APPENDIX IV

CHEMICAL SUBSTANCE INDEX NAMES

NOTE: REPRINTS OF THIS APPENDIX ARE AVAILABLE AT NO COST UNDER THE TITLE *NAMING AND INDEXING OF CHEMICAL SUBSTANCES FOR CHEMICAL ABSTRACTS.* INQUIRIES SHOULD BE ADDRESSED TO MARKETING COMMUNICATIONS, CHEMICAL ABSTRACTS SERVICE, P.O. BOX 3012, COLUMBUS, OHIO 43210-0012 USA.

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 Chemical Abstracts Service (CAS) Registry Numbers. These substances include specific chemical elements, alloys, minerals, mixtures, polymers, enzymes, polysaccharides, and elementary particles.

The chemical nomenclature used by 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 *CA 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. 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) of this Appendix. The nomenclature of fullerenes is more fully documented in ¶ 163A of Section B.

The main part of the *Index Guide* must be consulted before any search is conducted in the *CA Chemical Substance* and *General Subject Indexes*.

The arrangement of sections in "Chemical Substance Index Names" 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. Chemical Abstracts Service 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

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103. Introduction. Many names may be employed in scientific publications for a single compound. Even so simple a compound as $H_2NCH_2CH_2OH$ can be named 2-Aminoethanol, 2-Aminoethyl alcohol, 2-Hydroxyethylamine, β-Hydroxyethylamine, 2-Hydroxyethanamine, 1-Amino-2-hydroxyethan 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. The main part of the *Index Guide* provides cross-references from trivially named index headings employed before *CA* Volume 76 (1972), as well as for most of the trivial or author names of chemical substances encountered in the scientific literature.

104. Inversion of names. Ordering in the *Chemical Substance Index* (see Appendix II, ¶ 10C) 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-butanesulfonic acid, and of the ester, ethyl 2,4-diamino-3-chloro-1-butanesulfonate. The latter appears in the *Chemical Substance Index* as follows:

1 2

1-Butanesulfonic acid, 2,4-diamino-3-chloro-
ethyl ester

3

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** (see Appendix II, ¶ 10B).

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:

(*a*) determine the most senior compound class;
(*b*) determine the type of nomenclature that is appropriate;
(*c*) determine the preferred index heading parent;
(*d*) name the remainder of the structure as substituents, and/or as functional derivatives by modification phrases;
(*e*) 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:

(*a*) Free radicals and compounds for which substituent prefixes are unavailable, e.g., **Sulfur diimide** (¶ 200).

(*b*) Cationic compounds: coordination cations, onium, aminium, ylium cations.

(*c*) Neutral coordination compounds, including metallocenes.

(*d*) Anionic compounds, e.g., **Borate(1-)**.

(*e*) 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.

(*f*) 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).

(*g*) Amides, in the same order as the parent acids (see (*e*), above).

(*h*) Nitriles, in the same order as the parent acids (see (*e*), above).

(*i*) Aldehydes, Thials, Selenals, Tellurals.

(*j*) Ketones, Thiones, Selones, Tellones.

(*k*) Alcohols and Phenols (of equal rank), Thiols, Selenols, Tellurols.

(*l*) Hydroperoxides.

(*m*) Amines.

(*n*) 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.**

(*q*) Arsenic compounds (in similar order).

(*r*) Antimony compounds (in similar order).

(*s*) Bismuth compounds (in similar order).

(*t*) Boron compounds: carbapolyboranes, hetero polyboranes, polyboranes, heterocyclic, **Borane.**

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

(*v*) Germanium compounds (in similar order).

(*w*) Tin compounds (in similar order).

(*x*) Lead compounds (in similar order).

(*y*) 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.**

(*aa*) Selenium and tellurium compounds (in similar order).

(*bb*) Carbon compounds: carbocyclic, acyclic hydrocarbons.

107. Spelling. CAS accepts *Webster's New World Dictionary of American English*[2] as the primary authority for spelling; e.g. sulfur (not sulphur); aluminum (not aluminium). *Webster's Third New International Dictionary* (unabridged)[3] is used for words not found in the *New World 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 perylo, and the terminal “a” of cyclobuta, etc., are elided before vowels, e.g., **Benz**[*cd*]**indole**, **5*H*-Cyclobut**[*f*]**indene**. 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 Carbonthioic 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, and modifications. Different *types* of functional derivatives are separated by commas in the text of the modification.

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

[2] *Webster's New World Dictionary of American English*, 3rd college ed., Webster's New World, N.Y., 1988.

[3] *Webster's Third New International Dictionary of the English Language*, unabridged. Merriam, Springfield, Massachusetts, 1961.

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

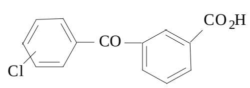
Hyphens separate locants from the words and syllables of a name; when used between locants, the intention is to indicate that such locants refer to different parts of the name; e.g., in **Acetamide,** ***N*****-2-naphthalenyl-**, the "*N*-" places the 2-naphthalenyl substituent on the nitrogen of the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

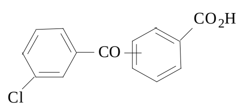
109. Enclosing marks are placed around compound substituent radicals and around and within complex radicals (¶ 162). Their presence or absence frequently removes ambiguity, especially when locants are omitted through lack of precise structural information.
Examples:

$MeSiH_2Cl$ — **Silane, chloromethyl-**

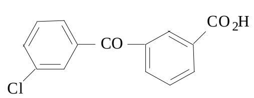
$ClCH_2SiH_3$ — **Silane, (chloromethyl)-**



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., $Cl(CH_3)N$-. The alternative structure, $ClCH_2NH$- 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)
Thioperoxydiphosphoric acid ($[(HO)_2P(O)]_2S_2$)

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*H*-[1,3]Oxathiolo[5,4-*g*]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]

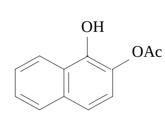
110. Multiplicative prefixes. Generally, prefixes derived from the Greek (di, tri-, etc.) are used, rather than the Latin (bi-, ter-, etc.); exceptions are nona- (not ennea-) for nine, and undeca- (not hendeca-) for eleven. (For lists of Latin and Greek prefixes, see ¶ 309.) The Latin prefixes bi-, ter-, etc., are used for ring assemblies, and bi- is employed in the term "bimol. monoanhydride."
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)
bis(2-aminoethyl)
[1,2-ethanediylbis(oxymethylene)]
bis(*O*-methyloxime)
bis(cyclohexaneacetate)
tris(dihydrogen phosphate)
bis(aziridinyl)
bis(diazo)
bis([1,1′-biphenyl]-4-yl)
bis(bicyclo[2.2.1]hept-2-yl)
tris(decyl)
tetrakis(1-aziridinyl)
bis(anhydrosulfide)
bis(benz[*a*]anthracen-1-yl)
Benzo[1,2-*c*:3,4-*c*′]bis[1,2,5]oxadiazole
Biscyclopenta[5,6]pyrido[4,3-*b*:3′,4′-*c*]pyridine
Benzoic acid, 2,2′-silylenebis-
Phosphonic acid, 1,4-phenylenebis-

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. It is not used if a locant is necessary, or when all functions are modified by the same class of derivative, or when only one functional group is present. The term "hydrogen" in an uninverted ester name precludes the use of "mono."
Examples:

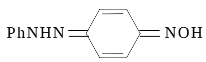
$MeC(=NOH)Me$ — **2−Propanone oxime**

$MeO_2C(CH_2)_2CO_2H$ — **Butanedioic acid monomethyl ester**



1,2−Naphthalenediol 2−acetate

$EtOP(O)(OMe)_2$ — **Phosphoric acid ethyl dimethyl ester**



2,5-Cyclohexadiene-1,4-dione mono(phenylhydrazone), oxime (note that the term "mono" is not repeated unless needed)

$EtOP(O)(OH)_2$

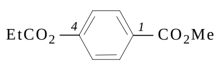
Phosphoric acid monoethyl ester (index name)

Ethyl dihydrogen phosphate (uninverted name)

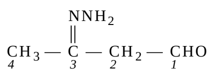
112. Functional derivatives of the principal reactive chemical groups of systematically-named index heading parents are cited in the modification; these derivatives, as defined for indexing purposes, are restricted to acyclic anhydrides, esters, hydrazides, hydrazones, and oximes. Other derivatives, 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.

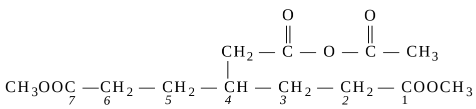
Examples:



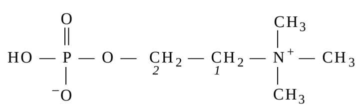
Benzoic acid, 4-(1-oxopropoxy)- methyl ester (not Benzoic acid, 4-hydroxy-, methyl ester, propanoate)



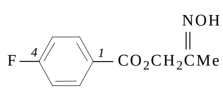
Butanal, 3-hydrazono- (not Butanal, 3-oxo-, 3-hydrazone)



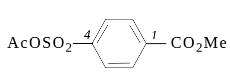
Heptanedioic acid, 4-[2-(acetyloxy)-2-oxoethyl]- dimethyl ester (not Heptanedioic acid, 4-(carboxymethyl)-, 4-anhydride with acetic acid, dimethyl ester)



Ethanaminium, *N*,*N*,*N*-trimethyl-2-(phosphonooxy)- 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:

(*a*) ionic terms relating to the heading parent, e.g., "chloride" at an "-aminium" heading;

(*b*) functional derivatives in the order: anhydrides, esters, hydrazides, hydrazones, oximes; multiplicative terms are cited before simple terms, e.g., 1,3-propanediyl dimethyl ester, otherwise alphabetic order is followed;

(*c*) additive terms describing fragments covalently attached to the index heading compound, e.g., N-oxide;

(*d*) ionic terms, e.g., ion(1-), radical ion(1-), then metal salts, followed by other salts alphabetically, e.g., acetate, hydrochloride;

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

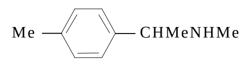
114. Locants. When a choice is necessary, italic Roman letters are placed before Greek letters, and Arabic numerals are placed last, e.g., *As*, *N*, *P*, *S*, α, β, γ, 1, 2, 3. (For the Greek alphabet see ¶ 310.)

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

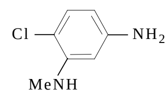
Examples:

$MeP(=NMe)(NHMe)_2$

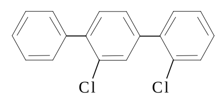
Phosphonimidic diamide, *N*,*N*′,*N*″,*P*-tetramethyl-



Benzenemethanamine, *N*,α,4-trimethyl-



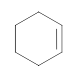
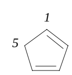
1,3-Benzenediamine, 4-chloro-N^3-methyl- (not 1,3- Benzenediamine, 6-chloro-N^1-methyl-)



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

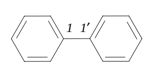
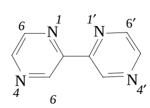
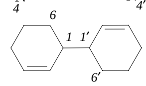
Locants for unsaturation in compounds named as index heading parents are always cited when the compound contains three or more skeletal atoms, except for monocyclic hydrocarbons with one multiple bond and no suffix.

Examples:

$HN{=}NNH_2$ (1 3)	**1-Triazene**
$H_2C{=}C{=}CH_2$	**1,2-Propadiene**
$H_2C{=}CHC{\equiv}CH$ (1 4)	**1-Buten-3-yne**
$H_2C{=}CH_2$	**Ethene**
	**Cyclohexene**
	**1,3-Cyclopentadiene**

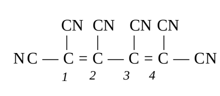
Locants denoting ring junctions of ring assemblies are always cited except for two-component assemblies of cycloalkenes, cycloalkadienes, etc.

Examples:

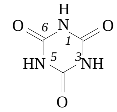
	**1,1′-Biphenyl**
	**2,2′-Bipyrazine**
	**Bi-2-cyclohexen-1-yl**

115. Locants for substituent suffixes of index heading parents are always cited if it is necessary to cite locants in the molecular skeleton for unsaturation, hetero atoms, indicated hydrogen, spiro or ring assembly junctions, bridges (in fused systems), or isotopic labeling. Locants for fusion sites, e.g., "[3,4-*d*]" (¶ 151), are disregarded in this connection. Locants are not cited for Geneva suffixes which terminate a chain, e.g., "-oic acid," "-dial," except when a monofunctional suffix is not at the 1-position of an "a"-named chain. Locants are always cited with cycloalkene names to which suffixes are attached.

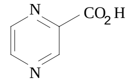
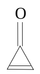
Examples:



1,3-Butadiene-1,1,2,3,4,4-hexacarbonitrile

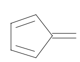
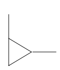
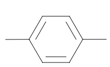


1,3,5-Triazine-2,4,6(1*H*,3*H*,5*H*)-trione

	**Pyrazinecarboxylic acid**
$HO_2CN{=}NCO_2H$	**Diazenedicarboxylic acid**
$H_2C{=}CHCO_2H$	**2-Propenoic acid**
$CH_3CH_2OCH_2CH_2OCH_2CH_2OCH_2CH_2OCH_2CH_2COOH$ 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15	**3,6,9,12-Tetraoxapentadecan-15-oic acid**
	**2-Cyclopropen-1-one**

116. Locants in substituent prefixes (radicals). Locants are assigned for multiple bonds in all unsaturated radicals containing three or more skeletal atoms. Locants are always cited for free valencies involving more than one position of a skeleton, except for the trivial names hydrazo, azino, azo, azoxy (¶ 193).

Examples:

HC≡CCH= 3 1	2-propynylidene
—N=NNH— 1 3	1-triazene-1,3-diyl
	2,4-cyclopentadien-1-ylidene
—C≡CC≡C—	1,3-butadiyne-1,4-diyl
$—CH_2CH_2—$	1,2-ethanediyl
═C=C═	1,2-ethenediylidene
	1,2-cyclopropanediyl
	1,4-phenylene

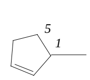
Locants are not cited for free valencies of radicals which have lost hydrogen from only one skeletal atom of an acyclic, or saturated monocyclic, homogeneous molecular skeleton.

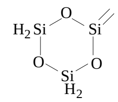
Examples:

$MeCH_2—$	ethyl
HN=N—	diazenyl
HP – P — | | HP – PH	tetraphosphetanyl
$H_2C{=}CHCH_2CH{=}$ 4 1	3-butenylidene
HN=NNH— 3 1	2-triazenyl

Locants are cited for free valencies of radicals from unsaturated homogeneous monocyclic systems, and from saturated heterogeneous monocyclic systems with cyclo...ane, cyclo...ene, etc., names.

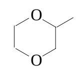
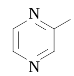
Examples:

	2-cyclopenten-1-yl

	cyclotrisiloxan-2-ylidene

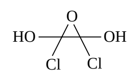
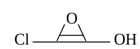
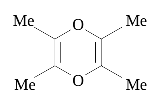
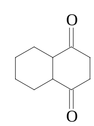
Locants for free valencies are cited for monocyclic radicals which possess locants for indicated hydrogen, hetero atoms, unsaturation, spiro or ring assembly junctions or bridges (in fused systems).

Examples:

	1,4-dioxan-2-yl
	pyrazinyl (not 2-pyrazinyl)

117. Locants for substituents on index heading parents and parent radicals are cited when the parent names possess locants for substituent suffixes, unsaturation, hetero atoms, indicated hydrogen, spiro or ring assembly junctions, or bridges (in fused systems). Locants are dispensed with for "hydro" prefixes in fully saturated ring systems unless ambiguity could result, e.g., because of a remaining etheno or other unsaturated bridge.

Examples:

	**2,3-Oxiranediol, 2,3-dichloro-**
	**Oxirenol, chloro-**
$MeCOCOCH_2Cl$	**2,3-Butanedione, 1-chloro-**
$H_2NCONHMe$	**Urea, methyl-**
	**1,4-Dioxin, 2,3,5,6-tetramethyl-**
PhC≡CC≡C— 4 1	(4-phenyl-1,3-butadiynyl)
	**1,4-Naphthalenedione, octahydro-**

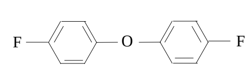
When one or more locants are needed for substituents on a heading parent or parent radical, all are cited.

Examples:

$F_3CCF_2CF\ I\ CF_3$	**Butane, 1,1,1,2,2,3,4,4,4-nonafluoro-3-iodo-**
CF_3 | CF_3 –CF—	[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]
$HO_2CCHCl\ SCHCl\ CO_2H$	**Acetic acid, 2,2′-thiobis[2-chloro-**

118. Locants in multiplicative nomenclature are cited for the positions of attachment on the heading parent if it consists of more than one skeletal atom, e.g., **Benzene, Acetic acid**, or contains an additional position for substitution, e.g., **Silanamine, Phosphonamidic acid**. Locants are otherwise not cited for heading parents which contain only one skeletal atom, e.g., **Methane, Silane, Methanone**, or for heading parents which are functional parent compounds (¶ 130), e.g., **Phosphonic acid**.

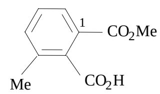
Examples:

PhOPh	**Benzene, 1,1′-oxybis-**
	**Benzene, 1,1′-oxybis[4-fluoro-**

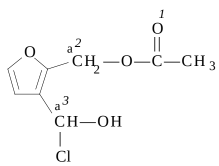
$HO_2CCH_2NHNHCH_2CO_2H$	**Acetic acid, 2,2′-hydrazobis-**
$HO_2CNHSiH_2NHCO_2H$	**Carbamic acid, silylenebis-**
MeSMe	**Methane, thiobis-**
$HOSiH_2CH_2SiH_2OH$	**Silanol, methylenebis-**
$H_2NSiH_2CH_2SiH_2NH_2$	**Silanamine, 1,1′-methylenebis-**

119. Locants for functional derivatives are used when needed to define the structure unambiguously. The terms “mono,” “di,” etc., are preferred to locants, but if a locant is necessary, “mono” is omitted.

Examples:



1,2-Benzenedicarboxylic acid, 3-methyl-
1-methyl ester



2,3-Furandimethanol, α^3-chloro-
α^2-acetate

MeOP(O) (OH)OP(O) (OH) OMe
P *P′*

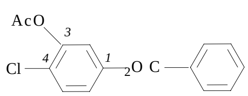
Diphosphoric acid
***P,P′*-dimethyl ester**

$HO_2C(CH_2)_2CONHNH_2$ — **Butanedioic acid monohydrazide**

MeC(=NOH)CMe = NNHPh — **2,3-Butanedione mono(phenylhydrazone), oxime**

Locants for all derivatives are cited if one or more are needed.

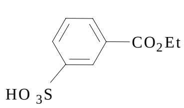
Example:



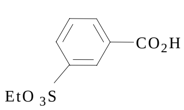
1,3-Benzenediol, 4-chloro-
3-acetate 1-benzoate

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 “monosodium 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.
Benzeneacetic 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:

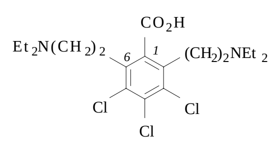
Naphthalene, chloro-2-methyl-

An indefinite name like P**iperidine, 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.

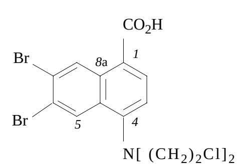
121. Alphabetization of substituent prefixes affects the position in the index where an inverted chemical substance name will be found (see Appendix II, ¶ 10C). Simple prefixes are placed in alphabetic order according to their names; only then are multiplicative prefixes (di-, tri-, etc.) placed in front 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 “tribromochlorodinitro,” 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, tetrachloro-**.

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.

