. L. Loening, "Hydrocarbons: Nomenclature" in *Kirk-Othmer Encyclopedia of Chemical Technology*, 3rd ed., John Wiley and Sons, New York, Vol. 12, 1980, pp. 892-900; 2nd ed., Vol. 11, 1966, pp. 288-293.
20. D. Eckroth, "Nitrogen's Hydrido Oxo Acids", *J. Chem. Inf. Comput. Sci.* **1983**, 23, 157-159.
21. A. L. Goodson, "Application of Graph-Based Chemical Nomenclature to Theoretical and Preparative Chemistry", *Croat. Chem. Acta* **1983**, 56, 315-324.
22. N. Lozac'h and A. L. Goodson, "Nodal Nomenclature II - Specific Nomenclature for Parent Hydrides, Free Radicals, Ions, and Substituents", *Angew. Chem.* **1984**, 96, 1-15; *Angew. Chem., Int. Ed. Engl.* **1984**, 23, 33-46.
23. A. D. McNaught and P. A. S. Smith, "Nomenclature of Heterocyclic Compounds" in *Comprehensive Heterocyclic Chemistry*, A. R. Katritzky and C. W. Rees, eds., Pergamon Press, Oxford, UK, 1984, pp. 7-45.
24. A. L. Goodson and N. Lozac'h, "Advantages of Nodal Nomenclature for Uniquely Identifying Atoms in Chemical Nomenclature", *Croat. Chem. Acta* **1986**, 59, 547-563.
25. W. V. Metanomski, "Unusual Names Assigned to Chemical Substances", *Chem. Int.* **1987**, 9, 211-215; *Irish Chem. News* **1988** (Spring), 31-34; *Biochim. Clin.* **1990**, 14, 58-62.
26. A. L. Goodson, "Nomenclature of Chemical Compounds" in *Chemical Graph Theory, Introduction and Fundamentals*, D. Bonchev and D. H. Rouvray, eds., Gordon and Breach Science Publishers, New York, 1991, Chapter 3, pp. 97-132.
27. H. A. Smith, Jr., "The Centennial of Systematic Organic Nomenclature", *J. Chem. Educ.* **1992**, 69, 863-865.
28. P. A. S. Smith, "Trivial Names for Chemical Substances: Will They Be Taught or Forgotten in the Twenty-First Century", *J. Chem. Educ.* **1992**, 69, 877-878.
29. J. G. Traynham, "Organic Nomenclature: The Geneva Conference and the Following Fifty Years" in *Organic Chemistry: Its Language and its State of the Art*, M. Volkan Kisakürek, ed., Verlag Helvetica Chimica Acta, Basel, 1993, pp. 1-8.
30. K. L. Loening, "Organic Nomenclature: The Geneva Conference and the Second Fifty Years: Some Personal Observations" in *Organic Chemistry: Its Language and its State of the Art*, M. Volkan Kisakürek, ed., Verlag Helvetica Chimica Acta, Basel, 1993, pp. 35-45.
31. E. W. Godly, "Chemical Nomenclature in the Government Laboratory" in *Organic Chemistry: Its Language and Its State of the Art*, Verlag Helvetica Chimica Acta, Basel, 1993, pp. 117-132.
32. J. H. Stocker, "Tomorrow's Organic Nomenclature" in *Organic Chemistry: Its Language and its State of the Art*, M. Volkan Kisakürek, ed., Verlag Helvetica Chimica Acta, Basel, 1993, pp. 161-171.
33. B. C. L. Weedon and G. P. Moss, "Carotenoids, Structure and Nomenclature", in *Carotenoids: Isolation and Analysis*, Vol. 1A, G. Britton, S. Liaaen-Jensen, and H. Pfander, eds., Birkhäuser Verlag, Basel, 1995, Chapter 3, pp. 27-70.
34. R. Guitart, P. Puig, and J. Gómez-Catalán, "Requirement for a Standardized Nomenclature Criterion for PCBs; Computer-Assisted Assignment of Correct Congener Denominations and Numbering", *Chemosphere* **1993**, 27, 1451-1459.
35. J. Kahovec, "Segment Nomenclature of Organic Compounds", *J. Chem. Inf. Comput. Sci.* **1996**, 36, 1-6.
36. W. H. Koppenol and J. G. Traynham, "Say NO to Nitric Oxide: Nomenclature for Nitrogen- and Oxygen-Containing Compounds", *Methods Enzymol.* **1996**, 268(Nitric Oxide, Part A), 3-7. Related commentary, *ibid.* p. 291.
37. S. Kopp-Kubel, "Drug Nomenclature" in *The Practice of Medicinal Chemistry*, 2nd ed., C. G. Wermuth, ed., Elsevier, London, 2003, pp. 697-705. Superseded 1996 edition.
38. A. Srikrishna, "A Rapid Way of Computing the Number of Rings Present in a Polycyclic Organic Compound", *J. Chem. Educ.* **1996**, 73, 428.
39. K. Mislow and C. Liang, "Knotted Structures in Chemistry, Biochemistry, and Molecular Biology", *Croat. Chem. Acta* **1996**, 69, 1385-1403.
40. D. Boring, "The Development and Adoption of Nonproprietary, Established, and Proprietary Names for Pharmaceuticals", *Drug Inf. J.* **1997**, 31, 621-634.
41. U. K. Deiters, "Some Remarks on the Nomenclature of Refrigerants", *Fluid Phase Equilib.* **1997**, 132, 265-270.
42. S. B. Elk, "Fundamental Difference That Exists between Synthetic versus Analytic Chemical Literature", *J. Chem. Inf. Comput. Sci.* **1997**, 37, 162-164.
43. S. B. Elk, "Uniparametricity - Why a Canonical Ordering (and a Consistent Nomenclature) for Organic Compounds Continues to Evade Us", *J. Chem. Inf. Comput. Sci.* **1997**, 37, 696-700.
44. P. G. Wester, H.-J. de Geus, J. de Boer, and U. A. Th. Brinkman, "Simple Nomenclature for Chlorinated Bornanes, Bornenes and Bornadienes from Which Structural Information Can Be Directly Deduced", *Chemosphere* **1997**, 35, 1187-1194; *Organohalogen Compd.* **1997**, 33, 47-52.
45. P. G. Wester, H.-J. de Geus, J. de Boer, and U. A. Th. Brinkman, "Simple Nomenclature for Chlorinated Camphenes and Dihydrocamphenes From Which Structural Information Can Be Directly Deduced", *Chemosphere* **1997**, 35, 2857-2880.
46. J. E. Merritt and B. J. Bossenbroek, "Basic Resources for Assigning Chemical Names within the Field of Chemical Nomenclature" in *Handbook of Terminology Management*, Vol. 1, *Basic Aspects of Terminology Management*, S. E. Wright and G. Budin, compilers, John Benjamins, Amsterdam, 1997, Section 2.2.5, pp. 218-242.
47. T. Yu. Astakhova and G. A. Vinogradov, "Fullerene Notation and Isomerization Operations", *Fullerene Sci. Technol.* **1997**, 5, 1545-1562.
48. R. G. Harvey, "Polycyclic Aromatic Hydrocarbons: Nomenclature" in *Polycyclic Aromatic Hydrocarbons*, Wiley-VCH Verlag, New York, 1997, pp. 12-20.
49. P. F. Rusch, "Nomenclature Searching" in *Encyclopedia of Computational Chemistry*, P. von Rague Schleyer, ed., John Wiley & Sons, New York, 1998, Vol. 3, pp. 1876-1881.
50. K. J. Thurlow, "IUPAC Nomenclature Part 1, Organic" in *Chemical Nomenclature*, K. J. Thurlow, ed., Kluwer Academic Publishers, Dordrecht, The Netherlands, 1998, pp. 103-126.
51. K. J. Thurlow, "IUPAC Nomenclature Part 2, Organic, Inorganic and Others" in *Chemical Nomenclature*, K. J. Thurlow, ed., Kluwer Academic Publishers, Dordrecht, The Netherlands, 1998, pp. 127-145.
52. R. B. Triggs, "Trivial Nomenclature: the INN and ISO Systems" in *Chemical Nomenclature*, K. J. Thurlow, ed., Kluwer Academic Publishers, Dordrecht, The Netherlands, 1998, pp. 208-234.
53. S. B. Elk, "A Modern Topological Perspective of Ring Compound Taxonomy Created by Re-examining Taylor's Nomenclature System", *THEOCHEM* **1998**, 453, 29-42.
54. —, "Graph Theoretical Logic of Organic Chemistry Nomenclature: Why Eulerian Paths Are Better Suited for Aliphatic Compounds Versus Hamiltonian Paths for Benzenoids", *THEOCHEM*, **1999**, 489, 189-194.
55. P. Stolz, N. Weis, and J. Krooss, "Nomenclature and Occurrence of Glycols and Their Derivatives in Indoor Air" in *Organic Indoor Air Pollutants*, T. Salthammer, ed., Wiley-VCH Verlag, Weinheim, Germany, 1999, pp. 117-125.
56. O. Safarowsky, B. Windisch, A. Mohry, and F. Vogtle, "Nomenclature for Catenanes, Rotaxanes, Molecular Knots, and Assemblies Derived from These Structural Elements", *J. Prakt. Chem.* **2000**, 342, 437-444.
57. S. H. Leung, "Amino Acids, Aromatic Compounds, and Carboxylic Acids: How Did They Get Their Common Names", *J. Chem. Educ.* **2000**, 77, 48-49.
58. J. Chimento, "How to Make Learning Chemical Nomenclature Fun, Exciting, and Palatable", *J. Chem. Educ.* **2000**, 77, 144-145.
59. T. D. Crute, "Classroom Nomenclature Games - BINGO", *J. Chem. Educ.* **2000**, 77, 481-482.
60. R. A. Gossage (letter); S. D. Kinrade, A.-M. E. Gillson, and C. T. G. Knight (reply), "Organosilicon Compounds - A Comment on Nomenclature Usage. Letter and Reply", *J. Chem. Doc., Dalton Trans.* **2002**, (10), 2256-2257.

61. H. Favre and W. H. Powell, "Phane Nomenclature" in *Cyclophane Chemistry for the 21st Century*, H. Takemura, ed., Research Signpost, Trivandrum, India, 2002, pp. 1-9.

Books

- R. Stelzner and H. Kuh, *Nomenklatur-Fragen in der Organischen Chemie*, G.m.b.H., Leipzig-Berlin, 1921.
- A. P. Terent'ev, A. N. Kost, A. M. Tsukerman, and V. M. Potapov, *Nomenklatura Organicheskikh Soedinenii, Obzor, Kritika, Predlozheniya* (Nomenclature of Organic Compounds, Review, Comments, Proposals), Izdatel'stvo Akademii Nauk SSSR, Moscow, 1955, 302 pp.
- N. Lozac'h, *La Nomenclature en Chimie Organique*, Masson et Cie Editeurs, Paris, 1967, 294 pp. (*Monographs de Chimie Organique*, Vol. VI; Complements au *Traite de Chimie Organique*).
- R. B. Fox and W. H. Powell, *Nomenclature of Organic Compounds. Principles and Practice*, 2nd ed., American Chemical Society/Oxford University Press, New York, 2001, 437 pp. Superseded J. H. Fletcher, O. C. Dermer, and R. B. Fox, *Nomenclature of Organic Compounds, Principles and Practice*, American Chemical Society, Washington, D.C., 1974, 337 pp. (*Advances in Chemistry Series No. 126*).
- D. Hellwinkel, *Die systematische Nomenklatur der organischen Chemie* (Systematic Nomenclature of Organic Chemistry), 4th ed., Springer-Verlag, Berlin, 1998, 227 pp. Superseded 3rd ed. of 1982.
- P. E. Verkade, *A History of the Nomenclature of Organic Chemistry*, F. C. Alderweireldt, et al., eds., D. Reidel Publishing Co., Dordrecht, Netherlands, 1985, 528 pp. A collection of translated articles which appeared as follows in *Bull. Soc. Chim. Fr.*: I. "La naissance de la nomenclature de Geneve (1892) et des propositions de nomenclature de Saint-Etienne (1897) et la litterature afferente", *Bull. Soc. Chim. Fr.* **1966**, 1807-1812; II. "Le developpement de la nomenclature de chimie organique pendant la periode de 1889-1897", *ibid.*, **1967**, 4009-4020; III. "Faits et evenements relatifs a la nomenclature de la chimie organique pendant la periode 1897-1911", *ibid.*, **1968**, 1358-1367; IV. "L'activite de l'Association Internationale de Societes Chimiques dans le domaine de la nomenclature de la chimie organique, 1911-1914", *ibid.*, **1969**, 3877-3881; V. "Activites individuelles dans le domaine de la nomenclature de la chimie organique pendant la periode de 1914 a 1930", *ibid.*, **1969**, 4297-4308; VI. "La creation de la nomenclature de Liege", *ibid.*, **1970**, 2739-2746; VII. "Le contenu de la nomenclature de Liege compare a celui de la nomenclature de Geneve", *ibid.*, **1971**, 1634-1647; VIII. "Faits et evenements relatifs a la nomenclature de la chimie organique pendant la periode de 1930 a 1946", *ibid.*, **1971**, 4299-4307; IX. "Sur l'activite de la Commission Internationale pendant la periode de 1946 a 1957", *ibid.*, **1973**, 1961-1971; X. "Sur la contenu des Sections A et B de l'IUPAC Nomenclature of Organic Chemistry", *ibid.*, **1975**, 555-570; XI. "Sur le procede de Combes (1892) pour la nomenclature des composes acycliques a fonction complexe", *ibid.*, **1975**, 1119-1126; XII. "Sur l'histoire de la creation de la Section C de l'IUPAC Nomenclature of Organic Chemistry", *ibid.*, **1975**, 2029-2036; XIII. "Un Livre Roumain tres remarquable sur la nomenclature de la chimie organique, publie en 1913 par C. I. Istrati", *ibid.* **1976**, 1445-1464; XIV. "Sur le contenu de la Section C de l'IUPAC Nomenclature of Organic Chemistry", *ibid.*, **1977**, 457-478; XV. "L'oeuvre de Siboni, sur la nomenclature de la chimie", *ibid.*, **1978**, II, 13-31; XVI. "Historique de la Section D de l'IUPAC Nomenclature of Organic Chemistry", *ibid.*, **1979**, 215-229.
- Handbuch zur Anwendung der Nomenklatur Organisch-Chemischer Verbindungen*, Wolfgang Liebscher, ed., Akademie-Verlag, Berlin, 1979.
- "Guiding Principles for Coining U.S. Adopted Names for Drugs" in *USAN and the USP Dictionary of Drug Names*, C. A. Fleeger, ed., United States Pharmacopeial Convention, Inc., Rockville, Maryland, 1993, I, pp. 781-790. (USAN 1994; 1961-1993 cumulative list.)
- K. Hirayama, *The HIRN System: Nomenclature of Organic Chemistry*, Springer-Verlag, Berlin, 1984, 149 pp.
- J. Heger, *Ako Tvorit Nazvy Organickych Zlucenin* (How to Name Organic Compounds), Slovenske Pedagogicke Nakladatel'stvo, Bratislava, 1985, 163 pp.
- A. Nickon and E. F. Silversmith, *Organic Chemistry: The Name Game, Modern Coined Terms and their Origins*, Pergamon Press, New York, 1987, 347 pp.
- P. Fresenius, *Organisch-chemische Nomenklatur: Grundlagen, Regeln, Beispiele* (Organic Chemical Nomenclature: Principles, Rules, Examples), 4th ed., Wissenschaftliche Verlagsgesellschaft, Stuttgart, Germany, 1998, 343 pp. Superseded 3rd ed. of 1991 and 2nd ed. of 1991. *Organic Chemical Nomenclature: Introduction to the Basic Principles*, trans. by A. J. Dundson, Ellis Harwood Ltd., Chichester, UK, 1989, 294 pp.
- E. W. Godly, *Naming Organic Compounds: A Systematic Instruction Manual*, Ellis Harwood Ltd., Chichester, UK, 1989, 267 pp.
- K. Loening, J. Merritt, D. Later, and W. Wright, *Polynuclear Aromatic Hydrocarbons Nomenclature Guide*, 1st ed., Battelle Press, Columbus, Ohio, 1990, 87 pp.
- F. G. Alcaraz, *Nomenclatura de Quimica Organica* (Nomenclature of Organic Chemistry), Universidad de Murcia, Murcia, Spain, 1991, 686 pp.
- H. Favre, *La Nomenclature pour la Chimie Organique; Les Noms Substitutifs et Les Noms de Classes Fonctionnelles* (Nomenclature for Organic Chemistry: Substitutive Names and Names of Functional Classes), Order des Chimistes du Québec, Montréal, 1992, 138 pp.
- M. V. Kisakürek, ed., *Organic Chemistry: Its Language and Its State of the Art*. Verlag Helvetica Chimica Acta, Basel, 1993. 196 pp. (Proceedings: Cen-

tenary of the 'Geneva Conference' of 1892. Geneva, Switzerland, 23 April 1992.)

- D. J. Polton, *Chemical Nomenclatures and the Computer*, Research Studies Press, Taunton, UK, John Wiley & Sons, New York, 1993. 264 pp. (Computers and Chemical Structure Information Series No. 4).
- G. Kruse, *Nomenklatur der organischen Chemie* (Nomenclature of Organic Chemistry), Wiley-VCH Verlag, Weinheim, Germany, 1997, 260 pp.
- K.-H. Hellwich, *Chemische Nomenklatur. Die systematische Benennung organisch-chemischer Verbindungen* (Chemical Nomenclature. The Systematic Naming of Organic Chemical Compounds), Govi-Verlag-Pharmazeutischer Verlag, Eschborn, Germany, 1998. 144 pp.
- H. Bartsch, *Die systematische Nomenklatur organischer Arzneistoffe* (Systematic Nomenclature of Organic Pharmaceuticals), Springer-Verlag, Wien, 1998, 112 pp.
- H. Reimlinger, *Nomenklatur organisch-chemischer Verbindungen* (Nomenclature of Organic Chemical Compounds), De Gruyter, Berlin, Germany, 1998, 606 pp.
- D. Hellwinkel, *Systematic Nomenclature of Organic Chemistry: A Directory to Comprehension and Application of Its Basic Principles*, Springer-Verlag, Berlin, Germany, 2001, 228 pp.
- U. Bünzli-Trepp, *Handbuch für die systematische Nomenklatur der organischen Chemie*, Logos Verlag, Berlin, Germany, 2001, 559 pp.

Algorithmic Generation of Chemical Names

- K. Conrow, "Computer Generation of Baeyer Systems Names of Saturated Bridged Bicyclic, Tricyclic, and Tetracyclic Hydrocarbons", *J. Chem. Doc.* **1966**, 6, 206-212.
- D. van Binnendyk and A. C. MacKay, "Computer-assisted Generation of IUPAC Names of Polycyclic Bridged Ring Systems", *Can. J. Chem.* **1973**, 51, 718-723.
- J. Mockus, A. C. Isenberg, and G. G. Vander Stouw, "Algorithmic Generation of Chemical Abstracts Index Names. 1. General Design", *J. Chem. Inf. Comput. Sci.* **1981**, 21, 183-195.
- D. E. Meyer and S. R. Gould, "Microcomputer Generation of Chemical Nomenclature from Graphic Structure Input", *Am. Lab.* **1988**, 20, 92-96.
- S. Davidson, "An Improved IUPAC-based Method for Identifying Alkanes", *J. Chem. Inf. Comput. Sci.* **1989**, 29, 151-155.
- A. M. Marconi, N. Proietti, and E. Zeuli, "Computer Aided Nomenclature: The MARK Algorithm for Organic Chemistry", *Tetrahedron Comput. Methodol.* **1990**, 3, 297-303.
- G. Rücker and C. Rücker, "Nomenclature of Organic Polycycles out of the Computer - How to Escape the Jungle of Secondary Rings", *Chimia* **1990**, 44, 116-120.
- J. L. Wisniewski, "AUTONOM: System for Computer Translation of Structural Diagrams into IUPAC-compatible Names. 1. General Design", *J. Chem. Inf. Comput. Sci.* **1990**, 30, 324-332.
- L. Goebels, A. J. Lawson, and J. L. Wisniewski, "AUTONOM: System for Computer Translation of Structural Diagrams into IUPAC-compatible Names. 2. Nomenclature of Chains and Rings", *J. Chem. Inf. Comput. Sci.* **1991**, 31, 216-225.
- K. W. Raymond, "A LISP Program for the Generation of IUPAC Names from Chemical Structures", *J. Chem. Inf. Comput. Sci.* **1991**, 31, 270-274.
- J. Navech and C. Despax, "Computer Processing and Nomenclature Construction of the IUPAC Name Using the SCN Code Number", *New J. Chem.* **1992**, 16, 1071-1076.
- J. L. Wisniewski, "AUTONOM - A Chemist's Dream: System for (Micro) computer Generation of IUPAC-Compatible Names from Structural Input", in *Chemical Structures 2*, (proceedings: 2nd International Conference on Chemical Structures. Noordwijkerhout, Netherlands, June, 1990), W. A. Warr, ed. Springer-Verlag, Berlin, 1993, pp. 55-63.
- J. Wisniewski, "AUTONOM: A Computer Program for the Generation of IUPAC Systematic Nomenclature Directly From the Graphic Structure Input", *Spec. Publ. - R. Soc. Chem.* **1993**, 120, 77-87. (Recent Advances in Chemical Information II).
- Y. Yoneda, "CHEMO Notation. A Line Notation for Organic Compounds Following IUPAC Nomenclature", *J. Chem. Inf. Comput. Sci.* **1996**, 36, 299-309.
- S. Yuan, C. Zheng, and J. Yao, "Chemical Abstracts Index Names: Automatic Generation", *Ind. Inf. Des. Issues* **1996**, 279-284.
- J. L. Wisniewski, "Nomenclature: Automatic Generation and Conversion" in *Encyclopedia of Computational Chemistry*, P. von Rague Schleyer, ed., John Wiley & Sons, New York, 1998, Vol. 3, pp. 1881-1894.
- S. B. Walker, "Computer-Generated Chemical Nomenclature" in *Chemical Nomenclature*, K. J. Thurlow, ed., Kluwer Academic Publishers, Dordrecht, The Netherlands, 1998, pp. 235-242.
- J. Brecher, "Name=Struct: A Practical Approach to the Sorry State of Real-Life Chemical Nomenclature", *J. Chem. Inf. Comput. Sci.* **1999**, 39, 943-950.
- , "Applying Interpretations of Chemical Names", U.S. Patent **6,584,412 B1**, June 24, 2003.
- "Online Naming Services" are available through a working relationship between IUPAC and two companies:

Advanced Chemistry Development (ACD) <http://www.acdlabs.com/>

Beilstein Information - AutoNom <http://www.beilstein.com/>

305. Biochemistry

1. Reports of the International Union of Chemistry. Commission on the Reform of the Nomenclature of Biological Chemistry:
 - (1) C. Belgium, "La nomenclature de chimie biologique: une reforme heureuse", *Schweiz. Apoth. Z.* **1928**, 66, 193-197.
 - (2) G. Bertrand, "Project de reforme de la nomenclature de chimie biologique (rapport presente a la Commission Internationale en 1922)", *Bull. Soc. Chim. Biol.* **1923**, 5, 96-109.
 - (3) G. Bertrand, "Propositions relatives a la nomenclature des glucides", *Bull. Soc. Chim. Biol.* **1927**, 9, 854-856.
 - (4) M. Bridel, "La reforme de la nomenclature de chimie biologique. Etat de la question a la fin de 1926", *Bull. Soc. Chim. Biol.* **1926**, 8, 1211-1216.
2. J. E. Courtois, "Work of Commission on Nomenclature of Biological Chemistry" in *Chemical Nomenclature*, American Chemical Society, Washington, D.C., 1953, pp. 83-94. (*Advances in Chemistry Series* No. 8.)
3. W. E. Chon "Representation of Macromolecules and Polymers of Biological Importance", *J. Chem. Doc.* **1969**, 9, 235-241.
4. N. A. Nelson, "Prostaglandin Nomenclature," *J. Med. Chem.* **1974**, 17, 911-918.
5. B. M. Benjamin, "Nomenclature in Genetic Engineering", *CBE Views* **1986**, 9, 48-50.
6. *The Terminology of Biotechnology: A Multidisciplinary Problem* (Proceedings of the 1989 International Chemical Congress of Pacific Basin Societies, PACIFICHEM '89), K. L. Loening, ed., Springer-Verlag, Berlin, 1990, 216 pp. This publication includes:
 - (1) K. L. Loening, "Activities of the IUPAC/IUB Joint Commission on Biochemical Nomenclature (JCBN) and the Nomenclature Committee of IUB (NC-IUB)", pp. 1-8.
 - (2) A. Tsugita, "Nomenclature and Protein Databases", pp. 9-16.
 - (3) J. A. Secrist III, "Nomenclature of Altered Proteins", pp. 17-24.
 - (4) J. E. Merritt, B. M. Benjamin, and W. F. Hackett, "Nomenclature and Representation of Biopolymer Sequences by Chemical Abstracts Service", pp. 25-40.
 - (5) D. Horton, "Development of Carbohydrate Nomenclature", pp. 41-50.
 - (6) E. C. Webb, "Enzyme Nomenclature", pp. 51-60.
 - (7) M. I. Johnston, R. J. Black, and M. W. Myers, "Interferon Nomenclature", pp. 61-70.
 - (8) L. Blaine, "The Nomenclature of Monoclonal Antibodies", pp. 71-84.
 - (9) A. L. Willis, W. L. Smith, D. L. Smith, and R. Eglon, "Nomenclature in the Field of Eicosanoids", pp. 93-108.
 - (10) D. O. Schiffman, "United States Adopted Names for Drugs", pp. 109-114.
 - (11) C. H. Barnstein and W. M. Heller, "Nomenclature of Pharmaceuticals", pp. 207-214.
7. J. Ferré, K. B. Jacobsen, and W. Pfeleiderer, "Proposal Towards a Normalization of Pteridine Nomenclature", *Pteridines* **1991**, 2, 129-132.
8. J. E. Merritt and K. L. Loening, "Enzyme Nomenclature" in *Polynuclear Aromatic Hydrocarbons: Measurements, Means, and Metabolism* (11th International Symposium on Polynuclear Aromatic Hydrocarbons, Gaithersburg, Maryland, Sept. 24, 1987), M. Cook, K. Loening, and J. E. Merritt, eds., Battelle Press, Columbus, Ohio, 1991, pp. 583-599.
9. A. F. Hoffman, J. Sjövall, G. Kurz, A. Radomska, C. D. Schteingart, G. S. Tint, Z. R. Vlahcevic, and K. D. R. Setchell, "A Proposed Nomenclature for Bile Acids", *J. Lipid Research*, **1992**, 33, 599-604.
10. K. F. Tipton, "The Naming of Parts", *Trends Biochem. Sci.* **1993**, 18, 113-115.
11. E. C. Webb, "Enzyme Nomenclature: A Personal Retrospective", *FASEB J.* **1993**, 7, 1192-1194.
12. E. Beutler, V. A. McKusick, A. G. Motulsky, C. R. Scriver, and F. Hutchinson, "Mutation Nomenclature: Nicknames, Systematic Names, and Unique Identifiers", *Hum. Mutat.* **1996**, 8(3), 203-206.
13. R. G. H. Cotton and H. H. Kazazian, Jr., "Mutation Nomenclature", *Hum. Mutat.* **1996**, 8(3), iv.
14. R. G. H. Cotton, Ad Hoc Committee on Mutation Nomenclature, "Update on Nomenclature for Human Gene Mutations", *Hum. Mut.* **1996**, 8(3), 197-202; *Hum. Mutat.* **1996**, 8(3), iv (editorial). For related website see <http://ariel.ucsc.unimelb.edu.au:80/~cotton/proposals.htm>
15. L. T. McGlade, B. A. Milot, and J. Scales, "Lipid Terminology", *Am. J. Clin. Nutr.* **1996**, 64, 668.
16. International Union of Pharmacology. Subcommittee on Opioid Receptors, "XII. Classification of Opioid Receptors", *Pharmacol. Rev.* **1996**, 48, 567-592.
17. International Union of Pharmacology. Committee on Receptor Nomenclature and Drug Classification, "XIV. Nomenclature in Nitric Oxide Research", *Pharmacol. Rev.* **1997**, 49, 137-142.
18. Hartig, P. R., "A Genome-Based Receptor Nomenclature", *Ann. N.Y. Acad. Sci.* **1997**, 812, 85-91.
19. J. M. Jez, T. G. Flynn, and T. M. Penning, "A Nomenclature System for the Aldo-Keto Reductase Superfamily", *Adv. Exp. Med. Biol.* **1997**, 414, 579-589.
20. D. F. Taber, J. D. Morrow, and L. J. Roberts, II, "A Nomenclature System for the Isoprostanes", *Prostaglandins* **1997**, 53, 63-67.
21. International Society for Interferon and Cytokine Research. Nomenclature Committee, "Nomenclature of Interferon Receptors and Interferon- σ ", *J. Interferon Cytokine Res.* **1997**, 17, 315-316.
22. C. A. Allen, "A Brief History of the Discovery of the Immunoglobulins and the Origin of the Modern Immunoglobulin Nomenclature", *Immunol. Cell Biol.* **1997**, 75, 65-68.
23. J. W. Bodnar, J. Killian, M. Nagle, and S. Ramchandani, "Deciphering the Language of the Genome", *J. Theor. Biol.* **1997**, 189, 183-193.
24. J. M. Jez, T. G. Flynn, and T. M. Trevor, "A New Nomenclature for the Aldo-Keto Reductase Superfamily", *Biochem. Pharmacol.* **1997**, 54, 639-647.
25. J. Rokach, S. P. Khanapure, S.-W. Hwang, M. Adiyaman, J. A. Lawson, and G. A. FitzGerald, "Nomenclature of Isoprostanes: A Proposal", *Prostaglandins* **1997**, 54, 853-873.
26. A. C. de Groot and J. W. Weijland, "Conversion of Common Names of Cosmetic Allergens to the INCI Nomenclature", *Contact Dermatitis* **1997**, 37, 145-150.
27. "Common Names of Pesticides Recently Approved by the BSI [British Standards Institution]", *Pestic. Sci.* **1997**, 49, 402-405.
28. S. E. Antonarakis, "Recommendations for Human Gene Mutations", *Hum. Mutat.* **1998**, 11, 1-3.
29. J. Buckingham, "Natural Products" in *Chemical Nomenclature*, K. J. Thurlow, ed., Kluwer Academic Publishers, Dordrecht, The Netherlands, 1998, pp. 162-207.
30. D. R. Flower, "A Topological Nomenclature for Protein Structure", *Protein Eng.* **1998**, 11, 723-727.
31. P. J. Moynihan, "Update on the Nomenclature of Carbohydrates and Their Dental Effects", *J. Dent.* **1998**, 26, 209-218.
32. M. Saffran, "Amino Acid Names and Parlor Games: From Trivial Names to a One-Letter Code, Amino Acid Names Have Strained Students' Memories. Is a More Rational Nomenclature Possible?", *Biochem. Educ.* **1998**, 26, 116-118.
33. B. R. Larsen, M. Lahaniati, A. Calogirou, and D. Kotzias, "Atmospheric Oxidation Products of Terpenes: A New Nomenclature", *Chemosphere* **1998**, 37, 1207-1220.
34. S. F. O'Keefe, "Nomenclature and Classification of Lipids", *Food Sci. Technol. (N.Y.)* **2002**, 117 (Food Lipids), 1-40. Superseded *ibid.* **1998**, 88, 1-36.
35. A. J. Kenny, "Introduction: Nomenclature and Classes of Peptidases" in *Proteolytic Enzymes*, E. E. Sterchi and W. Stoecker, eds., Springer-Verlag, Berlin, Germany, 1999, pp. 1-8.
36. A. E. Manzi and H. van Halbeek, "Saccharide Structure and Nomenclature" in *Essentials of Glycobiology*, A. Varki, ed., Cold Spring Harbor Laboratory Press, Cold Spring Harbor, NY, 1999, pp. 17-29.
37. International Union of Pharmacology. Committee on Receptor Nomenclature and Drug Classification, "XX. Current Status of the Nomenclature for Nicotinic Acetylcholine Receptors and Their Subunits", *Pharmacol. Rev.* **1999**, 51, 397-401.
38. Weed Science Society of America. Terminology Committee, "Common and Chemical Names of Herbicides Approved by the Weed Science Society of America", *Weed Sci.* **2003**, 51, 1022-1028. Superseded *ibid.* **2002**, 50, 824-829; **2002**, 50, 130-136; **2000**, 48, 786-792; **1999**, 47, 764-769; **1998**, 46, 729-734.
39. H. Luders, "Structure and Nomenclature of Surface-Active Alkyl Glucosides", *Surfactant Sci. Ser.* **2000**, 91, 7-18.
40. P. Gegeheimer, "Enzyme Nomenclature: Functional or Structural", *RNA* **2000**, 6, 1695-1697.
41. International Union of Pharmacology. Nomenclature Committee, "XXII. Nomenclature of Chemokine Receptors", *Pharmacol. Rev.* **2000**, 52, 145-176.
42. A. Zlotnik and O. Yoshie, "Chemokines: A New Classification System and Their Role in Immunity", *Immunity* **2000**, 12, 121-127.
43. K. Lobb and C. K. Chow, "Fatty Acid Classification and Nomenclature", *Food Sci. Technol. (N.Y.)* **2000**, 96, 1-15.
44. K. Tipton and S. Boyce, "History of the Enzyme Nomenclature System", *Bioinformatics* **2000**, 16, 34-40.
45. I. H. Mather, "A Review and Proposed Nomenclature for Major Proteins of the Milk-Fat Globule Membranes", *J. Dairy Sci.* **2000**, 83, 203-247.
46. S. B. Walker, "Common Names of Pesticides Recently Approved by the BSI [British Standards Institution]", *Pest Manage. Sci.* **2001**, 57, 653-654.
47. International Union of Immunological Societies. World Health Organization Subcommittee on Chemokine Nomenclature, "Chemokine/Chemokine Receptor Nomenclature", *J. Leukocyte Biol.* **2001**, 70, 465-466; *J. Immunol. Methods* **2002**, 262, 1-3.
48. International Union of Pharmacology. Nomenclature Committee, "XXV. Nomenclature and Classification of Adenosine Receptors", *Pharmacol. Rev.* **2001**, 53, 527-552.
49. S. Fields and M. Johnston, "A Crisis in Postgenomic Nomenclature", *Science* **2002**, 296, 671-672.
50. H. M. Wain, M. Lush, F. Ducluzeau, and S. Povey, "Genew: the Human Gene Nomenclature Database", *Nucleic Acids Res.* **2002**, 30, 169-171.
51. H. M. Wain, E. A. Bruford, R. C. Lovering, M. L. Lush, M. W. Wright, and S. Povey, "Guidelines for Human Gene Nomenclature", *Genomics* **2002**, 79, 464-470.
52. L. J. Maltais, J. A. Blake, T. Chu, C. M. Lutz, J. T. Eppig, and I. Jackson, "Rules and Guidelines for Mouse Gene, Allele, and Mutation Nomenclature: A Condensed Version", *Genomics* **2002**, 79, 471-474.
53. R. Aasland *et al.*, "Normalization of Nomenclature for Peptide Motifs as Ligands of Modular Protein Domains", *FEBS Letters* **2002**, 513, 141-144.
54. Lynch, K. R., "Review - Lysophospholipid Receptor Nomenclature", *Biochem. Biophys. Acta* **2002**, 1582, 70-71.
55. E. Banin, Y. Neuberger, Y. Altshuler, A. Halevi, O. Inbar, D. Nir, and A. Dukler, "A Novel Linear Code Nomenclature for Complex Carbohydrates", *Trends Glycosci. Glycotechnol.* **2002**, 14, 127-137.

56. D. S. Nichols and K. Sanderson, "The Nomenclature, Structure, and Properties of Food Lipids" in *Chemical and Functional Properties of Food Lipids*, Z. E. Sikorski and A. Kolakowska, eds., CRC Press, Boca Raton, FL, 2003, pp. 29-59.

57. D. Tsikas, "Incorrect and Inconsistent Use of Homocysteine's Nomenclature: A Potential Source of Misunderstandings", *Eur. J. Clin. Invest.* **2003**, *33*, 1095-1096.

58. S. V. Filip and F. Cavalier, "A Contribution to the Nomenclature of Depsipeptides", *J. Peptide Sci.* **2004**, *10*, 115-118.

306. Inorganic chemistry

1. A. Werner, *New Ideas on Inorganic Chemistry*, translated by E. P. Headley from 2nd German ed., Longmans, Green, and Co., London, 1911. (See also A. Werner, *Z. Anorg. Chem.* **1897**, *14*, 23, and A. Werner and A. Klein, *Z. Anorg. Chem.* **1897**, *14*, 28.)

2. A. Stock, "Einige Nomenclaturfragen der Anorganischen Chemie", *Z. Angew. Chem.* **1919**, *32*(1), 373-376.

3. R. J. Meyer and A. Rosenheim, "Die Vorschlaege der Deutschen Nomenclaturkommission fuer Anorganische Chemie", *Z. Angew. Chem.* **1925**, *38*, 713-715. (See also *Chem. Weekbl.* **1926**, *23*, 93-96.)

4. M. Delepine, "Revision of Inorganic Chemical Nomenclature, Report of the IUPAC Committee for the Reform of the Nomenclature of Inorganic Chemistry", *Chem. Weekblad.* **1926**, *23*, 86-93. (Minutes of the meeting of the Commission for the Reform of Inorganic Chemical Nomenclature, October 6-7, 1925, appear in *Chem. Weekbl.* **1926**, *23*, 96-99.)

5. E. J. Crane, "Report of the Committee on Nomenclature in Inorganic Chemistry, Washington, D.C., September, 1926", *Chem. Weekbl.* **1926**, *23*, 486-487.

6. W. P. Jorissen, H. Bassett, A. Damiens, F. Fichter, and H. Remy, "Rules for Naming Inorganic Compounds. Report of the Committee of the International Union of Chemistry for the Reform of Inorganic Chemical Nomenclature, 1940", *J. Am. Chem. Soc.* **1941**, *63*, 889-897. Also published in *J. Chem. Soc.* **1940**, 1404-1415. (See also R. J. Meyer, "Report on the Nomenclature of Inorganic Compounds", *Chem. Weekbl.* **1936**, *33*, 722-729.)

7. J. D. Scott, "The Need for Reform in Inorganic Chemical Nomenclature", *Chem. Rev.* **1943**, *32*, 73-97.

8. R. V. G. Ewens and H. Bassett, "Inorganic Chemical Nomenclature", *Chem. Ind.* **1949**, *27*, 131-139.

9. H. Bassett, "Some General Principles of Inorganic Chemical Nomenclature" in *Chemical Nomenclature*, American Chemical Society, Washington, D.C., 1953, pp. 5-8. (*Advances in Chemistry Series No. 8.*)

10. W. C. Fernelius, "Nomenclature of Coordination Compounds and Its Relation to General Inorganic Nomenclature" in *Chemical Nomenclature*, American Chemical Society, Washington, D.C., 1953, pp. 9-37. (*Advances in Chemistry Series No. 8.*)

11. W. C. Fernelius, "Principles of Inorganic Nomenclature", in *Treatise on Analytical Nomenclature*, I. M. Kolthoff and P. J. Elving, eds., Interscience, New York, 1961, Vol. 1, Pt. 2, Section A, pp. 1-33.

12. W. C. Fernelius, "Nomenclature of Coordination Compounds: Present Status", *J. Chem. Doc.* **1964**, *4*, 70-83; **1965**, *5*, 200-205.

13. P. M. McDonnell and R. F. Pasternak, "Line-Formula Notation System for Coordination Compounds", *J. Chem. Doc.* **1965**, *5*, 56-60.

14. W. C. Fernelius, "The Nomenclature of Coordination Compounds from Pre-Werner Times to the 1966 IUPAC Report" in *Werner Centennial*, American Chemical Society, Washington, D.C., 1967, pp. 147-160. (*Advances in Chemistry Series No. 62.*)

15. R. M. Adams, "Inorganic Nomenclature in 1966, Problems and Progress", *J. Chem. Doc.* **1967**, *7*, 67-71.

16. F. A. Cotton, "Proposed Nomenclature for Olefin-Metal and Other Organometallic Complexes", *J. Am. Chem. Soc.* **1968**, *90*, 6230-6232.

17. J. E. Huheey, "The Rules of Inorganic Nomenclature", in *Inorganic Chemistry: Principles of Structure and Reactivity* by J. E. Huheey. Harper & Row, New York, 1972. Appendix E, pp. 674-690.

18. W. C. Fernelius, "Present Status of Inorganic Chemical Nomenclature", *J. Chem. Inf. Comput. Sci.* **1981**, *21*, 213-218.

19. J. B. Casey, W. J. Evans, and W. H. Powell, "A Descriptor System and Principles for Numbering Closed Boron Polyhedra with at Least One Rotational Symmetry Axis and One Symmetry Plane", *Inorg. Chem.* **1981**, *20*, 1333-1341; "A Descriptor System and Suggested Numbering Procedures for Closed Boron Polyhedra Belonging to D_n , T , and C_s Symmetry Point Groups", *ibid.* **1984**, *23*, 3556-3561.

20. J. B. Casey, W. J. Evans, and W. H. Powell, "Structural Nomenclature for Polyboron Hydrides and Related Compounds. 1. Closed and Capped Polyhedral Structures", *Inorg. Chem.* **1983**, *22*, 2228-2235; "2. Nonclosed Structures", *ibid.* **1984**, *23*, 4132-4143.

21. W. C. Fernelius, "Some Reflections on the Periodic Table and Its Use", *J. Chem. Educ.* **1986**, *63*, 263-266.

22. D. H. Busch, "Labelling Columns of the Long Form Periodic Table", *Chem. Int.* **1987**, *9*(2), 49-50; "Column Labelling for the Long Form of the Periodic Table", *Chem. Int.* **1989**, *11*(2), 57-60.

23. E. K. Hyde, D. C. Hoffman, and O. L. Keller, Jr., "A History and Analysis of the Discovery of Elements 104 and 105", *Radiochim. Acta* **1987**, *42*, 57-102.

24. W. C. Fernelius, "Correct Methods for Naming Inorganic Compounds", *J. Chem. Educ.* **1987**, *64*, 901-903.

25. W. H. Powell and T. E. Sloan, "Inorganic Ring Nomenclature: Past, Present, and Future", *Phosphorus, Sulfur Silicon, Relat. Elem.* **1989**, *41*, 183-191.

26. International Union of Crystallography. Commission on Crystallographic Nomenclature. Subcommittee on the Nomenclature of Inorganic Structure Types, "Nomenclature of Inorganic Structure Types", *Acta Cryst.* **1990**, *A46*, 1-11.

27. Particle Data Group "The Naming Scheme for Hadrons", Section III of the Introduction of *Review of Particle Properties*, *Phys. Lett. B*, 1990, 239, 1.6-1.11 (an update of the scheme originally published as "A New Naming Scheme for Hadrons", *ibid.*, 1986.)

28. B. E. Douglas, "Nomenclature of Inorganic Chemistry", in *Concepts and Models of Inorganic Chemistry* by B. E. Douglas, D. H. McDaniel, J. J. Alexander. 3rd ed., John Wiley & Sons, New York, 1994. Appendix B, pp. B1-B17.

29. G. T. Seaborg, "Terminology of the Transuranium Elements", *Terminology* **1994**, *1*, 229-252.

30. G. T. Seaborg, "Transuranium Elements: Past, Present, and Future", *Acc. Chem. Res.* **1995**, *28*, 257-264.

31. N. N. Greenwood, "Recent Developments Concerning the Discovery of Elements 110-111", *Pure Appl. Chem.* **1997**, *69*, 179-184.

32. H. Strunz, "Chemical-Structural Mineral Classification Principles and Summary of System", *Neues Jahrb. Mineral. Monatsch.* **1997**, *(10)*, 435-445.

33. International Mineralogical Association. Commission on New Minerals and Mineral Names, "Recommended Nomenclature for Zeolite Minerals", *Can. Mineral.* **1997**, *35*, 1571-1606; *Mineral. Mag.* **1998**, *62*, 533-571; *Eur. J. Mineralog.* **1998**, *10*, 1037-1081.

34. Y. P. Jeannin, "The Nomenclature of Polyoxometalates: How To Connect a Name and a Structure", *Chem. Rev. (Washington, D.C.)* **1998**, *98*, 51-76.

35. R. Metselaar, "Terminology for Compounds in the Si-Al-O-N System", *J. Eur. Ceramic Soc.* **1998**, *18*, 183-184.

36. P. E. Childs, "From Hydrogen to Meitnerium: Naming the Chemical Elements" in *Chemical Nomenclature*, K. J. Thurlow, ed., Kluwer Academic Publishers, Dordrecht, The Netherlands, 1998, pp. 27-66.

37. K. J. Thurlow, "IUPAC Nomenclature Part 2, Organic, Inorganic and Others" in *Chemical Nomenclature*, K. J. Thurlow, ed., Kluwer Academic Publishers, Dordrecht, The Netherlands, 1998, pp. 127-145.

38. W. Liescher and E. Fluck, *Die systematische Nomenclatur der anorganischen Chemie* (Systematic Nomenclature of Inorganic Chemistry), Wiley-VCH Verlag, Weinheim, Germany, 1998, 388 pp.

39. E. H. Nickel and J. D. Grice, "The IMA Commission on New Minerals and Mineral Names: Procedures and Guidelines on Mineral Nomenclature, 1998", *Can. Mineral.* **1998**, *36*, 913-926; *Mineral. Petrol.* **1998**, *64*, 237-263; *Mineral. Rec.* **1999**, *30*, 163-176.

40. J. L. Jambor, "Nomenclature of the Alunite Supergroup", *Can. Mineral.* **1999**, *37*, 1323-1341; K. L. Scott, "Nomenclature of the Alunite Supergroup: Discussion", *Can. Mineral.* **2000**, *38*, 1295-1297; J. L. Jambor, "Nomenclature of the Alunite Supergroup: Reply", *Can. Mineral.* **2000**, *38*, 1298-1303.

41. M. Rieder, "Mineral Nomenclature in the Mica Group: the Promise and the Reality", *Eur. J. Mineral.* **2001**, *13*, 1009-1012.

42. D. L. Bish and J. M. Boak, "Clinoptilolite-Heulandite Nomenclature", *Rev. Mineral. Geochem.* **2001**, *45*, 207-216.

43. T. Armbruster, "Revised Nomenclature of Högbomite, Nigerite, and Taaffeite Minerals", *Eur. J. Mineral.* **2002**, *14*, 389-395.

44. R. Oberti, G. Della Ventura, L. Ottolini, F. C. Hawthorne, and P. Bonazzi, "Re-definition, Nomenclature and Crystal-Chemistry of the Hellandite Group", *Am. Mineral.* **2002**, *87*, 745-752.

45. N. V. Chukanov, I. V. Pekov, and A. P. Khomyakov, "Recommended Nomenclature for Labuntsovite-Group Minerals", *Eur. J. Mineral.* **2002**, *14*, 165-173.

46. W. H. Koppenol, "NO Nomenclature", *Nitric Oxide* **2002**, *6*, 96-98.

47. O. Johnsen, G. Ferraris, R. A. Gault, J. D. Grice, A. R. Kampf, and I. G. Pekov, "The Nomenclature of Eudialyte-Group Minerals", *Can. Mineral.* **2003**, *41*, 785-794.

48. J. D. Grice and G. Ferraris, "New Minerals Approved in 2002 and Nomenclature Modifications Approved in 1998-2002 by the Commission on New Minerals and Mineral Names, International Mineralogical Association", *Am. Mineral.* **2003**, *88*, 1620-1624; *Can. Mineral.* **2003**, *41*, 795-802.

49. B. E. Leake *et al.*, "Nomenclature of Amphiboles: Additions and Revisions to the International Mineralogical Association's Amphibole Nomenclature", *Eur. J. Mineral.* **2004**, *16*, 191-196.

307. Macromolecular chemistry

1. M. L. Huggins, "Macromolecular Nomenclature: General Background and Perspective", *J. Chem. Doc.* **1969**, *9*, 230-231.