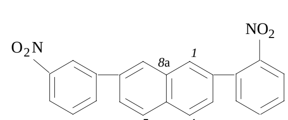
Examples:



Benzoic acid, 3,4,5-trichloro-2,6-bis[2-(diethylamino)ethyl]-(letter "c" is placed before "d", the initial letter of the complex radical)



1-Naphthalenecarboxylic acid, 4-[bis-(2-chloroethyl)amino]-6,7-dibromo- (the multiplicative prefix "bis-" is part of the name of the complex substituent prefix and this is therefore placed before "bromo")



Naphthalene, 2-(2-nitrophenyl)- 7-(3-nitrophenyl)- (the radicals are placed in order, according to the locants they contain, before locants relating to the heading parent are inserted)

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

Unless a structure at variance with the index name selected for a particular tautomer, e.g., **2,4-Pyrimidinediol** as the structure of Uracil, is emphasized by an author, information on tautomeric systems is collected in *CA Chemical Substance Indexes* at the preferred names to which the cross-references lead. Index names for related tautomers not possessing common names are selected by similar principles.

The necessity for many tautomeric structures to be redrawn to accord 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 (see Appendix II, ¶ 13) and *CA Chemical Substance Index* name.

When the author of an original document emphasizes a tautomeric structure different from that represented by the usual preferred index name, the normalization algorithm is bypassed and a different Registry Number and index name are assigned.

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:

$$\mathrm{M{=}Q{-}ZH} \rightleftharpoons \mathrm{HM{-}Q{=}Z}$$

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:

—NH–C=N–C=N–C=N— ⇌ —N=C–NH–C=N–C=N— ⇌

—N=C–N=C–NH–C=N— ⇌ —N=C–N=C–N=C–NH—

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

—NH–C=N— ⇌ —N=C–NH—

(amidine tautomerism)

—NH–N=N— ⇌ —N=N–NH—

(diazoamino tautomerism)

—NH–C=O(S, Se, Te) ⇌ —N=C–O(S, Se, Te)H

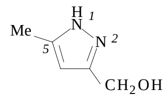
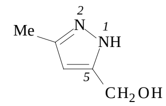
(lactam-lactim tautomerism)

—NH–P=N— ⇌ —N=P–NH—

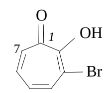
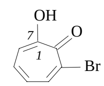
$—S(=O)_2–NH_2$ ⇌ $—S(=O)(OH)=NH$

A unique *CA Chemical Substance Index* name is selected for each compound containing a normalized tautomeric structure by application *first* of the structural rules which follow, and then of the nomenclature rules (see III, 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

 ⇌ 

1*H*-Pyrazole-3-methanol, 5-methyl- (principle: lowest locant for principal group) NOT **1*H*-Pyrazole-5-methanol, 3-methyl-**

 ⇌ 

2,4,6-Cycloheptatrien-1-one, 3-bromo-2-hydroxy- (principle: lowest locants for substituents) NOT **2,4,6-Cycloheptatrien-1-one, 2-bromo-7-hydroxy-**

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

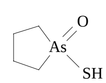
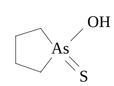
II. *Structural rules.* These rules are used to select the particular structure of a tautomer from which the unique *CA Chemical Substance Index* name is then derived. They are applied before the nomenclature rules (see III, below) are considered.

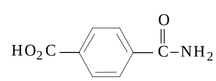
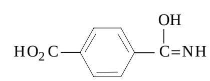
1. The maximum number of oxygen (or other chalcogen) atoms are doubly bonded to the central atom Q. If it is necessary to make a choice, the descending order of precedence for double-bond formation is O, S, Se, Te.

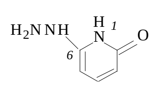
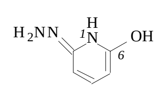
Examples:

$CH_3–C(=O)–NH_2$ NOT $CH_3–C(OH)=NH$

$HS–P(=S)(SH)–NH_2$ NOT $HS–P(SH)_2=NH$

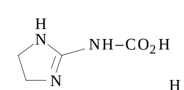
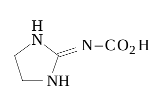
 NOT 

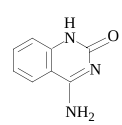
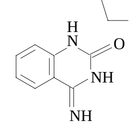
 NOT 

 NOT 

2. For a compound which contains a nitrogenous heterocycle bonded to one or more acyclic nitrogen atoms in such a way that a normalized tautomer results, the preferred structure is that which has the maximum number of single bonds between the heterocycle and the nitrogen atoms. *This rule is not applied* when the nitrogen atom is part of a hydrazone or oxime which is a derivative of the principal function (*see nomenclature rule* III, (*a*) *below*).

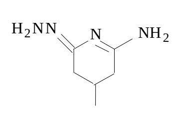
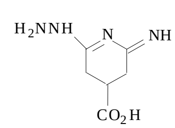
Examples:

 NOT 

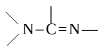
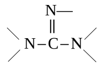
 NOT 

When it is necessary to choose between amino and hydrazino, amino is preferred.

Example:

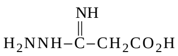
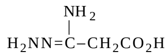
 NOT 

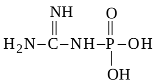
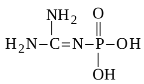
3. For a compound which contains a completely *acyclic*

 or 

fragment which is capable of being structured with an unsubstituted imino (=NH) group, that tautomeric form is preferred over any other, even when the fragment is bonded to an amino, hydrazino, or other nitrogen-containing radical.

Examples:

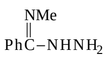
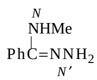
 NOT 

 NOT 

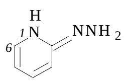
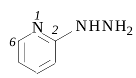
III. *Nomenclature rules*. When the structural rules, above, are insufficient to enable a choice of preferred tautomeric form to be made, the following nomenclature rules are successively applied until a decision is reached:

(a) The preferred index heading parent expresses the maximum number of the principal chemical functional group.

Examples:

 ⇌ 

Benzenecarboximidic acid, *N*-methylhydrazide NOT **Benzenecarbohydrazonamide, *N*-methyl-**

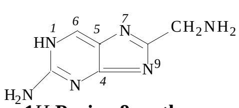
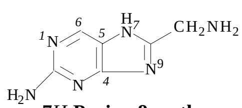
 ⇌ 

2(1*H*)-Pyridinone hydrazone NOT **Pyridine, 2-hydrazino-**

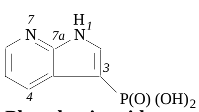
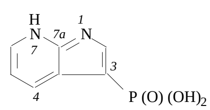
(NOTE: Hydrazones and oximes of principal functional groups are exceptions to structural rule II. 2, above.)

(b) The lowest locant for indicated hydrogen (see ¶ 135) is expressed in the preferred index name for nitrogenous heterocycles which are normalized, whether such heterocycles are expressed in the index heading parent, substituent prefix, or index modification.

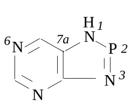
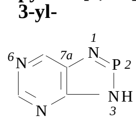
Examples:

 ⇌ 

1*H*-Purine-8-methanamine, 2-amino- NOT **7*H*-Purine-8-methanamine, 2-amino-**

 ⇌ 

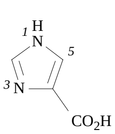
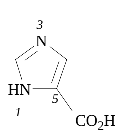
Phosphonic acid, 1*H*-pyrrolo[2,3-*b*]pyridin-3-yl- NOT **Phosphonic acid, 7*H*-pyrrolo[2,3-*b*]pyridin-3-yl-**

 ⇌ 

1*H*-1,3,2-Diazaphospholo[4,5-*d*]pyrimidine NOT **3*H*-1,3,2-Diazaphospholo[4,5-*d*]pyrimidine**

(c) Lowest locants are expressed for (i) suffixes, i.e., principal groups of index heading parents and free valencies of substituent radicals, and (ii) multiple bonds in parents and radicals.

Examples:

 ⇌ 

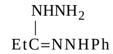
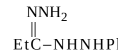
1*H*-Imidazole-4-carboxylic acid NOT **1*H*-Imidazole-5-carboxylic acid**

$Ph-NH-N=N-CH_2CO_2H$ ⇌ $Ph-N=N-NH-CH_2CO_2H$

Acetic acid, (3-phenyl-1-triazenyl)- NOT **Acetic acid, (3-phenyl-2-triazenyl)-**

(d) The maximum number of substituents are cited as prefixes in the index heading.

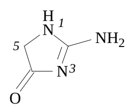
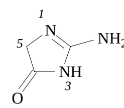
Example:

 ⇌ 

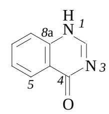
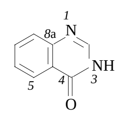
Propanehydrazonic acid, *N*-phenylhydrazide NOT **Propanehydrazonic acid 2-phenylhydrazide**

(e) Substituent prefixes and added hydrogen (see ¶ 136) are assigned lowest locants (see ¶ 137) to denote positions of attachment to an index heading parent or a substituent radical.

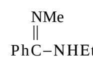
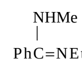
Examples:

 ⇌ 

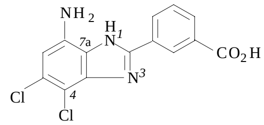
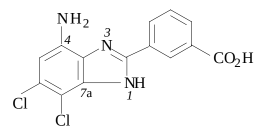
4*H*-Imidazol-4-one, 2-amino-1,5-dihydro- NOT **4*H*-Imidazol-4-one, 2-amino-3,5-dihydro-**

 ⇌ 

4(1*H*)-Quinazolinone NOT **4(3*H*)-Quinazolinone**

 ⇌ 

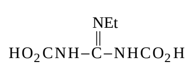
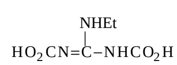
Benzenecarboximidamide, *N*-ethyl-*N′*-methyl- NOT **Benzenecarboximidamide, *N′*-ethyl-*N*-methyl-**

 ⇌ 

Benzoic acid, 3-(7-amino-4,5-dichloro-1*H*-benzimidazol-2-yl)- NOT **Benzoic acid, 3-(4-amino-6,7-dichloro-1*H*-benzimidazol-2-yl)-**

(f) The index heading parent expresses the maximum number of occurrences by use of multiplicative nomenclature (see ¶ 125).

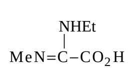
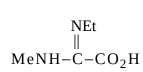
Example

 ⇌ 

Carbamic acid, (ethylcarbonimidoyl)bis- NOT **Carbamic acid, [(carboxyamino)(ethylamino)methylene]-**

(g) The preferred *CA* index name is that which occurs earliest in the index arrangement as determined by the rules for ordering of *Chemical Substance Index* entries (see Appendix II, ¶ 10C).

Examples:

 ⇌ 

Acetic acid, (ethylamino)(methylimino)- NOT **Acetic acid, (ethylimino)(methylamino)-**

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

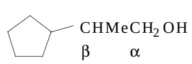
For salts and molecular addition compounds, see ¶¶ 192, 198.

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.

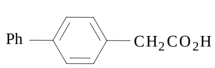
A conjunctive name is employed when any ring system (including a polyhedral borane) is attached by single bonds to one or more saturated acyclic hydrocarbon chains, each of which bears only one functional substituent corresponding to the principal chemical group of the compound. When a second or third 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

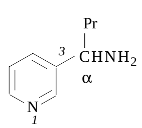
$PhCH_2OH$ — **Benzenemethanol**



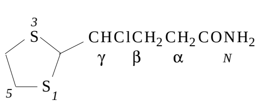
Cyclopentaneethanol, β-methyl-



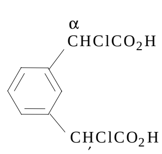
[1,1′-Biphenyl]-4-acetic acid



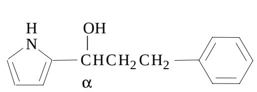
3-Pyridinemethanamine, α-propyl-



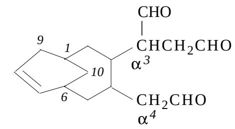
1,3-Dithiolane-2-butanamide, γ-chloro-



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



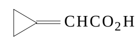
1*H*-Pyrrole-2-methanol, α–(2–phenylethyl)- (the heading parent which expresses the preferred ring system, not the preferred acyclic chain, is chosen)



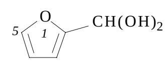
Bicyclo[4.3.1]dec-7-ene-3,4-diacetaldehyde, α^3-(2-oxoethyl) (not Bicyclo[4.3.1]dec-7-ene-3-propanol, β-formyl-4-(2-oxoethyl)-; the preferred heading parent expresses the maximum number of principal groups and, because it also expresses a ring system, is preferred to **Butanedial)**

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.

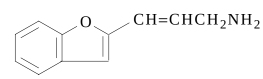
Examples



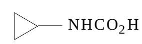
Acetic acid, cyclopropylidene-



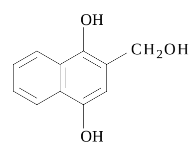
Methanediol, 2-furanyl-



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



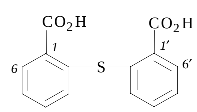
Carbamic acid, cyclopropyl-



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:



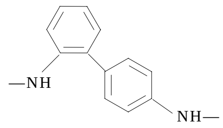
Benzoic acid, 2,2′-thiobis-

In the example above, a simple one-part polyvalent radical, thio, was employed as a multiplier; other such radicals are oxy, -O-; methylene, $-CH_2-$; 1,4-phenylene, 1,4-C_6H_4=; imino, -NH-; nitrilo, -N=; and 1,3-disiloxanediyl, SiH_2OSiH_2-. In general, any simple multivalent radical may be used as a multiplicative radical, and may itself be substituted; e.g., (methylimino), $-N(CH_3)-$; (1-methyl-1,3-propanediyl), $-CH(CH_3)CH_2CH_2-$.

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.

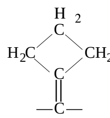
Examples of permissible multiplying radicals:

$—CH_2OCH_2—$	[oxybis(methylene)]
$CH_2–CHCl—$ above N of $—CHCl–CH_2–N–CH_2–CHCl—$	[nitrilotris(1-chloro-2,1-ethanediyl)]
$—OCH_2CHClO—$	[(1-chloro-1,2-ethanediyl)bis(oxy)]
SiH_2 (above) and SiH_2 (below) on C of $—SiH_2CH_2CH_2\,C–SiH_2—$	(1-propanyl-3-ylidynetetrasilylene)

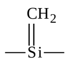


([1,1′-biphenyl]-2,4′-diyldiimino)

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

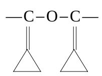


(cyclobutylidenemethylene)

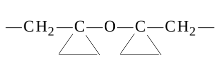


(methylenesilylene)

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



[oxybis(cyclopropylidenemethylene)]

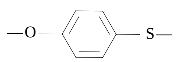


[oxybis[(cyclopropylidene)(methylene)]]

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

— CH_2NH —

—CH_2CH= NCH_2 CH=



—CHCl $CH_2PHCHCl$ CH_2—

— CH_2OO —

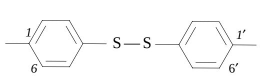
—SiH_2—O—SiH=

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:

—CHCl CH_2 OCH_2CHCl— (locants 1 2 2 1)

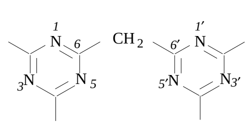
[oxybis(1-chloro-2,1-ethanediyl)]



(dithiodi-4,1-phenylene)

—CH_2CH=CHSe CH=CHCH_2— (locants 3 2 1)

(selenodi-2-propene-3,1-diyl)



[methylenebis(1,3,5-triazine-6,2,4-triyl)] (the 2- and 4-positions are equally close to the heading parent and are therefore cited in normal sequence)

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.

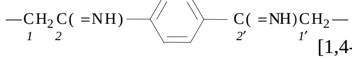
Examples:

—CH_2 NHCOCH_2 CONHCH_2— (locants 1 2 3)

[(1,3-dioxo-1,3-propanediyl)bis(iminomethylene)]

—COCO—

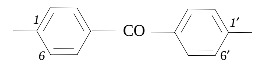
(1,2-dioxo-1,2-ethanediyl)



[1,4-phenylenebis(2-imino-2,1-ethanediyl)]

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

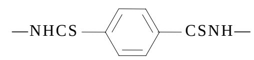
Examples:



(carbonyldi-4,1-phenylene)

—NHC(= NH) NH—

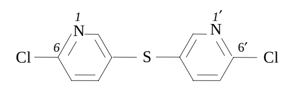
(carbonimidoyldiimino)



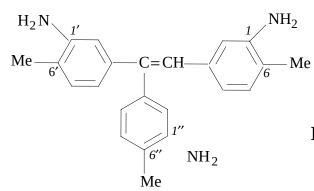
[1,4-phenylenebis(carbonothioylimino)]

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:



Pyridine, 3,3′-thiobis[6-chloro- (not Pyridine, 5,5′-thiobis[2-chloro-; multiplicative radicals are given lowest locants) (The uninverted form of this name is 3,3′-Thiobis[6-chloropyridine].)



Benzenamine, 3,3′,3″-(1-ethenyl-2-ylidene)tris[6-methyl-

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:

$HOCH_2$ CH_2 OCH_2 Si H_2 OSi HOSi H_2 CH_2 OCH_2 CH_2 OH (locants 1′ 2′ … 2 1)
|OSi H_2 CH_2 OCH_2 CH_2 OH

Ethanol, 2,2′-[[3-[[[(2-hydroxethoxy)methyl]silyl]oxy]-1,5-trisiloxanediyl]bis(methyleneoxy)]-bis- (not Ethanol, 2,2′,2″-[silylidynetris(oxysilylenemethyleneoxy)]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, 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- (azo); -SiH_2-O-SiH_2-(1,3-disiloxanediyl); -SiH_2-NH-SiH_2-(1,3-disilazanediyl). The above are all single hetero units, but -HP-NH-, -S-O-, and -O-SiH_2-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.)

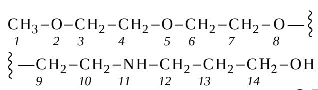
TABLE I
REPLACEMENT PREFIXES IN DESCENDING ORDER OF PRECEDENCE

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

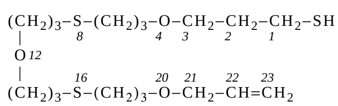
The replacement prefixes are placed in descending order of precedence ahead of the name of the carbon skeleton with locants to indicate the positions of the atoms replaced. Lowest locants are assigned to the hetero atoms, not to functional groups or unsaturation.

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.

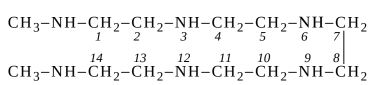
Examples:



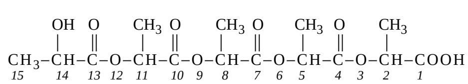
2,5,8-Trioxa-11-azatetradecan-14-ol



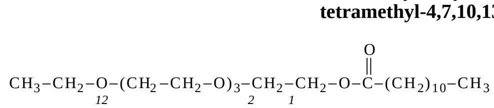
4,12,20-Trioxa-8,16-dithiatricos-22-ene-1-thiol



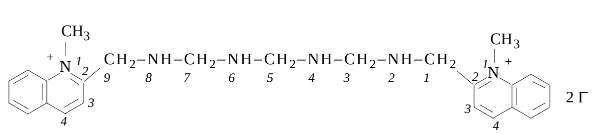
3,6,9,12-Tetraazatetradecane-1,14-diamine, N,N′-dimethyl-



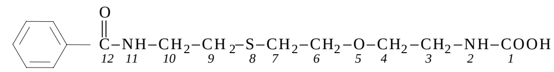
3,6,9,12-Tetraoxapentadecanoic acid, 14-hydroxy-2,5,8,11-tetramethyl-4,7,10,13-tetraoxo-



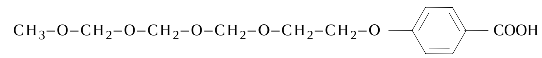
Dodecanoic acid 3,6,9,12-tetraoxatetradec-1-yl ester



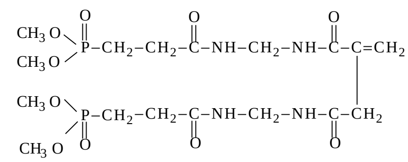
Quinolinium,2,2′-(2,4,6,8-tetraazanonane-1,9-diyl)bis[1-methyl-, diiodide



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



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



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

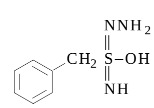
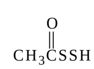
129. Replacement nomenclature for functions is a method of describing the replacement of hydroxyl and oxo functional groups by nitrogen, chalcogens, halogens, or halogenoids such as isocyanato. The replacement may be carried out in substituent suffixes, e.g., -thioic acid from -oic acid; in substituent 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 $-NH_2$), azido (for $-N_3$), chlorido (for -Cl) (and similarly for other halo atoms), cyanatido (for -OCN), hydrazido (for $-NHNH_2$), 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 $=NNH_2$), 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 peroxo, (thioperoxo), and (dithioperoxo).