2. H. K. Livingston and R. B. Fox, "Nomenclature of Organic Polymers", *J. Chem. Doc.* **1969**, *9*, 232-234.

3. N. M. Bikales, "Polymer Nomenclature in Industry", *J. Chem. Doc.* **1969**, *9*, 245-247.

4. R. B. Fox, "Nomenclature of Macrocyclic Compounds by Sequential Citation", *J. Chem. Inf. Comput. Sci.* **1984**, *24*, 266-271.

5. N. M. Bikales, "Nomenclature" in *Encyclopedia of Polymer Science and Engineering*, 2nd ed., J. I. Kroschwitz, ed., John Wiley & Sons, New York, Vol. 10, 1987, pp. 191-204.

6. K. L. Loening and A. D. Jenkins, "Nomenclature for Polymers", in *Comprehensive Polymer Science*, C. Booth and C. Price, eds., Pergamon Press, Oxford, UK, 1988, Vol. 1: Polymer Characterization, Chapter 2, pp. 13-54.

7. N. M. Bikales, "Nomenclature" in *Concise Encyclopedia of Polymer Science and Engineering*, J. I. Kroschwitz, ed., John Wiley & Sons, New York, 1990, pp. 653-654.
8. R. B. Fox, "Naming Organic Polymers" in *Handbook of Chemistry and Physics*, 77th ed., D. R. Lide, ed., CRC Press, Boca Raton, Florida, 1996, Section 13, pp. 1-2.
9. W. V. Metanowski, "Structure-Based Polymer Nomenclature", *J. Polym. Sci., Part C: Polym. Lett.* **1990**, 28(5), 173-174.
10. W. V. Metanowski, J. E. Merritt, and K. L. Loening, "Macromolecules: Structure Representation and Nomenclature" in *Chemical Structures 2* (Proceedings: 2nd International Conference on Chemical Structures, Noordwijkerhout, The Netherlands, June, 1990), W. Warr, ed., Springer-Verlag, Berlin, 1993, pp. 65-85.
11. G. R. Newkome, G. R. Baker, J. K. Young, and J. G. Traynham, "A Systematic Nomenclature for Cascade Polymers", *J. Polym. Sci., Part A*, **1993**, 31, 641-651.
12. L. H. Sperling and W. V. Metanowski, "Nomenclature in Polymer Science and Engineering", *Polym. Mater. Sci. Eng.* **1993**, 68, 341.
13. L. H. Sperling and W. V. Metanowski, "Polymer Nomenclature II: Engineering and Novel Multicomponent Polymer Structures". *Polym. Mater. Sci. Eng.* **1993**, 69, 575.
14. G. R. Baker, R. Gregory, and J. K. Young, "A Systematic Nomenclature for Cascade (Dendritic) Polymers" in *Advances in Dendritic Macromolecules*, Vol. 1, George R. Newkome, editor. JAI Press, Greenwich, Connecticut, 1994, pp. 169-186.
15. Fox, R. B., "Nomenclature of Polymeric Materials", *Rubber Chem. Technol.* **1995**, 68, 547-550.
16. A. D. Jenkins, "Problems in Composing Definitions of Terms for Polymer Chemistry", *Terminology* **1995**, 2, 351-364.
17. J. A. Patterson, J. L. Schultz, and E. S. Wilks, "Enhanced Polymer Structure, Searching, and Retrieval in an Interactive Database". *J. Chem. Inf. Comput. Sci.* **1995**, 35, 8-20.
18. J. L. Schultz and E. S. Wilks, "Orientation and Nomenclature of Multiple Radicals in Comb, Star, and Other Polymers with Multichain End Groups". *J. Chem. Inf. Comput. Sci.* **1996**, 36, 510-515.
19. —, "A Nomenclature and Structural Representation System for Ladder and Spiro Polymers". *J. Chem. Inf. Comput. Sci.* **1996**, 36, 786-793.
20. —, "Nomenclature and Structural Representation for Linear, Single-Strand Polymers Aftertreated to Hyperconnected Networks". *J. Chem. Inf. Comput. Sci.* **1996**, 36, 955-966.
21. —, "Symmetrical 'I'-Shaped Hyperbranched Structural-Repeating-Unit (SRU) Polymers: Converting Unregistrable SRUs to SRUs Registrable by Chemical Abstracts Service's Registry System". *J. Chem. Inf. Comput. Sci.* **1996**, 36, 967-972.
22. —, "A Nomenclature and Structural Representation System for Asymmetrical 'I'-Shaped Hyperbranched Polymers". *J. Chem. Inf. Comput. Sci.* **1996**, 36, 1109-1117.
23. L. H. Sperling, "Nomenclature and Notational Problems in the Phase Separation Characteristics of Block Copolymers". *Polym. Mat. Sci. Eng.* **1996**, 74(Spring), 445.
24. E. S. Wilks, "Polymer Nomenclature and Structure: A Comparison of Systems Used by CAS, IUPAC, MDL, and duPont. 1. Regular Single-Strand Organic Polymers", *J. Chem. Inf. Comput. Sci.* **1997**, 37, 171-192.
25. —, "2. Aftertreated (Post-treated), Alternating/Periodic, and Block Polymers", *J. Chem. Inf. Sci.* **1997**, 37, 193-208.
26. —, "3. Comb/Graft, Cross-Linked, and Dendritic/Hyperconnected/Star Polymers", *J. Chem. Inf. Comput. Sci.* **1997**, 37, 209-223.
27. —, "4. Stereochemistry, Inorganic, Coordination, Double-Strand, Polysiloxanes, Oligomers, Telomers". *J. Chem. Inf. Comput. Sci.* **1997**, 37, 224-235.
28. J. L. Schultz and E. S. Wilks, "Hierarchical Polymer Registration and Source-Based/Structure-Based Correlative Search Capability via a 'Hub Concept'", *J. Chem. Inf. Comput. Sci.* **1997**, 37, 425-435.
29. —, "Improved Indexing of Chemical Abstracts Service Post-Treated Polymers", *J. Chem. Inf. Comput. Sci.* **1997**, 37, 436-442.
30. —, "Polymers: Structural Representation" in *Encyclopedia of Computational Chemistry*, P. von Rague Schleyer, ed., John Wiley & Sons, New York, 1998, Vol. 3, pp. 2135-2150.
31. —, "Dendritic and Star Polymers: Classification, Nomenclature, Structure Representation, and Registration in the DuPont SCION Database", *J. Chem. Inf. Comput. Sci.* **1998**, 38, 85-89.
32. E. S. Wilks, "Nomenclature and Structure Representation for Dendritic Polymers", *Polym. Prepr.* **1998**, 39(2), 6-11.
33. A. D. Jenkins, "Nomenclature for Polymer Chemistry" in *Chemical Nomenclature*, K. J. Thurlow, ed., Kluwer Academic Publishers, Dordrecht, The Netherlands, 1998, pp. 146-161.
34. E. S. Wilks, "Whither Nomenclature?", *Polym. Prepr.* **1999**, 40(2), 6-11.
35. L. H. Sperling and W. V. Metanowski, "Modern Nomenclature and Terminology for Polymer Science and Technology", *Polym. Prepr.*, **1999**, 40(1), 6-11; *Polym. Mater. Sci. Eng.* **1999**, 80(Spring), 640-641.
36. W. V. Metanowski, "Nomenclature" in *Polymer Handbook*, 4th ed., J. Brandrup, E. H. Immergut, and A. E. Grulke, eds., John Wiley & Sons, New York, 1999, pp. 1/1-1/12.
37. L. H. Sperling, W. V. Metanowski, and C. E. Carraher, Jr., "Polymer Nomenclature" in *Applied Polymer Science 21st Century*, C. D. Craver and C. E. Carraher, Jr., eds., Elsevier Science Ltd., Amsterdam, 2000, pp. 49-54.
38. E. S. Wilks, "Polymer Nomenclature: the Controversy between Source-Based and Structure-Based Representations (A Personal Perspective)", *Prog. Polym. Sci.* **2000**, 25, 1-100.
39. —, "Polymer Nomenclature" in *Industrial Polymers Handbook* E. S. Wilks, ed., Wiley-VCH Verlag, Weinheim, Germany, 2001, Vol. 1, pp. 205-243.
40. K. Hatada, R. G. Jones, I. Mita, and E. S. Wilks, "Proposed Shorthand Notation for Nomenclature and Graphic Representation of Modified Polymers", *Polym. Prepr.* **2001**, 42(2), xxvi-xxxii.
41. R. B. Fox and E. S. Wilks, "Nomenclature for Organic Polymers" in *CRC Handbook of Chemistry and Physics 2001-2002*, 82nd ed., D. R. Lide, ed., CRC Press, Boca Raton, Florida, 2001, Section 13, pp. 1-5 (superseded item 8, above).
42. E. S. Wilks, "Terminology and Nomenclature for Rotaxanes - A Progress Report", *Polym. Prepr.* **2003**, 44(1), 1281-1287.
43. R. B. Fox, E. S. Wilks, and A. Yerin, "An Alternative Approach to Nomenclature for Macrocyclic Components of Rotaxanes and Catenanes", *Polym. Prepr.* **2003**, 44(2), 956-961.
44. E. S. Wilks, "Nomenclature for Single-Strand and Quasi-Single-Strand Inorganic and Coordination Polymers", *Polym. Prepr.* **2004**, 45(1).

308. Stereochemistry

Organic Compounds

1. R. S. Cahn, C. K. Ingold, and V. Prelog, "Specification of Molecular Chirality", *Angew. Chem., Int. Ed. Engl.* **1966**, 5, 385-414 (errata: **1966**, 5, 511); *Angew. Chem.* **1966**, 78, 413-447.
2. R. S. Cahn, "An Introduction to the Sequence Rule", *J. Chem. Educ.* **1964**, 41, 116-125 (errata: **1964**, 41, 508).
3. R. S. Cahn, C. K. Ingold, and V. Prelog, "The Specification of Asymmetric Configuration in Organic Chemistry", *Experientia* **1956**, 12, 81-94.
4. R. S. Cahn and C. K. Ingold, "Specification of Configuration about Quadrivalent Asymmetric Atoms", *J. Chem. Soc.* **1951**, 612-622.
5. E. L. Eliel, "Recent Advances in Stereochemical Nomenclature", *J. Chem. Educ.* **1971**, 48, 163-167.
6. Beilstein Institut, "Stereochemical Conventions in the Beilstein Handbook of Organic Chemistry", *Beilsteins Handbuch der Organischen Chemie*, Vierte Auflage, Drittes und Viertes Ergänzungswerk, Einundzwanzigster Band, Dritter Teil, Springer-Verlag, Berlin, 1978, pp. xx-xxviii.
7. V. Prelog and G. Helmchen, "Basic Principles of the CIP-System and Proposals for a Revision", *Angew. Chem.* **1982**, 94, 614-631; *Angew. Chem., Int. Ed. Engl.* **1982**, 21, 567-583.
8. K. Mislow and J. Siegel, "Stereoisomerism and Local Chirality", *J. Am. Chem. Soc.* **1984**, 106, 3319-3328.
9. J. H. Brewster, "On the Distinction of Diastereoisomers in the Cahn-Ingold-Prelog (RS) Notation", *J. Org. Chem.* **1986**, 51, 4751-4753.
10. P. Mata, A. M. Lobo, C. Marshall, and A. P. Johnson "The CIP Sequence Rules: Analysis and Proposal for a Revision", *Tetrahedron: Asymmetry*, **1993**, 4, 657-668.
11. E. L. Eliel, S. H. Samuel, and L. N. Lewis, *Stereochemistry of Organic Compounds*, John Wiley & Sons, New York, 1994. (Chapter 5. Configuration, pp. 101-113. Glossary. pp. 1191-1210).
12. G. Helmchen, "Glossary of Problematic Terms in Organic Stereochemistry", *Enantiomer* **1996**, 1(1), 84A-84D; *ibid.* **1997**, 2, 315-318.
13. S. Reichelt, A. Reichelt, N. Muller, and I. Ugi, "Topology and Group Theory-Tools for Determining the Stereochemistry of Molecules", *Croat. Chem. Acta* **1996**, 69, 813-825.
14. C. Thilgen, A. Herrmann, and F. Diederich, "Configurational Description of Chiral Fullerenes and Fullerene Derivatives with a Chiral Functionalization Pattern", *Helv. Chim. Acta* **1997**, 80, 183-189.
15. E. L. Eliel, "Infelicitous Stereochemical Nomenclature", *Chirality* **1997**, 9, 428-430.
16. E. L. Eliel and M. B. Ramirez, "(-)-Quinic Acid: Configurational (Stereochemical) Descriptors", *Tetrahedron: Asymmetry* **1997**, 8, 3551-3554.
17. S. B. Elk, "Redefining the Terminology of Stereoisomerism To Produce a Mathematics-Based Taxonomy Paradigm", *THEOCHEM* **1998**, 431, 237-247.
18. J. Gal, "Problems of Stereochemical Nomenclature and Terminology. 1. The *Homochiral* Controversy. Its Nature and Origins, and a Proposed Solution", *Enantiomer* **1998**, 3, 263-273.
19. J. Michl and R. West, "Conformations of Linear Chains. Systematics and Suggestions for Nomenclature", *Acc. Chem. Res.* **2000**, 33, 821-823.
20. A. Berces, D. M. Whitfield, and T. Nukada, "Quantitative Description of Six-Membered Ring Conformations Following the IUPAC Conformational Nomenclature", *Tetrahedron* **2001**, 57, 477-491.
21. J. Caldwell and I. W. Wainer, "Stereochemistry: Definitions and a Note on Nomenclature", *Hum. Psychopharmacol. Clin. Exp.* **2001**, 16, S105-S107.
22. K. C. Nicolau, C. N. C. Boddy, and J. S. Siegel, "Does CIP Nomenclature Adequately Handle Molecules with Multiple Stereoelements? A Case Study of Vancomycin and Cognates", *Angew. Chem., Int. Ed.* **2001**, 40, 701-704.

Inorganic Compounds

1. W. Thewalt, K. A. Jensen, and C. E. Schaeffer, "A Nomenclature Symbolism for Chiral and Achiral Isomers of Bridged Inorganic Complexes", *Inorg. Chem.* **1972**, 11, 2129-2136.
2. T. E. Sloan and D. H. Busch, "Stereochemical Description and Notation for Coordination Systems" in *Stereochemistry of Optically Active Transition Metal Compounds*, B. E. Douglas and Y. Saito, eds., American Chemical Society, Washington, D.C., 1980, pp. 397-419. (*ACS Symposium Series* No. 119.)
3. T. E. Sloan, "Stereochemical Nomenclature and Notation in Inorganic Chemistry" in *Topics in Inorganic and Organometallic Stereochemistry*, G. Geoffroy, ed., John Wiley & Sons, New York, 1981, pp. 1-36.
4. T. Damhus and C. E. Schaeffer, "Three Reference Systems for Chirality Specification, Application, Geometric Properties, and Mutual Relationships", *Inorg. Chem.* **1983**, 22, 2406-2412.
5. M. Brorson, T. Damhus, and C. E. Schaeffer, "Exhaustive Examination of Chiral Configurations of Edges on a Regular Octahedron: Analysis of the Possibilities of Assigning Chirality Descriptors within a Generalized Δ/Λ System", *Inorg. Chem.* **1983**, 22, 1569-1573.
6. T. E. Sloan, "Nomenclature of Coordination Compounds" in *Comprehensive Coordination Chemistry*, G. Wilkinson, R. D. Gillard, and J. A. McCleverty, eds., Pergamon Press, London, 1987, Part 1, Vol. 1, Chapter 3, pp. 109-134.

K. CHEMICAL PREFIXES

309. Miscellaneous chemical prefixes. The following list of prefixes most often encountered in the chemical literature (though not necessarily employed in CA index names) is intended to supplement Section H (Illustrative List of Substituent Prefixes); items in Section H are therefore not repeated here. Also excluded are prefixes derived from individual element or compound names, e.g., phospho-, ferri-, aceto-, oxa-, thiazolo-. Prefixes usually italicized are so shown.

The lower-case Greek alphabet is supplied in a separate list below (¶ 310). Greek and Latin multiplicative prefixes are also listed separately (¶ 311).

ac- abbreviation of *alicyclic*; as, *ac*-amino derivatives of Tetralin. Cf. *ar-*.
ace- from *acetylene*; as, *acenaphthene*.

aci- the *acid* form: as *aci*-acetoacetic ester, $\text{CH}_3\text{C}(\text{OH})\text{:CHCOOC}_2\text{H}_5$; *ac*-nitro group HON(O):.

aldo-, *ald-* from *aldehyde*; as, *aldohexose*, *aldoxime*.

allo- (Greek *allos*, other) indicating *close relation*; as, *allo*-telluric acid, *allo*-cimene (a structural isomer of ocimene). Specifically, designating the more stable of two geometrical isomers; as, *allomaleic acid* (fumaric acid).

amphi- (Greek, both, around) relating to both sides or both kinds; as, *amphi*-naphthoquinone (2,6-naphthalenedione), *amphiphile*.

andro-, *andr-* (Greek) relating to *man*, *male*; as *androgen*, *androsterone*.

ang- having an *angular* alignment of rings; as, *ang*-2',3'-naphth-1,2-anthracene (pentaphene). Cf. *lin-*.

anhydro- (Greek *anhydros*, without water) denoting *abstraction of water*, *anhydride of*; as, *anhydroglucose*. Cf. *dehydro-*.

antho-, *anth-* (Greek) of *flowers*; as, *anthocyanin*, *anthoxanthin*.

antra-, *antr-* (Greek, *anthrax*, coal) of *coal* or *anthracene*; as, *anthracite*, *antraquinone*, *anthrapyrole*.

anti- (Greek, against) *opposite*, *opposed to*; as, *antioxidant*; specifically, equivalent to *trans-* (which see) as, *anti*-benzaldehyde.

apo- (Greek, from) denoting formation from, or relationship to, another compound; as, *apomorphine*, $\text{C}_{17}\text{H}_{17}\text{NO}_2$ (morphine is $\text{C}_{17}\text{H}_{19}\text{NO}_3$).

ar- abbreviation of *aromatic*; as, *ar*-derivatives of Tetralin.

as- abbreviation of *asymmetric*; as, *as*-trichlorobenzene (1,2,4- $\text{Cl}_3\text{C}_6\text{H}_3$).

benzo-, *benz-* of *benzene*; as, *benzoic*; specifically, denoting fusion of a benzene ring; as, *benzoquinoline*.

bi- (Latin) *twice*, *two*, *double*; specifically: (a) in double proportion; as, *bicarbonate* (no longer considered good usage); (b) denoting the doubling of an organic radical or molecule; as, *biphenyl*, $\text{C}_6\text{H}_5\text{C}_6\text{H}_5$; *bipyridine*, $\text{C}_5\text{H}_4\text{N}_2$.

bicyclo- of *two rings*; specifically, designating certain *bicyclic* bridged compounds; as, *bicyclo*[2.2.1]heptane.

bili- (Latin) of *bilirubin*, as, *biliverdin*.

bisnor-, *dinor-* indicating removal of two CH_2 groups; as, *bisnor*cholic acid or *dinor*cholic acid $\text{C}_{22}\text{H}_{36}\text{O}_2$ (cholic acid is $\text{C}_{24}\text{H}_{40}\text{O}_2$).

bufo-, *buf-* (Latin *bufo*, toad) derived from the *toad*; as, *bufotalin*.

chole-, *cholo*, *chol-* (Greek) of *bile*; as, *cholesterol*, *choline*.

chromo- (Greek *chroma*, color) *color*, *colored*; as, *chromophore*, *chromoprotein*, *chromoisomer* (a colored isomer of a colorless compound).

chryso-, *chrys-* (Greek) *gold*, *golden yellow*, *yellow*; as *chrysophanic acid*, *chryszazin*.

cincho-, *cinch-* of *cinchona* or *cinchonine*; as *cinchomeric acid*, *cinchonan*.
cis- (Latin, on this side) an isomer in which certain atoms or groups are on the *same side* of a plane; as, *cis*-1,4-cyclohexanediol.

copro- (Greek) of *dung* or *excrement*; as, *coprosterol*.

cyclo- (Greek *kyklos*, circle) of ring structure, *cyclic*; as, *cyclohexane*.

D- denoting configurational relationship to D-glyceraldehyde; as, D-fructose.

d- (a) abbreviation of *dextro* or *dextrorotatory*; as, *d*-strychnine; (b) less properly = D.

de-, *des-* (Latin) indicating *removal* of something from the molecule; as, *deoxybenzoin*, $\text{C}_6\text{H}_5\text{CH}_2\text{COC}_6\text{H}_5$ (benzoin with one oxygen atom removed).

dehydro- denoting (a) *removal of hydrogen*; as, *dehydrocholic acid*; (b) sometimes, *removal of water*; as, *dehydro*mic acid.

dextro- (Latin *dexter*, right) rotating the plane of polarization to the right; as, *dextro*pinene. Abbreviation, *d*; as, *d*-valine.

dl-; *d,l-* denoting a *racemic form*. Cf. *dextro-*, *levo-*.

dvi- (Sanskrit, two, twice) designating provisionally an element of the same family, in the *second place beyond*; as *dvi*-manganese (rhenium).

eka- (Sanskrit, one) designating provisionally an element of the same family, in the *first place beyond*; as, *eka*-manganese (technetium).

endo- (Greek, within) indicating an *inner position*, specifically: (a) in the ring and not in a side chain; (b) attached as a bridge within a ring; as, 1,4-*endo*-methylene-cyclohexane (bicyclo[2.2.1]heptane).

epi- (Greek, upon, on, to) denoting (a) the 1,6-positions in naphthalene; as, *epi*-dichloronaphthalene; (b) in aldoses and related compounds identity of structure except arrangement about the α -carbon atom; as, *epi*thamnose (epimer of rhamnose); (c) a bridge connection; as, 9,10-*epi*dioxanthracene (anthracene 9,10-peroxide).

ergo-, *ergot-* relating to *ergot*; as, *ergosterol*, *ergotamine*.

erythro-, *erythr-* (Greek) *red*; as *erythromycin*, *erythrosine*.

eso- (Greek, within) denoting immediate attachment to a ring atom. Cf. *exo-*.

etio-, *aetio-* (Greek *aitia*, cause) denoting a *degradation product*; as, *etio*cholic acid, *etio*cobalamin.

exo- (Greek) *outside*, *out of*; as, *exotoxin* (an excreted toxin); specifically, denoting attachment in a side chain. Cf. *endo*, *eso-*.

flavo-, *flav-* (Latin *flavus*, yellow) *yellow*; as, *flavoprotein*, *flavone*; specifically, designating certain series of coordination compounds.

fuco-, *fuc-* of *fucus* (a seaweed); as, *fucoxanthin*, *fuco*se.

gala-, *galacto-*, *galact-* (Greek, milk, milky) relating to: (a) *milk*; as, *galactase*, *galactose*; (b) *galactose*; as, *galactocerebroside*, *galactolipin*.

gallo-, *gall-* relating to *gallnuts* or *gallic acid*; as, *gallotannic acid*, *gallo*catechin.

gem- abbreviation of *geminate* (said of two groups attached to the same atom); as, a *gem*-diol (e.g., 1,1-ethanediol), the *gem*-dimethyl grouping in camphor.

gluco-, *gluc-* (a) of *glucose*; as, *glucopyranose*, *glucuronic acid*; (b) less properly = *glyco-*, *glyc-*.

glyco-, *glyc-* (Greek) *sweet*, or relating to *sugars* or *glycine*; as, *glycogen*, *glycoside*, *glycocholic acid*.

hemato-, *hemat-*, *hemo-*, *hem-* (also *haemato-*, etc.) (Greek) of *blood* or its color; as, *hematoporphyrin*, *hematein*, *hemoglobin*, *hemin*.

hetero-, *heter-* (Greek *heteros*, other) *other*, *different*; as, *heteropoly acids*, *heterocyclic*.

holo- (Greek) *whole*, *complete*; as, *holocellulose*; *holophosphoric acid*, H_3PO_5 .

homo- (Greek) *same*, *similar*; as, *homocyclic*, *homologous* (differing by an increase of CH_2); as, *homophthalic acid*.

hydro-, *hydr-* (Greek) (a) denoting presence or addition of *hydrogen*; as, *hydrochloric*, *hydracrylic*; (b) sometimes, relating to *water*; as *hydrate*.

hyo- (Greek) of *swine*; as, *hyodeoxycholic acid* (from hog bile), *hyoscyamine* (from *Hyoscyamus* (hog bean)).

hypo- (Greek, under, beneath) indicating a lower (or the *lowest*) state of oxidation; as, *hypochlorous acid*, *hypoxanthine*.

i- abbreviation of (a) *inactive*; as, *i*-tartaric acid; (b) *iso-*; as, *i*-pentane.

iso- (Greek) *equal*, *alike*; as, *isomer*; usually, denoting an *isomer* of a compound; as, *isocyanic acid*; specifically, denoting an isomer having a single, simple branching at the end of a straight chain; as, *isopentane*, $(\text{CH}_3)_2\text{CHCH}_2\text{CH}_3$.

keto-, *ket-* from *ketone*; as, *ketohexose*, *ketoxime*.