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:

$MeCS_2H$	**Ethane(dithioic) acid** (not Acetic acid, dithio-)
PhC(=NH) OH	**Benzenecarboximidic acid** (the tautomeric **Benzamide** is preferred, except for esters and anhydrides; see ¶ 122)
	**Benzenemethanesulfonohydrazonimidic acid** (derived from the conjunctive name **Benzenemethanesulfonic acid)**
	**Ethane(dithioperoxoic) acid**

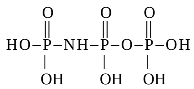
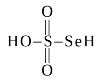
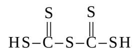
In replacement names from phosphorus and arsenic functional parent compounds (¶ 197), all the affixes except hydrazono may be employed as part of the suffix. For **Carbonic acid** and its relatives (¶ 183) all but hydrazido and nitrido may be used.

Examples:

$ClP(O)(OH)_2$	**Phosphorochloridic acid**
$MeAs(NH_2)OH$	**Arsonamidous acid, *As*-methyl-**
$P(S)(NH_2)_3$	**Phosphorothioic triamide**
$(HO)_2C{=}NNH_2$	**Carbonohydrazonic acid**
$(HOO)_2CO$	**Carbonodiperoxoic 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**
HO_2CNHCO_2H	**Imidodicarbonic acid**
	**Selenosulfuric acid (H_2SO_3Se)**
	**Thiodicarbonic acid([(HS)C(S)]$_2$S)**

Nondetachable prefixes are used in a few other cases.
Examples:

$ClSO_3H$	**Chlorosulfuric acid**
$S(O)(=NH)(NH_2)_2$	**Imidosulfamide**
$(H_2N)_2CS$	**Thiourea**
H_2NSH	**Thiohydroxylamine**
AcOSAc	**Thioperoxide, diacetyl**
EtOSH	**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.

(*b*) *Molecular-skeleton parent compounds* are nonfunctional. They are chains or rings of atoms with only hydrogen atoms attached and possessing names which express or imply the substitutive valency and bonding of the skeletal atoms. (**Methane** and monoatomic hydrides of the Group IVA elements and the Group VA elements (except nitrogen) are treated as molecular skeletons.) Examples include **Ethane**, **Distannane**, **Diazene**, **3,6,9,12,15-Pentaoxaheptadecane**, **Cyclohexane, Morpholine**, **Phosphine**, **Stannane**. They are transformed into index heading parents by appending, as a suffix, the substituent which represents the principal functional group of the compound; other substituents are expressed as prefixes.

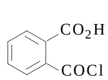
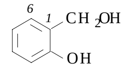
131. Substituent suffixes of molecular-skeleton parent compounds are chosen to represent the principal chemical functional group (or groups) in accordance with the order of precedence of compound classes (¶ 106). When no suffix is available to represent the preferred compound class, either a substitutive functional parent compound (¶ 130) is used as a heading parent, or another system of nomenclature, e.g., coordination or radicofunctional, is adopted.

Examples:

$EtP(O)(OH)_2$	**Phosphonic acid, ethyl-**(Phosphonic acid is a functional parent compound.)
$PhSF_3$	**Sulfur, trifluorophenyl-**, (*T*-4)- (a coordination name)
F_3COOCF_3	**Peroxide, bis(trifluoromethyl)** (a radicofunctional name)

The particular suffixes used for various classes of compounds in descending order of precedence from acids through imines (¶ 106) are described in the sections of this Guide dealing with these classes. Only one class may be expressed as a suffix in a single index heading parent; less preferred classes are denoted by prefixes. Multiplicative prefixes are employed to indicate the number of principal groups present.

Examples (in descending order of compound classes):

	**Benzoic acid, 2-(chlorocarbonyl)-**
$EtCO_2H$	**Propanoic acid**
$MeCHMeSO_3H$ (1 2)	**2-Propanesulfonic acid**
$MeCOCH_2CSMe$ (1 5)	**2-Pentanone, 4-thioxo-**
$HOSiMe_2OSiMe_2OH$	**1,3-Disiloxanediol, 1,1,3,3-tetramethyl-**
	**Benzenemethanol, 2-hydroxy-**
$CH_3CH_2NH_2$	**Ethanamine**

132. Substituent prefixes (commonly called "radicals") are employed to denote atoms and chemical groups attached to an index heading parent. The following substituents are never expressed as suffixes; they may be termed "compulsory" or "mandatory" prefixes: astato (At-), astatyl (AtO_2-), azido (N_3-), bromo (Br-), chloro (Cl-), chlorosyl (OCl-), chloryl (O_2Cl-), diazo (N_2-), fluoro (F-), iodo (I-), iodosyl (OI-), iodyl (O_2I-), isocyanato (OCN-), isocyano (CN-), nitro (O_2N-), *aci*-nitro ((HO)(O)N=), nitroso (ON-), perchloryl (O_3Cl-). In addition, all thio, sulfinyl, and sulfonyl radicals, (RS-), (RS(O)-), and ($RS(O)_2$-), and their seleno and telluro analogs, are mandatory substituent prefixes; so are hydrocarbon radicals and other radicals derived from molecular skeletons, e.g., ethyl, furanyl, disiloxanediyl, when attached to a more preferred heading parent.

Radicals may be simple, compound, or complex. A compound radical is made up of two or more simple radicals, e.g., (chlorothio), (diaminomethyl). A complex radical is composed of a simple radical to which at least one compound radical is attached; e.g., [(chloromethyl)amino], [1-(trichloromethyl)-2-butenyl]. In these examples, amino and 2-butenyl are parent radicals, and methyl (in both cases) is a subsidiary radical. This procedure may be repeated indefinitely. (Chlorothio) is obtained by *addition* of the two components, (aminomethyl) by *substitution* of methyl by amino. Substitution is the preferred method where a substitutive simple radical is available; e.g., (aminomethylene) is (NH_2CH=), not (NH_2CH_2-). Substitution in certain radicals, including the following, is not permitted: hydroxy, mercapto, selenyl, telluryl, hydroperoxy, sulfeno, diazenyl, formyl, carboxy, sulfo, phosphono, and carbonothioyl.

Examples:

$Me(CH_2)_4O$—	(pentyloxy)	NOT	(pentylhydroxy)
PhN=N—	(phenylazo)	NOT	(phenyldiazenyl)
ClCO—	(chlorocarbonyl)	NOT	(chloroformyl)
PhO_2C—	(phenoxycarbonyl)	NOT	(phenylcarboxy)
$(MeO)_2P(O)$—	(dimethoxyphosphinyl)	NOT	(dimethylphosphono)
MeOCS—	(methoxythioxomethyl)	NOT	(methoxycarbonothioyl)

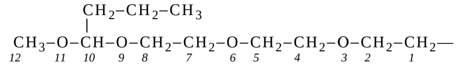
All compound radicals are enclosed in parentheses. Simple radicals are so enclosed when two locants of like type fall together; e.g., **Benzoic acid**, **3-(4-pyridinyl)-**; for clarity, when one locant has been omitted in the name of an indefinite compound; e.g., **1,2-Propanediol, 3-(thienyl)-**; and when "bis" or "tris" has been employed to remove ambiguity (see ¶ 110); e.g., tris(decyl), bis(benzanthracenyl), bis(azepinyl). Brackets are used in complex radicals, e.g., [2-(dimethylamino)ethoxy]. Spaces in a name often permit the dropping of one set of enclosing marks around radicals in substituents and modifications; e.g., **Disulfide, 2-chloroethyl ethyl; Propanoic acid, 2-ethylbutyl ester.**

133. Compound radicals. Selection of names for compound radicals is usually simple, but, when chain branching is present, can sometimes become perplexing. The following rules are successively applied; ((*a*) through (*e*) lead to selection of the preferred parent radical, (*f*) through (*h*) to a particular occurrence of this radical).

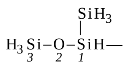
(*a*) Greatest number of acyclic hetero atoms.
(*b*) Greatest number of skeletal atoms.
(*c*) Greatest number of most preferred acyclic hetero atoms (see Table I, ¶ 128).
(*d*) Greatest number of multiple bonds.
(*e*) Lowest locants in the simple radical for replacement atoms in "a" names, then for multiple bonds of any kind, and finally for double bonds.
(*f*) Greatest number of substituents attached to the simple radical.
(*g*) Lowest locants for such substituents.
(*h*) Earliest index position of the total radical as it appears within the index name.

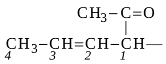
Examples (the italic letters on the left indicate the particular rule (above) that is exemplified):

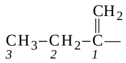
(*a*)

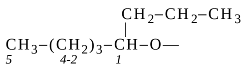


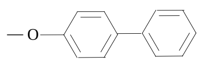
(10-propyl-3,6,9,11-tetraoxadodec-1-yl)

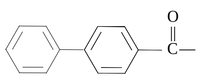
(*a*)  (1-silyldisiloxanyl)

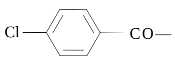
(*b*)  (1-acetyl-2-butenyl)

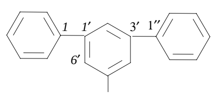
(*b*)  (1-methylenepropyl)

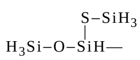
(*b*)  [(1-propylpentyl)oxy](not (1-butylbutoxy))(the selection principles are applied before elision is performed; another example follows)

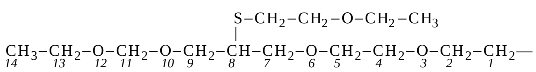
(*b*)  ([1,1′-biphenyl]-4-yloxy)(not (4-phenylphenoxy))

(*b*)  ([1,1′-biphenyl]-4-ylcarbonyl)-(not (4-phenylbenzoyl))(the simple radical benzoyl is retained for (phenylcarbonyl) only when the rules lead to this name)

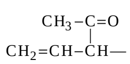
(*b*)  (4-chlorobenzoyl)(not [(4-chlorophenyl)carbonyl])

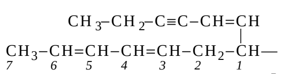
(*b*)  [1,1′:3′,1″-terphenyl]-5′-yl

(*c*)  [1-(silylthio)disiloxanyl]

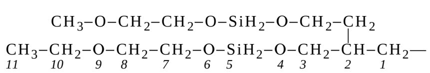
(*c*) 

[8-[(2-ethoxyethyl)thio]-3,6,10,12-tetraoxatetradec-1-yl]

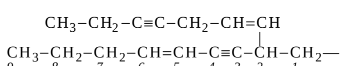
(*d*)  (1-acetyl-2-propenyl)

(*d*) 

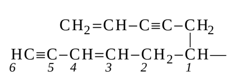
[1-(1-hexen-3-ynyl)-3,5-heptadienyl] (double bonds are preferred over an equal number of triple bonds)

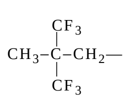
(*e*) 

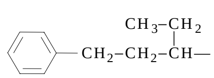
[2-(3,5,8-trioxa-4-silanon-1-yl)-4,6,9-trioxa-5-silaundec-1-yl]

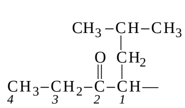
(*e*) 

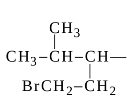
[2-(1-hepten-4-ynyl)-5-nonen-3-ynyl]

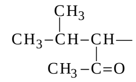
(*e*)  [1-(4-penten-2-ynyl)-3-hexen-5-ynyl]

(*f*)  [3,3,3-trifluoro-2-methyl-2-(trifluoromethyl)propyl]

(*f*)  (1-ethyl-3-phenylpropyl)(not [1-(2-phenylethyl)propyl])

(*g*)  [1-(2-methylpropyl)-2-oxobutyl](not [3-methyl-1-(1-oxopropyl)butyl])

(*g*)  [1-(2-bromoethyl)-2-methylpropyl] (not [3-bromo-1-(1-methylethyl)propyl])

(*h*)  (1-acetyl-2-methylpropyl)(not[1-(1-methylethyl)-2-oxopropyl])

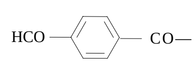
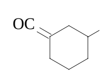
134. Carbonyl radicals which form part of a carbon chain are expressed by oxo substituents on the chain; the only exceptions are carboxy (-C(O)OH) and acetyl (-C(O)CH$_3$) radicals. The latter is used whenever (1-oxoethyl) would otherwise be called for. All chalcogen, imido and hydrazono analogs of carbonyl in a chain are treated similarly by use of thioxo, selenoxo, telluroxo, imido, and hydrazono 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-thioxoethyl),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:

HO_2CCH_2—	(carboxymethyl)
$HCOCH_2$—	(2-oxoethyl)(not (formylmethyl))
EtCO—	(1-oxopropyl)
$ClCOCH_2$	(2-chloro-2-oxoethyl)
H_2NCH_2CO—	(aminoacetyl)(glycyl is permitted in peptide nomenclature)
ClCOCO—	(chlorooxoacetyl)
AcNH—	(acetylamino)
EtCONH—	[(1-oxopropyl)amino]
$\underset{4}{Ph}C(=NH)(CH_2)_2\underset{1}{C}S$—	(4-imino-4-phenyl-1-thioxobutyl)
MeC(=NH)NH—	[(1-iminoethyl)amino]

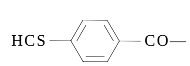
Isolated carbonyl radicals, other than carboxy, are expressed as carbonyl (as a doubling radical, or when both free valencies are attached to a single atom), formyl (if unsubstituted), benzoyl (if attached to a phenyl group which is not itself attached to another phenyl), or as a compound radical in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

Examples:

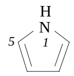
HO_2CCO—	(carboxycarbonyl)
H_2NCO—	(aminocarbonyl)(not carbamoyl)
ClCO—	(chlorocarbonyl)(not chloroformyl)
—NHCONH—	(carbonyldiimino)
	(4-formylbenzoyl)
	(3-carbonylcyclohexyl)

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, carbonohydrazonoyl, carbonothioyl, etc., are employed.

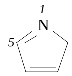
Examples:

HS_2CNH—	[(dithiocarboxy)amino]
	[4-(thioxomethyl)benzoyl]
HOC(=NH) —	(hydroxyiminomethyl)
$H_2NC(=NH)NH$ —	[(aminoiminomethyl)amino]
HN=C=N —	(carbonimidoylamino)

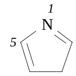
135. Indicated hydrogen is a designation comprising a locant followed immediately by an italic capital *H* placed before a ring system name to express the position of each of the saturated atoms necessary for formation of a definable, stable ring system. Thus, Pyrrole always has one saturated atom (an 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:



1*H*-Pyrrole



2*H*-Pyrrole

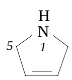


3*H*-Pyrrole

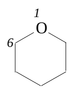
In the *Chemical Substance Index* only a single illustrative structural diagram is provided for each ring system, viz., the diagram which shows the saturated center(s) in the lowest-numbered nonangular position(s).

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.

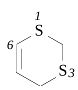
Examples:



1*H*-Pyrrole, 2,5-dihydro- (not 2*H*-Pyrrole, 1,5-dihydro-)



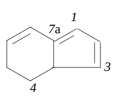
2*H*-Pyran, tetrahydro- (not 4*H*-Pyran, tetrahydro-)



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

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

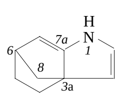
Example:



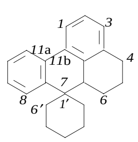
4*H*-Indene, 3a,5-dihydro- (not 3a*H*-Indene, 4,5-dihydro- or 5*H*-Indene, 3a,4-dihydro-)

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.

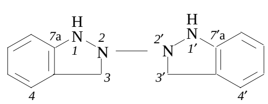
Examples:



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



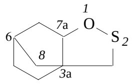
Spiro[7*H*-benz[*de*]anthracene-7,1′-cyclohexane], 4,5,6,6a-tetrahydro-



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.

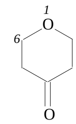
Example:



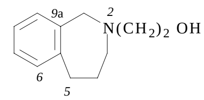
4H-3a,6-Methano-3H-1,2-benzoxathiole, tetrahydro- (3a*H*-1,2-Benzoxathiole cannot exist; the lowest available locant is therefore cited and the "extra" hydrogen for the bridge cited as additional indicated hydrogen, not in the "added" hydrogen form (see below), 3a(4*H*),6-Methano....)

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.)

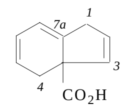
Examples:



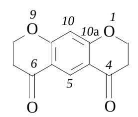
4*H*-Pyran-4-one, tetrahydro-



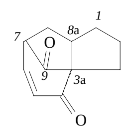
2*H*-2-Benzazepine-2-ethanol, 1,3,4,5-tetrahydro-



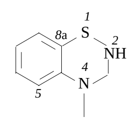
3a*H*-Indene-3a-carboxylic acid, 1,4-dihydro-



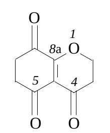
4*H*,6*H*-Benzo[1,2-*b*:5,4-*b*′]dipyran-4,6-dione, 2,3,7,8-tetrahydro-



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

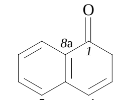


(2,3-dihydro-4*H*-1,2,4-benzo thiadiazin-4-yl)(not 2*H*-1,2,4-benzothiadiazin-4(3*H*)-yl)



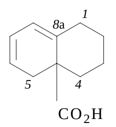
2*H*-1-Benzopyran-4,5,8(3*H*)-trione, 6,7-dihydro- (not 4*H*-1-Benzopyran-4,5,8-trione, 2,3,6,7-tetrahydro-)

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.

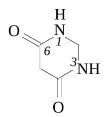


When principal functions or free valencies require added hydrogen, it is assigned to the lowest-numbered available angular or nonangular position; e.g., **1(2*H*)-Naphthalenone, 3,4-dihydro-** (not 1(4*H*)-Naphthalenone, 2,3-dihydro-); **2(4a*H*)-Naphthalenone, 5,6,7,8-tetrahydro-**. When the ring system 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.

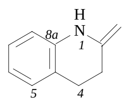
Examples:



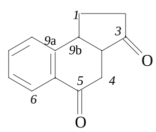
4a(2*H*)-Naphthalenecarboxylic acid, 1,3,4,5-tetrahydro- (a 4a(1*H*)-isomer cannot exist)



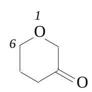
4,6(1*H*,5*H*)-Pyrimidinedione, dihydro-



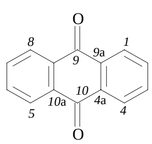
(3,4-dihydro-2(1*H*)-quinolinylidene) (not (1,4-dihydro-2(3*H*)-quinolinylidene))



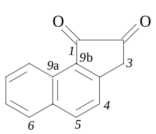
1*H*-Benz[*e*]indene-3,5(2*H*,4*H*)-dione, 3a,9b-dihydro-



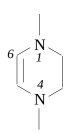
2*H*-Pyran-3(4*H*)-one, dihydro- (3*H*-Pyran cannot exist)



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



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

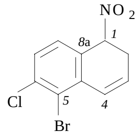


(2,3-dihydro-1,4-pyrazinediyl) (not (1,4(2*H*,3*H*)-pyrazinediyl))

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-)

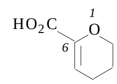
Lowest locants for various kinds of structural features in cyclic and acyclic molecular skeletons are assigned, in order, to:

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

Examples

$CH_3{-}O{-}CH_2{-}CH_2{-}O{-}CH_2{-}CH_2{-}O{-}CH_2{-}CH_2{-}O{-}CH_2{-}CH_2{-}OH$
1 2 3 4 5 6 7 8 9 10 11 12 13

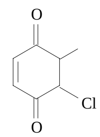
2,5,8,11-Tetraoxatridecan-13-ol- (not 3,6,9,12-Tetraoxatridecan-1-ol)



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

$CH_2{=}CH{-}C({=}O){-}CH_3$
4 3 2 1

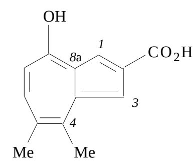
3-Buten-2-one (not 1-Buten-3-one)



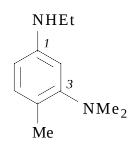
(6-chloro-2,5-dioxo-3-cyclohexen-1-yl)

$MeCH{=}CHC{\equiv}CCF_3$
1 6

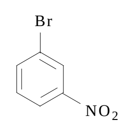
2-Hexen-4-yne, 6,6,6-trifluoro- (double bond given preference over triple bond)



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



1,3-Benzenediamine, *N*[1]-ethyl-*N*[3],-*N*[3],4-trimethyl- (not 1,3-Benzenediamine, *N*[3]-ethyl-*N*[1],*N*[1],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.

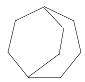
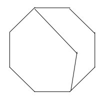
(*a*) Greatest number of the principal chemical functional group.

(*b*) 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.)

(*c*) 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:

(1) be a nitrogenous heterocycle;
(2) be a heterocycle;
(3) contain the largest number of rings;
(4) be a cyclic system occurring earliest in the following list of systems; spiro, bridged fused, bridged nonfused (Von Baeyer), fused;
(5) contain the largest individual ring (applies to fused carbocyclic systems);
(6) contain the greatest number of ring atoms;

(7) contain the greater number of ring atoms common to two or more rings (applies to Von Baeyer ring systems); thus

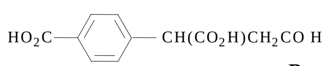
 is senior to 

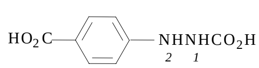
(8) contain lowest locants for bridges;
(9) contain the largest number of hetero atoms;
(10) contain the most preferred hetero atom other than nitrogen, according to the order in Table I, ¶ 128, i.e., O, S, Se, Te, P, As, Sb, Bi, Si, Ge, Sn, Pb, B.
(11) possess the most linear arrangement of rings (thus,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

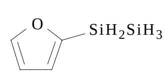
If the preferred heading parent occurs more than once in the total compound, further principles must be applied, as follows:
(*i*) Centrality. For three or more occurrences of the heading parent, at least one of which must be nonterminal, the basis of the name is the central occurrence (or one of the 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):

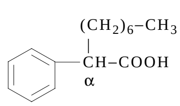
(*a*)
OH $CH_2-CH_2-CH_2-CH_2-CH_3$
$CH_3-CH-CH-CH_2-OH$
4 3 2 1
1,3-Butanediol, 2-pentyl-

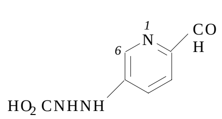
(*a*)

Butanedioic acid, (4-carboxyphenyl)-

(*b*)

Hydrazinecarboxylic acid, 2-(4-carboxyphenyl)-

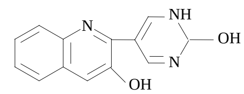
(*b*)

Disilane, 2-furanyl-

(*b*)
PhN=NH
Diazene, phenyl- (not Benzenamine, *N*-imino-) (homogeneous hetero chains are never broken to obtain a higher function or more preferred parent)

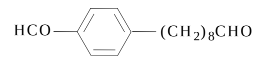
(*b*)

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*)
$O-CH_2-CH_2-O-CH_2-CH_3$
$CH_3-O-CH_2-CH_2-O-CH_2-CH_2-O-CH-CH_2-NHNH-CH_2-CH_2-CH_3$
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15
2,5,8-Trioxa-11,12-diazapentadecane, 9-(2-ethoxyethoxy)-

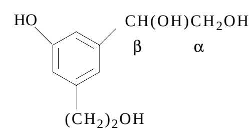
(*c*)

3-Quinolinol, 2-(1,2-dihydro-2-hydroxy-5-pyrimidinyl)-

(*d*)
$CH_2-CH_2-CH_2$
$CH_3-O-CH-O-CH_2-O-CH_2-O-CH_2-O-CH_3$
1 2 3 4 5 6 7 8 9 10 11
2,4,6,8,10-Pentaoxaundecane, 3-propyl-

(*e*)

Benzenenonanal, 4-formyl- (not Benzaldehyde, 4-(9-oxononyl)-)

(*e*)
$CH{=}CH-CH_2-OH$
$HO-CH_2-CH_2-CH_2-CH_2-CH-CH{=}CH-CH_2-CH_2-OH$
9 8 7 6 5 4 3 2 1
3-Nonene-1,9-diol, 5-(3-hydroxy-1-propenyl)-(not 2,5-Octadiene-1,8-diol, 5-(4-hydroxybutyl-)

(*e*)
CH_2
$CH_3-CH_2-CH_2-C-CH_2-CH_3$
6 5 4 3 2 1
Hexane, 3-methylene- (not 1-Pentene, 2-ethyl-)

(*e*)

1,3-Benzenediethanol, β, 5-dihydroxy- (see ¶ 124)

(*f*)
$H_3SiOSiH_2SiH_2SSiH_3$
3 2 1
Disiloxane, disilathianyl-

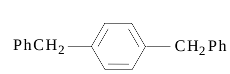
(*g*)
CH_3
$CH_2{=}C-CH{=}CH_2$
1 2
1,3-Butadiene, 2-methyl-

(*g*)
$C{\equiv}C-CH_2-CH_2-OH$
$HO-CH_2-CH{=}CH-CH_2-CH-CH_2-CH{=}CH-CH_2-OH$
9 8 7 6 5 4 3 2 1
2,7-Nonadiene-1,9-diol, 5-(4-hydroxy-1-butynyl)- (double bonds are preferred over an equal number of triple bonds)

(*h*)
$O-CH_2-CH_3$
$CH_3-O-CH_2-CH-O-CH_2-O-CH_2-O-CH_2-CH_2-COOH$
1 2 3 4 5 6 7 8 9 10 11 12
2,5,7,9-Tetraoxadodecan-12-oic acid, 4-ethoxy- (not 3,5,7,9-Tetraoxadodecan-12-oic acid, 4-(methoxymethyl)-

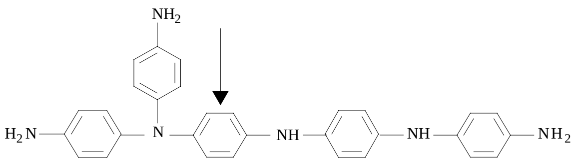
(*h*)
$HO-CH_2-CH_2-CH_2$ OH
$HO-CH_2-CH_2-CH_2-CH_2-CH-CH_2-CH-CH_3$
1 2 3 4 5 6 7 8
1,7-Octanediol, 5-(3-hydroxypropyl)- (not 1,8-Octanediol, 4-(2-hydroxypropyl)-)

(*h*)
$CH_2-CH{=}CH-CH_2-OH$
$HO-CH_2-CH{=}CH-CH_2-CH-CH{=}CH-CH_2-CH_2-OH$
1 2 3 4 5 6 7 8 9
2,6-Nonadiene-1,9-diol, 5-(4-hydroxy-2-butenyl)- (not 2,7-Nonadiene-1,9-diol, 5-(4-hydroxy-1-butenyl)-)

(*i*)

Benzene, 1,4-bis(phenylmethyl)-

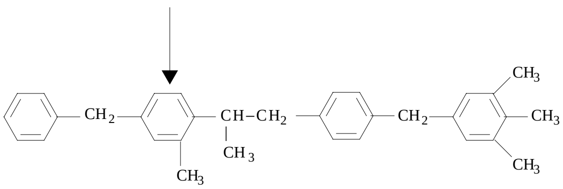
(*i*)
$Cl_2CHCH_2O(CH_2)_2O(CH_2)_2Cl$
Ethane, 1-(2-chloroethoxy)-2-(2,2-dichloroethoxy)-

(*i*)



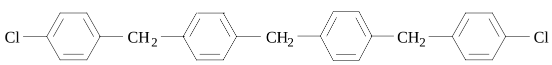
1,4-Benzenediamine, *N*,*N*-bis(4-aminophenyl)-*N′*-[4-[(4-aminophenyl)amino]phenyl]-

(*i*,*j*)



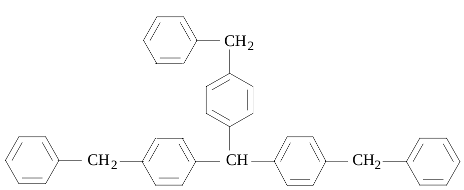
Benzene, 2-methyl-1-[1-methyl-2-[4-[(3,4,5-trimethylphenyl)-methy l]phenyl]ethyl]-4-(phenylmethyl)- (of the two central occurrences of the preferred heading parent, the one with the maximum number (three) of substituents is chosen; note that the centrality principle prevents choice of the tetrasubstituted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

(*i*,*l*)



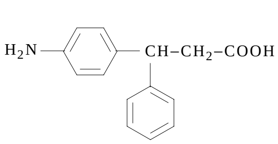
Benzene, 1,1′-methylenebis[4-[(4-chlorophenyl)methyl]-

(*i*,*l*)



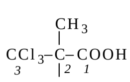
Benzene, 1,1′,1′′-methylidynetris[4-(phenylmethyl)- (when multiplication of the heading parent is permitted, occurrences directly attached to the central connecting radical are included in the same operation if possible)

(j)



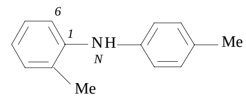
Benzenepropanoic acid, 4-amino-β-phenyl-

(*j*)



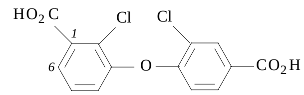
Propanoic acid, 3,3,3-trichloro-2-methyl-2-(trichloromethyl)- (not Propanoic acid, 2,2-bis(trichloromethyl)-) (like treatment of like groups is discontinued (¶ 255))

(*k*)



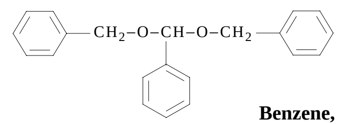
Benzenamine, 2-methyl-*N*-(4-methylphenyl)-

(*k*)



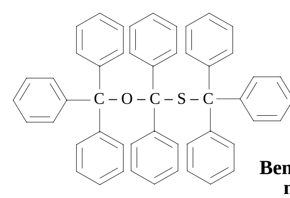
Benzoic acid, 3-(4-carboxy-2-chlorophenoxy)-2-chloro-

(*l*)



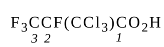
Benzene, 1,1′-[(phenylmethylene)bis(oxymethylene)]bis- (note that all occurrences of benzene are terminal and that the principle of centrality is therefore not applicable)

(*l*,*m*)



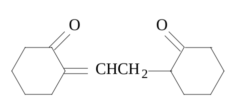
Benzene, 1,1′,1′′-[[[diphenyl(triphenylmethoxy)methyl] thio]methylidyne]tris- (not Benzene, 1,1′,1′′-[[diphenyl[(triphenylmethyl)thio]methoxy]methyldynetris-)

(*m*)



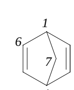
Propanoic acid, 2,3,3,3-tetrafluoro- 2-(trichloromethyl)- (not Propanoic acid, 3,3,3-trichloro-2-fluoro-2-(trifluoromethyl)-)

(*m*)

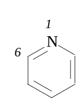


Cyclohexanone, 2-[2-(2-oxocyclohexyl)ethylidene]- (not Cyclohexanone, 2-[2-(2-oxocyclohexylidene)ethyl]-)

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

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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**

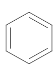
AsH_5 **Arsorane**

$H_3SiOSiH_2OSiH_2$ **Trisiloxane**

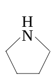
H_3SnSnH_3 **Distannane**

$CH_3\text{-}CH_2\text{-}O\text{-}CH_2\text{-}CH_2\text{-}O\text{-}CH_2\text{-}CH_2\text{-}O\text{-}CH_2\text{-}CH_2\text{-}O\text{-}CH_2\text{-}CH_3$
14 13 12 11 10 9 8 7 6 5 4 3 2 1

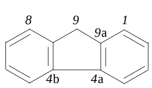
3,6,9,12-Tetraoxatetradecane



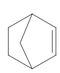
Benzene



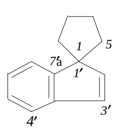
Pyrrolidine



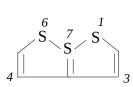
9*H*-Fluorene



Bicyclo[2.2.1]hept-2-ene



Spiro[cyclopentane-1,1′-[1*H*]-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 C_9H_{20}, **Hexadecane** for $C_{16}H_{34}$, **Eicosane** for $C_{20}H_{42}$, **Heneicosane** for $C_{21}H_{44}$, and **Tritriacontane** for $C_{33}H_{68}$.

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., “-enyne,” “-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:

$MeCH{=}CHCH_2CH{=}CH_2$ **1,4-Hexadiene** (not 2,5-Hexadiene)

$H_2C{=}C{=}CH_2$ **1,2-Propadiene**

$MeCH_2C{\equiv}CCH_2Me$ (6 … 1) **3-Hexyne**

$HC{\equiv}CC{\equiv}CH$ (1 … 4) **1,3-Butadiyne**

$HC{\equiv}CCH_2CH{=}CH_2$ (5 … 1) **1-Penten-4-yne**

$MeCH{=}CH(CH_2)_3C{\equiv}CH$ (… 1) **6-Octen-1-yne** (not 2-Octen-7-yne)

$H_2C{=}CHCH_2OH$ **2-Propen-1-ol** (not 1-Propen-3-ol)

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). These locants are *not* affected by the presence of a principal chemical group. Unsaturation is indicated as for the hydrocarbon chain, with lowest locants compatible with the low numbering of the hetero atoms.

Examples:

$CH_3\text{-}CH_2\text{-}O\text{-}CH_2\text{-}CH_2\text{-}O\text{-}CH_2\text{-}CH_2\text{-}O\text{-}CH_2\text{-}CH_2\text{-}O\text{-}CH_3$
13 12 11 10 9 8 7 6 5 4 3 2 1

2,5,8,11-Tetraoxatridecane

$CH_3{-}O{-}SiH_2{-}CH_2{-}CH_2{-}SiH_2{-}S{-}CH_3$
1 2 3 4 5 6 7 8

2-Oxa-7-thia-3,6-disilaoctane (not 7-Oxa-2-thia-3,6-disilaoctane)

$CH_3\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}CH_3$
1 2 3 4 5 6 7 8 9 10 11 12 13 14

3,6,9,12-Tetrasilatetradecane

$H_2C{=}CHCH_2[O(CH_2)_2]_3OMe$ (14 12 … 2 1) **2,5,8,11-Tetraoxatetradec-13-ene**

$H_2C{=}CH(OCH{=}CH)_3OCH{=}CH_2$ (14 13 … 3 1) **3,6,9,12-Tetraoxatetradeca-1,4,7,10,13-pentaene**

143. Homogeneous hetero chains are considered to include the mononuclear hydrides **Phosphine** (PH_3), **Phosphorane** (PH_5), **Arsine** (AsH_3), **Arsorane** (AsH_5), **Stibine** (SbH_3), **Bismuthine** (BiH_3), **Silane** (SiH_4), **Germane** (GeH_4), **Stannane** (SnH_4), and **Plumbane** (PbH_4). Chains composed of two or more of these hydride residues are named by prefixing the hydride name with “Di,” “Tri,” etc.

Examples:

H_2BiBiH_2 **Dibismuthine**

H_4PPH_4 **Diphosphorane**

$H_3SnSnH_2SnH_3$ **Tristannane**

$H_3Si(SiH_2)_3SiH_3$	**Pentasilane**

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:

HAs=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:

$H_3SiOSiH_2OSiH_3$ (1 2 3 4 5)	**Trisiloxane**
$H_3GeSeGeH_3$ (1 2 3)	**Digermaselenane**
$H_3SnSSnH_2SSnH_3$ (1 2 3 4 5)	**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., disilazanyl for SiH_3NHSiH_2-, are employed in the presence of higher functions (see ¶161).

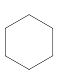
"A" names for hetero chains are avoided unless carbon substituents can be included in the chain. Otherwise the preferred parent is a homogeneous hetero chain, hydride, or element name.

Examples:

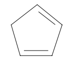
$H_3GeOSiH_2SPbH_3$	**Silane, (germyloxy)(plumbylthio)-**
$H_3GeOPbH_2SeMe$ (1 2 3 4)	**2-Oxa-4-selena-1-germa-3-plumbapentane**

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.

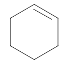
Examples:



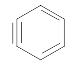
Cyclohexane



1,3-Cyclopentadiene



Cyclohexene

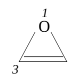


1,3-Cyclohexadien-5-yne (not Benzyne)

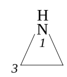
146. Monocyclic hetero systems.

(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 Dioxaazole.

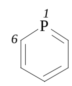
Examples:



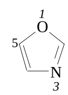
Oxirene



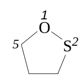
Aziridine



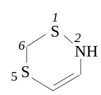
Phosphorin



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)



2*H*-1,5,2-Dithiazine (not 1*H*-2,4,1-Dithiazine; not 6*H*-1,3,6-Dithiazine; not 4*H*-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 "2*H*" signifies indicated hydrogen (see ¶ 135)).

TABLE II
HANTZSCH-WIDMAN STEMS FOR MONOCYCLIC HETERO SYSTEMS OF THREE THROUGH TEN MEMBERS[1]

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

[1]The symbols denoting the ring sizes for 3, 4, 7, 8, 9, 10 members are derived from numerical prefixes as follows: "ri" from t*ri*; "et" from t*et*ra; "ep" from h*ep*ta; "oc" from *oc*ta; "on" from n*on*a; and "ec" from d*ec*a.

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

[3]When 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.

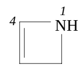
[4]Saturation is expressed by detachable prefixes such as "tetrahydro-," "hexahydro-," etc. The prefix "perhydro-" is not used.

[5]This 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.

[6]Saturation 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.

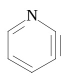
Example:



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., **1*H*-Pyrrole, 2*H*-Pyrrole, 3*H*-Pyrrole.** Presence of a triple bond in addition to the maximum number of noncumulative double bonds is expressed by the subtractive prefix "didehydro."

Example:



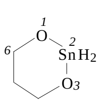
Pyridine, 2,3-didehydro-

TABLE III
MONOCYCLIC HETERO SYSTEMS WITH TRIVIAL NAMES

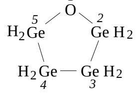
Hantzsch-Widman name	*Index name*
Azine	**Pyridine**
Azine, hexahydro-	**Piperidine**
Azole	**Pyrrole (1*H*-, 2*H*-,** or **3*H*-)**
Azolidine	**Pyrrolidine**
1,2-Diazine	**Pyridazine**
1,3-Diazine	**Pyrimidine**
1,4-Diazine	**Pyrazine**
1,4-Diazine, hexahydro-	**Piperazine**
1,2-Diazole	**Pyrazole (1*H*-, 3*H*-,** or **4*H*-)**
1,3-Diazole	**Imidazole (1*H*-, 2*H*-,** or **4*H*-)**
1,2-Diazolidine	**Pyrazolidine**
1,3-Diazolidine	**Imidazolidine**
2*H*-1,4-Oxazine, tetrahydro-	**Morpholine**
1,2-Oxazole	**Isoxazole**
Oxin	**Pyran (2*H*-** or **4*H*-)**
Oxole	**Furan**
1,2-Selenazole	**Isoselenazole**
Selenole	**Selenophene**
Tellurole	**Tellurophene**
2*H*-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).

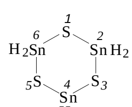
Examples:



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



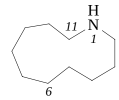
Oxatetragermolane



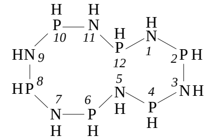
1,3,5,2,4,6-Trithiatristannin

(*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.