L- configurationally related to L-glyceraldehyde; as, L-fructose.

l- (a) abbreviation of *levo* or *levorotatory*; as, *l*-strychnine; (b) less properly = L.

lano- (Latin) of *wool*; as, *lanosterol* (from wool fat).

leuco-, *leuc-* (Greek) *colorless*, *white*; as, *leucine*; specifically, a colorless reduced derivative of a triphenylmethane dye; as, *leucomethylene blue*.

levo-, *laevo-* (Latin *laevus*, left) rotating the plane of polarization to the left; as, *levo*valine. Abbreviation, *l*; as, *l*-valine.

lin- denoting a straight, *linear* alignment of rings; as *lin*-naphthanthracene (pentacene). Cf. *ang-*.

litho-, *lith-* (Greek *lithos*, stone) related to *stone* or *calculus*; as, *litharge*, *lithocholic acid* (from gallstones).

luteo- (Latin *luteus*) *orange-yellow*, *brownish yellow*; as *luteolin*; specifically, the coordination compounds $[\text{M}(\text{NH}_3)_6]\text{Cl}_3$.

m- abbreviation of *meta* (sense c).

meso-, *mes-* (Greek) *middle*, *intermediate*; specifically: (a) an intermediate hydrated form of an inorganic acid; as, *mesoperiodic acid*, H_3IO_6 ; (b) optically inactive owing to internal compensation; as, *mesotartaric acid*; (c) (abbreviated μ -) centrally substituted; as, *meso*-chloroanthracene (9-chloroanthracene), *meso*-phenylimidazole (2-phenylimidazole); (d) (abbreviated *ms*-) centrally fused; as, *mesonaphthodianthrene* (phenanthro[1,10,9,8-opqra]perylene).

meta-, *met-* (Greek) indicating *changed relation*; specifically, designating (a) a low hydrated form of an acid (usually that derived from the "ortho" form by loss of one molecule of water); as, *metaphosphoric acid*, HPO_3 ; (b) a closely related compound (sometimes, a polymer); as, *metaldehyde* (trimer of ordinary (acet)aldehyde); (c) (abbreviated *m*-) the 1,3-positions in benzene; as, *m*-xylene.

n- abbreviation of *normal* (unbranched); as, *n*-butane, *n*-butyl.

naphtho-, *naphth-* (Greek *naphtha*) relating to *naphthalene*; as, *naphthoquinone*.

neo- (Greek) *new*; designating new or recent; as, *neosphenamine*; (of a hydrocarbon) having one carbon atom connected directly to four others; as, *neopentane*, $(\text{CH}_3)_4\text{C}$.

nor- from *normal*; (a) a lower homologue; as, *nor*camphane (of which camphane is a trimethyl derivative); (b) a normal (straight-chain) isomer; as, *nor*leucine.

o- abbreviation of *ortho* (sense d).

oligo-, *olig-* (Greek *oligos*, small) meaning few; as, *oligosaccharide*.

ortho- (Greek, straight, right, true) (a) the fully hydrated form of an acid; as, *orthonitric acid*, H_2NO_5 ; (b) the highest-hydrated stable form; as, *orthophosphoric acid*, H_3PO_4 ; (c) the common or symmetrical molecular form of an element; as, *orthohydrogen*; (d) (abbreviated *o*-) the 1,2-positions in benzene; as, *o*-xylene.

p- abbreviation of *para* (sense c).

para-, *par-* (Greek, beside, alongside of, beyond) indicating a relationship; as *paraxanthine* (1,7-dimethylxanthine). Specifically, (a) a higher hydrated form of an acid; as, *paraperiodic acid*, H_2IO_5 (preferably called orthoperiodic); (b) a polymer; as, *paraldehyde*; (c) (abbreviated *p*-) the 1,4-positions in benzene; as, *p*-xylene.

per- (Latin) *complete*, *thorough*, *extreme*; (a) the highest (or a high) state of oxidation; as, *perchloric acid*, *manganese peroxide* (better, dioxide); (b) pres-

ence of the peroxide group (O₂); as, barium *peroxide*, *perbenzoic acid*, *per acid* (better, peroxy acid); (c) exhaustive substitution or addition; as, *perchloroethylene*, C₂Cl₄; *perhydronaphthalene*, C₁₀H₁₈.

peri- (Greek, around, about) (a) the 1,8-positions in naphthalene; as *peri-dinitronaphthalene* (b) in polycyclic ring systems, fusion of a ring to two or more adjoining rings: as, *perinaphthindene* (phenalene).

peroxy- containing the *peroxide* group (O₂); as, *peroxymonosulfuric acid*, HOSO₂OOH.

pheno-, phen- (from *phene*, benzene) related to *phenyl* or *benzene*; as, *phenacyl*; specifically, an anthracene analogue having two hetero atoms in the central positions; as, *phenazine*, *phenothiazine*.

phloro-, phlor- relating to *phlorizin*; as, *phloroglucinol*, *phloretin*.

phthalo-, phthal- relating to *phthalic acid*; as, *phthalocyanine*, *phthalide*.

phyllo-, phyll- (Greek *phyllos*) of *leaves*; as, *phylloporphylin*.

phyto-, phyt- (Greek) relating to *plants*; as, *phytosterol*, *phytohormones*.

picro-, picr- (Greek) *bitter*; as, *picrotoxin*, *picric acid*.

pino-, pin- (Latin *pinus*, pine) relating to *pine* or *pinene*; as, *pinic acid*, *pinocavone*.

poly- (Greek) many; as, *polymer*, *polysulfide*, *polysaccharide*.

pro- (Greek, before) a precursor; as *proenzyme*, *provitamin*.

proto-, prot- (Greek) *first*; specifically, designating: (a) first in an inorganic series; as, *protoxide* (lowest in oxygen content); (b) parent or immediate antecedent; as, *protactinium*, *protochlorophyll*.

pseudo-, pseud- abbreviated ψ or *ps* (Greek, false) indicating *resemblance* to, or *relation* (especially isomerism) with; as, ψ -cumene, *pseudacotine*, *pseudobase*. Abbreviation: as, ψ -cumene.

purpuro- (Latin *purpura*, purple) indicating *purple* or *red* color; as, *purpurogallin*.

pyo- py- (Greek) relating to *pus*; as, *pyocyanine*.

pyro-, pyr- (Greek *pyr*, fire) indicating *formation by heat*; as, *pyrocinchonnic acid*, *pyrene*; specifically, designating an acid derived from two molecules of an "ortho" acid by loss of H₂O; as, *pyrophosphoric acid*, H₄P₂O₇ (2H₃PO₄-H₂O).

pyrrolo-, pyrro-, pyr- containing the *pyrrole* ring; as, *pyrrolopyridine*, *pyrrocoline*.

reso-, res- relating to *resorcinol*; as, *resorufin*, *resazurin*.

rhodo-, rhod- (Greek *rhodon*, rose) *rose-red*; as, *rhodoporphylin*, *rhodamine*.

s- abbreviation of (a) *symmetric(al)*; (b) *secondary*.

sapo- (Latin, soap) relating to *soap* or *soap bark*; as *saponin*, *sapogenin*.

sec- abbreviation of *secondary*; as, *sec-butyl*.

seco- (Latin *secare*, to cut) denoting ring cleavage; as, 16,17-*seco*androstane.

sub- (Latin, under, below) denoting (a) a *low proportion* (or deficiency, as in a basic salt); as, *subiodide*, *suboxide*, aluminum *subacetate*.

super- (Latin, above, over) denoting a *high proportion* (or superfluity, as in an acid salt); as, *superoxide* (peroxide), *superphosphate*.

sym- abbreviation of *symmetric(al)*; as *sym-dichloroethylene* (1,2-dichloroethene).

syn- (Greek, with, together) equivalent to *cis* (which see); as, *syn-benzaldoxime*.

t- abbreviation of *tertiary*; as, *t-butyl*.

tauro- (Latin *taurus*, bull) relating to *bulls* or to *taurine*; as, *taurocholic acid*, *taurocyamine*.

tere- (Latin *terebinthus*, terebinth) relating to *terebene* or *terpenes*; as, *terephthalic*, *teresantalic*.

tert- abbreviation of *tertiary*; as, *tert-butyl*.

thymo-, thym- relating to (a) *thyme*; as, *thymoquinone*, *thymol*; (b) the *thymus*; as, *thymonucleic*.

trans- (Latin, across) an isomer in which certain atoms or groups are on *opposite sides* of a plane; as, *trans-cinnamic acid*.

uns-, *unsym-* abbreviations of *unsymmetrical*; as, *uns-dichloroethane*, CH₃CHCl₂.

uro-, ur- (Greek *ouro-*, *our-*) relating to *urine* or *urea*; as, *urobilin*, *urethane*, *uric acid*.

urso-, urs- (Latin *ursus*, bear) relating to *bears* or the *bearberry*; as, *ursolic acid*.

v- abbreviation of *vicinal*; as, *v-triazine*.

verdo- (French, *verd*, *vert*, green) indicating *green* color; as, *verdohemim*.

vic- abbreviation of *vicinal*; as, *vic-triazole*.

xantho-, xanth- (Greek) *yellow*; as, *xanthotoxin*, *xanthic acids*, *xanthine*.

xylo-, xyl- (Greek *xylon*, wood) relating to *wood*, *xylene*, or *xylose*; as, *xylan*, *xyloidine*, *xyloquinone*, *xylocaine*.

zymo-, zym- (Greek *zyme*, leaven) relating to a *ferment* or *fermentation*; as, *zymosterol*, *zymase*.

310. Greek alphabet. Lower-case Greek letters are employed in the chemical literature to number carbon chains and to indicate the size of lactone rings (a γ -lactone generally contains a furan ring, a δ -lactone a pyran ring, and so on). In CA names, Greek letters are reserved for the *acyclic* portion of conjunctive index parents (see ¶ 124), while cyclic portions are numbered with arabic numbers. Of Greek capital letters, Δ (delta) is sometimes encountered in the literature to denote a double bond; T (tau) indicates a triple bond. Some lower-case letters have additional meanings; ϕ (phi) is a shorthand version of "phenyl" or "Ph"; see also "meso" and "pseudo" in ¶ 309.

α -	alpha	ν -	nu
β -	beta	ξ	xi
γ	gamma	\omicron	omicron
δ -	delta	π -	pi
ϵ -	epsilon	ρ -	rho
ζ	zeta	σ -	sigma
η -	eta	τ -	tau
θ -	theta	υ -	upsilon
ι -	iota	ϕ	phi
κ -	kappa	χ -	chi
λ -	lambda	ψ -	psi
μ -	mu	ω -	omega

311. Multiplicative prefixes. In CA index names, Greek prefixes are preferred, except for nona- (for nine), and undeca- (for eleven). The terms hemi- (Greek) and sesqui- (Latin) were employed by CA in hydrate and ammoniate names prior to the Twelfth Collective period (1987-1991) (see ¶¶ 192, 265A). For use of the special terms bis-, tris-, tetrakis-, etc., with complex terms and to avoid ambiguity, see ¶¶ 110 and 266.

	Greek	Latin
1/2	hemi-	semi-
1	mono-, mon-	uni-
1 1/2		sesqui-
2	di-	bi-
3	tri-	tri-, ter-
4	tetra-, tetr-	quadri-, quadr-, quater-
5	penta-, pent-	quinque-, quinqu-
6	hexa-, hex-	sexi-, sex-
7	hepta-, hept-	septi-, sept-
8	octa-, oct-, octo-, octi-	
9	ennea-, enne-	nona-, non-, novi-
10	deca-, dec-, deci-	
11	hendeca-, hendec-	undeca-, undec-
12	dodeca-, dodec-	
13	trideca-, tridec-	
14	tetradeca-, tetradec-	
15	pentadeca-, pentadec-	
16	hexadeca- hexadec-	
17	heptadeca-, heptadec-	
18	octadeca-, octadec-	
19	nonadeca-, nonadec-	
20	eicosa-, eicos-	
21	heneicosa-, heneicos-	
22	docosa-, docos-	
23	tricos-, tricos-	
24	tetracosa-, tetracos-	
25	pentacosa-, pentacos-	
26	hexacosa-, hexacos-	
27	heptacosa-, heptacos-	
28	octacosa-, octacos-	
29	nonacosa-, nonacos-	
30	triaconta- triacont-	
31	hentriaconta-, hentriacont-	
32	dotriaconta-, dotriacont-	
33	tritriaconta-, tritriacont-	
40	tetraconta-, tetracont-	
50	pentaconta-, pentacont-	
60	hexaconta-, hexacont-	
70	heptaconta-, heptacont-	
80	octaconta-, octacont-	
90	nonaconta-, nonacont-	
100	hecta-, hect-	
101	henhecta-, henhect-	
102	dohecta-, dohect-	
110	decahecta-, decahect-	
120	eicosahecta-, eicosahect-	
132	dotriacontahecta-, dotriacontahecta-	
200	dicta-, dict-	
300	tricta ¹	
400	tetracta ¹	
1000	kilia ¹	

¹ International Union of Pure and Applied Chemistry, Organic Chemistry Division, Commission on Nomenclature of Organic Chemistry, "Extension of Rules A-1.1 and A-2.5 Concerning Numerical Terms Used in Organic Chemical Nomenclature (Recommendations 1986)", *Pure Appl. Chem.* **1986**, 58, 1693-6.

L. CHEMICAL STRUCTURAL DIAGRAMS FROM CA INDEX NAMES

Introduction	¶ 312
Form of CA index names	313
Deriving a chemical structural diagram	314
Index heading parents	315

Substituent prefixes	¶ 316
Modifications	317
Stereochemistry	318

312. Introduction. The foregoing sections of this document are concerned with selection of index names for chemical substances, but the user of CA printed indexes and computer-readable files often needs to proceed from a CA index name to the structure diagram of a chemical substance. The aim of this section is therefore to describe succinctly the form of CA index names, to illustrate the procedure for deriving a chemical structural diagram from a CA index name, and to show where in CAS publications structural data can be found. The structural diagrams accurately represent the positions of atoms relative to each other in a molecule but because of molecular flexibility, crowding, and/or the need to draw a three-dimensional structure in two dimensions, some structural diagrams are, of necessity, distorted. For example, some bond lengths and angles may differ from those in the molecule represented.¹

313. Form of CA index names. The complexity of chemical substances generally dictates the complexity of CA index names. The CA index name consists of up to five fragments, namely, the *index heading parent* alone or followed successively by the *substituent*, *modification*, and *stereochemistry* fragments (compare ¶104), as necessary. Some index heading parents are followed by *synonym line formulas* (compare ¶219, 315.II). Every name contains an index heading parent and it is by citing the *parent* first (i.e., in an inverted format) that the names of related chemical substances are listed together in the printed indexes.

314. Deriving a chemical structural diagram from a CA index name proceeds by taking each name fragment sequentially, converting it into a structural fragment, and then placing each structural fragment in its proper position in the diagram, using the appropriate positional information. The complete derivation of a chemical structural diagram may require up to four steps, depending upon the complexity of the chemical substance, each based on one of the four possible CA index name fragments. This process is illustrated in the remaining paragraphs of this section.

315. Index heading parents include the largest or most important molecular skeleton and (when present) the highest function in a chemical substance (see ¶¶ 130, 164).

I. Index heading parents that stand alone.

The simplest *index heading parents* may be illustrated by examples such as the following:

Butane

Chlorine

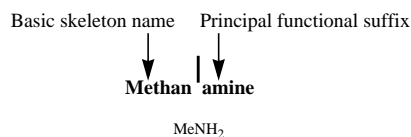
2-Hexene

Nickel

The names of acyclic hydrocarbons are discussed in ¶ 141 and the multiplicative terms that indicate the number of carbon atoms in a hydrocarbon are listed in ¶ 311. Element names are discussed in ¶ 219.

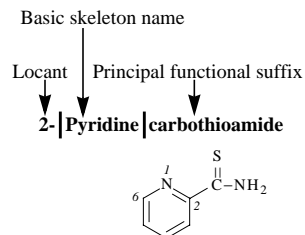
Some index heading parents are made up of two parts: a *basic skeleton name* and a *principal functional suffix*. Principal functional suffixes are discussed in detail in Section C (¶¶ 164-177).

Example:



The basic skeleton is the one-carbon unit "Methane" (¶ 141), the final "e" being elided before a vowel. The principal (here, the only) functional group is the amine (¶ 176).

Example:



The *Chemical Substance Index* contains the following entry for pyridine.

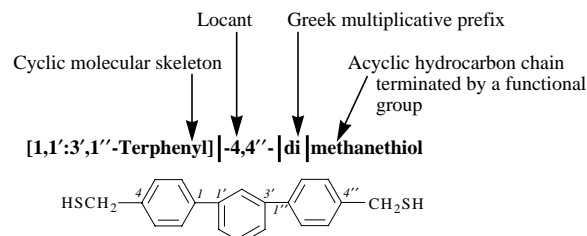
Pyridine



The carbothioamide principal function suffix is discussed in detail with other amide groups in ¶¶ 171 and 233. The locant, 2, indicates where the carbothioamide group is attached to the pyridine ring (¶ 115).

Another type of two-part name, known as a "conjunctive name" (see ¶ 124), is a combination of the name of a cyclic molecular skeleton and the name(s) of one or more identical, saturated acyclic hydrocarbon chains, each terminated by the same functional group.

Example:

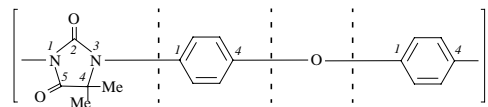


The structure of the phenyl group is found in the Illustrative List of Substituent Prefixes (¶ 294). That "ter" is a Latin prefix meaning "three" is found in ¶ 311. The first set of locants (1,1':3',1'') indicates that the three benzene rings are connected as shown. The second set of locants (4,4'') shows that the two methanethiol groups (see ¶¶ 141 and 175) are attached as shown to the first and third benzene rings. Such "ring assembly" names are described in ¶ 157.

Polymers are named either on the basis of the monomers from which they are formed (see ¶ 317) or on the basis of their structure, as represented by a structural repeating unit (compare ¶ 222). In the latter, the multivalent radicals are cited in sequence, following the term "Poly", and can be drawn from left to right. Each radical retains its own numbering and is oriented, if possible, so that the point of attachment at the left of the radical is assigned the lowest possible locant.

Example:

Poly[(4,4-dimethyl-2,5-dioxo-1,3-imidazolidinediyl)-1,4-phenyleneoxy-1,4-phenylene]



In this chemical structural diagram, the multivalent radicals are separated by dashed vertical lines and the numbering of each radical is shown, where appropriate. The structures of the radicals (e.g., oxy, phenylene) are found in ¶ 294 or can be inferred from the chemical structural diagrams associated with parent names (e.g., imidazolidine) in the *Ring Systems Handbook* or the *Chemical Substance Index*. The meanings of the methyl and oxo terms can also be determined from ¶ 294.

¹A. L. Goodson, "Graphical Representation of Chemical Structures in Chemical Abstracts Service Publications", *J. Chem. Inf. Comput. Sci.* **1980**, 20, 212-217.

II. Index heading parents with synonym line formulas.

Synonym line formulas are molecular formulas which follow the index heading parent. They are printed in boldface and are enclosed in parentheses. They are often useful for resolving ambiguity, where two or more substances, usually inorganic (see ¶ 219), have the same name.

Examples:

Aluminum calcium titanium oxide (Al₂CaTiO₆)

Aluminum calcium titanium oxide (Al₂Ca₄Ti₂O₁₁)

Lack of a synonym line formula in such a case means that the author did not provide the necessary specificity in the original document.

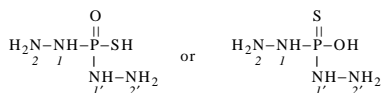
Example:

Aluminum calcium titanium oxide

III. Index heading parents with chemical structural diagrams.

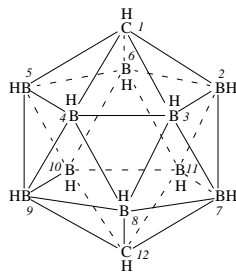
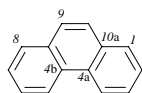
A *chemical structural diagram* is provided in the *Chemical Substance Index* where the structure of an inorganic substance (¶ 219) may not be readily apparent from the name.

Example:

Phosphorodihyrazidothioic acid

A similar procedure is followed for other types of index heading parents such as *cage parents*, *ring parents*, and *stereoparents*. Here, however, the structural diagrams are published in the *Ring Systems Handbook* as well as the *Chemical Substance Index*.

Examples:

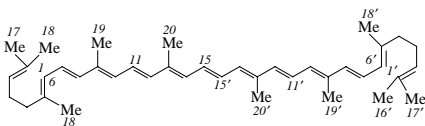
Cage Parent:**1,12-Dicarbadoecaborane(12)****Ring Parent:****Phenanthrene**

As stated in ¶ 313, the complexity of chemical substances generally dictates the complexity of CA index names. This is particularly true for natural products whose names must imply standard orientation and stereochemical representation as well as structure and numbering (compare ¶ 318). Such complexity makes it desirable to use a simple, nonsystematic (“trivial”) name, or *stereoparent name*, as the index heading parent and to define the *stereoparent name* by means of a chemical structural diagram.

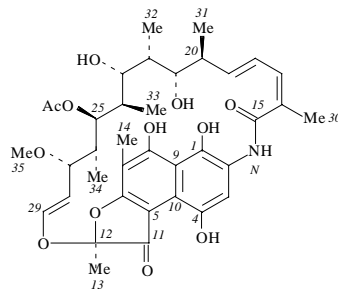
Examples:

Acyclic stereoparent:**ψ,ψ-Carotene**

((6E,8E,10E,12E,14E,16E,18E,20E,22E,24E,26E)-2,6,10,14,19,23,27,31-octamethyl-2,6,8,10,12,14,16,18,20,22,24,26,30-dotriacontatriecaene)

**Cyclic stereoparent:**

Rifamycin ((2S,12Z,14E,16S,17S,18R,19R,20R,21S,22R,23S,24E)-21-(acetyloxy)-5,6,9,17,19-pentahydroxy-23-methoxy-2,4,12,16,18,20,22-heptomethyl-2,7-(epoxypentadeca[1,11,13]trienimino)naphtho[2,1-b]furan-1,11(2H)-dione)



316. Substituent prefixes (see ¶ 10A) follow the “comma of inversion” (see ¶ 104) in CA index names and their structures can be determined from ¶ 294, the Illustrative List of Substituent Prefixes.