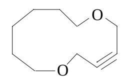
Examples:



Azacycloundecane



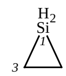
1,3,5,7,9,11-Hexaaza-2,4,6,8,10,12-hexaphosphacyclododecane



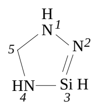
1,6-Dioxacyclododec-3-yne

(*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.

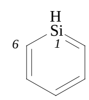
Examples:



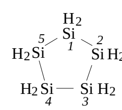
Silacyclopropane



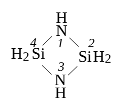
1,2,4-Triaza-3-silacyclopent-2-ene



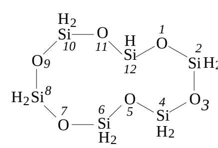
Silabenzene



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.

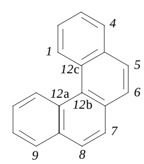
(*c*) *Spiro systems* have pairs of rings (or ring systems) with only one common atom.

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

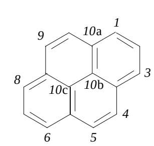
In the following sections, methods of naming ring systems of all these types will be described. The names of more complicated cases are built up from base components which may be described as "fundamental" systems.

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 2*n* 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:



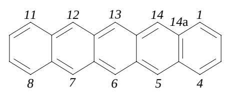
An ortho-fused system (3 common faces; 6 common atoms)



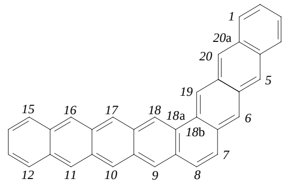
An ortho- and peri-fused system (5 common faces; 6 common atoms)

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:



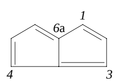
Pentacene



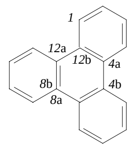
Octaphene

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.*

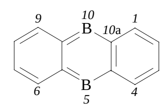
The following ring systems require citation of indicated hydrogen (¶ 135) to complete the name: **Indene, Fluorene, Phenalene, Trindene.**

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
as-**Indacene**	C_5-C_5-C_6
s-**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	C_5-C_5-C_6-C_6-C_6-C_6-C_6
Coronene	C_6-C_6-C_6-C_6-C_6-C_6-C_6
Trinaphthylene	C_6-C_6-C_6-C_6-C_6-C_6-C_6
Heptaphene	C_6-C_6-C_6-C_6-C_6-C_6-C_6
Heptacene	C_6-C_6-C_6-C_6-C_6-C_6-C_6
Pyranthrene	C_6-C_6-C_6-C_6-C_6-C_6-C_6-C_6
Ovalene	C_6-C_6-C_6-C_6-C_6-C_6-C_6-C_6-C_6-C_6

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.

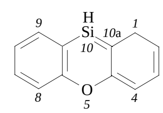
Example:



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:



1*H*-Phenoxasilin

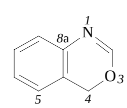
An exception is **Phenazine** for the analog that contains nitrogen in *both* central positions.

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.**

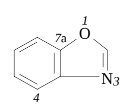
The replacement of the oxygen in **Xanthene** by sulfur or selenium has been denoted by the appropriate chalcogen functional replacement prefix: **Thioxanthene, Selenoxanthene.**

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).

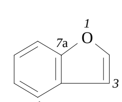
Examples:



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



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

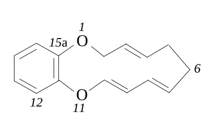


Benzofuran (the isomer is named Isobenzofuran)

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:



2*H*-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 SYSTEMS[1]

Index Name	*Ring Analysis*
Isoarsindole[2]	C_4As-C_6
Arsindole[2]	C_4As-C_6
Isoarsinoline	C_5As-C_6
Arsinoline	C_5As-C_6
Arsanthridine	$C_5As-C_6-C_6$
Acridarsine	$C_5As-C_6-C_6$
Arsanthrene	$C_4As_2-C_6-C_6$
Isophosphindole[2]	C_4P-C_6
Phosphindole[2]	C_4P-C_6
Isophosphinoline	C_5P-C_6
Phosphinoline	C_5P-C_6
Tellurophene	C_4Te
Selenophene	C_5Se
Selenanthrene	$C_4Se_2-C_6-C_6$
Thiophene	C_4S
Thianthrene	$C_4S_2-C_6-C_6$
Furan	C_4O
Pyran[2]	C_5O
Isobenzofuran	C_4O-C_6
Xanthene[2]	$C_5O-C_6-C_6$
Phenoxastibinin	$C_4OSb-C_6-C_6$
Phenoxarsine[2]	$C_4AsO-C_6-C_6$
Phenoxaphosphine[2]	$C_4OP-C_6-C_6$
Phenoxatellurin	$C_4OTe-C_6-C_6$
Phenoxaselenin	$C_4OSe-C_6-C_6$
Phenoxathiin	$C_4OS-C_6-C_6$
Pyrrole[2]	C_4N
Imidazole[2]	C_2N_2
Pyrazole[2]	C_3N_2
Isothiazole	C_3NS
Isoxazole	C_3NO
Pyridine	C_5N
Pyrazine	C_4N_2
Pyridazine	C_4N_2
Pyrrolizine[2]	C_4N-C_4N
Indolizine	C_4N-C_5N
Isoindole[2]	C_4N-C_6
Indole[2]	C_4N-C_6
Indazole[2]	$C_3N_2-C_6$
Purine[2]	$C_3N_2-C_4N_2$
Isoquinoline[3]	C_5N-C_6
Quinoline[3]	C_5N-C_6
Quinolizine[3]	C_5N-C_5N
Phthalazine	$C_4N_2-C_6$
Naphthyridine[4]	C_5N-C_5N
Quinoxaline	$C_4N_2-C_6$
Quinazoline	$C_4N_2-C_6$
Cinnoline	$C_4N_2-C_6$
Pteridine	$C_4N_2-C_4N_2$
Carbazole[2]	$C_4N-C_6-C_6$
Phenanthridine	$C_5N-C_6-C_6$
Acridine	$C_5N-C_6-C_6$
Perimidine[2]	$C_4N_2-C_6-C_6$
Phenanthroline[5]	$C_5N-C_5N-C_6$
Phenazine	$C_4N_2-C_6-C_6$
Anthyridine	$C_5N-C_5N-C_5N$
Phenarsazine	$C_4AsN-C_6-C_6$
Phenophosphazine	$C_4NP-C_6-C_6$
Phenotellurazine[2]	$C_4NTe-C_6-C_6$
Phenoselenazine[2]	$C_4NSe-C_6-C_6$
Phenothiazine[2]	$C_4NS-C_6-C_6$
Phenoxazine[2]	$C_4NO-C_6-C_6$
Thebenidine	$C_5N-C_6-C_6-C_6$
Quindoline[2]	$C_4N-C_5N-C_6-C_6$
Quinindoline[2]	$C_4N-C_5N-C_6-C_6$
Phthaloperine[2]	$C_5-C_4N_2-C_6-C_6-C_6$
Acrindoline[2]	$C_4N-C_5N-C_6-C_6-C_6$
Triphenodithiazine	$C_4NS-C_4NS-C_6-C_6-C_6$
Triphenodioxazine	$C_4NO-C_4NO-C_6-C_6-C_6$
Phenanthrazine	$C_4N_2-C_6-C_6-C_6-C_6-C_6-C_6$
Anthrazine	$C_4N_2-C_6-C_6-C_6-C_6-C_6-C_6$

[1]The 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).

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

[3]Because 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.

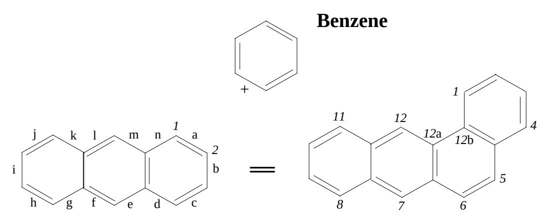
150. Selection of a base component is facilitated by use of Tables IV, ¶ 148 and V, ¶149; the appropriate component listed *latest* in these Tables is used. The system must contain at least two rings of five or more atoms, although such rings need not be directly fused to one another; i.e., they may 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:

(a) be a heterocycle;
(b) be a nitrogenous heterocycle;
(c) be a nonnitrogenous heterocycle containing a hetero atom of highest precedence (see Table I, ¶ 128);
(d) contain the greatest number of rings;
(e) contain the largest individual ring; **Benzindene (**not Cyclopenta-naphthalene) is an exception based on established usage;
(f) contain the greatest total number of hetero atoms;
(g) contain the greatest variety of hetero atoms, e.g., one nitrogen and one oxygen rather than two nitrogens;
(h) contain the greatest number of hetero atoms of highest precedence;
(i) possess the most linear structure;
(j) 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:



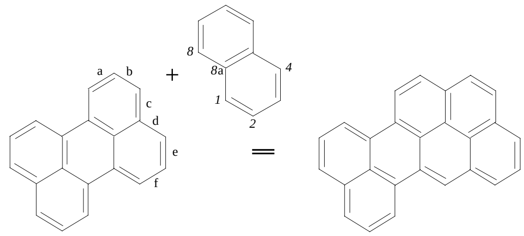
Benzene

Anthracene (base component) **Benz[*a*]anthracene**

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.

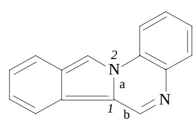
Angular positions of base components involved in fusion are not cited.
Example:

Naphthalene



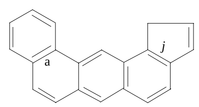
Perylene **Naphtho[8,1,2-*bcd*]perylene** (not "[8,8a,1,2-*bcd*]")

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:



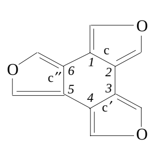
Isoindolo[2,1-*a*]quinoxaline (not "[2,3-*a*]"; not "[1,2-*c*]")

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:

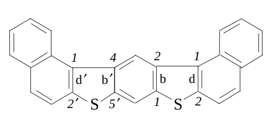


Benzo[*a*]cyclopent[*j*]anthracene

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:

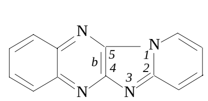


Benzo[1,2-*c*:3,4-*c*′:5,6-*c*′′]trifuran

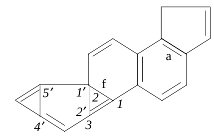


Dinaphtho[1,2-*d*:1′,2′-*d*′]benzo-[1,2-*b*:5,4-*b*′]dithiophene (not Dinaphtho[2,1-*b*:2′,1′-*b*′]benzo-[1,2-*d*:5,4-*d*′]dithiophene)

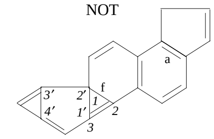
Ring systems fused to base components are designated primary components; a ring system (other than a base component) fused only to a primary component is a secondary component, and primed numerical locants are used to denote its fusion sites. Primed and unprimed locant sets are separated by colons. Lowest 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:



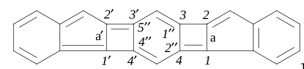
Pyrido[1′,2′:1,2]imidazo[4,5-*b*]-quinoxaline



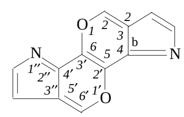
NOT



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.)



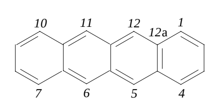
Benzo[1′′,2′′:3,4;5′′,4′′:3′,4′]dicyclobuta[1,2-*a*:1′,2′-*a*]diindene (Note that a semicolon separates locant sets which already contain colons.)



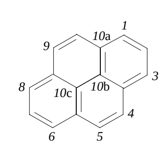
Pyrrolo[2′′,3′′:4′,5′]pyrano-[2′,3′:5,6]pyrano[4,3-*b*]pyrrole

152. Orientation and numbering of fused systems.

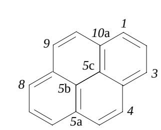
(*a*) *Hydrocarbons*. The component rings are normally drawn as regular polygons. The cyclopropane ring may point left or right, and cyclopentane and cycloheptane rings may point up or down. The total system is oriented so that (*a*) a maximum number of rings are in a horizontal row, and (*b*) a maximum 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:



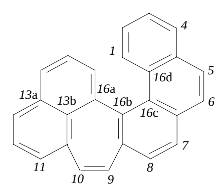
Naphthacene



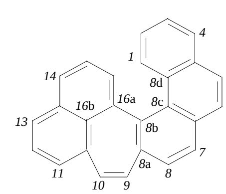
NOT



Pyrene

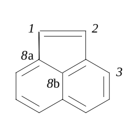


NOT

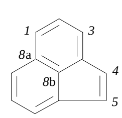


Naphtho[1′,8′:3,4,5]cyclohepta[1,2-*c*]phenanthrene

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

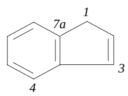


NOT



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

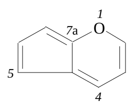
Indicated hydrogen is assigned the lowest locant.
Example:



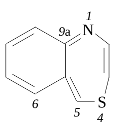
1*H*-Indene (not 3*H*-Indene)

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

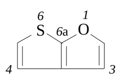
(*b*) *Heterocycles*. The ring systems are oriented as for hydrocarbons. When a choice is necessary, lowest locants are assigned to (*a*) all hetero atoms; (*b*) most preferred hetero atom (Table I, ¶ 128); (*c*) carbon atoms common to two or more rings; (*d*) positions bearing indicated hydrogen; (*e*) 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:



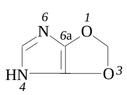
Cyclopenta[*b*]pyran



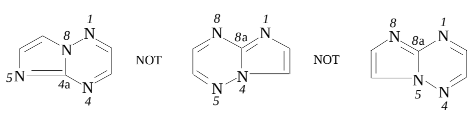
4,1-Benzothiazepine



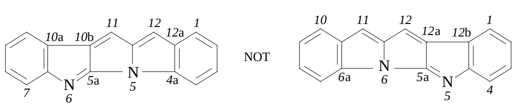
Thieno[2,3-*b*]furan



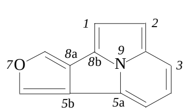
4*H*-1,3-Dioxolo[4,5-*d*]imidazole



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



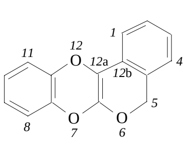
Pyrrolo[1,2-*a*:5,4-*b*′]diindole



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

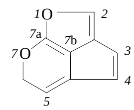
The following heterocyclic systems have special numbering systems: **Acridine, Carbazole, Purine, Xanthene,** and Epoxy- and Epithiocyclopenta[*a*]phenanthrenes (steroid numbering).

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:

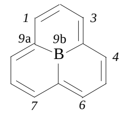


5*H*-[2]Benzopyrano[3,4-*b*][1,4]-benzodioxin (Note: The locants "2" and "1,4," which relate to the components, are bracketed to indicate that they do not conform to the peripheral numbering of the total system)

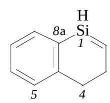
153. Replacement ("a") nomenclature for fused systems is employed when fusion names fail to express all interfaces (fusion sites) between component systems. This occurs when two or more components that are expressed as prefixes are fused to one another as well as to the base component. "A" names are 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:



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



9b-Boraphenalene

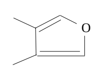


1-Silanaphthalene, 3,4-dihydro-

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 (–CH_2–), ethano (–CH_2–CH_2–), etheno (–CH=CH–), propano (–$CH_2CH_2CH_2$–), 2-buteno (–CH_2CH=-$CHCH_2$–), and benzeno (–C_6H_4–). Trivalent bridges, e.g., metheno (–CH=), 1-propanyl-3-ylidene (–CH_2CH_2CH=), 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- (–SiH_2–). Heterocyclic rings may also be used as bridges.
Example:



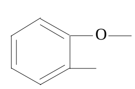
3,4-furano (cf. "furo" for the fusion prefix)

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:

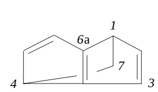
–NH$(CH_2)_2$– (iminoethano)

–OSO– (epoxythioxy)

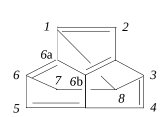


(epoxy[1,2]benzeno)

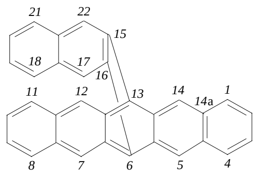
Indicated hydrogen of a fused system is cited, if possible, to accommodate a bridge. When this is unnecessary or impossible, the lowest-numbered nonangular indicated hydrogen is cited for the fused system, and additional indicated hydrogen, when needed, is cited ahead of the bridge locants.
Examples:



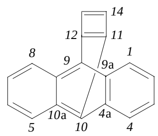
1,4-Methanopentalene, 1,4-dihydro-



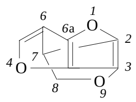
6,1,3-Ethanylylidenecyclopenta[*cd*] pentalene



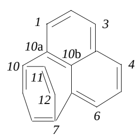
6,13[2′,3′]-Naphthalenopentacene



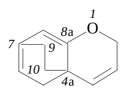
9,10[1′,2′]-*endo*-Cyclobutanthracene



3,2,6-(Epoxyethanylylidene)furo-[3,2-*b*]furan



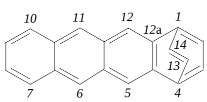
7,10-Ethenocyclohepta[*de*]-naphthalene



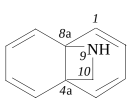
5*H*-4a,7-Ethano-2*H*-1-benzopyran (4a*H*-1-Benzopyran cannot exist)

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.

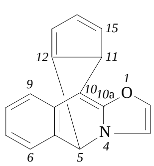
Examples:



1,4-Ethenonaphthacene

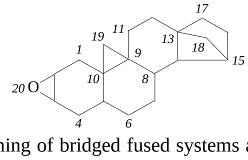


8a,4a-(Iminomethano)naphthalene (not 4a,8a-(Iminomethano)-naphthalene)



11*H*-5,10[1′,2′]-*endo*-Cyclopent-5*H*-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.



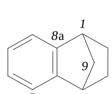
Criteria for the naming of bridged fused systems are applied successively as follows:

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

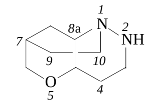
(*b*) The bridges are as simple as possible; e.g., two simple bridges are preferred to one compound bridge, and saturated bridges are preferred to unsaturated ones.

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

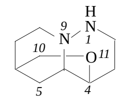
Examples:



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



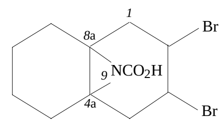
NOT



1,7-Ethano-1*H*-pyrano[3,2-*c*]-pyridazine, octahydro- (not 4,6-(Epoxymethano)-1*H*-pyrido[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.)

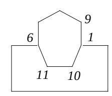
Example:



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.

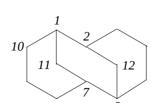
Example:



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.

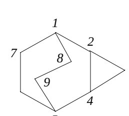
(*a*) The main ring contains the maximum number of atoms, two of which must serve as bridgeheads for the main bridge.

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

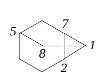
(*c*) The main ring is divided as symmetrically as possible by the main bridge.

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

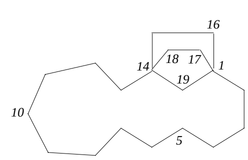
Examples:



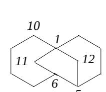
Tricyclo[3.2.2.0^{2,4}]nonane (not Tricyclo[2.2.2.1^{2,3}]nonane)



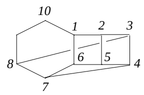
Tricyclo[3.2.1.0^{2,7}]octane (not Tricyclo[2.2.2.0^{2,6}]octane)



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

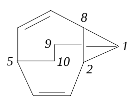
Unsaturation is denoted by "-ene" and "-yne" suffixes. A second locant in parentheses is cited for a double bond at a bridgehead when it does not proceed to the next atom in the numbered path. Multiple-bond locants are determined by the following criteria applied successively:

(*a*) The numbering proceeds in a clockwise sequence.

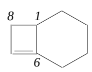
(*b*) The cases in which both locants for a double bond are cited are minimized.

(*c*) Lowest locants are employed.