Example:

**2H-Pyran-2,4(3H)-dione,
3-[[[(4-aminophenyl)amino]phenylmethylene]-
6-phenyl-**

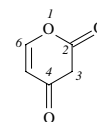
The structure of the chemical substance represented by this name is derived by first obtaining the structure of **2H-Pyran** from the *Chemical Substance Index* or, better, from the *Ring Systems Handbook*. The Ring Name Index of the 1993 edition of the *Ring Systems Handbook* reveals that the Ring File (RF) number for **2H-Pyran** is RF 2133. Entry RF 2133 in the *Ring Systems Handbook* is as follows:

RF 2133
2H-Pyran
C₅H₆O

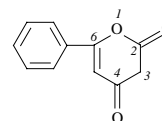


289-66-7

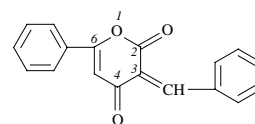
The *index heading parent* contains two functional groups which ¶ 174 identifies as ketone groups. However, putting an oxygen on position 4 requires “adding” a hydrogen at position 3. The indicated and added hydrogen terms (see ¶¶ 135 and 136) in the index heading parent thus define the bonding in the ring (the bonding could also be defined by “3,4-dihydro” but that would be part of the *substituent* fragment of the name and not of the index heading parent, which must be able to stand alone). The complete index heading parent (**2H-Pyran-2,4(3H)-dione**) is therefore:



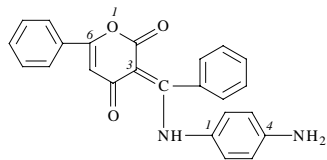
The *substituent* fragment of the name indicates that a simple substituent (i.e., “phenyl”, see ¶ 294) is attached to the ring at position 6:



A complex substituent is attached to the ring at position 3. The second phenyl group is attached through the methylene group (see ¶ 294) to position 3 to yield:



The third phenyl group has an amino group (¶ 294) attached to the 4-position and is itself attached through an amino group to the methylene group of the partial structure. The complete structure is therefore:

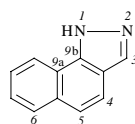


317. Modifications of the principal functions or other groups follow the substituent(s) (¶ 104). Where derivatives of more than one functional group must be named, the derivative terms are cited in the order described in ¶ 113. Example:

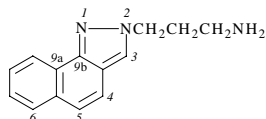
2*H*-Benzo[*g*]indazole-2-propanamine, 3,3a,4,5-tetrahydro-*N,N*-dimethyl-3-phenyl-, hydrochloride (1:3)

Only the form **1*H*-Benzo[*g*]indazole** is illustrated in the *Chemical Substance Index* and the *Ring Systems Handbook*:

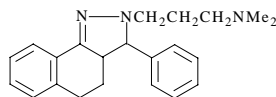
1*H*-Benz[*g*]indazole



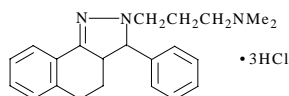
The structure is converted into the *2H*-isomer and the propanamine group (¶ 141 and 176) is attached at the 2-position. (It should be noted that, in conjunctive nomenclature, the function is located at the end of the saturated, acyclic chain furthest from the ring system of the index heading parent (see ¶ 124).)



The four hydrogens are added to the 3, 3a, 4, and 5 positions to saturate the two double bonds; then, when the phenyl and two methyl substituents (see ¶ 294) are attached, the structure becomes:



The “hydrochloride (1:3)” modification completes the structure:

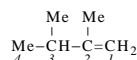


The modification is also used in naming *polymers* (¶ 222) on the basis of the monomers from which they are formed.

Example:

1-Butene, 2,3-dimethyl-, homopolymer

The structure of 1-Butene is deduced from ¶ 141. When the two methyl groups (¶ 294) are attached at positions 2 and 3, the structure becomes:



The homopolymer is represented as follows:

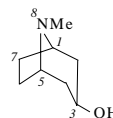


318. Stereochemistry for the heading parent is the last structural information described in a *CA* name. The various symbols used to describe the spatial arrangement of atoms are discussed in ¶ 203.

Example:

8-Azabicyclo[3.2.1]octan-3-ol, 8-methyl-, (3-*exo*)-

The structure corresponding to the basic skeleton name, principal functional suffix, and substituent is determined as described above. The stereochemistry of the hydroxy group (the methyl group rocks back and forth about the nitrogen atom, eliminating the effects of asymmetry there) is denoted by “(3-*exo*)-”, the meaning of which is determined from ¶ 203 I. The structure is therefore:



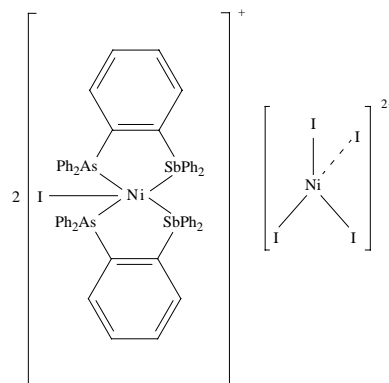
As stated in ¶ 315, *stereoparent names* (see ¶ 203 II) in the *Chemical Substance Index* imply (in the absence of cited stereochemical descriptors) a standard structure, including specific stereochemistry, as illustrated by an accompanying structural diagram complete with the numbering system from which locants for substituents and derivatives are derived. With the exception of monosaccharide and some peptide stereoparents, italicized systematic names (and in some cases one or more trivial names) appear as synonyms in parentheses immediately following the (preferred) boldface stereoparent name. In the following examples these systematically named synonyms (1) illustrate the various types of stereochemical descriptors found in *CA* indexes and (2) show how the use of stereoparents as the preferred *CA* names for many natural products avoids citation of (often necessarily complicated) stereochemical descriptors.

Stereochemical descriptors in the *CA* index names of *coordination compounds* reflect the geometry of ligand attachments around one or more central metal atoms (compare ¶ 215).

Example:

Nickel(1+), bis[[2-(diphenylstibino- κ Sb)phenyl]diphenylarsine- κ As]iodo-, (T-4)-tetraiodonickelate(2-) (2:1)

In this example, the central atom is nickel. The structure of the two large ligands can be determined by reference to ¶ 294. The italicized element symbols (*As*, *Sb*) identify the ligating atoms. The stereochemistry symbol (*T*-4) along with the Kappa indicates that the anion is tetrahedral (see ¶ 203 III). The structure of this coordination compound is therefore:



M. INDEX

The references are to paragraphs, not to pages. Trivial and former CA names, general terms and name fragments are listed along with current CA index names. Locants and other numerals, etc., have generally been omitted.

- Abeo**, 212
Acenaphthylene, 148, 152
Acetaldehyde, 173
hydrate, 192
oximes, 195
Acetals, 169, 196
of carbohydrates, 208
retrospective index searching for, 226
of stereoparents, 202
Acetamide, 171
Acetate fibers, 222
Acetates
of amines, 198
Acetato, 215
Acetic acid, 165
anhydride-esters, 186
anhydrides, 179
esters, 185
hydrazides, 189
locants for substituents, 117
molecular addition compds., 192
multiplication of, 118
order of precedence of, 106
polymers containing, 222
Acetoacetic acid, 167
Acetone, 174
hydrazone, 190
retrospective index searching for, 262
Acetonitrile, 172
Acetoxy, 175, 283
Acetyl, 134, 168, 174
free radical, 1-oxoethyl as name for, 187
Acetylamino, 134, 171
Acetyl chloride, 170
as substituent, 134
Acetylides, 180
of elements, 219
Acetyloxy, 175, 283
Acid azides, 170
order of precedence of, 106
Acid chlorides. See *Acid halides*
Acid halides, 170
of arsenic and phosphorus acids, 197
of carbohydrates, 208
inorganic, 219
order of precedence of, 106
retrospective index searching for, 227
Acid isocyanates, 183
order of precedence of, 106
Acid radicals, 134, 168, 287
from amino acids, 205
from arsenic acids, 197
from phosphorus acids, 197, 219, 276
hetero-atom-attached, 163, 171, 174
Acids. See also *Carboxylic acids*; *Imidic acids*;
Sulfonic acids; etc.
acyclic, with cyclic substituents, 166
anhydrides—see *Anhydrides*
of arsenic end phosphorus, 197
of carbohydrates, 208
of chlorine, nitrogen, phosphorus, etc., order
of precedence of, 106
Class I and Class II, 185
conjunctive names for, 166
epoxy derivs., 166
expressed as suffixes, 164-177
functional derivs., 169
halogen oxo, 188
inorganic "oxo", 219, 273
isopoly end heteropoly, 219
labeled, 220
ligands from, 215
of metals, 219, 273
order of precedence of, 106, 167
radicals from—see *Acid radicals*
retrospective index searching for, 228, 273
as substituents, 167
Acinitro, 132, 193
Acridine
analogs, 149
numbering of, 152
ACS. See *American Chemical Society*
Actinomycins, 206
Acyclic compounds, 141-144
nonfunctional, order of precedence of, 106
Acyl radicals. See *Acid radicals*
Added hydrogen, 136, 256
in cyclic ketones, 174
in ring assemblies, 157
in spiro systems, 156
Additional index entries
for anions, 198, 281A
for coordination compds., 215
for cyclic peptides, 206
for molecular addition compds., 192, 265A
Addition compounds. See *Molecular addition
compounds*
Additive nomenclature, 123, 228A
Additive terms, 113
locants for, 119
Adducts, 192
Adenine, 122
Adenosine, 210
Adenosine triphosphatase, 218
Adenylic acid, 210
homopolymer, 222
Agar, 208
-al, 173
Alanine, 205
peptides containing, 206
Alanine aminotransferase, 218
Alcohols, 175
carbohydrates as, 208
Class 1, 185
esters, 185
labeled, 220
metal salts, 198
order of precedence of, 106
retrospective index searching for, 229
Aldaric acids, 208
Aldehydes, 173
order of precedence of, 106
oximes, 195
retrospective index searching for, 230
Aldehydic acids, 167, 228
Alditols, 208
Aldonic acids, 208
Aldoses, 208
Alkaline earth metals, 219
Alkaloids, 204
retrospective index searching for, 231
stereochemistry of, 202
steroidal, 211
Alkanes, 141
locants for, 113
Alkenyl radicals
locants for, 116
Alkoxy radicals
elision in names of, 107
Alkyl radicals, 161
1-imino and 1-oxo derivs., 134, 168
allo, 209
Alloys, 214
labeled, 220
retrospective index searching for, 232
 α (*alpha*), 203, 208, 212
Alphabetization
of index names, 121
Alpha particle, 217
Alternating polymers, 222, 277
Aluminate, 215, 219
Aluminum
labeled complexes, 220
Aluminum chloride
and dimer, 215, 219
Alums, 219
American Chemical Society
nomenclature reports of, 302
nomenclature rules of, 296-300
American Mineralogist, 219
Amic acids, 167, 228
Amides, 171
of amino acids, 205
of arsenic and phosphorus acids, 197
of carbohydrate acids, 208, 240
N-hydroxy, 193
order of precedence of, 106
oxides, 268
oximes, 171
peptides, 206
radicals from, 134, 171
retrospective index searching for, 233
tautomerism with imidic acids, 122, 165
unexpressed, 171
Amidines. See *Imidamides*
Amidine tautomerism, 122
Amido, 215
Amidodiphosphoric acid, 219
Amidodiphosphoryl chloride, 219
Amidogen, 187, 219
Amidoimidodisulfuric acid, 219
Amidoimidodisulfurous chloride, 219
Amidoselenic acid, 219
Amidoselenonyl fluoride, 219
Amidosulfonyl chloride, 200, 219
Amidosulfoxylic acid, 219
Amidothiiodiphosphoric acid, 219
Amidoximes, 171
Amines, 176
boron complexes, 182
N-hydroxy, 193
order of precedence of, 106, 271
retrospective index searching for, 235
salts with acids, 198
Aminium compounds, 184
hydroxides, inner salts, 112
present and former indexing rules for, 270
salts, 198
ylides, 201
Amino, 176
Amino acids, 205
ACS rules for, 302
amides of, 171
homopolymers, 206
polymers, 222
IUPAC-IUB tentative nomenclature rule for,
297
retrospective index searching for, 236
Aminobutyryl
in peptide names, 206
Aminocarbonyl, 134
Amino group
tautomerism of, 122
Ammines, 215
labeled, 220
Ammonia, 219
Ammoniates, 192
of inorganic salts, 219
Ammonio, 184
Ammonium chloride, 219
Ammonium salts
inorganic, 219
organic, 184, 270
Ammoniumyl, 184, 219
Amylopectin, 208
-an
in mineral names, 219
Androstane, 211
Androstanol
esters, 202
-ane, 146
Aneurine, 224
Angiotensins, 206
Anhydride-esters, 186
Anhydrides, 179
of amino acids, 205
of carbohydrates, 208
of carbonic acid derivs., 183
of cyanic acid, 183
of halogen oxo acids, 188
of inorganic with organic acids, 219
as modification terms, 112, 113

- with partial esters, 186
retrospective index searching for, 237
- anhydro*, 208
- Anhydro**, 139
- Anhydrosulfides**, 179, 197, 200
"bis" and parentheses used with, 110
of inorganic acids, 219
of thiocyanic acid, 183
- Anilic acids**, 167, 228
- Anilides**, 171, 233
- Anils**, 176
- Anions**, 180
additional index entries, 198, 281A
citation in modifications, 113
common, 198, 281A
complex, 215
of elements, 219
in modifications, 198
- anium**, 184
- "a" nomenclature**. See *Replacement nomenclature*
- Anthracene**
in fused systems, 148, 151
numbering of, 152
preferred to phenanthrene, 138
- Anthracenedione**, 136
- anti*, 203
- Antielements**, 217
- Antihelium**, 217
- Antimonate**, 215
- Antimonide**, 180
- Antimony**
defined as metal, 101, 181, 215, 219, 257
- Antimony compounds**, 181
monocyclic, 146
order of precedence of, 106
Von Baeyer systems, 155
- Antimony hydroxide**, 181, 219
- Antiparticles**, 217
- Antiproton**, 217
- Apamin**, 206
- Apiose**, 208
- Apocarotenes**, 212
- Aqua**, 219
- ar*, 120
- Arabanan**, 208
- arabinose**, 208
- Arrow nomenclature**, 208, 210
- Arsenamldic acid**, 197
- Arsenic acid**, 197
- Arsenous acid**, 197
- Arsenic acids**, 197, 273
anhydrides, 179
inorganic, and salts, 219
- Arsenic compounds**, 197
order of precedence of, 106
tautomeric, 122
- Arsenic triamide**, 197
- Arsenides**, 180
of elements, 219
- Arsenido**, 215
- Arsenous acid**, 197
- Arsindole**, 149
- Arsine**, 143, 197
- Arsine selenide**, 197
- Arsine sulfide**, 197, 200
- Arsinic acid**, 197
- Arsino**, 161, 197
- Arsinous acid**, 197
- Arsinous cyanide**, 197
- Arsinyl**, 197
- Arsonic acid**, 197
derivs., 271
- Arsonimidous acid**, 129
- Arsonium compounds**, 184
- Arsonous acid**, 197
- Arsorane**, 140, 143, 197
- as*, 108
- Ascorbic acid**, 208, 224
- ase**, 218
- Asparaginase**, 218
- Aspartic acid**
peptides containing, 206
- Aspartoyl**, 205
- Assumptions**
for amino acid end peptide stereochemistry, 205, 206
for biline stereochemistry, 223
for coordination stereochemistry, 203
for polymer SRU names, 222
- ate**, 219
- Atisane**, 212
- ato ligands**, 215
- Aurate**, 215
- Aza**, 128
- Azacycloundecane**, 146
- Azahomoandrostan**, 211
- Azete**, 146
- Azi**, 161
- Azides**
acid, 170
acid, order of precedence of, 106
- Azidodisulfuric acid**, 219
- Azidosulfuric acid**, 219
- Azines**, 190
- Azino**, 161, 193
- Aziridine**, 146
- Azo**, 161, 193
- Azo compounds**, 193, 218
dyes, 216
retrospective index searching for, 238
- Azomethines**, 176
- Azonia**, 184
- Azoxy compounds**, 193
retrospective index searching for, 238
- Balata**, 222
- Barbituric acid**, 122
- Baryon**, 217
- Base components**
carbocyclic, of fused systems, 148
heterocyclic, of fused systems, 149, 281
selection of, 150
- Benzaldehyde**, 173
- Benzenamine**, 176
- Benzenaminium**
hydroxide, inner salts, 201
- Benzene**
alkoxy derivs., 196
in fused systems, 149, 151
multiplication of, 118
preferred to cyclohexane, 138
radicals from, 161
ring assemblies of, 157, 163
- Benzenecarbothioic acid**
hydrazide, 189
- Benzenecarbothioyl chloride**, 170
- Benzenecarboximidic acid**, 129, 165
- Benzenediactic acid**
derivs., 124
- Benzenediazonium compounds**, 198
- Benzenedicarboxylic acid**
polymers, 222
- Benzenedipropanoic acid**, 166
- Benzenemethanol**, 124
derivs., 131
- Benzenepropanal**
hydrazones, 190
- Benzenesulfonamide**, 171
- Benzenesulfonic acid**
anhydrides, 179
- Benzenethiol**
esters, 185
- Benzenide**, 180
- Benzeno**, 154
- Benzimidazole**
tautomers, 122
- Benzimidazolium compounds**, 184
- Benzindene**, 150
- Benzisothiazole**
abnormal valency in, 158
- Benzo**, 149
elision of, 107
- Benzodioxaborole**, 182
- Benzofuran**, 149
- Benzogermole**, 194
- Benzoic acid**, 165
anhydrides, 179
derivs., 131
esters, 185
order of precedence of, 106
- Benzonitrile**, 172
- Benzopyran**
as fusion component, 152
- Benzopyranol**
vitamin E derivs., 224
- Benzopyranone**, 185
- Benzothiazolium compounds**, 184
dyes, 216
- Benzothienyl**, 161
- Benzoxazine**, 149
- Benzoxazole**, 149
- Benzoyl**, 134, 168, 174
- Benzoyl isocyanide**, 170
- Benzyl alcohol**, 124
derivs., 131
- Benzynes**, 145
- Beryllium chloride**, 219
- β (*beta*), 203, 208, 212
- Beta particle**, 217
- Bibicyclo**, 157
- Bibliography**
of nomenclature of chemical substances, 295-308
- Bicyclodecasilane**, 155
- Bicycloheptyl**
"bis" and parentheses used with, 110
- Bicyclohexadienyldiylidene**, 161
- Bicyclohexenyl**, 157
- Bicyclohexyl**, 157
- Bicyclo systems**. See *Von Baeyer systems*
- Bicyclotetrasilazane**, 155
- Bicyclotetrasiloxanyl**, 157
- Bicycloundecane**, 155
- Biguanidine**, 251
- Biisoquinoline**, 157
- Bile pigments**, 223
retrospective index searching for, 278
- Biline**, 223, 278
- "Bimol."**
in anhydride names, 179
- Bi names**. See *Ring assemblies*
- Binaphthalene**, 157, 266, 281
- Binaphthalenediyl**, 161
- Binary compounds**, 219
- Biochemistry**
nomenclature of, history and development of, 305
nomenclature rules for, 297
- Bipentaborane**, 159
- Biphenyl**, 114, 157, 281
locants in, 113
- Biphenyldiyl**, 125, 161
- Biphenyl**, 161
punctuation for, 109, 110
- Biphenylcarbonyl**, 168
- Bipiperidine**, 157
- Bipyridinediyl**, 161
- Bis**, 110, 266
alphabetization rules for names containing, 121
enclosing marks following, 109
in multiplicative names, 125
in ordering of substituents, 121
- Bismuth compounds**, 181
monocyclic, 146
order of precedence of, 106
- Bismuth hydroxide**, 181
- Bismuthine**, 143, 181
- Bismuthine imide**, 181
- Bismuthine oxide**, 181
- Bismuthino**, 161, 181
- Bisulfite addition compounds**, 192
- Bithiazole**
polymers, 222
- Bithiazolyl**, 161
- Bitriazole**, 157
- Block polymers**, 222, 277
- Bohrium**, 219
- Bonds**
metal-metal, 203
multiple—see *Unsaturated compounds*
- Bora**, 128
- Boranamine**, 182
- Borane**, 159, 182
free radicals from, 187
order of precedence of, 106
oxybis-, derivs., 179
trifluoro-, 257
- Boranetriamine**, 182
- Boranthrene**, 149
- Borate (1-)**, 106, 182
- Borates**
aminium, 201
complex, 215
- Borazine**, 146, 182
- Boric acid**, 182, 219
anhydride-esters, 186
anhydrides, 179
- Borinic acid**, 182

- Borole**, 182
- Boron acids**, 182
anhydrides, 179, 182
esters, 185
hydrazides, 182
- Boron complexes**, 201
- Boron compounds**, 159, 182
inorganic, IUPAC report on, 298
molecular skeletons, 159
order of precedence of, 106
retrospective index searching for, 239
zwitterionic, 201
- Boronic acid**, 182
- Boron metaphosphate**, 219
- Boron phosphate**, 219
- Boroxin**, 146
- Borhiin**, 146
- Boryl**, 161
- Boson**, 217
- Boughton system**
for isotopes, 220
- Brackets**, 109
around complex radicals, 132
around locants in spiro names, 156
in multiplicative names, 125
- Bradykinin**, 206
- Brass**, 214
- Bridged fused systems**, 154
- Bridged systems**, 140, 147, 155
choice between, 138
fused, 154
indicated hydrogen in, 135
Von Baeyer names for, 155
- Bromic acid**, 188
- Bromo**, 131
- Bromous acid**, 219
- Bronze**, 214
- Bufanolide**, 211
- Butanedioic acid**
anhydride-esters, 186
- Butanediol**
fibers from dioic acids and, 222
- Butenone**, 137
- Butyne**
metal derivs., 219
- Butyryl**
in peptide names, 206
- ¹⁴C, 220
- CA. See *Chemical Abstracts*
- Cadinane**, 212
- Caerulein**, 206
- Caffeine**, 122
- Cahn-Ingold-Prelog rule**. See *Sequence rule*
- Calciferol**, 224
- Calcitonin**, 206
- Calcium carbide**, 219
- Camphor**, 212
- Carbaboranes**, 160, 182
- Carbamic acid**, 183
conjunctive names not formed from, 124
as elided name, 107
esters, 185
hydroxy, 193
multiplication of, 118
- Carbamic chloride**, 183
- Carbamimidic acid**, 183
- Carbamoyl**, 134
- Carbapolyboranes**
order of precedence of, 106
- Carbazole**
numbering of, 152
- Carbide**, 219
- Carbocyclic compounds**, 145, 147, 148
monocyclic, radicals from, 161
order of precedence of, 106
spiro, 156
- Carbodiimide**, 177, 191
- Carbodithioic acids**, 165, 200
- Carbohydrates**, 208
ACS nomenclature rules for, 302
IUPAC tentative nomenclature rules for, 296
retrospective index searching for, 240
- Carbohydrazide**, 252
- Carbohydrazones**, 190
- Carbohydrazonic acids**, 165
- Carbon compounds**. See also *Carbocyclic compounds*
acyclic, 141
acyclic and cyclic, order of precedence of, 106
ions, 180, 184, 219
- Carbon dioxide**, 219
- Carbon disulfide**, 219
- Carbonic acid**, 183
cyclic esters, 196
anhydrides, 179
anhydride with silicic acid, 199
derivs., retrospective index searching for, 241
order of precedence of, 106, 271
and related compounds, 183
replacement names from, 129
- Carbonic bromide chloride**, 183
- Carbonic dihydrazide**, 183, 189
- Carbonimidic acid**, 183
- Carbonimidoyl**, 134, 168, 174
in multiplicative names, 125
- Carbonitriles**, 172
- Carbonium compounds**, 184
- Carbon monoxide**, 219
- Carbochloridic acid**, 183
- Carbochloridothioic acid**
anhydrosulfides, 170
- Carbonodiperoxoic acid**, 129, 183
- Carbonodithioic acid**
anhydrosulfides, 200
- Carbonohydrazoneic acid**, 129
- Carbonohydrazoneoyl**, 134
- Carbothioic dichloride**, 183
- Carbothioyl**, 134, 168, 174
in multiplicative names, 125
- Carbon oxide sulfide**, 219
- Carbon tetrachloride**, 272
- Carbonyl**, 134, 168, 174
free radicals containing, 187
hetero-atom-attached, 163
in multiplicative names, 125
- Carbonyldiimino**, 134
- Carbonyls**
metal, 215, 219
- Carbostyryl**, 122
- Carbothioamides**
elision in names of, 107
- Carbothioic acids**, 165
- Carboxaldehydes**, 173, 230
- Carboxamides**, 171, 233
tautomerism of, 122
- Carboximides**, 191
- Carboximidic acids**, 129, 165
tautomerism of, 122
- carboxy, 220
- Carboxy**, 134
- Carboxy-amino**, 183
- Carboxylato**, 215
- Carboxylic acids**, 165
acyclic with cyclic substituents, 166
aminium salts, 198
anhydrides with inorganic acids, 219
of carbohydrates, 208
esters, 185
free radicals from, 187
functional derivs., 169
labeled, 220
molecular addition compds., 192
order of precedence of, 106, 167
retrospective index searching for, 228
salts, 198
as substituents, 167
- Cardanolide**, 211
- Carotene**, 212
- Carotenoids**, 212
ACS report on nomenclature of, 302
IUPAC tentative nomenclature rules for, 296
- Carrageenan**
mixtures containing, 221
- Cast iron**, 214
- Categories**
for elements, 219
- Catena compounds**, 192
- Cations**, 184
complex, 215
elementary and inorganic, 219
order of precedence of, 106
present and former indexing rules for, 270
salts, 198
- Cellulose**, 208, 240
- Centrality**
in amines, 176
in index name selection, 138, 255
- Cephalosporins**
stereochemistry of, 203
- Cermets**, 214
- Cevane**, 211
- Chemical Abstracts*
index nomenclature for, reports on, 301
- Chicle**, 222
- Chirality**. See *Stereochemistry*
- chiro, 209
- Chloramido**, 215
- Chloramine**, 219
- Chloric acid**, 219
metal salts, 219
- Chlorides**
of arsenic and phosphorus acids, 197
of elements, 219
glycosyl, 208
- Chlorine compounds**, 188
- Chlorine nitrate**, 219
- Chlorine oxide**, 219
- Chloro**, 132
- Chlorocarbonyl**, 131
- Chloroimidisulfuric acid**, 219
- Chloronium**, 219
- Chlorophylls**, 233
- Chlorosulfuric acid**, 129, 219
- Chlorosyl**, 219
- Chloryl**, 188, 219
- Chloryl fluoride**, 219
- Chloryloxy**, 188
- Cholane**, 211
- Cholecalciferol**, 224
- Cholestane**, 211
- Chromates**
complex, 215
- Chromatite**, 219
- Chrome alums**, 219
- Chromic acid**, 219, 273
- Chromium carbonyl**, 219
- Chromium hydroxide**, 219
- Chromyl**, 219
- Chymotrypsin**, 218
- cis, 203, 209
- C.I. names**, 216
- Cinchonanol**
salts, 202
- Cinnoline**, 149
- ³⁵Cl, 220
- Class I acids**, 185, 247
- Class I alcohols and thiols**, 185, 247
- Cluster compounds**, 203, 215, 219
- Cobalamin**, 224
- Cobalt**
labeled complexes, 220
- Cobaltate**, 219
- Cobalt nitrate sulfate**, 219
- Cobamic acid**, 224
- Cobamide**, 224
- Cobinamide**, 224
- Cobinic acid**, 224
- Cobyric acid**, 224
- Cocarbonylase**, 224
- Coenzyme A**, 210
- Colons**, 108
in coordination names, 215
in index names, 108
- Colour Index*, 216
- Commas**, 108
of inversion, 104
in modifications, 108
- Common components**
of addition compds., 192, 265A
of salts, 198, 281A
- Complexes**. See *Coordination compounds*
- Complexity**
principle of, discontinuance of, 255
- Compound classes**
order of precedence of, 106
- Compound radicals**, 133, 162
- Conanine**, 211
- Configuration**. See *Stereochemistry*
- Configuration numbers**
for coordination compds., 203
- Conjugate acids**, 184
labeled, 220
- Conjunctive nomenclature**, 124, 315
for acids, 166