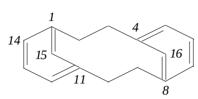
Examples:



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



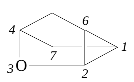
Bicyclo[4.2.0]oct-6-ene (not Bicyclo[4.2.0]oct-1(8)-ene)



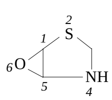
Tricyclo[9.3.1.1^{4,8}]hexadeca-1-(15),4,6,8(16),11,13-hexaene (not Tricyclo[9.3.1.1^{4,8}]hexadeca-4,6,8-(16),11(15),12,14-hexaene)

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.

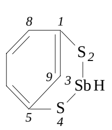
Examples:



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)



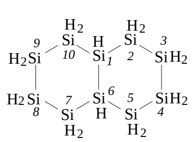
6-Oxa-2-thia-4-azabicyclo[3.1.0]-hexane (not 6-Oxa-4-thia-2-azabicyclo[3.1.0]hexane)



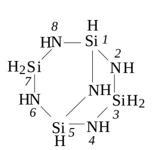
2,4-Dithia-3-stibabicyclo[3.3.1]-nona-1(9),5,7-triene (not 2,4-Dithia-3-stibabicyclo[3.3.1]nona-1(8),5(9),6-triene)

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.

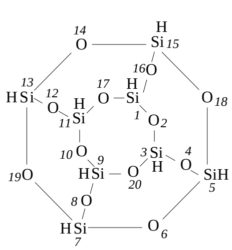
Examples:



Bicyclo[4.4.0]decasilane



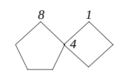
Bicyclo[3.3.1]tetrasilazane



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.

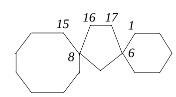
Example:



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.

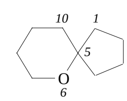
Example:



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.

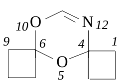
Example:



6-Oxaspiro[4.5]decane

Unsaturation is expressed by "-ene" and "-yne" suffixes.

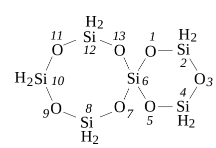
Example:



5,10-Dioxa-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.

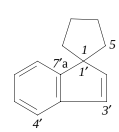
Example:



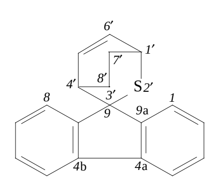
Spiro[5.7]hexasiloxane

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:



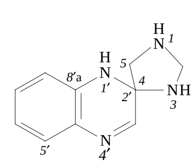
Spiro[cyclopentane-1,1′-[1*H*]-indene] (not Spiro[cyclopentane–1,1′-1′*H*-indene])



Spiro[9*H*–fluorene-9,3′-[2]thia-bicyclo[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.

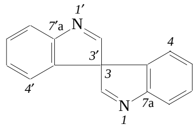
Example:



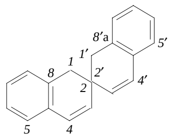
Spiro[imidazolidine-4,2′(1′*H*)-quinoxaline]

Monospiro systems containing identical fused components are given "Spirobi-" 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′-Spirobi[3*H*-indole]

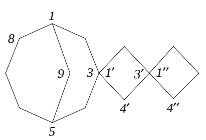


2,2′(1*H*,1′*H*)-Spirobinaphthalene

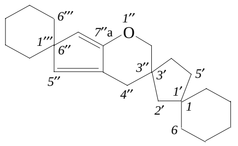
Di-, tri-, etc., spiro systems containing at least one fused or bridged component are named by extension of these policies. If terminal components are identical, citation is determined by earliest index position of the complete name. Serially primed locants are used for successive components.

"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.

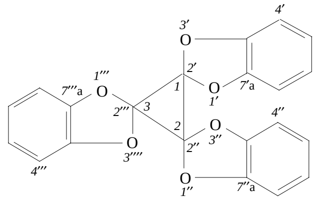
Examples:



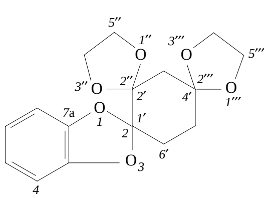
Dispiro[bicyclo[3.3.1]nonane–3,1′–cyclobutane–3′,1′′–cyclobutane]



Trispiro[cyclohexane-1,1′-cyclopentane–3′,3′′(2′′*H*)–cyclopenta–[*b*]pyran–6′′(4′′*H*),1′′′–cyclohexane]



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

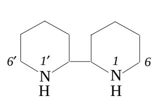


Trispiro[1,3-benzodioxole-2,1′-cyclohexane-2′,2′′:4′,2′′′-bis-[1,3]dioxolane]

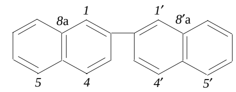
157. Ring assemblies contain a multiplicity of the same cyclic system joined by single bonds, not necessarily in equivalent positions. They are treated as molecular skeletons in substitutive nomenclature and rank just above the component ring. Except for assemblies of benzene, and two-component assemblies 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.*

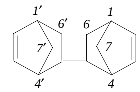
Examples:



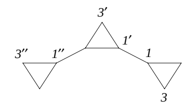
2,2′-Bipiperidine



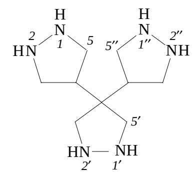
2,2′-Binaphthalene



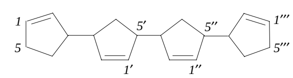
5,5′-Bibicyclo[2.2.1]hept-2-ene (not 2,2′-Bibicyclo[2.2.1]hept-5-ene)



1,1′:2′,1′′-Tercyclopropane



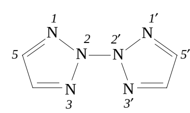
4,4′:4′,4′′-Terpyrazolidine



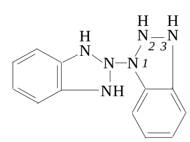
3,3′:5′,3′′:5′′,3′′′-Quatercyclopentene

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.

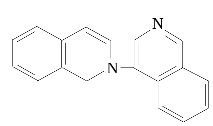
Example:



2,2′-Bi-2*H*-1,2,3-triazole



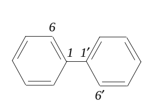
1*H*-Benzotriazole, 1-(1,3–dihydro-2*H*-benzotriazol-2-yl)-2,3-dihydro- (not 1*H*-Benzotriazole, 2-(2,3-dihydro-1*H*-benzotriazol-1-yl)-2,3-dihydro-; not 1(3*H*),2′-Bi-2*H*-benzotriazole, 1′,3′-dihydro-)



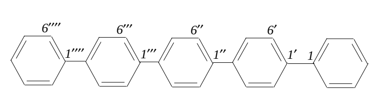
2(1*H*),4′-Biisoquinoline

Linear benzene assemblies (*polyphenyls*) are named by prefacing "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.

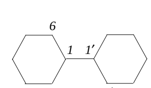
Examples:



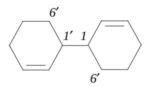
1,1′-Biphenyl



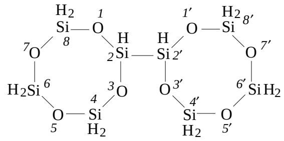
1,1′:4′,1′′:4′′,1′′′:4′′′,1′′′′-Quinquephenyl



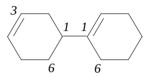
1,1′-Bicyclohexyl (not Bicyclohex–1-yl)



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



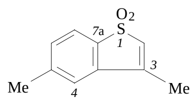
Bicyclotetrasiloxan-2-yl



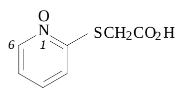
Cyclohexene, 1-(3-cyclohexen-1-yl)- (not Cyclohexene, 4-(1-cyclohexen-1-yl)- (lowest locant for the substituent prefix is preferred (¶ 138))

158. Neutral hetero atoms with abnormal valencies in ring systems are expressed (*a*) by additive terms, e.g., "oxide," "sulfide," in the modification; (*b*) by the greek letter "λ" followed by a superscript numeric (*c*) by the prefix "hydro" (in molecular skeletons not treated normally in substitutive nomenclature); (*d*) by superscript Roman numerals attached to the italicized element symbol, e.g. S^{IV}; (*e*) by substituent prefixes, e.g. "oxido"; (*f*) by a combination of methods *a, b, c, d* or *e* above.

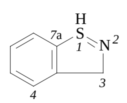
Examples:



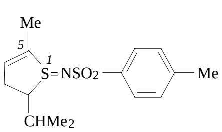
Benzo[*b*]thiophene, 3,5-dimethyl-1,1-dioxide



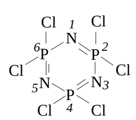
Acetic acid [(1-oxido-2-pyridinyl)thio]-
(former modification *N*-**oxide)**



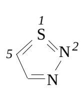
3*H*-1λ⁴-1,2-Benzisothiazole



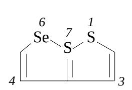
Thiophene, 1,1,2,3-tetrahydro-5-methyl-2-(1-methylethyl)-1-[[(4-methylphenyl)sulfonyl]imino]- (because the abnormal valency cannot be expressed in a substituent by an approved method, the higher (sulfonamide) function is "overstepped")



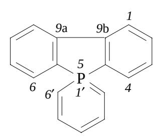
1,3,5,2,4,6-Triazatriphosphorine, 2,2,4,4,6,6-hexachloro-2,2,4,4,-6,6-hexahydro-



1,2,3-Thia(S^{IV})diazole



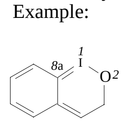
7λ⁴-[1,2]Dithiolo[5,1-*e*][1,2]thiaselenole



Spiro[5*H*-dibenzophosphole-5,1′λ⁵-phosphorin]

In a few cases, abnormal valency is implied rather than expressed, e.g. cyclic iodine systems, in which iodine is usually trivalent.

Example:



3*H*-1,2-Benziodoxin

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 BH_3.) 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, the higher hydrides as heterocyclic compounds. **Borane(1)** is BH, **Borane(2)** is BH_2. In higher boranes, the number of boron atoms is expressed by multiplicative prefixes.

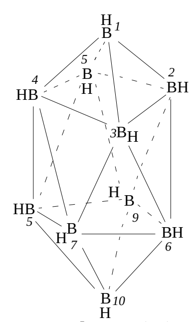
Examples:

B_2H_4	**Diborane(4)**
B_2H_6	**Diborane(6)**
B_3H_7	**Triborane(7)**
B_4H_{10}	**Tetraborane(10)**
B_5H_9	**Pentaborane(9)**
B_6H_{10}	**Hexaborane(10)**
$B_{10}H_{14}$	**Decaborane(14)**

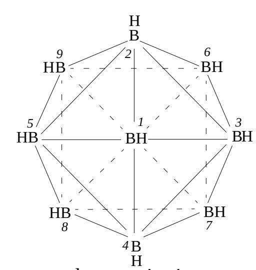
Until structures have been determined, author terms such as "*iso*" and "*neo*" are cited in index modifications to differentiate isomers.

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)

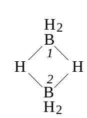


planar projection

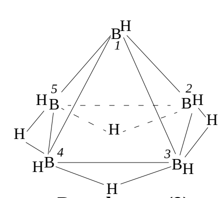
(Note that atom "6" (in the lower plane) is nearest to atom "2" in the direction of numbering.)

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.

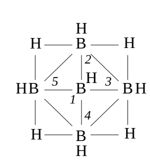
Examples:



Diborane(6)

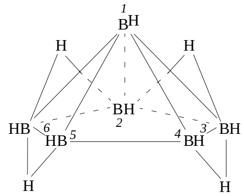


Pentaborane(9)

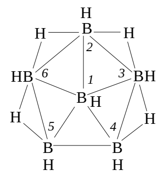


planar projection

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



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:

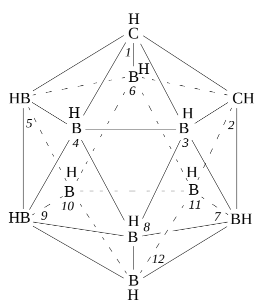
1,1′-Bipentaborane(9)

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-**.

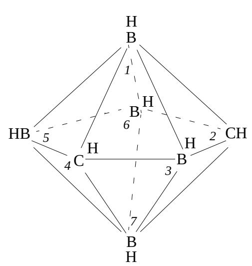
Polyboranes joined along an edge, or with a triangular face in common, are named like fused ring systems; e.g., **Decaborano(14)[5′,6′:5,6]decaborane(14), Undecaborano[2′,7′,11′:1,2,3]dodecaborane(17).**

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 "-ylidyne" 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 "-ylidyne." Stibine and bismuthine may have the "-ine" ending replaced by "-ino," "-ylene," and "-ylidyne." 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_2B–	boryl	HC≡	methylidyne
H_2C=	methylene	HSi≡	silylidyne
=Sn=	stannanetetrayl	HAs=	arsinidene
H_2P–	phosphino	As≡	arsinidyne
HP=	phosphinidene	H_2Sb–	stibino
P≡	phosphinidyne	HSb=	stibylene
H_4P–	phosphoranyl	Sb≡	stibylidyne
H_3P=	phosphoranylidene	H_2Bi–	bismuthino
H_2P≡	phosphoranylidyne	HBi=	bismuthylene
H_2As–	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 "-ylidyne" to indicate two or three atoms lost at one position. (Methylene is an exception.) Locants are not cited for monovalent radicals (the free valency position is always "l"), 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_2C=$CHCH_2$–	2-propenyl (not allyl)
EtCH=	propylidene
PrC≡	butylidyne
H_2C=C=	ethenylidene
H_2C=CHCH=	2-propenylidene
MeC≡CCH_2CH=CHCH=	2-hepten-5-ynylidene
–$(CH_2)_2$–	1,2-ethanediyl
–CH_2CH=	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_2CHCH_2—	1,2,3-propanetriyl
‖ —CH_2CCH_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 (not necessarily that of the molecular skeleton) 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$(CH_2)_2$] OCH_2CH_2–	3,6,9,12-tetraoxatridec-1-yl (not [2-[2-[2-(2-methoxyethoxy)-ethoxyl]ethoxy]ethyl])
$MeSiH_2CH_2SiH_2$CH=$CHSiH_2CH_2SiH_2$CH= 10 9 7 4 2 1	2,4,7,9-tetrasiladec-5-en-1-ylidene
—CH_2CH_2[S$(CH_2)_2$]$_2$SCH=CHNHCH$_2$CH$_2$- 1 2 9 12 14	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–	diazenyl (the substituted radical is named azo)
H_2NNHNH–	triazanyl
HN=NNH–	2-triazenyl

$H_2NN{=}NN{=}N–$	1,3-pentazadienyl
$H_2PPH–$	diphosphinyl
–PHPH–	1,2-diphosphinediyl
=AsAs=	1,2-diarsinediylidene
–Sb=Sb–	1,2-distibenediyl
$H_2NNH–$	hydrazino
$H_2NN=$	hydrazono
–NHN=	1-hydrazinyl-2-ylidene
–NHNH–	hydrazo (to different atoms) hydrazi (to the same atom)
–N=N–	azo (to different atoms) azi (to the same atom)
=NN=	azino

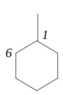
(*e*) *Heterogeneous heteroacyclic radicals* are named analogously to hydrocarbon radicals.

Examples:

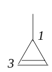
$H_3SiOSiH_2–$	disiloxanyl
$H_3SiOSiH=$	disiloxanylidene
$H_3SnOSn≡$	distannoxanylidyne
$–SiH_2NHSiH_2–$	1,3-disilazanediyl
$—SiH_2OSiHOSiH_2—$	1,3,5-trisiloxanetriyl

(*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 ("l" 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 "l") 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.

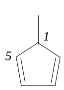
Examples:



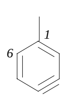
cyclohexyl



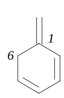
2-cyclopropen-1-yl



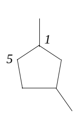
2,4-cyclopentadien-1-yl



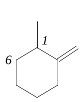
1,5-cyclohexadien-3-yn-1-yl



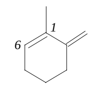
2,4-cyclohexadien-1-ylidene



1,3-cyclopentanediyl (not 1,3-cyclopentylene)



1-cyclohexanyl-2-ylidene (not 1-cyclohexyl-2-ylidene)

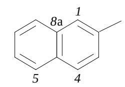


6-cyclohexen-1-yl-2-ylidene

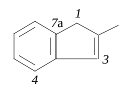
Radicals from *benzene* are named phenyl (C_6H_5-), 1,2-, 1,3-, and 1,4-phenylene (-C_6H_4-), 1,2,3-benzenetriyl, 1,2,3,4-benzenetetrayl, etc.

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.

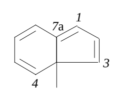
Examples:



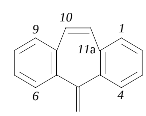
2-naphthalenyl (not 2-naphthyl)



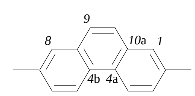
1*H*-inden-2-yl



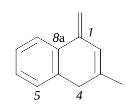
3a*H*-inden-3a-yl (a hydro derivative would be named, e.g., 2,3-dihydro-3a*H*-inden-3a-yl, not 2*H*-inden-3a(3*H*)-yl)



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



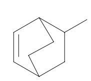
2,7-phenanthrenediyl



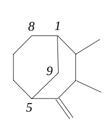
3-naphthalenyl-1(4*H*)-ylidene (not 2-naphthalenyl-4(1*H*)-ylidene)

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.

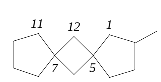
Examples:



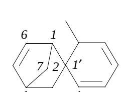
bicyclo[2.2.2]oct-5-en-2-yl (not bicyclo[2.2.2]oct-2-en-5-yl)



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



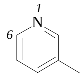
dispiro[4.1.4.1]dodec-2-yl

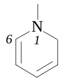


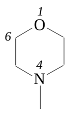
spiro[bicyclo[2.2.1]hept-5-ene-2,1′-[3,5]cyclohexadien]-2′-yl (note: lowest locants are assigned, in order, to spiro atoms, free valencies, all multiple bonds, double bonds)

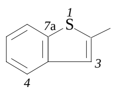
(*g*) *Heterocyclic radicals* from ring systems not named by organic replacement ("a") nomenclature are named analogously to fused-hydrocarbon radicals (above). Radicals involving free valencies at hetero atoms in abnormal valency states are not normally employed, unless the valency is expressed by indicated hydrogen (¶ 158). Instead, the compound is named at the abnormal-valency parent (see last example below). The shortened form thienyl is used for thiophene radicals and all their fused derivatives; selenophene-yl (not selenophenyl) is the name of the seleno analog.

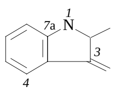
Examples:

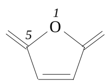

3-pyridinyl (not 3-pyridyl)

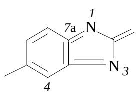

1(2*H*)-pyridinyl

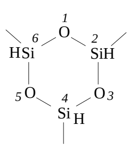

4-morpholinyl (not morpholino)

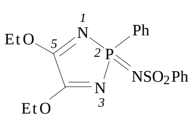

benzo[*b*]thien-2-yl (not benzo[*b*]-thiophen-2-yl)


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


2,5-furandiylidene

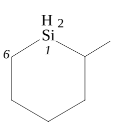

2*H*-benzimidazol-5-yl-2-ylidene

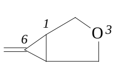

cyclotrisiloxane-2,4,6-triyl


2*H*-1,3,2-Diazaphosphole, 4,5-diethoxy-2,2-dihydro-2-phenyl-2-[(phenylsulfonyl)imino]- (not Benzenesulfonamide, *N*-(4,5-diethoxy-2-phenyl-2*H*-1,3,2-diazaphosphol-2(2*H*)-ylidene)-)

"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).

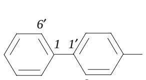
Examples:

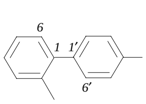

silacyclohex-2-yl (not 2-silacyclohexyl)

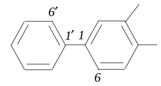

3-oxabicyclo[3.1.0]hex-6-ylidene

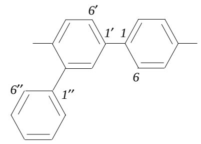
(*h*) *Ring-assembly radicals* are derived by bracketing the assembly name, eliding a final "e" if "y" is to follow, and appending the radical endings "-yl," "-ylidene," "-diyl," etc., as appropriate. The free valencies need not be on the terminal rings of the assembly.