- present and former policies of, 255
- Constitutional repeating units**, 222
- Coordination compounds**, 215
- amino acid transition metal salts as, 205
 - labeled, 220
 - order of precedence of, 106
 - polymers of, 222
 - porphyrin complexes, 223
 - retrospective index searching for, 242
 - stereochemistry of, 203
 - structural diagram derivation for, 318
 - sulfur complexes as, 200
- Copolymers**, 222
- Copper**
- monocysteine complex, 205
- Corrin**, 224
- Corrinoids**. See also *Vitamin B₁₂*
- IUPAC-IUB tentative nomenclature rules for, 297
- Corticosteroids**, 206
- Coumarins**, 185
- Cuprates**
- complex, 215
- Cyanamide**, 183, 267
- Cyanates**
- of arsenic and phosphorus acids, 197
- Cyanato**, 183, 188, 215
- Cyanic acid**, 183, 188, 219
- anhydrides, 170, 179
 - esters, 185, 188
- Cyanides**
- of arsenic and phosphorus acids, 197
- Cyanine dyes**, 216
- Cyano**, 172
- Cyanocobalamin**, 224
- Cyanosulfuric acid**, 219
- Cyclic(glycylglycylglycyl)**, 206
- Cyclitols**, 209
- IUPAC tentative nomenclature rules for, 296
- Cycloalkanes**, 145
- Cycloalkenes**, 145
- Cycloalkenyl radicals**
- locants for, 116
- Cycloandrostanane**, 211
- Cyclodisilazane**, 146
- Cyclohexadienyne**, 145
- Cyclohexanamine**
- salts, 198
- Cyclohexane**, 130
- benzene preferred to, 138
 - polyhydroxy derivs., 209
 - terpene derivs., 212
- Cyclohexasiloxane**, 146
- Cyclohexastannane**, 199
- Cyclohexene**, 145
- no locant used with, 113
- Cyclohexenone**, 174
- Cyclohexenylidene**, 161
- Cyclohexyl**, 161
- Cyclopentadiene**, 145
- Cyclopentadienide**, 180
- Cyclopentadienyl**, 161
- in metal complexes, 215
- Cyclopentane**
- fused derivs., 151
- Cyclopentaphenanthrene**
- bridged derivs., 154
 - derivs., 211
 - and derivs., numbering of, 152
- Cyclopregnane**, 211
- Cyclopropenyl**, 161
- Cyclocopregnane**, 211
- Cyclosiloxanes**, 146
- Cyclotrisiloxanol**, 199
- Cysteine**, 205
- Cytidine**, 210
- Cytidylic acid**, 210
- Cytochalasan**, 202
- Cytochrome c**, 207
- Cytosine**, 122
- d*
- in deuterium-labeled compds., 220
- D, 108, 205, 208, 209
- De**, 206
- Decaborane**, 159
- Decaborano**, 159
- Decyl**
- "tris" and parentheses used with, 110
- Dehydro**, 139, 146, 158, 208
- in phorbine names, 223
- Dehydrogenase**, 218
- Deoxo**, 204
- Deoxy**, 139, 204, 208
- Depsipeptides**, 206
- Derivatives**. See *Functional derivatives*
- Desulfo**, 206
- Deuterium**, 220
- Di**, 110
- Diarsene**, 143
- Diarsine**, 197
- Diarsinous acid**, 179
- Diazadiphosphetidine**, 197
- Diazane**. See *Hydrazine*
- Diazaporphine**, 223
- Diazene**
- and derivs., 193
 - order of precedence of, 106
- Diazene-carboxaldehyde**
- hydrazones, 190
- Diazene-carboxylic acid**
- hydrazides, 189
- Diazenyl**, 161
- Diazenyloxy**
- free radical, 187
- Diazo**, 132
- "bis" and parentheses used with, 110
- Diazoamino tautomerism**, 122
- Diazo compounds**, 193
- retrospective index searching for, 243
- Diazonio**, 184
- Diazonium compounds**, 184
- double salts, 216
 - salts, 198
- Dibismuthine**, 143
- Diborane**, 159, 182
- Dicarbododecaborane**, 160, 182
- Dicarbahaheptaborane**, 160
- Dicarbonyl acid**, 179
- Dicarbonyl dichloride**, 183
- Dicarbonyl acid**
- esters and hydrazides, 119
- Didehydro**, 139, 146, 208
- in phorbine names, 223
- Diels-Alder adducts**, 192
- Diene adducts**, 192
- Diethylamino**
- alphabetization of, 121
- Digermaselenane**, 144
- Diimidotricarbonimidic acid**, 183
- Diimidotriphosphoramide**, 197
- Dilimidotrisulfuric acid**, 219
- Dimers**
- of aluminum chloride, 215, 219
 - of boranamines, 182
- Dinorcholestanic acid**, 211
- Dioic acids**, 165
- Diols**
- esters, 119, 185
- Diones**, 174
- cyclic, 136
 - derivs., 119
- Dioxaaazadispirododecene**, 156
- Dioxacyclopentindene**, 153
- Dioxagermanin**, 199
- Dioxastannin**, 146
- Dioxy**, 196
- in free radical names, 187
- Diphosphine**, 197
- order of precedence of, 106
 - sulfides, 200
- Diphosphinediyl**, 161
- Diphosphinium**, 219
- Diphosphinyl**, 161, 197
- Diphosphonic acid**, 179
- Diphosphorane**, 143
- Diphosphoric acid**, 197, 219
- esters, 119
 - nucleotide esters, 210
- Diphosphoric(III,V) acid**, 219
- Diphosphorous acid**, 219
- Diphosphorous tetramide**, 219
- Diphosphoryl**, 219
- Diphosphoryl chloride**, 197
- Diphosphoryl chloride fluoride**, 219
- Diplumbosilane**, 199
- Diselenides**, 200
- Diselenious acid**, 219
- Disilane**, 199
- order of precedence of, 106
- Disilanehexol**, 219
- Disilathiane**, 199
- order of precedence of, 106
- Disilazane**, 144, 199
- radicals from, 144
- Disilazanediyli**, 161
- Disilanyl**, 199
- Disilazanyl**, 144, 199
- Disilene**, 143
- Disiloxane**, 199
- order of precedence of, 106
- Disiloxanediol**, 131
- Disiloxanediyl**, 125
- as hetero unit, 127
- Disiloxanyl**, 161
- Distannane**, 140
- Distannazane**
- radicals from, 144
- Distibene**, 181
- Distibenediyl**, 161
- Distibine**, 181
- Disulfamide**, 219
- (Disulfate)**, 109
- Disulfides**, 200
- acyl, 179
 - chloro, 170
 - order of precedence of, 106
 - phosphono sulfo, 219
- Disulfones**
- order of precedence of, 106
- Disulfonothioic acids**, 165
- Disulfonyl**, 219
- Disulfoxides**, 200
- order of precedence of, 106
- Disulfuric acid**
- and salts, 109, 219
- Dithiastibabicyclononatriene**, 155
- Dithiazine**, 146
- Dithiin**, 135
- Dithio**
- as hetero unit, 127
- Dithiocarboxy**, 134
- Dithioperoxy acids**, 165, 200
- Diylidene**, 161
- Diyl**, 161
- DL, 108, 205, 208
- Double bonds**. See *Unsaturated compounds*
- Double salts**, 219
- Dyes**, 216
- retrospective index searching for, 244
- E*, 203
- report on, 301
- Earliest index position**
- principle of, 122
 - of radical names, 133
 - of total index names, 138
- E.C.**, 218
- ecane**, 146
- ecin**, 146
- ecine**, 146
- Egg White**
- mixtures containing, 221
- Element**, 104, 219
- Element**, 105, 219
- Elementary particles**, 217
- retrospective index searching for, 245
- Elements**, 219
- of atomic number 104 and higher, 101
 - isotopes of, 220
- Elision**
- of vowels and syllables, 107, 283
- enantio*, 206
- Enclosing marks**, 109
- in complex radicals, 132
 - in indefinite names, 132
 - in labeled radicals, 220
 - in ligand names, 215
 - in uninverted multiplicative names, 192
- endo*, 154, 203, 206
- ene**, 139, 141, 155
- no elision of "a" before, 142
- enyl**, 161
- Enzymes**, 218
- retrospective index searching for, 246
- epane**, 146
- epi*, 209
- Epidoxy**, 154, 211
- epin**, 146
- epine**, 146

- Epithio**, 154, 208
- Epoxides**
oxirane names for, 166
- Epoxy**, 154, 211
- Ergocalciferol**, 224
- Ergostane**, 211
- erythro*, 108, 208
- Ester-anhydrides**, 186
- Esters**, 185. See also *Functional derivatives*
of amino acids, 205
anions of, 180
of carbohydrates, 208
of halogen oxo acids, 188
of hetero-atom-attached hydroxyl groups, 175
as modification terms, 112, 113
of polyalkylene glycols, 222
retrospective index searching for, 247
of stereoparents, 202
of thio acids, 200
- η (*eta*)
for pi-bonded ligands, 215
- etane**, 146
- ete**, 146
- Ethanamine**, 131
- Ethane**, 130, 163
- Ethanedinitrile**, 172
- Ethanedioic acid**, 165
- Ethanediol**
esters, 185
- Ethanedione**, 190
- Ethanedithioic acid**, 129
- Ethane(dithioperoxoic) acid**, 129
- Ethanediyil**, 125
- Ethanthioamide**
S-oxide, 200
- Ethanimidic acid**, 165
- Ethanamine**, 177
- Ethano**, 154
- Ethanol**, 175
esters, 185
- Ethanylylidene**, 154
- Ethenol**
polymers, 222
- Ethenone**, 174
- Ethers**, 196
"a" names for poly, 142
of polyalkylene glycols, 222
retrospective index searching for, 248, 271
- Ethoxy**
elision in spelling of, 107
free radical, 187
- Ethyl**, 161
free radical, 187
- Ethylene glycol**
polymers, 222
- Ethylides**, 201
- Ethylum**, 184
- Ethyne**
metal derivs., 219
- etidine**, 146
- Eudesmane**, 212
- Ewens-Bassett numbers**, 215, 219
in vitamin B₁₂ names, 224
- exo*, 203
- Farnoquinone**, 224
- Fermion**, 217
- Ferrates**, 215
porphine complexes, 223
- Ferrocene**, 215
order of precedence of, 271
retrospective index searching for, 264
- Fibers**
synthetic, 222
- Fibrinopeptide B**, 206
- Fluoresceins**, 216
- Fluorimide**, 219
- Fluorine compounds**, 117, 188
- Fluorocarbons**
locants for, 117
- Fluoroselenious acid**, 219
- Formaldehyde**, 183
oximes, 195
polymers, 222
- Formamide**, 183
- Formamidine**, 234, 280
- Formazan**, 193
retrospective index searching for, 249
- Formazano**, 193
- Formazanyl**, 193
- Formic acid**, 183
anhydrides, 179
order of precedence of, 106
replacement analogs, 183
formyl, 220
- Formyl**, 134, 173
- Formyl isocyanate**, 183
- Free radicals**, 187
cationic, 184
- Friedo**, 212
- Fructose**, 208
valine deriv., 202
- Fullerenes**, 163A
- Fulminic acid**, 188, 219
- Functional compounds**
described by suffixes, 164-177
- Functional derivatives**
of acids, 169
of amino acids, 205
commas between names of, 108
locants for, 119
order of citation of, 113
retrospective index searching for, 250
of stereoparents, 202, 204
of steroids, 286
- Functional parent compounds**, 130, 131
acids, order of precedence of, 106
- Functions**
order of precedence of, 106
- Furan**, 146
in fused systems, 149, 151
- Furandione**
polymers containing, 222
- Furandiylylidene**, 161
- Furanimine**, 185
- Furanium compounds**, 184
- Furano**, 154
- furanose**, 208
- Furanosides**, 208
- Furazan**, 281
- Furostan**, 211
- Furylium compounds**, 184
- Fused ring systems**, 147, 148
- Fused systems**
base components for, 148, 149, 150, 281
boron-containing, 159
bridged, 154
carbocyclic, 148, 151
heterocyclic, 149, 151, 281
numbering of, 152
replacement nomenclature for, 153
- Galactitol**, 208
- Galactose**, 208
- Gammacerane**, 212
- Gastrin**, 206
- Geometry**
of coordination complexes, 203
- Germanamine**, 199
- Germanate**, 215
- Germane**, 143, 199, 219
- Germanium compounds**, 199
cyclic, 146, 194
order of precedence of, 106
- Germanium hydroxide**, 199
- Germaselenanes**, 144
- Gibbane**, 212
- Glucagon**, 206
- Glucitol**, 208
gluco, 208
- Gluconyl chloride**, 208
- Glucopyranose**, 208
- Glucopyranosyl**, 208
- Glucopyranosylamine**, 208
- Glucopyranuronic acid**, 208
- Glucose**, 208
mixtures containing, 221
polymers, 222
- Glucosides**, 208
- Glucuronan**, 208
- Glutamic acid**, 205
peptides containing, 206
- Glutamoyl**, 205
- Glycerides**, 185
glycero, 208
- Glycerol**
esters, 185
- Glycine**, 205
peptides containing, 206
- Glycols**
polymers, 222
- Glycolic acid**, 167
- Glycosides**, 208, 240
- Glycosylamines**, 208
- Glycosyl halides**, 208
- Glycosyl radicals**, 208
in nucleosides and nucleotides, 210
- Glycyl**, 205
- Gonane**, 211
- Gonatriene**, 211
- Gorgostane**, 211
- Graft polymers**, 222, 277
- Gramicidin S**, 206
- Graphite**, 219
- Graphite nitrate**, 219
- Graphitic acid**, 219
- Greek letters**
alphabet, 310
order of citation of, 113
- Guanidine**, 183
derivs., retrospective index searching for, 251
- Guanine**, 122
- Guanosine**, 210
- Guanlylic acid**, 210
polymers, 222
- gulo*, 208
- Gutta-percha**, 222
- H*. See *Added hydrogen*; *Indicated hydrogen*
- Hadron**, 217
- Hahnium**, 219
- Halides**. See also *Acid halides*
of germanium, lead, etc., 272
of metals, 219
of silicon, 282
- Halogen compounds**, 188
- Halogenoid compounds**, 188
- Halogens**, 219
- Hantzsch-Widman system**, 146
order of precedence of, 138
- Helium-group gases**, 219
- Hematin**, 223
- Hemi**, 192, 265A, 311
- Hemiacetals**
of carbohydrates, 208
- Heptene**
polymers, 222
- Hetero-atom chains**
acyclic, 142
acyclic, radicals from, 161
heterogeneous, 144
homogeneous, 143
homogeneous, breaking of, avoided, 138
- Hetero atoms**
lowest locants for, 137
order of precedence of compds. containing, 106, 138
- Heterocyclic compounds**
fused, 149, 281
numbering of, 152
spelling of names of, 107
order of precedence of, 106
preferred to carbocycles, 138
- Heterogeneous hetero chains**, 144
- Heteropoly acids**, 219
- Hetero polyboranes**, 160
- Hetero units**, 127, 176, 196, 279
- Hexaborane**, 159
- Hexadiene**, 141
- Hexanedioic acid**
polymers with diols, 222
- Hexapropylene glycol**, 222
- Hexene**
polymers, 222
- Hexodialdose**, 208
- Hexopyranosulose**, 208
- Hexoses**, 208
- Hexosulofuranose**, 208
- Hexosulose**, 208
- Hexulose**, 208
- Hexyne**, 141
- Histidine**
numbering of, 205
- Homo**, 204, 211
- Homocysteine**, 205
- Homogeneous hetero chains**, 143

- Homoglycans**, 208
Homonorpregnane, 211
Homonorursene, 212
Hormones, 206
Hydantoin, 122
Hydrates, 192, 265A, 311
 citation in modification, 113
 labeled, 220
 of metal salts, 219
Hydrazine, 161, 211
Hydrazide
 as index parent, 180, 219
Hydrazides, 189. See also *Functional derivatives*
 of amino acids, 205
 of arsenic and phosphorus acids, 197
 of boron acids, 182
 of elements, 219
Hydrazine, 143, 193, 219
 acyl—see *Hydrazides*
 alkylidene—see *Hydrazones*
 alkylthio, 189
 boryl, 182
 derivs., 189, 193
 derivs., retrospective index searching for, 252
 order of precedence of, 106
Hydrazinecarbothioamide
 derivs., 190
Hydrazinecarboxamide
 derivs., 193, 202
Hydrazinecarboxylic acid, 183, 189, 193
Hydrazinedicarboxylic acid, 165
Hydrazinedisulfonyl dichloride, 219
Hydrazinium, 184, 219
Hydraziniumyl, 184
Hydrazino, 161, 189, 193
 tautomerism of, 122
Hydrazinosulfonyl, 189
Hydrazinylylidene, 161, 193
Hydrazo, 161, 193
Hydrazoic acid, 219
Hydrazonamides, 171
Hydrazones, 190. See also *Functional derivatives*
 of carbohydrates, 208
 of stereoparents, 204
 tautomerism of, 122
Hydrazonic acids, 165, 169, 190
 hydrazides, 122
 tautomerism with hydrazides, 165
Hydrazono, 161, 190, 193
Hydrazyl, 187
Hydride
 as index parent, 219
Hydrides, 219
 labeled, 220
Hydriodic acid, 219
Hydro
 abnormal-valency ring systems, 158
 locants for, 117
Hydrobromic acid, 219
Hydrocarbons
 acyclic, 141
 fused systems, 148, 152
 labeled, 220
 monocyclic, 145
 monocyclic, radicals from, 161
 order of precedence of, 106
 polycyclic, 147
 spiro, 156
Hydrochloric acid
 and dimer, 219
Hydrochlorides, 198
Hydrocyanic acid, 183
Hydrodisulfides, 200
Hydrofluoric acid, 219
Hydrogen
 added—see *Added hydrogen*
 indicated—see *Indicated hydrogen*
 isotopes of, 220
 in partial ester names, 185
 subtraction of, from ring systems, 139
Hydrogenase, 218
Hydrogenobyrinic acid, 224
Hydrogen peroxide, 219
Hydrogen sulfide, 219
Hydrogen triiodide, 219
Hydrogen trioxide, 219
Hydroisocyanic acid, 219
Hydrolytic polymers, 222, 277
Hydroperoxides, 126, 196
 of elements, 219
 order of precedence of, 106
Hydroperoxo, 219
 free radical, 187
Hydroperoxy, 196
Hydrotrioxides, 196
Hydrotrioxo, 219
Hydrotrisulfides, 200
Hydroxamic acids, 167, 228
Hydroxides
 inner salts, 293A
 inorganic, 219
Hydroxamic acids, 167, 228
Hydroxyl, 219
 free radical, 187
 hetero-atom-attached, 163, 175
Hydroxylamine, 193, 219
 O-acyl, 171
 N-alkyl and N-aryl, 176
 N-alkylidene—see *Oximes*
 derivs., retrospective index searching for, 253
 order of precedence of, 106
Hydroxylaminesulfonic acid, 193, 195
Hydroxylase, 218
Hypernuclei, 217
Hyperon, 217
Hyphens, 108
 in hydroperoxide names, 126
Hypoboric acid
 esters, 182, 185
Hypochlorous acid, 188, 219
Hypofluorous acid, 188
Hypiodous acid
 anhydrides, 188
Hyponitric acid, 219
Hyponitrous acid
 and metal salts, 219
Hypophosphoric acid, 197, 219

-ian
 in mineral names, 219
-ide, 219
ido, 208
Illustrated structural diagrams, 135
 for stereoparents, 204, 211
Imidamides, 171
 N-hydroxy, 171
 radicals from, 134
 retrospective index searching for, 234
 tautomerism of, 122
Imidazole, 146
Imidazolidine, 146
Imides, 191
 of arsenic and phosphorus acids, 197
 oxides, 268
Imidic acids, 129, 183, 228
 amides preferred to, 122
 radicals from, 134
 tautomerism of, 122, 165
Imido, 215
Imidodicarbonic acid, 129
Imidodiphosphoric acid, 197, 219
Imidodiselenic diamide, 219
Imidodisulfuryl fluoride
 metal salts, 219
Imidogen, 187
Imidosulfamic acid, 219
Imidosulfamide, 129, 219
Imidosulfurous acid, 200
Imidotetraphosphoric acid, 219
Imidotriphosphoric acid, 129
-imine
 in fused systems, 154
Imines, 177
 N-alkyl derivatives, 176
 order of precedence of, 106
 retrospective index searching for, 254
Iminio, 184
Iminium compounds, 184
Imino
 as bridge, 154
 in multiplicative nomenclature, 125
 as substituent, 177
 in tautomers, 122
Iminodiimidotriphosphoramidate, 219
Iminomethyl, 168, 177
-in, 146, 149
Indefinite compounds, 120
 cationic, 184
 coordination compds., 215
Indene, 135
Index names
 choice of, 101, 103, 105, 138
 with functional suffixes, 164-177
 inversion of, 104
 preferred, definition of, 192
 retrospective searching of, 225-293
 structural diagrams from, 312-318
Index name selection. See also *Order of precedence*
 CAS policies (previous and present) for, 255, 301
 CAS policy revision for, 101, 255
 for compds., 138
 for fused ring systems, 151
 necessity of rules for, 103
 principles of, 105
 for radicals, 133
Index parents
 definition of, 130, 164, 315
 inversion of substituent prefixes at, 104
 nonfunctional, molecular skeletons as, 140, 163
 nonfunctional, order of precedence of, 106, 271
 structural diagrams from, 312-318
Indicated hydrogen, 135, 317
 in abnormal-valency ring systems, 158
 to accommodate bridges, 154
 ACS report on, 302
 for cyclic ketones, 174
 for cyclic sulfur compds. with abnormal valencies, 158
 of fusion components, ignored, 152
 lowest locants for, 122, 137, 138
 present and former rules for, 256
 in ring assemblies, 157
 in spiro systems, 156
Indole
 analogs, 149
Indolylidene, 161
-ine, 146, 149
Inner salts, 112, 201, 224, 293A
 vitamin B₁₂ derivs., 224
Inorganic compounds, 219
 indexing policy changes for, 225, 239, 257, 273
 labeled, 220
 nomenclature of, history and development of, 306
 nomenclature rules for, 298
Inosine, 210
Inosinic acid, 210
Inositols, 209
 retrospective index searching for, 258
Inosose, 209
Insulins, 206, 274
Intermetallic compounds, 219
 labeled, 220
International Mineralogical Association, 219
International Union of Biochemistry, 218
 nomenclature rules of, 296-297
International Union of Pure and Applied Chemistry, 101, 219
 nomenclature rules of, 296-300
Inversion
 of index names, 104
Iodate
 dichloro, 219
Iodic acid, 219
Iodine
 as index parent, 188
Iodine acids, 219
 anhydrides, 188
Iodine compounds
 with abnormal valencies, 259
 addition compds., 192
 cyclic, 158
 retrospective index searching for, 259
Iodonium, 184
Iodyl, 188
Ion(1-)
 as modification term, 113, 198
Ions
 complex, 215
 inorganic, 219
 negative, 180

- negative, in modifications, 198
negative, of elements, 219
order of citation of, in modifications, 113
positive, 184, 219, 270
- io radicals**
from metals, 215
- irane**, 146
- irene**, 146
- iridine**, 146
- irine**, 146
- Iron compounds**, 215, 219
hemes, 223
- Iron oxide**, 219
- Iron zinc oxide**, 219
- Iso**
in boron-compd. names, 159
- Isobenzofurancarboxylic acid**, 186
- Isobenzofurandione**, 179
- Isocyanates**
acid, 170
acid, order of precedence of, 106
- Isocyanato**, 183, 188
- Isocyanides**, 188
of arsenic and phosphorus acids, 197
retrospective index searching for, 260
- Isocyano**, 188
- Isocytidylic acid**, 210
- Isoguanilyc acid**, 210
- Isohypophosphoric acid**, 197, 219
- Isoindole**
in fused systems, 149, 151
- Isonauraminic acid**, 208
- Isopoly acids**, 219
- Isoselenazole**, 146
- Isosemicarbazones**, 190
- Isothiazole**, 146
- Isotopes**, 220
in alloys, 214
compds. labeled with, 220
elementary particles, 217
of hydrogen, ACS report on, 302
metastable, 220
- Isoxazole**, 146
- Italics**, 108
- ite**, 219
- itol**, 208
- IUB**. See *International Union of Biochemistry*
- Ium compounds**, 184, 215
borates, 201
retrospective index searching for, 270
salts, 198
zwitterionic, 201
- iumdiyl**, 184
- iumyl**, 184
- IUPAC**. See *International Union of Pure and Applied Chemistry*
- Kaurane**, 212
- Ketenes**, 174
thio, 183
retrospective index searching for, 261
- Keto-enol tautomers**
stereochemistry of, 203
- Ketones**, 174
added hydrogen in cyclic, 136
hetero-atom-attached, 163
indicated hydrogen in cyclic, 135
nitrogen-containing cyclic, 171
of nitrogenous heterocycles, 122
order of precedence of, 106
oximes, 195
retrospective index searching for, 262
- Ketoses**, 208
- Kraystay K**, 221
- Kromycin**, 202
- Krypton fluoride**, 219
- L, 108, 205, 208, 209
- Labeled compounds**. See *Isotopes*
- Lactam-lactim tautomerism**, 122
- Lactams**
carbohydrates, 208
- Lactate dehydrogenase**, 218
- Lactoflavine**, 224
- Lactones**, 185
of amino acids, 205
of carbohydrate acids, 208
cyclic peptides, 206
steroidal, 211
- Lactose**, 208
- Lactoyl**
in peptides, 206
- Ladder polymers**, 222
- Lakes**, 216
- λ (*lambda*)
in heterocyclic ring systems, 158
- Langham, Cecil C.**, 102
- Lanostane**, 212
- Latin prefixes**, 311
- Lead compounds**, 199
cyclic, 158
monocyclic, 146
order of precedence of, 106
- Lepton**, 217
- Leptonic molecules**, 217
- Letter locants**
in coordination names, 215
in labeled compds., 220
order of citation of numerals and, 114
- Leucomycin V**, 202
- Ligands**, 215, 242
- Like treatment of like things, discontinuance of**, 138, 255
- Linearity**
of bridged fused systems, 154
of fused systems, 138, 150
- Line formulas**
with binary names, 219
for carbonic anhydride sulfur analogs, 183
containing isotope symbols, 220
for inorganic compds., 219, 257, 315
with polyphosphorus acids, 197
synonym line formulas, 109, 129
- Lipids**
IUPAC-IUB tentative rules for nomenclature of, 297
- Lithian**, 219
- Lithio**, 215
- Lithium compounds**
organic, 194
- Locants**, 114
all cited when one is needed, 117, 119
in "a" names, 128
effect on alphabetization, 121
for bridged fused systems, 154
capital italic letters, in coordination nomenclature, 215
enclosing marks between like, 132
in ester names, 185
for functional derivs., 119
for fused systems, 115, 152
for indefinite compds., 120
for isotopes, 220
lowest, definition of, 137
lowest, principle of, 255
in modifications, 185
for molecular skeletons, 137, 138
in multiplicative nomenclature, 118
present and former rules for, 263
primed, 114, 151, 152
in radicals, 116, 133
in rings and chains, 137
for suffixes, 115
for sulfides of hetero atoms, 200
- Lowest locants**, 137, 255
for indicated hydrogen, 122, 135, 152
for multiple bonds, 138
in radicals, 133
in tautomers, 122
- Lupane**, 212
- Lysozyme**, 218
- Macromolecular chemistry**
nomenclature of, history and development of, 307
nomenclature rules for, 299
- Magnesate**
phorbine complexes, 223
- Magnesium**
cations, 219
- Magnesium compounds**
chlorophylls, 223
- Malonic acid**. See *Propanedioic acid*
- Manganese hydroxide oxide**, 219
- Manganic acid**, 219, 273
- Mannan**, 208
- Mannopyranosyl bromide**, 208
- Maximum substitution**, 122, 133, 138
- Melamine**, 122
polymers with formaldehyde, 222
- Melanocyte-stimulating hormone**, 206
- Menthane**, 212
- Mercapto**
free radical, 187
hetero-atom-attached, 175
- Mercury**
organic derivs., 194
- Mercury chloride**, 219
- Meso-ionic compounds**, 201, 293A
- Meson**, 217
- Mesonic atom**, 217
- Metaborates**
cyclic, 219
- Metal complexes**. See *Coordination compounds*
- Metal carbonyls**, 215
- Metallic compounds**
organo-, 194
monocyclic, 146
retrospective index searching for, 272
- Metalloenes**, 215
retrospective index searching for, 264, 271
stereochemistry of, 203
- Metal-metal bonds**, 203, 215
- Metal oxides**
radicals from, 219
- Metal radicals**, 215
- Metals**, 215
complexes of, 215
definition of, 219
hydroxides and oxides, 219
isotopes, 217
- Metal salts**, 198
of amino acids, 205
- Metaphosphinic acid**, 197
- Metaphosphoric acid**, 197, 219
- Metaphosphorous acid**, 197
- Methanamine**, 176
boron complexes, 182
- Methanaminium**, 184
salts, 198
ylides, 201
- Methane**, 130, 140, 141
multiplication of, 118
- Methanediumine**, 177
- Methane(dithioic) acid**, 183
- Methaneperoxoic acid**, 183
- Methanethial**, 183
- Methanethioamide**, 183
- Methanethione**, 174, 183
- Methanimidoyl isocyanate**, 183
- Methanimine**, 183
- Methano**, 154
- Methanoic acid**
replacement analogs, 183
- Methanone**, 174, 183
oximes, 195
- Metheno**, 154
- Methines**, 216
- Methiodides**, 184
- Methoxides**, 180
- Methoxy**, 107, 287
free radical, 187
- Methyl**, 161
free radical, 187
- Methylene**, 125, 161
parentheses around, 110
- Methylethyl**, 162
- Methylides**, 201
- Methylidyne**, 161
free radical, 187
- Methylum**, 184
- Methyliumyl**, 184
- Methylthio**
free radical, 187
- Methylphenyl**, 162
- Minerals**, 219
labeled, 220
- (-)** (*minus*), 203
- Mixed salts**, 219
- Mixtures**, 221
of dyes, 216
order of citation of, in modifications, 113
retrospective index searching for, 265
of stereoisomers, 203
- Modifications**
enclosing marks in, 109
format of, 104, 317
locants for terms in, 119
order of citation of terms in, 113
- Molecular addition compounds**, 192, 265A

- See also *Salts*
of amino acids, 205
of borane, 182, 239
citation in modification, 113
of polymers, 222
stereochemistry of, 203
of stereoparents, 202
- Molecular skeletons**, 140-163
boron, 159
definition of, 140, 315
as index parents, 130
numbering of, 137
order of precedence of, 106, 271
radicals from, 161
- Molybdate**
iron sodium oxide, 219
- Mono**, 111, 120, 192, 311
in anhydride names, 179
in ester names, 185
- Monoprotonated**
as modification term, 184
- Morpholine**, 146
- Morpholinyl**, 161
- μ (*mu*), 215
in polyborane names, 182
- muco*, 209
- Multiple bonds**. See also *Unsaturated compounds*
maximum number of, in parent radicals, 133
- Multiplicative nomenclature**, 125
brackets around parent in, 109
for ester names, 185
locants in, 118
for fused systems, 151
preferred, 138
retrospective index searching for, 255
ylidene radicals in, 125, 255
- Multiplicative prefixes**, 110, 311
alphabetization rules for, 121
present and former rule for, 266
- Muonic molecule**, 217
- Muonium**, 217
- Muramic acid**, 208
myo, 209
- N*, 108
order of citation of, in locant sets, 114
- ¹⁵*N*, 220
- Name selection**. See *Index name selection*
- Naphthacene**
numbering of, 152
- Naphthalene**
in fused systems, 148, 151
numbering of, 137
- Naphthalenedione**
vitamin K derivs., 224
- Naphthalenimine**, 154
- Naphthaleno**, 154
- Naphthalenone**
added hydrogen in, 136
- Natural products**. See *Stereoparents neo*, 209
- Neo**
in boron compd. names, 159
in terpene names, 212
- Neogammacerane**, 212
- Neonocerane**, 212
- Neuraminic acid**, 208
- Neutrino**, 217
- Neutron**, 217
- Nickelbyrinic acid**, 224
- Nielsbohrium**, 219
- Ninth Collective Index**
substance name revision in, 101
- Niobate**, 215
- Nitramide**, 219
- Nitrate**
as index parent, 219
- Nitric acid**
and metal salts, 219
- Nitric acidium**, 219
- Nitrides**
of arsenic and phosphorus acids, 197
- Nitrido**, 215
- Nitridotriphosphoric acid**, 219
- Nitriles**, 172
of carbohydrate acids, 208
order of precedence of, 106
retrospective index searching for, 267
- Nitrilimine**, 172, 201, 267
- Nitrilio**, 184
- Nitrilo**, 125
- aci-Nitro*, 193
- Nitrogen acids**, 219
- Nitrogen compounds**, 193
N-glycosyl derivs., 208
heterocyclic, *N*-acyl derivs., 171
monocyclic, 146
order of precedence of, 106
peptides as, 206
phosphorus-, 197
order of precedence of, 106
quaternary, 184, 270
salts, 198
tautomeric, 122
- Nitrogen hydrides**, 219
- Nitrolic acids**, 167, 228
- Nitrone**
retrospective index searching for, 268
- Nitrosamide**, 219
- Nitrosolic acids**, 228
- Nitrososulfonyl fluoride**, 219
- Nitrosyl**, 219
- Nitrosyl chloride**, 219
- Nitrosyl (disulfate)**, 219
- Nitrosyls**
metal, 215
- Nitrous acid**, 219
anhydrides, 179
- Nitroxide**, 187
- Nitryl**, 219
- NNO*, 193
- Nomenclature**
history of chemical, 303-308
IUPAC, IUB, and ACS rules of chemical, 296-300
retrospective index searching of CAS, 225
- Nonfunctional compounds**
order of precedence of, 106
- Nor**, 139
in alkaloid names, 204
in peptide names, 206
in steroid names, 211
in terpene names, 212
- Norcholenedioic acid**, 211
- Norlupane**, 202
- Normalization**
of tautomeric structures, 122, 184
- Nucleon**, 217
- Nucleosides**, 210
retrospective index searching for, 269
- Nucleotides**, 210
polymers, 222
retrospective index searching for, 269
- Numbering**. See also *Locants*
of fused systems, 152
of molecular skeletons, 137
- Numerals**
in alphabetization, 121
order of citation of letters and, 114
- Nylon**, 222
- o**
elision of, 107
- o*, 108
- ¹⁷*O*, 220
- oan**
in mineral names, 219
- ocane**, 146
- Occurrences**
maximum number of parent, 122, 125, 138
- ocin**, 146
- ocine**, 146
- Octaphene**, 148
- oic acids**, 165
- olane**, 146
- ol**, 175
- ole**, 146
- Oleanane**, 212
- olidine**, 146
- Oligomers**, 222
of arsenic and phosphorus acids, 197
of boranamines, 182
of carbohydrates, 208
clusters, 219
of nucleotides, 210
- Oligonucleotides**, 210
- Oligosaccharides**, 208
- onane**, 146
- one**, 174
- elision of "e" before, 107
- onin**, 146
- onine**, 146
- Onium compounds**, 184. See also *Cations*
inner salts, 112, 293A
present and former indexing rules for, 270
salts, 198
ylides, 201
- ONN*, 193
- Ophiobolane**, 212
- Optical rotation**. See *Stereochemistry or*, 120
- Order of citation**. See also *Alphabetization*
of locants, 114
of modification terms, 113
of substituent prefixes, 121
- Order of precedence**
of acids, 167
of arsenic and phosphorus acids, 197
of base components in ring systems, 148, 281
of carbonic acid and related compds., 183
of cations, 184
of compd. classes, 106
in index name selection, 105
present and former, 271
of ring systems, 138
of silicon compds., 106, 199
- Organic chemistry**
nomenclature of, history and development of, 304
nomenclature rules for, 296
- Organic hetero chains**, 142
- Organometallic compounds**, 194
monocyclic, 146
retrospective index searching for, 272
- Orientation**. See also *Linearity*
of fused ring systems, 152
- Orotidylic acid**, 210
- Ortho acids**
esters, 185
- Ortho-fusion**, 148
- Ortho-peri fusion**, 148
- Osazones**, 190
- osyl**, 208
- Oxa**, 128
- "Oxa-aza" nomenclature**. See *Replacement nomenclature*
- Oxadiazolidinone**, 201
- Oxaspirodecane**, 156
- Oxatetragermolane**, 146
- Oxathiaazabicyclohexane**, 155
- Oxathiadisilaoctane**, 142
- Oxathiolane**, 146
- Oxatricycloheptane**, 155
- Oxazole**, 146
- Oxetane**, 196
- Oxetanone**, 196
- Oxidase**, 218
- Oxides**. See also *Additive terms*
of amides and imides, 268
of amines, 176
of azo compds., 193
of cyclic nitrogen and sulfur compds., 158
of cyclic phosphorus compds., 185
of cyclic sulfur compds., 171, 179
of elements, 219
of hetero atoms, 158
locants for, 119
of nitrogen atoms, 113, 176, 193, 268
of phosphorus compds., 175
of thioacids, thioamides and thiones, 200
of thio esters, 185
- Oximes**, 195. See also *Functional derivatives*
of amides, 171
of carbohydrates, 208
of stereoparents, 204
tautomerism of, 122
- Oxirane**, 196
polymers, 222
- Oxirene**, 146
- Oxirenol**
and derivs., no locants used with, 117
- Oxireno systems**, 281
- Oxo**, 174
in terminal positions, 173
- Oxo acids**. See *Acids*
- Oxonia**, 184
- Oxonium chloride**, 219
- Oxonium compounds**, 184

- Oxy**, 125
free radical, 187
- Oxygen compounds**, 196
monocyclic, 146
order of precedence of, 106
- Oxytocin**, 206
- Ozonides**, 192
of elements, 219
- P*-, 108, 219
- Papain**, 218
- Pantothenic acid**, 224
- Paraformaldehyde**, 222
- Parent compounds**, 130
- Parentheses**, 109
around compound radicals, 132
- Particle resonances**, 217
- Pectic substances**
ACS report on nomenclature of, 302
- Penicillins**
stereochemistry of, 203
- Pentaborane**, 159
- Pentacene**, 148
- Pentacycloctasiloxane**, 155
- Pentalene**, 148
- Pentanedioic acid**, 165
- Pentaheptadecanediol**, 222
- Pentasilane**, 143
- Pentazadienyl**, 161
- Pentoses**, 208
- Pentuloses**, 208
- Pentyloxy**, 132
- Peptides**, 206, 222
"a" names not used for, 127
IUPAC-IUB tentative rules for nomenclature of, 297
retrospective index searching for, 274
- Perchlorato**, 215
- Perchloric acid**
and ammonium salt, 219
esters, 185
- Perchloryl**, 188, 219
- Perhalic acids**, 188
- Periodic acid**, 219
- Periods**
in spiro and Von Baeyer names, 108
- Permanganic acid**, 219, 273
- Peroxides**, 126, 131, 196
carboxy, 179
of elements, 219
order of precedence of, 106
retrospective index searching for, 275
- Peroxoic acids**, 165
- Peroxy acid halides**, 170
- Peroxy acids**, 165
of arsenic and phosphorus, 197
from carbonic acid, 183
esters, 185, 196
inorganic, 219
order of precedence of, 106, 167
retrospective index searching for, 271, 280
of sulfur, 200
- Peroxychromic acid**, 219
- Peroxydicarbonic acid**, 183, 219
- Peroxydicarbonic difluoride**, 196
- Peroxydiphosphonic acid**, 196
- Peroxydiphosphoramidic acid**, 219
- Peroxydisulfuric acid**, 219
- Peroxyhypofluorous acid**
esters, 196
- Peroxymonosulfuric acid**, 219
- Perylene**
in fused systems, 148, 151
- Phenanthrene**
anthracene preferred to, 138
numbering of, 152
- Phenazine**, 149
amino derivs., 216
- Pheno**, 149
- Phenol**
polymers with formaldehyde, 222
- Phenolphthalein**, 216
- Phenols**, 175
Class I, 185
metal salts, 198
order of precedence of, 106
retrospective index searching for, 229, 271
salts, 198
- Phenolsulfonephthalein**, 216
- Phenothiazine**
amino derivs., 216
- Phenothiazinium**, 184
- Phenoxasilin**, 149
- Phenoxazine**
amino derivs., 216
- Phenoxide**, 180
- Phenoxy**
elision in spelling of, 107
- Phenylalaninamide**, 206
- Phenylalanine**, 205
peptides containing, 206
- Phenylalanyl**, 205
- Phenylazo**, 131
- Phenylene**, 125
- Phenylenedicarbonyl**, 168
- Phenylsulfinyl**
free radical, 187
- Phenylsulfonyl**, 168
- Phenylthio**, 168
- Phorbine**, 223
- Phospha**, 128
- Phosphaborocine**, 182
- Phosphatase**, 218
- Phosphate**, 180
as index parent, 219
as modification term, 180
- Phosphazines**, 190
- Phosphenic acid**, 197
- Phosphenimidous chloride**, 197
- Phosphenous acid**, 197
- Phosphide**
as modification term, 180
- Phosphides**
of elements, 219
- Phosphido**, 215
- Phosphine**, 130, 143, 197
order of precedence of, 106, 271
- Phosphinecarboxylic acid**, 197
- Phosphine imide**, 197
order of precedence of, 106, 271
- Phosphine oxide**, 197
order of precedence of, 106, 271
- Phosphine sulfide**, 200
order of precedence of, 106, 271
- Phosphinic acid**, 197
- Phosphinic cyanate**, 179
- Phosphinidene**, 161
- Phosphinidyne**, 161
- Phosphinimine**, 177
- Phosphino**, 161, 197
free radical, 187
- Phosphinyl**, 197
- Phosphinothioyl**, 197
- Phosphinous acid**, 197
- Phosphonate**, 180
- Phosphonia**, 184
- Phosphonic acid**, 197
anhydrides, 179
- Phosphonium**, 184
inorganic, 219
mercury derivs., 194
salts, 198
ylides, 201, 276
- Phosphonium cyanide**, 219
- Phosphonocyanatidic acid**, 197
- Phosphonous acid**, 197
- Phosphorane**, 143, 197
order of precedence of, 106, 271
and phosphonium ylides, 201
- Phosphoranyl**, 161
- Phosphoric acid**, 197
anhydrides, 179
esters, 185
inorganic salts, 219
replacement names from, 129
- Phosphorin**, 146
- Phosphorochloridic acid**, 129
- Phosphorodiamidic acid**, 197
- Phosphorodithioic acid**
esters, 185
- Phosphorothioic acid**
esters, 185
- Phosphorothioic triamide**, 129
- Phosphorous acid**, 197, 219
esters, 185
- Phosphorous trichloride**, 197
- Phosphorus(1+)**, 215
- Phosphorus acids**, 197, 219
anhydride-esters, 186
anhydrides, 179
inorganic, and salts, 219
nucleotide esters, 210
replacement names for, 129
salts, 198
- Phosphorus compounds**, 197
monocyclic, 146
order of precedence of, 106, 271
retrospective index searching for, 276
spiro, abnormal valency in, 158
tautomeric, 122
- Phosphoryl**, 276
- Phosphoryl chloride**, 276
- Phthaleins**, 216
- Phthalocyanine**, 223, 278
copper complex, 215
- Phylloquinone**, 224
- Physicochemical units**
manual of, 300
- Pi-bonded ligands**, 215
- Picrasane**, 202
- Picrates**, 180, 192
- Pigments**
organic, 216
- Pinane**, 212
- Piperazine**, 146
- Piperazinium**, 184
- Piperidine**
pyridine preferred to, 138
- Platinum metals**, 219
- Plumba**, 158
- Plumbane**, 143, 199
iodo derivs., 219
- Plumboxanes**, 199
(+) (*plus*), 203
- Plutonyl ion**, 219
- Polyalkylene glycols**, 222
- Polyamides**
"a" names for, 171
fibers, 222
- Polyboranes**, 159
hetero, 160
radicals from, 161
- Polycyclic systems**, 147. See also *Ring systems*
- Poly(dioxobutanediyl)**, 222
- Polyesters**, 222
- Polyethylene glycols**, 222
- Polymers**, 222
of amino acids, 206
"a" names not used for, 127
of carbohydrates, 208
of coordination compds., 215
nomenclature of, history and development of, 307
order of citation of, in modifications, 113
retrospective index searching for, 277
stereochemistry of, 203
structural diagram derivation for, 315
- Poly(methylene)**, 220
- Polynucleotides**, 222
IUPAC-IUB recommendations for nomenclature of, 297
- Poly(oxyethanediyl)**, 222
- Poly(oxymethylene)**, 222
- Polyphenyls**, 157
branched, 163
functional derivs., 163
radicals from branched, 162
radicals from unbranched, 161
- Polypropylene glycols**, 222
- Polysaccharides**, 208
- Polysulfides**, 200
order of precedence of, 106
- Polyvalent radicals**
in multiplicative names, 125
- Porphine**, 223
- Porphyrazine**, 223
- Porphyryns**, 223
retrospective index searching for, 278
- Positron**, 217
- Positronium**, 217
- Potassium phosphate sulfate**, 219
- P, P'*, 219
- Precedence**
order of—see *Order of precedence*
- Preferred index names**
definition of, 192
- Prefixes**
miscellaneous, 309
multiplicative—see *Multiplicative prefixes*