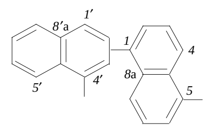
Examples:

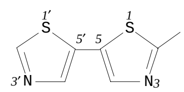

[1,1′-biphenyl]-4-yl (not 4-biphenylyl)

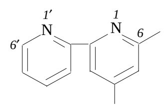

[1,1′-biphenyl]-2,4′-diyl (not 2,4′-biphenylylene)

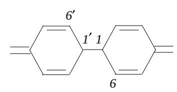

[1,1′-biphenyl]-3,4-diyl (not (4-phenyl-1,2-phenylene))


[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-dicarbadodecaboran(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).

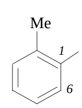
Examples:

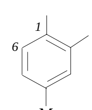
Me_2CH–	(1-methylethyl)
H_2C=CMe–	(1-methylethenyl) (the unsaturated parent radical is preferred)

$$\underset{11}{CH_3}-\underset{10}{CH}=\underset{9}{CH}-\underset{8}{CH}=\underset{7}{CH}-\underset{6}{\overset{\overset{CH=CH-C\equiv C-CH_3}{|}}{CH}}-\underset{5}{CH}=\underset{4}{CH}-\underset{3}{CH}=\underset{2}{CH}-\underset{1}{CH_2}-$$

[6-(1-penten-3-ynyl)-2,4,7,9-undecatetraenyl]

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:

(*a*) longest chain of rings containing all of the free valencies, which need not be on terminal rings;

(*b*) lowest locants in the radical name for (1) ring junctions, and (2) free valencies;

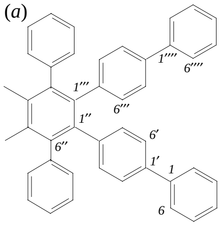
(*c*) maximum number of substituent prefixes;

(*d*) lowest locants for substituent prefixes;

(*e*) earliest index position of the radical name.

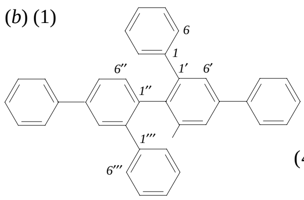
Examples (the letters on the left refer to the principles above):

(*a*)



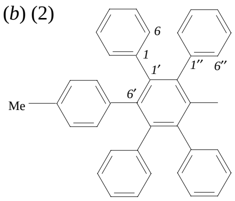
(3″,6″-diphenyl[1,1′:4′,1″:2″,1‴:-4‴,1⁗-quinquephenyl]-4″,-5″-diyl)

(*b*) (1)



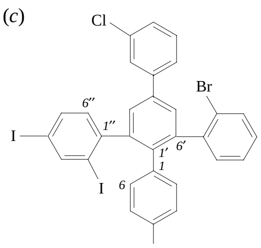
(4″,5′-diphenyl[1,1′:2′,1″:2″,1‴-quaterphenyl]-3′-yl)

(*b*) (2)

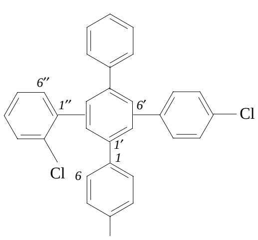


[6′-(4-methylphenyl)-4′,5′-diphenyl-[1,1′:2′,1″-terphenyl]-3′-yl]

(*c*)

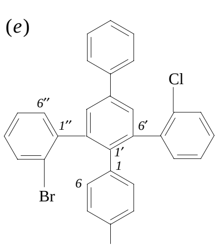


[6′-(2-bromophenyl)-4-(3-chloro-phenyl)-2″,4″-diiodo[1,1′:2′,1″-terphenyl]-4-yl]



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

(*e*)



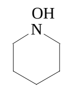
[2″-bromo-6′-(2–chlorophenyl)-4′-phenyl[1,1′:2′,1″-terphenyl]-4-yl](not [6′-(2–bromophenyl)-2″-chloro-4′-phenyl[1,1′:2′,1″-ter-phenyl]-4-yl])

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:

$H_3C–CH_3$ **Ethane**

$PhNO_2$ **Benzene, nitro**- ("nitro" is a mandatory prefix (¶ 132))

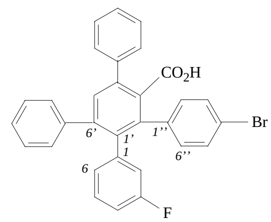


Piperidine, 1-hydroxy- ("hydroxy" is considered nonfunctional when attached to a hetero atom other than silicon)

$Me_3SiCOMe$ **Silane, acetyltrimethyl**- (not Ethanone,1-(trimethylsilyl)-: an acyclic ketone function is not recognized unless it has two carbonlinkages)

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-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 patent fullerene. Incompletely described fullerenes, i.e., where ring sizes and/or point group symmetries are not know 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-)-C_{60}-I_h

[5,6]Fullerene-C_{60}-I_h
ion(1+)

[5,6]Fulleren-C_{60}-I_h-1(2*H*)-ylium

[5,6}Fulleren-C_{60}-I_h-1(2*H*)-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-C_{60}-I_h
compd. with potassium (1:1), ion(1+)

[2] *Science* **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.

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-C_{60}-I_h.**

Fullerenes containing substituents require that hydrogen be added before the substituents can be named.[5] For example, $C_{60}F_{60}$ is named **[5,6]Fullerane-C_{60}-I_h, hexacontafluoro**- (the hydrogen being part of the parent name). $C_{60}Br_2$ is named as a dibromodihydrofullerene, and $C_{60}H_6Ph_6$ is named as a dodecahydrohexaphenylfullerene.

Addition of hydrogen is not necessary when a fullerene contains two functional groups, as in **[5,6]Fullerene-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-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]fulleren-C_{60}-I_h-2- yl.**[5]

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[5]International 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)

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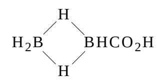
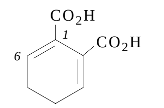
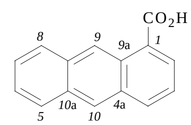
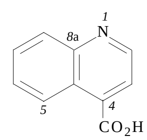
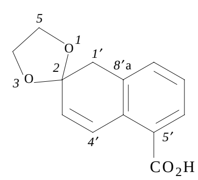
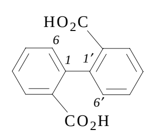
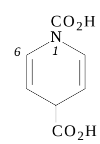
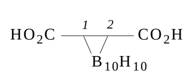
164. Introduction. In substitutive nomenclature, a principal chemical group is that substituent of a molecular skeleton which is selected for expression as a suffix. Only one kind of substituent may be cited as a suffix, viz., the most senior one as determined by the Order of Precedence of Compound Classes (¶ 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 **Carbonic 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 heteroacyclic 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.)

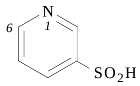
Examples:

$MeCH_2CO_2H$	**Propanoic acid** (not Propionic acid)
$\underset{5}{M}e(CH_2)_3\underset{1}{C}O_2H$	**Pentanoic acid** (not Valeric acid)
$H_2\underset{3}{C}{=}CH\underset{1}{C}O_2H$	**2-Propenoic acid** (not Acrylic acid)
$\underset{18}{M}e(CH_2)_4\underset{13}{C}H{=}CHCH_2CH{=}\underset{9}{C}H(CH_2)_7\underset{1}{C}O_2H$	**9,12-Octadecadienoic acid**
$HO_2\underset{1}{C}\underset{2}{C}O_2H$	**Ethanedioic acid** (not Oxalic acid)
$HO_2\underset{1}{C}(CH_2)_3\underset{5}{C}O_2H$	**Pentanedioic acid** (not Glutaric acid)
$H_3\underset{1}{C}{-}\underset{2}{C}H_2{-}\underset{3}{O}{-}\underset{4}{C}H_2{-}\underset{5}{C}H_2{-}\underset{6}{O}{-}\underset{7}{C}H_2{-}\underset{8}{C}H_2{-}\underset{9}{O}{-}\underset{10}{C}H_2{-}\underset{11}{C}H_2{-}\underset{12}{O}{-}\underset{13}{C}H_2{-}\underset{14}{C}H{=}\underset{15}{C}H{-}(CH_2)_7{-}\underset{23}{C}OOH$	**3,6,9,12-Tetraoxatricos-14-en-23-oic acid** (The hetero atoms are given preference for lowest locants; the locant for the “-oic acid” suffix is cited if it is not “1.”)
$HOO\underset{1}{C}{-}\underset{2}{C}H_2{-}\underset{3}{C}H(COOH){-}CH_2{-}COOH$	**1,2,3-Propanetricarboxylic acid** (numbering excludes the carboxyl groups)
$(HO_2C)_2C{=}C(CO_2H)_2$	**Ethenetetracarboxylic acid**
$HO_2C\underset{1}{N}H\underset{2}{N}HCO_2H$	**1,2-Hydrazinedicarboxylic acid** (not Bicarbamic acid)
H_2PCO_2H	**Phosphinecarboxylic acid** (not Formic acid, phosphino-)
$HO_2CSnH_2OSnH_2CO_2H$ (locants 1, 2, 3)	**1,3-Distannoxanedicarboxylic acid**
	**Diborane(6)carboxylic acid**
	**2,6-Cyclohexadiene-1,2-dicarboxylic acid** (lowest locants for principal groups are preferred)
	**1-Anthracenecarboxylic acid**
	**4-Quinolinecarboxylic acid**
	**Spiro[1,3-dioxolane-2,2′(1′H)-naphthalene]-5′-carboxylic acid**
	**[1,1′-Biphenyl]-2,2′-dicarboxylic acid**
	**1,4(4*H*)-Pyridinedicarboxylic acid** (the added hydrogen is expressed after the final locant but relates to the 1-carboxyl group; see ¶ 136)
	**1,2-Dicarbadodecaborane(12)-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:

$EtSO_3H$	**Ethanesulfonic acid**
$\underset{5}{C}H_3{-}\underset{4}{C}H_2{-}\underset{3}{C}H_2{-}\underset{2}{C}H(SO_3H){-}\underset{1}{C}H_3$	**2-Pentanesulfonic acid**

$PhSO_3H$	**Benzenesulfonic acid**
	**3-Pyridinesulfinic acid**
MeSOH	**Methanesulfenic acid**
$H_2NN{=}NSO_3H$ (3 2 1)	**1-Triazene-1-sulfonic acid**
H_2NNHSO_2H	**Hydrazinesulfinic acid**
$CH_3-CH_2-O-CH_2-CH_2-O-CH_2-CH_2-O-CH_2-CH_2-O-CH_2-CH(SO_3H)-CH_3$ (1 2 3 4 5 6 7 8 9 10 11 12 13 14 15)	**3,6,9,12-Tetraoxapentadecane-14-sulfonic acid** (hetero atoms are preferred over principal groups for lowest locants)
H_2PSO_3H	**Phosphinesulfonic acid**
$PhSeO_3H$	**Benzeneselenonic acid**
$CH_3-CH_2-CH_2-CH_2-CH(SeO_2H)-CH_3$ (6 5 4 3 2 1)	**2-Hexaneseleninic acid**
$CH_3-CH_2-CH(TeO_2H)-CH_3$ (4 3 2 1)	**2-Butanetellurinic acid**
PhTeOH	**Benzenetellurenic acid**

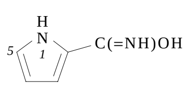
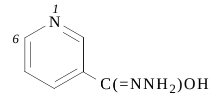
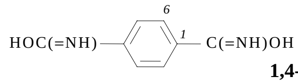
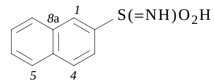
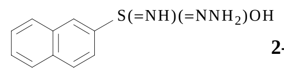
(*c*) *Imidic and hydrazonic acids.* Names for these are formed from the parent carboxylic, sulfonic, sulfinic, selenonic, etc., acid names by functional replacement nomenclature (¶ 129). Some modification of the formal endings is made; thus, an "-oic acid" becomes an "imidic acid", not an "-imidoic acid". **Acetic acid** affords systematically named Ethanoic acid replacement analogs, while **Benzoic acid** is treated as Benzenecarboxylic acid in a similar manner. The suffixes appended to the molecular skeleton name in each case are as follows:

Parent Acid	*Imidic acid*	*Hydrazonic acid*
-oic	-imidic	-hydrazonic
-carboxylic	-carboximidic	-carbohydrazonic
-sulfonic	-sulfonimidic	-sulfonohydrazonic
-sulfinic	-sulfinimidic	-sulfinohydrazonic

The group -S(:NH)$_2$OH is named by the suffix "-sulfonodiimidic acid," and -S(:NH)(:NNH$_2$)OH by "-sulfonohydrazonimidic acid." Selenium and tellurium acids are named analogously.

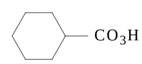
Note: Imidic acids are tautomeric with amides; except for derivatives in which an acid proton has been replaced, e.g., esters and anhydrides, amides are preferred for index entries; see ¶ 122. Hydrazonic acids are tautomeric with hydrazides, which are preferred as index entries.

Examples:

MeC(=NH)OH	**Ethanimidic acid** (not Acetimidic acid)
PhC(=NH)OH	**Benzenecarboximidic acid** (not Benzimidic acid)
$Me(CH_2)_4C(=NH)OH$ (6 1)	**Hexanimidic acid**
	**1*H*-Pyrrole-2-carboximidic acid**
$HOC(=NH)(CH_2)_4C(=NH)OH$	**Hexanediimidic acid**
$H_2NNHC(=NH)OH$	**Hydrazinecarboximidic acid**
$MeC(=NNH_2)OH$	**Ethanehydrazonic acid**
	**3-Pyridinecarbohydrazonic acid**
	**1,4-Benzenedicarboximidic acid**
	**2-Naphthalenesulfonimidic acid**
$EtS(=NH)_2OH$	**Ethanesulfonodiimidic acid**
	**2-Naphthalenesulfonohydrazonimidic acid**
EtS(=NH)OH	**Ethanesulfinimidic acid**
$PhSe(=NH)O_2H$	**Benzeneselenonimidic acid**

(*d*) *Peroxy acids* are named by use of the suffixes "-peroxoic acid" (from "-oic acid") and "-carboperoxoic acid" (from "-carboxylic acid"). **Acetic acid** and **Benzoic acid** afford systematically named peroxy acids. Sulfonic, sulfinic, and sulfenic acids and their selenium and tellurium analogs are named by use of the suffixes "-sulfonoperoxoic acid", etc. Combinations with imidic and hydrazonic suffixes are made, in alphabetic order, by the normal rules.

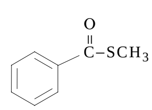
Examples:

$CH_3-C(=O)-OOH$	**Ethaneperoxoic acid** (not Peroxyacetic acid)
	**Cyclohexanecarboperoxoic acid**
$HO_3C(CH_2)_2CO_3H$	**Butanediperoxoic acid**
MeC(=NH)OOH	**Ethanimidoperoxoic acid** (not Peroxyacetimidic acid)
PhC(=NH)OOH	**Benzenecarboximidoperoxoic acid** (not Peroxybenzimidic acid)

Peroxy analogs of acids expressed as heading parents, e.g., **Carbonoperoxoic acid** (¶ 183), **Phosphoroperoxoic acid** (¶ 197), are ranked with the acids, e.g., **Carbonic acid**, **Phosphoric acid**, from which they are derived.

(*e*) *Thio acids* derived from carboxylic, sulfonic, sulfinic, and sulfenic acids and their imidic, hydrazonic, and peroxy replacement analogs are named by incorporating "thio" (or "dithio") into the suffixes of the oxygenated acid names. The terms "seleno" and "telluro" are used similarly when appropriate. Selenonic, telluronic, etc., acids are handled like sulfonic acids. The names do not distinguish between replacement of oxygen in =O and -OH groups in the unesterified acids. This information is usually given in the ester name, or by a substituent prefix.

Examples:

	**Benzenecarbothioic acid, *S*-methyl ester**
$CH_3CH_2O-C(=S)CH_2CH_2C(=O)-OH$ (4 3 2 1)	**Butanoic acid, 4-ethoxy-4-thioxo-** (for order of precedence of acid groups, see ¶ 167)

When a specific name for a single form is imperative, an italicized element symbol is used in the heading parent, e.g., **Ethanethioic *O*-acid** for $CH_3C(S)$-OH.

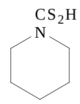
Replacement by two sulfur atoms in a monocarboxylic acid named by the suffix "-oic acid" is denoted by the suffix "-(dithioic) acid" and by one sulfur atom in each of the two groups in a "-dioic acid" by "-bis(thioic) acid." Ambiguity is absent from "-carboxylic" names, and parentheses are therefore not employed for the analogous "-carbodithioic acid" and "-dicarbothioic acid" suffixes.

Examples:

$Me(CH_2)_2COSH$ — **Butanethioic acid**

$H_2C{=}CHCS_2H$ (3, 1) — **2-Propene(dithioic) acid**

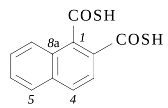
PhCOSH — **Benzenecarbothioic acid** (not Benzoic acid, thio-)



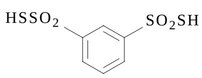
1-Piperidinecarbodithioic acid

$HOSCCH_2COSH$ — **Propanebis(thioic) acid**

$HS_2CCH_2CH{=}CHCH_2CS_2H$ (1, 6) — **3-Hexenebis(dithioic) acid**



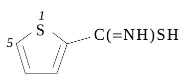
1,2-Naphthalenedicarbothioic acid



1,3-Benzenedisulfonothioic acid

MeCH[S(S)SH]Me (1 2 3) — **2-Propanesulfinodithioic acid**

MeSSH — **Methanesulfenothioic acid**



2-Thiophenecarboximidothioic acid

EtS(=NH)OSH — **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:

$HOSCCH_2CH_2CO_2H$ — **Propanoic acid, 3-(thiocarboxy)-**

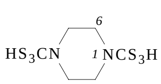
$EtOSCCO_2H$ — **Acetic acid, ethoxythioxo-**

Thio peroxy acids are named by similar principles; the replacement affixes "(thioperoxo)" and "(dithioperoxo)" 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:

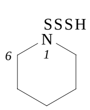
MeCOSSH — **Ethane(dithioperoxoic) acid**

PhC(=NH)OSH — **Benzenecarboximido(thioperoxoic) acid**



1,4-Piperazinedicarbo(dithioperoxo)thioic acid

$PhSO_2SSH$ — **Benzenesulfono(dithioperoxoic) acid**



1-Piperidinesulfeno(dithioperoxic) acid

MeCHMeSSOH (1 2) — **2-Propanesulfeno(thioperoxoic) acid**

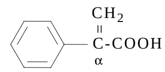
MeCSeOH — **Ethaneselenoic acid**

PhCSeSH — **Benzenecarboselenothioic acid**

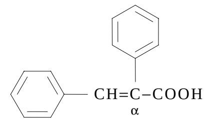
166. Acyclic acids with cyclic substituents may usually be named by conjunctive nomenclature (¶ 124).

Examples:

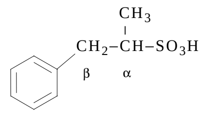
$PhCH_2CH_2CO_2H$ (β α) — **Benzenepropanoic acid** (not Hydrocinnamic acid)



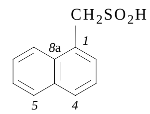
Benzeneacetic acid, α-methylene- (not Atropic acid)



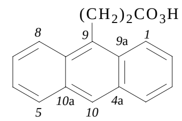
Benzeneacetic acid, α-(phenylmethylene)- (not Benzene-2-propenoic acid, α-phenyl-; conjunctive nomenclature is not used with unsaturated acyclic acids (¶ 124))



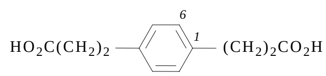
Benzeneethanesulfonic acid, α-methyl-



1-Naphthalenemethanesulfinic acid



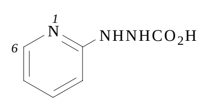
9-Anthracenepropaneperoxoic acid



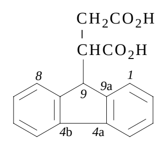
1,4-Benzenedipropanoic acid

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:



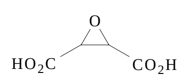
Hydrazinecarboxylic acid, 2-(2-pyridinyl)-



Butanedioic acid, 9*H*-fluoren-9-yl-

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

Example:



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

167. Order of precedence of acids. Acid suffixes are the most preferred of all non-cationic substituent suffixes as principal groups (¶ 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*).