- substituent—see *Substituent prefixes*
- Pregnane**, 211
and derivs., stereochemistry of, 203
- Pregnenedione**
mixtures containing, 221
- Primary components**
in fused systems, 151
- Primed locants**, 114
in fused systems, 151, 152
- Principal chemical groups**, 104, 164-177
esters of, 185
hetero-atom-attached, 163
lowest locant for, 137
as suffixes, 131
- Proline**, 205
salts, 202
- Pronunciation**
of chemical words, ACS report on, 302
- Propadiene**, 141
- Propanamine**, 176
- Propanebis(thioic) acid**, 165
- Propanedioic acid**
anhydride-esters, 186
anhydrides, 179
cyclic esters, 185
esters, 185
hydrazides, 189
- Propanesulfonic acid**, 131
- Propanetriol**
esters, 185
- Propanimine**, 177
- Propanoic acid**, 131, 165
anhydrides, 179
- Propanone**, 174
hydrazone, 190
retrospective index searching for, 262
- Propene(dithioic) acid**, 165
- Propenoic acid**
polymers containing, 222
- Propenol**, 141
- Propoxide**, 180
- Prostaglandins**, 202
- Prostane**, 202
- Proteinases**, 218
- Proteins**, 207
enzymes, 218, 246
- Proton**, 217
- Punctuation**, 108
- Purinamine**
derivs., 210
glycosyl, 208
- Purine**
nucleoside and nucleotide derivs., 210
numbering of, 152
tautomeric derivs. of, 122
- Purinium**, 184
- Purinone**
derivs., 210
- Pyran**, 135, 146
- Pyranone**, 135, 136
- Pyranoses**, 208
- Pyranosides**, 208
- Pyrazine**, 146
- Pyrazole**, 146
tautomeric derivs., 122, 180
- Pyrazolidine**, 146
- Pyrene**
numbering of, 152
- Pyridazine**, 146
- Pyridine**, 146
preferred to piperidine, 138
- Pyridinecarboxamide**, 224
- Pyridinium**, 184
acyloxy derivs., 185
ylides, 201
- Pyridinone**
hydrazones and oximes, 122
- Pyridinyl**, 161
- Pyridoxal**, 224
- Pyridoxamine**, 224
- Pyridoxol**, 224
- Pyrimidine**, 146
nucleoside and nucleotide derivs., 210
tautomeric derivs., 122
- Pyrimidine**, 281
- Pyrophosphoric acid**, 197, 273
- Pyrrole**, 135, 146
- Pyrrolidine**, 135, 146
- Pyrylium**, 184
- Quark**, 217
- Quater**, 157
- Quaterphenyl**
radicals from, 162
- Question marks**, 120
- Quinoline**
analogs, 149
- Quinolinium**, 184
- Quinolizinium**, 184
- Quinoxaline**
in fused systems, 149, 151
- Quinquephenyl**, 157
radicals from, 162
- R**, 203, 212
- Radical ions**, 180
- Radicals**. See *Free radicals*; *Substituent prefixes*
- Radical functional nomenclature**, 126
- Ratios**
in addition-compd. names, 192
in anhydride names, 179
in ester names, 185
- Rayon**, 222
- Reductase**, 218
- Replacement nomenclature**
for acids, 165
for acyclic skeletons, 127, 140, 142
for amides, 171
for amines, 176
for anhydrides, 179
for arsenic and phosphorus acids, 197
for boron compds., 182
for cations, 184
in cocarboxylase names, 224
for esters, 185
for ethers and peroxides, 196
for functional groups, 129
for fused systems, 149, 153
for hetero chains, 142, 144
for heterosteroids, 211
for hydrazides, 189
for ketones, 174
lowest locants in, 137
for minerals, 219
prefixes for, 128
present and former rules for, 279, 280
for radicals, 133, 161, 287
for silicon (etc.) compds., 199
for spiro systems, 156
for sulfur compds., 200
for urea derivs., 183
for Von Baeyer systems, 155
- Replacement prefixes**, 128
elision of "a" in, 146
- Resonance-stabilized compounds**
anions, 180
cations, 184
phenazine and phenothiazine amino derivs., 216
- Retinoic acid**, 212
- Retinol**, 212
retro, 206, 211, 212
- Retrocarotenes**, 212
- Retrospective searching**
for index names, 225-293
- Retrosteroids**, 211
- Ribitol**, 208
riboflavin deriv., 224
ribo, 208
- Riboflavin**, 224
- Ribofuranosyl**, 210
- Ribonic acid**, 208
- Ribonuclease A**, 207
- Ribose**, 208
- Ring assemblies**, 147, 157, 266, 281
added hydrogen in, 136
indicated hydrogen in, 135
locants for, 114
punctuation for, 109
radicals from, 161, 287
retrospective index searching for, 281
- Ring contraction**
in alkaloids, 204
in steroids, 211
in terpenes, 212
- Ring expansion**
in alkaloids, 204
in steroids, 211
in terpenes, 212
- Ring-size descriptors**, 108
- Ring systems**
additional index entries for, 138, 163, 281
base components of fused, 150, 281
bridged fused, 154
carbocyclic fused, 148
with functional side chains, 124
fused steroidal, 211
heterocyclic, 199
arsenic- and phosphorus-containing, 197
cyclic esters named as, 185
fused, 149
imides named as, 191
oxygen-containing, 196
indicated hydrogen in, 135
locants for, 137
metal-containing, 194
monocyclic hetero, 146
monocyclic hydrocarbon, 145
nitrogenous, *N*-acyl derivs., 171
order of precedence of, 138
polycyclic, 147
preferred to acyclic skeletons, 138, 271
radicals from, 161
replacement names for fused, 153
retrospective index searching for, 281
Von Baeyer, 155
- Roman letters**
as locants, order of citation of, 114
- Rotaxanes**, 192
- Rubber**, 222
- s*, 108
- S*, 203, 212
- ³⁵S, 220
- S*^{IV}, 140, 158
- Saccharides**, 208
in nucleosides and nucleotides, 210
- Salamandra alkaloids**, 211
- Salt-type parents**, 219
- Salts**, 198. See also *Molecular addition compounds*
of amino acids, 205
of cations, 180
citation of, in modifications, 113
common anions of, 198, 281A
double and mixed, 219
of germanium, lead, and tin, 199
inorganic, 219
locants not used for, 119
of stereoparents, 202
- Sanbornite**, 219
- Schiff bases**, 176
- scyllo*, 209
- Searching**
retrospective, for index names, 225-293
- Seco**, 204, 212
- Secocholestanol**, 211
- Secocholestatrienol**, 224
- Secoergostatetraenol**, 224
- Secostychnidinoic acid**, 204
- Selection**
of index names—see *Index name selection*
- Selenals**, 173
order of precedence of, 106
- Selenic acid**, 219
- Selenic diamide**, 219
- Selenides**, 200, 271
di and poly, order of precedence of, 106
of elements, 219
- Seleninic acids**, 165
- Selenious acid**, 219
- Selenium compounds**, 200
order of precedence of, 106
- Seleno**, 200
- Selenols**, 175
order of precedence of, 106
- Selenonic acids**, 165
- Selenonyl chloride**, 219
- Selenophene**, 146
- Selenosulfuric acid**, 129
- Selenotelluroarsenious acid**, 219
- Selenoxo**, 174
- Selenyl**, 219
free radical, 187
- Selones**, 174
order of precedence of, 106
- Semicarbazones**, 190
of stereoparents, 202

- Semicolons**, 108
Semioxamazones, 190
Septanoses, 208
Sequence rule, 203
Sesqui, 192, 265A, 311
Sigma-bonded ligands, 215
Sila, 128
Silabenzene, 146
Silacyclopentane, 199
Silacyclopropane, 146
Silanamine
 derivs., 144, 176
 multiplication of, 118
 N-silyl, 199
Silane, 143, 199
 acyl derivs., 163
 order of precedence of, 106
 polymers, 222, 277
 tetrachloro, 257
Silano, 154
Silanol, 175, 199
 multiplication of, 118
Silathianes, 199, 282
Silazanes, 144, 146, 199
 Spiro systems, 156
 Von Baeyer systems, 155
Silica, 219
Silicic acids, 199, 282
Silicide
 as index parent, 180
Silicon compounds, 199, 282
 “a” names for acyclic, 142
 fused systems, 149
 monocyclic, 146
 order of precedence of, 106
 polymers, 222, 277
 retrospective index searching for, 282
 Von Baeyer systems, 155
Siloxanes, 144, 199
 cyclic, 146
 polymers, 222, 277
 ring assemblies, 157
 Spiro systems, 156
 multiplicative radicals from, 125
 Von Baeyer systems, 155
Silylene
 free radical, 187
Silyldiyne, 161
Sodio, 215
Sodium chloride, 219
 labeled, 220
 mixtures containing, 221
Sodium chloride sulfate, 219
Sodium hydride, 219
Sodium oxide, 219
Sodium peroxide, 219
Solanidane, 211
Solanidenol, 211
Solanidine, 211
Solasodine, 211
Solid solutions
 of inorganic compds., 219
Solvates, 192
Spaces
 in uninverted names, 108
Species names
 for peptides, 206
Spelling, 107
 present and former rules for, 283
Spirobi, 156
Spirohexasiloxane, 156
Spirooctane, 156
Spirosolane, 211
Spirostan, 211
Spiro systems, 140, 147, 156
 added hydrogen in, 136
 cationic, 184
 indicated hydrogen in, 135
 punctuation in names of, 108, 109
 radicals from, 161
 steroidal, 211
SRUs, 222
Stainless steel, 214
Stannane, 130, 143, 199
Stannanetrayl, 161
Stannate
 dipotassium, 219
Stannathianes, 144
Stannazanes, 144
Stannoxanes, 199
Starch, 208
Steel, 214
Stereochemical descriptors, 203, 284, 318
 for alkaloids, 204
 for amino acids and peptides, 205, 206
 for carbohydrates, 208
 chirality symbols, 203
 for inositols, 209
 for polymers, 222
 for steroids, 211
 for terpenes, 212
Stereochemistry, 202-212, 284, 318
 ACS reports on, 302
 assumptions, 205
 of biline, 223
 at double bonds, reports on, 301, 302
 of inositols, 209
 IUPAC tentative rules for, 296
 of octahedral inorganic compds., IUPAC
 tentative proposals for, 298
 of polymers, IUPAC nomenclature report
 on, 299
 present and former rules for, 284
Stereoparents, 101, 202-212, 285, 318
 addition compds. of, 192
 copolymers, 222
 definition of, 202
 mixtures containing, 221
 modified stereochemistry cited for, 203
 present and former indexing rules for, 285
Steroids, 211
 with modified stereochemistry, 203
 retrospective index searching for, 286
Stibinamine, 181
Stibine, 143, 181
 boryl derivs., 182
Stibine oxide, 181
Stibine sulfide, 181, 200
Stibino, 161, 181
Stibole, 181
Stibylene, 161
Stigmastane, 211
Stock numbers, 219
 in vitamin B₁₂ names, 224
Streptamine, 209
Structural diagrams, 135
 in *CA* indexes, 315
 derivation from index names, 312-318
Structural repeating units, 222
Strychnidine, 204
Subdivisions
 of large index headings, 104
Substituent prefixes, 161, 294, 316
 from acids-see *Acid radicals*
 alphabetic list of, 294
 “a” names for, 128
 cationic, 184
 compound and complex, 133, 162
 elision in, 283
 enclosing marks for, 109
 ester groups as, 112
 functional groups expressed as, 250
 inversion of, 104
 locants for, 117
 locants in, 116
 lowest locants for, 137
 maximum number of, 122, 133, 138
 from metals, 215
 multivalent, as structural repeating units,
 222
 order of citation of, 121
 polyvalent, in multiplicative names, 125
 present and former rules for, 287
 from steroids, 211
Substituent suffixes, 131
 locants for, 115
 order of precedence of, 106
 principal groups as, 131, 164-177, 315
Substitutive nomenclature, 130, 139, 164
Substitutive parent compounds, 130
Subtractive nomenclature, 139
Succinic acid. See *Butanedioic acid*
Sucrose, 208
Suffixes. See *Substituent suffixes*
Sugars. See *Carbohydrates*
Sulfamic acid, 219
 as elided name, 107
 metal salts, 219
Sulfamide, 219
 derivs., 219
 as elided name, 107
Sulfanilic acid, 167
Sulfato, 215
Sulfenic acids, 165
 esters, 196
Sulfenoselenoic acids, 200
Sulfenothioic acids, 165, 188, 196, 200
Sulfides, 200, 271
 of elements, 219
 di and poly, order of precedence of, 106
 of hetero atoms, 158
 of nitrogen and phosphorus compds., 200
 retrospective index searching for, 288
Sulfilimine, 200
Sulfimide, 200, 219
Sulfinic acids, 165
Sulfinimide acids, 165, 200
Sulfinylyl, 168, 200, 219
Sulfinylamino, 200
Sulfinylsulfonyl, 200
Sulfonamides, 171
Sulfonefluorescein, 216
Sulfonephthaleins, 216
Sulfones
 retrospective index searching for, 289
 di and poly, order of precedence of, 106
Sulfonic acids, 165
 acyclic with cyclic substituents, 166
 anhydrides with inorganic acids, 219
 esters, 185
 free radicals from, 187
 order of precedence of, 106, 167
Sulfonimide acids, 165
Sulfonimidoyl, 200
Sulfonium, 184, 219
 ylides, 201
Sulfoniumyl, 184
Sulfonohydrazonic acids, 165
Sulfonohydrazonimide acids, 129
Sulfonothioic acids
 esters, 200
Sulfonyl, 168, 200, 219
Sulfonyl halides, 170
Sulfonyloxy
 in free radical names, 187
Sulfoxides, 200
 retrospective index searching for, 289
Sulfoximine, 200
Sulfoxylic acid, 219
 selenium analogs not recognized, 219
Sulfur
 coordination complexes, 131, 200
 tetravalent, in ring systems, 140
Sulfur acids, 219
 order of precedence of, 106
Sulfur compounds, 200
 cyclic, with abnormal valencies, 158
 dyes, 216
 retrospective index searching for, 288
 thio carbohydrates, 208
Sulfur diimide, 106, 200
Sulfur dioxide, 219
Sulfuric acid, 219
 ammonium iron salt, 219
 anhydrides, 179
 esters, 185
 and metal salts, 219
 uranium complex, 219
Sulfurous acid, 219
 monosodium salt, addition compds., 192
Sulfur oxides, 219
Sulfur trilmide, 200
Sulfur trioxide, 219
Sulfuryl, 219
Sulfuryl chloride, 219
Superoxides
 of elements, 219
Superoxido, 215
Superscripts
 abnormal valency indicated by, 158
 in Von Baeyer names, 155
Superscripts, 114, 137
Sydones, 201, 293A
syn, 203
Synonym line formulas. See *Line formulas*
Synthetic fibers, 222
System indicators

- for coordination compds., 203
- t*
in tritium-labeled compds., 220
- Tachyon**, 217
- Tacticity**
of polymers, 222
- Tantalate**
heptapotassium, 219
- Tartaric acid**
addition compds. of, 192
- Tautomeric compounds**, 122
acetoacetanilide and pyrazolinone dyes, 216
amides and imidic acids, 165
anions, 180
cations, 184
cyclic amines and imines, 177
histidine, 205
hydrazides and hydrazonic acids, 165
tropolones, 122, 180
urea and carbamimidic acid, 183
- Tellones**, 174
order of precedence of, 106
- Tellurals**
order of precedence of, 106
- Tellurenic acids**, 165
- Telluric acid**, 219
- Tellurides**, 200, 271
of elements, 219
order of precedence of, 106
- Tellurinic acids**, 165
- Tellurinyl**, 200
- Tellurium compounds**, 200
order of precedence of, 106
- Telluro**, 200
- Tellurols**, 175
order of precedence of, 106
- Tellurophene**, 146
- Telluroxo**, 174
- Telomers**, 222
- Tercyclopropane**, 157
- Terpenes**, 212
ACS proposed system of nomenclature for, 302
retrospective index searching for, 290
- Terphenyl**, 157
- Terphenylcarboxylic acid**, 163
- Terphenyldiyl**, 161
- Terphenylyl**, 162
- Terpyrazolidine**, 157
- Tetra**, 110
- tetrahedro*, 108
- Tetrakis**, 110
- Tetraoxatetradecapentaene**, 142
- Tetraoxatetradecene**, 142
- Tetraoxatridecane**, 142
- Tetraoxatridecyl**, 161
- Tetraoxides**, 196
- Tetrapyrroles**, 223
- Tetrasiladecenylidene**, 161
- Tetrasilatetradecane**, 142
- Tetrasiloxane**, 199
- Tetrazadiene**, 143
- Tetrazane**, 143
- Tetrazene**, 143
- Theophylline**, 122
- Thia**, 128
- Thiaandrostane**, 211
- Thiadiazole**
abnormal valency in, 158
- Thials**, 173
order of precedence of, 106
- Thiamine**, 224
- Thiaporphine**, 223
- Thiazolium**
vitamin B₁₂ deriv., 224
- Thiireno systems**, 281
- Thio**, 200
- Thio acids**, 165, 200
of arsenic and phosphorus, 197
esters, 200
esters, S-oxides, 185
retrospective index searching for, 280
- Thioamides**, 171
S-oxides, 200
- Thioboric acid**, 219
- Thiocyanic acid**, 183, 219
anhydrosulfides, 183, 188
- Thiodicarbonic acid**, 129, 200
- Thiodiphosphoric acid**, 179
- Thiodiphosphoric acid**, 219
- Thiohydroperoxides**, 129, 196
- Thiohypochlorous acid**
anhydrosulfides, 170, 188
- Thiohydroxylamine**, 129
order of precedence of, 106
- Thioic acids**, 129, 165
- Thiols**, 175
Class I, 185
order of precedence of, 106
retrospective index searching for, 291
- Thiometaphosphinic acid**, 197
- Thiomorpholine**, 146
- Thiones**, 174
order of precedence of, 106
S-oxides, 200
- thiono*, 108
- Thionyl**, 219
- Thionyl chloride cyanide**, 219
- Thionyl imide**, 200
- Thioperoxides**, 129, 196
- Thioperoxy acids**
esters, 185
- Thioperoxydicarbonic acid**, 183
- Thioperoxydicarbonic diamide**, 200
- Thioperoxydiphosphoric acid**, 197, 219
- Thioperoxydiphosphoric tetrafluoride**, 200
- Thioperoxymonosulfuric acid**, 219
and esters, 200
- Thiophene**, 146
abnormal valency in, 158
- Thiophene-ol**, 175
- Thiopheniumyl**, 184
- Thiophosphoryl chloride**, 276
- Thiosemicarbazones**, 190
- Thiosilicic acid**, 199, 219
- Thiosulfuric acid**
anhydrosulfides, 200
- Thiosulfuric acidium**, 219
- Thiosulfurous acid**, 219
- Thiosulfuryl chloride**, 219
- Thiotriiazyl**, 219
- Thiourea**, 129, 183
- Thioxanthene**, 149
- Thioxo**, 131, 174
in terminal position, 173
- Thioxomethyl**, 134, 173, 174
- Thorium hydride iodide**, 219
- threo*, 208
- Thromboxane**, 202
- Thymidine**, 210
- Thymidylic acid**, 210
- Tin chloride**, 219
- Tin compounds**, 199
cyclic, 139
monocyclic, 146
order of precedence of, 106
- Titanyl**, 219
- Tocopherols**, 224
- Tomatidine**, 211
- Trade names**
for polymers, 222
- trans*, 203
- Transition metals**, 219
amino acid salts of, 205
- Tri**, 110
- Triazane**, 143, 193
order of precedence of, 106
- Triazanium**, 184
- Triazanyl**, 161
- Triazatriphosphorine**, 158, 197
- Triazenyl**, 193
tautomerism of, 122
- Triazinetriamine**
polymers with formaldehyde, 222
- Tribismuthine**, 181
- Triborane**, 159
- Trichlorodiphosphoric acid**, 219
- Trichothecane**, 212
- Tricyclododecane**, 155
- Triguamide**, 280
- Triiodides**
of elements, 219
- Trimers**
of sulfimide, 219
- Trioxatriphosphorinane**, 197, 219
- Trioxides**, 196
order of precedence of, 106
- Trioxopropanediyl**, 168
- Triphenylene**, 148
- Triphosphonic acid**, 179
- Triphosphoric acid**, 219
- Triple bonds**. See *Unsaturated compounds*
- Tris**, 110
- Trisilane**
order of precedence of, 106
- Trisiloxane**, 140, 144
- Trisiloxanetriyl**, 161
- Tristannane**, 143
- Tristannathiane**, 144
- Tristannoxane**, 199
- Trisulfides**, 200
order of precedence of, 106
- Trisulfones**, 200
order of precedence of, 106
- Trisulfuric acid**, 219
- Trisulfuryl chloride**, 219
- Trithiaazatetradecenediyl**, 161
- Trithiatristannacyclohexane**, 146
- Trithiatriazine**
hexaoxide, 219
- Tritium**
compds. labeled with, 220
- Trivial names**, 101
for monocyclic hetero systems, 146
- Tropine**, 204
- Tropolones**, 122, 180
- Tyrosine**
peptides containing, 206
- Ulosaric acids**, 208
- Ulosonic acids**, 208
- Ulosuronic acids**, 208
- ulosyl**, 208
- Uninverted index names**, 104, 108
brackets around index parent in multiplicative, 109
of esters, 104
of salts, 198
- Unnilpentium**, 219
- Unsaturated compounds**
acyclic, 141
carbohydrates, 208
conjunctive names not formed from acyclic, 124
double vs. triple bonds in, 138
greater number of multiple bonds in parent of, 138
locants for, 114, 137
monocyclic hydrocarbons, 145
spiro systems, 156
steroids, 211
Von Baeyer systems, 155
- Ununnilium fluoride**, 219
- Uracil**, 122
- Uranate**, 219
- Uranium**
complexes, 219
- Uranium chloride oxide**, 219
- Uranyl**, 219
- Urea**, 183
derivs., retrospective index searching for, 292
hydroxy, 193
no locants for monosubstituted, 117
polymers with formaldehyde, 222
tautomerism of, 183
- Urethanes**, 185
- Ureylene**
carbonyldiimino as name for, 134
- Uric acid**, 122
- Uridine**, 210
- Uridylic acid**, 210
- Uronamides**, 208
- uronamidoyl**, 208
- Uronic acids**, 208
- uronosyl**, 208
- Ursane**, 212
- Valency**
abnormal, in ring systems, 158, 161, 163
- Valine**, 205
peptides containing, 206
- Vanadyl**, 219
- Vasopressin**, 206
- Veratraman**, 211
- Veratrum alkaloids**, 211
- Vinyl acetal polymers**, 222
- Vinyl alcohol polymers**, 222
- Vitamin A**, 212, 224

Vitamin B₁₂, 224. See also *Corrinoids*
Vitamins, 224
IUPAC-IUB tentative rules for, 297
retrospective index searching for, 293
Von Baeyer systems, 140, 155
cationic, 184
choice between, 138
oxygen-containing, 196
punctuation in, 108, 109, 155
radicals from, 161
Vowels
elision of, 107, 146
Water, 219
in coordination compds., 219
hydrates, 113, 192, 265A, 311
labeled, 220
Willemite, 219

Xanthene, 149
amino derivs., 216
numbering of, 152
Xanthic acids, 185
Xanthine, 210
derivs., 122
Xanthophylls, 212
Xanthosine, 210
Xanthylic acid, 210
Xenonate, 219
Xenon compounds, 219

-yl, 161
-ylene, 161
Ylic acids
nucleotides, 210
-ylidene, 161
added hydrogen for cyclic, 136

in multiplicative names, 125, 255
Ylides, 201, 276
-ylidyne, 161
-ylium, 184
-ylidene, 161
-yne, 139, 141, 155
-ynyl, 161

Z, 203
report on, 301
Zincate
dye derivs., 216
Zinc chloride
double salts with dyes, 216
Zinc sulfide, 219
Zirconyl, 219
Zwitterionic compounds, 201, 293A