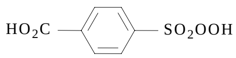
(*f*) *Sulfinic acids*, likewise.

(*g*) *Sulfenic acids*, likewise.

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

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

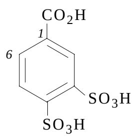
Examples:



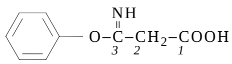
Benzenesulfonoperoxoic acid, 4-carboxy-

$HO-\underset{1}{\overset{S}{\overset{\|}{C}}}-\underset{2}{CH_2}-\underset{3}{CH_2}-\underset{4}{\overset{S}{\overset{\|}{C}}}-SH$

Propanethioic acid, 3-(dithiocarboxy)-



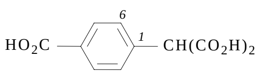
Benzoic acid, 3,4-disulfo-



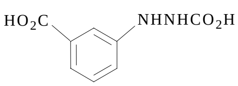
Propanoic acid, 3-imino-3-phenoxy-

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).

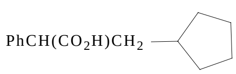
Examples:



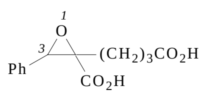
Propanedioic acid, (4-carboxyphenyl)- (principle: maximum number of the principal group)



Hydrazinecarboxylic acid, 2-(3-carboxyphenyl)- (principle: hetero acyclic parent preferred)



Benzeneacetic acid, α-(cyclopentylmethyl)- (principle: preferred ring system)



Oxiranebutanoic acid, 2-carboxy-3-phenyl- (principle: largest heading parent)

$\underset{3}{F_3C}-\underset{\underset{CF_3}{|}}{\overset{\overset{CH_3}{|}}{C}}{}_{2}-\underset{1}{COOH}$

Propanoic acid, 3,3,3-trifluoro-2-methyl-2-(trifluoromethyl)- principle: maximum number of substituent prefixes)

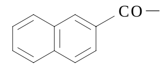
Aldehydic, amic, anilic, hydroxamic, hydroximic, nitrolic, and nitrosolic acids are indexed as compounds of mixed function (see ¶ 228). So are trivially named hydroxy and oxo acids, e.g., Glycolic acid, Acetoacetic acid, and amino acids, e.g., Sulfanilic acid, other than those which are of biological 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 (CH_3CO-) and benzoyl (C_6H_5CO-). Amino acid radicals, e.g., glycyl, L-alanyl, are restricted to use in peptide and depsipeptide names (¶ 206).

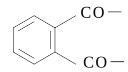
Radicals derived from monocarboxylic acids are in general named as (1-oxoalkyl) or (arylcarbonyl); carboximidic acids afford (1-iminoalkyl) and (aryliminomethyl) radicals; carbothioic acids give (1-thioxoalkyl) and (arylthioxomethyl) radicals (carbonimidoyl and carbonothioyl are used only as multiplicative 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:

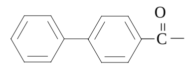
EtCO—	(1-oxopropyl)
MeCS—	(1-thioxoethyl)(not thioacetyl)
HN=CH—	(iminomethyl)(not formimidoyl)
—COCOCO—	(1,2,3-trioxo-1,3-propanediyl)
$HO_2C(CH_2)_2CO$—	(3-carboxy-1-oxopropyl)
HOC(=NH)C(=NH)—	(2-hydroxy-1,2-diiminoethyl)



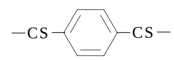
(2-naphthalenylcarbonyl)



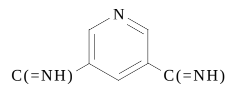
(1,2-phenylenedicarbonyl)



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



(1,4-phenylenedicarbonothioyl)



(3,5-pyridinediyldicarbonimidoyl)

$PhSO_2$—	(phenylsulfonyl)
PhSO—	(phenylsulfinyl)
PhS(=NH)—	(*S*-phenylsulfinimidoyl)
PhS—	(phenylthio)

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):NNH_2) (¶ 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:

$MeC(OH)_3$	**1,1,1-Ethanetriol** (not Orthoacetic acid)
$MeC(OMe)_2OH$	**Ethanol, 1,1-dimethoxy-**

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, -N_3, 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
-sulfonimidic	-sulfonimidoyl

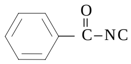
Examples:

$Me(CH_2)_3CONCS$ **Pentanoyl isothiocyanate**

$\underset{14}{CH_3}-\underset{13}{CH_2}-\underset{12}{O}-\underset{11}{CH_2}-\underset{10}{CH_2}-\underset{9}{O}-\underset{8}{CH_2}-\underset{7}{CH_2}-\underset{6}{O}-\underset{5}{CH_2}-\underset{4}{CH_2}-\underset{3}{O}-\underset{2}{CH_2}-\underset{1}{\overset{O}{\overset{\|}{C}}}-F$

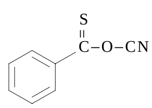
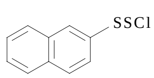
3,6,9,12-Tetraoxatetradecanoyl fluoride

$H_2NNHCOCl$ **Hydrazinecarbonyl chloride**

	**Benzoyl isocyanide**
PhC(=NH)Br	**Benzenecarboximidoyl bromide**
PhCSCl	**Benzenecarbothioyl chloride**
$CH_3{-}CH_2{-}CH_2{-}CH_2{-}SO_2{-}NCO$	**1-Butanesulfonyl isocyanate**
PhS(O)(=NH)Cl	**Benzenesulfonimidoyl chloride**
$ClCO(CH_2)_2COCl$	**Butanedioyl dichloride** (not Butanedioyl chloride)
$OCNSO_2CH_2(CH_2)_4CH_2SO_2NCO$	**1,6-Hexanedisulfonyl diisocyanate**
$PhCH_2CH_2CON_3$	**Benzenepropanoyl azide**

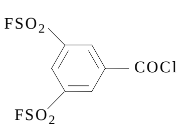
Halides, etc., of peroxy acids are generally indexed as anhydrides, anhydrosulfides, etc., with halogen or halogenoid "oxo" acids such as **Hypochlorous** or **Thiocyanic acid**. Halides, etc., of (thioperoxy)sulfenic acids are indexed at **Disulfide.**

Examples:

ClCOSCl	**Carbonochloridothioic acid, anhydrosulfide with thiohypochlorous acid**
	**Benzenecarbothioic acid, anhydride with cyanic acid**
	**Disulfide, chloro 2-naphthalenyl**

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, $-N_3$, -NCO, -NCS, -NCSe, -NCTe, -NC, -CN.

Examples:

	**Benzoyl chloride, 3,5-bis(fluorosulfonyl)-**
$FCO(CH_2)_2COI$	**Butanoyl fluoride, 4-iodo-4-oxo-**

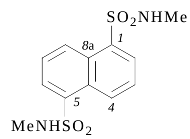
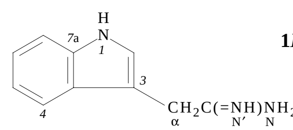
Functional derivatives of acid chlorides are indexed similarly to those of the parent acids (¶ 169).

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.

Examples:

$MeCONH_2$	**Acetamide**
$HN{=}NHCONH_2$	**Diazenecarboxamide**
$MeCSNH_2$	**Ethanethioamide**
$H_2NCS(CH_2)_4CSNH2$	**Hexanedithioamide**
$H_2NC(=NH)CH_2C(=NH)NH_2$	**Propanediimidamide**
$PhC(=NNH_2)NH_2$	**Benzenecarbohydrazonamide**
$MeS(=NH)_2NH_2$	**Methanesulfonodiimidamide**
	**1,5-Naphthalenedisulfonamide, *N,N′*-dimethyl-**
PhCSNHPh	**Benzenecarbothioamide, *N*-phenyl-**
	**1*H*-Indole-3-ethanimidamide**
MeCONHCOMe	**Acetamide, *N*-acetyl-** (not Diacetamide)
$PhSO_2NHSO_2Ph$	**Benzenesulfonamide, *N*-(phenylsulfonyl)-** (not Dibenzenesulfonamide)

Amides of peroxy acids and thio peroxy acids are indexed as *O*-acyl derivatives of **Hydroxylamine** and **Thiohydroxylamine** (¶ 193).

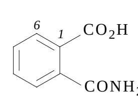
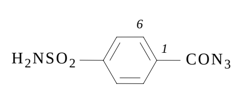
Amide radicals are named as compound or complex radicals based on "amino" or "imino," with acid radicals (¶ 168) as substituents.

Examples:

AcNH—	(acetylamino)(not acetamido)
BzN=	(benzoylimino)
$Me(CH_2)_4CONH$—	[(1-oxohexyl)amino](not hexanamido)
$PhSO_2NH$—	[(phenylsulfonyl)amino](not benzenesulfonamido)
PhC(=NH)NH—	[(iminophenylmethyl)amino]

The radicals above are employed as substituents when a more preferred amide or a higher function, e.g., an acid or acid chloride, is present in part of the molecule attached to the amide by way of the nitrogen atom. Other attachments call for use of amino and oxo, or (aminocarbonyl), (aminosulfonyl), etc., radicals.

Examples:

$H_2NCO(CH_2)_2CO_2H$	**Butanoic acid, 4-amino-4-oxo-**
	**Benzoic acid, 2-(aminocarbonyl)-**
	**Benzoyl azide, 4-(aminosulfonyl)-**

$H_2NCSCH_2CONHMe$ (3, 1, N)	**Propanamide, 3-amino-*N*-methyl-3-thioxo-**
$AcNHSO_2Ph$	**Acetamide, *N*-(phenylsulfonyl)-**

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

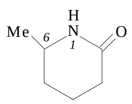
Example:

$H_2NCOCH_2CONH(CH_2)_2NHCOCH_2CONH(CH_2)_2NHCOCH_2CONH_2$ (1, 4, 7, 11, 14, 17)

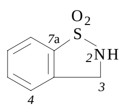
4,7,11,14-Tetraazaheptadecanediamide, 3,8,10,15-tetraoxo-

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.

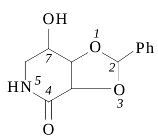
Examples:



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



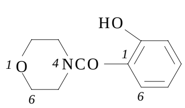
1,2-Benzisothiazole, 2,3-dihydro-1,1-dioxide (ranked as a non-functional cyclic nitrogen skeleton)



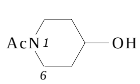
1,3-Dioxolo[4,5-*c*]pyridin-4(3*aH*)-one, tetrahydro-7-hydroxy-2-phenyl-

Amides of which only the nitrogen atom forms part of a ring system are indexed as *N*-acyl derivatives at the ring name. They are regarded as “unexpressed amides” and rank just below an “expressed amide” *of the same type of acid*. Lower functions are disregarded unless they can be expressed as suffixes at the name of the ring of which the amide nitrogen is part. Residues of formic acid, carbonic acid and related compounds are expressed at the nitrogen heterocycle by such suffixes as “-carboxaldehyde,” “-carboxylic acid,” “carboxamide,” etc., and the compounds are ranked accordingly.

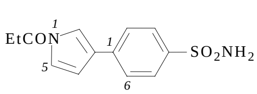
Examples:



Morpholine, 4-(2-hydroxybenzoyl)-



4-Piperidinol, 1-acetyl-



1*H*-Pyrrole, 3-[4-(aminosulfonyl)phenyl]-1-(1-oxopropyl)-(unexpressed carboxamide is favored over expressed sulfonamide)

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

Example:

$H_2NCH_2CONH_2$	**Acetamide, 2-amino-** (not Glycinamide)

Oximes of amides (amidoximes) ($R-C(:NOH)NH_2$) are tautomeric with *N*-hydroxy carboximidamides (R-C(:NH)NHOH) and are indexed at imidamide names:

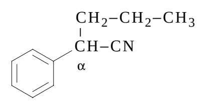
Example:

$Me(CH_2)_4C(=NH)NHOH$	**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 ($RC{\equiv}\overset{+}{N}{-}\overset{-}{N}{-}R'$) are named as substituted hydrazinium hydroxide inner salts (¶¶ 201, 267).

Examples:

MeCN	**Acetonitrile**
HC≡CCH=CHCN (5, 1)	**2-Penten-4-ynenitrile**
NCCN	**Ethanedinitrile** (not Cyanogen)
H_3GeCN	**Germanecarbonitrile**
H_2NNHCN	**Hydrazinecarbonitrile**
$(NC)_2C=C(CN)_2$	**Ethenetetracarbonitrile**
PhCN	**Benzonitrile**

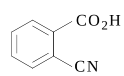


Benzeneacetonitrile, α-propyl-

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

Examples:

$NCCH_2CONH_2$ (2, 1)	**Acetamide, 2-cyano-** (not Propanamide, 3-nitrilo-)
MeCH(CN)COCl	**Propanoyl chloride, 2-cyano-**

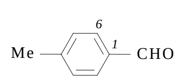


Benzoic acid, 2-cyano-

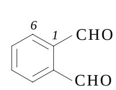
173. Aldehydes, RCHO, are named from “-carboxylic” and “-oic” acids by use of “-carboxaldehyde” and “-al” suffixes, respectively.

Examples:

AcH(MeCHO)	**Acetaldehyde**
MeCH=CHCHO	**2-Butenal**
$HCOCH_2CH=CHC{\equiv}CCH_2CHO$ (1, 3, 5, 8)	**3-Octen-5-ynedial**
$H_2P(O)CHO$	**Phosphinecarboxaldehyde oxide**



Benzaldehyde, 4-methyl-



1,2-Benzenedicarboxaldehyde

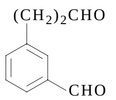
$PhCH_2CHO$	**Benzeneacetaldehyde**

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

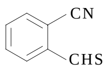
In the presence of more highly ranked compound classes (¶ 106) or more preferred aldehydes, the -CHO group is expressed by formyl (if it does not form part of an acyclic carbon chain) or by a terminal oxo radical. For thio aldehydes, the equivalent radicals are (thioxomethyl) and a terminal thioxo radical.

Examples:

$HCOCH_2CO_2H$	**Propanoic acid, 3-oxo-**



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



Benzonitrile, 2-(thioxomethyl)-

$TeCH(CH_2)_2CHS$ — **Butanethial, 4-telluroxo-**

Substitution of the aldehydic hydrogen atom by radicals derived from molecular skeletons is avoided; but radicals such as nitro and nitroso (or, for Formaldehyde and its chalcogen analogs only, a single sulfonyl or sulfinyl) are permitted.

Examples:

MeC(=NOH)NO — **Acetaldehyde, 1-nitroso-**
oxime (not Acetonitrosolic acid)

$BzNO_2$ — **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 -SeO_2- and -TeO_2-, respectively.) In acyclic ketones the group must generally be in a nonterminal position of a carbon or "a"-named chain and have two carbon attachments. Ketenes, in which a terminal unsaturated carbon bears a chalcogen atom, are exceptions; they are named by use of the same suffixes as ketones. 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 (attached at carbon atoms) consists only of a single carbon atom with a chalcogen attached, the heading parents **Methanone, Methanethione, Methaneselone** and **Methanetellone** are employed.

Examples:

MeCOMe (1 2 3) — **2-Propanone** (not Acetone)

$MeCH_2OSiH_2(CH_2)_2CO(CH_2)_2SiH_2OCH_2Me$ (1, 3 4, 7, 10, 11, 13)

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

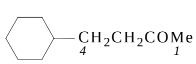
$MeCOCH_2COCH{=}CH_2$ (1, 6) — **5-Hexene-2,4-dione** (not 1-Hexene-3,5-dione)

$H_2C{=}C{=}O$ — **Ethenone** (not Ketene)

$Me(CH_2)_3CH{=}C{=}O$ (6, 1) — **1-Hexen-1-one**

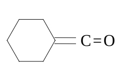
$MeCSeCH_2Me$ (1, 4) — **2-Butaneselone**

$MeCOCH_2CSCH_2Me$ (1, 6) — **2-Hexanone, 4-thioxo-** (not 2,4-Hexanedione, 4-thio-)



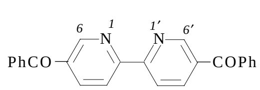
2-Butanone, 4-cyclohexyl-

$PhCO(CH_2)_4Me$ — **1-Hexanone, 1-phenyl-** (not Hexanal, 1-phenyl-)

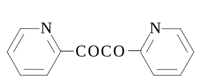


Methanone, cyclohexylidene-

Ph_2CO — **Methanone, diphenyl-** (not Benzophenone)



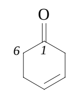
Methanone, [2,2′-bipyridine]-5,5′-diylbis[phenyl- (a multiplicative name (¶ 125))



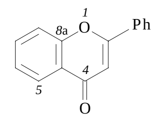
Ethanedione, di-2-pyridinyl-

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.

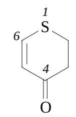
Examples:



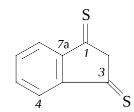
3-Cyclohexen-1-one



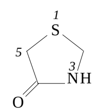
4*H*-1-Benzopyran-4-one, 2-phenyl- (not flavone)



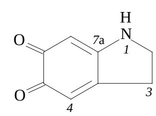
4*H*-Thiopyran-4-one, 2,3-dihydro- (not 2*H*-Thiopyran-4(3*H*)-one)



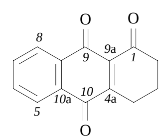
1*H*-Indene-1,3(2*H*)-dithione



4-Thiazolidinone



1*H*-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)

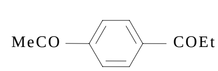


1,9,10(2*H*)-Anthracenetrione, 3,4-dihydro- (the added hydrogen is cited in the lowest-numbered available position)

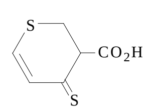
In the presence of higher functions or more preferred ketones, oxo, thioxo, selenoxo, and telluroxo radicals, are used. The =CO group, when not part of an acyclic chain or a ring, is expressed as carbonyl; the chalcogen analogs (carbonothioyl, carbonoselenoyl, and carbonotelluroyl) are used when they 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:

$MeCOCH_2COBr$ — **Butanoyl bromide, 3-oxo-** (not Acetyl bromide, acetyl-)

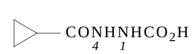


1-Propanone, 1-(4-acetylphenyl)-

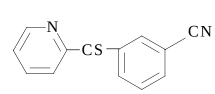


2*H*-Thiopyran-3-carboxylic acid, 3,4-dihydro-4-thioxo-

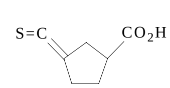
$HCOCH_2COCO_2H$ (4, 1) — **Butanoic acid, 2,4-dioxo-** (not Propanoic acid, 3-formyl-2-oxo-)



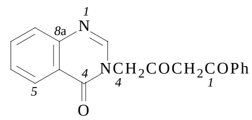
Hydrazinecarboxylic acid, 2-(cyclopropylcarbonyl)-



Benzonitrile, 3-(2-pyridinylthioxomethyl)- (not Benzonitrile, 3-(2-pyridinylcarbonothioyl)-)



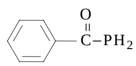
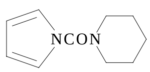
Cyclopentanecarboxylic acid, 3-carbonothioyl-



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

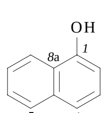
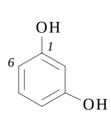
Carbonyl groups and their chalcogen analogs in heterocycles are named and ranked as ketones, thiones, etc., even when a neighboring ring atom is not carbon (see above), but acyclic carbonyl (etc.) groups attached to cyclic or acyclic hetero atoms (including silicon) are not recognized as ketones, and the functionality of the group is disregarded. It is expressed, not as a suffix, but as an appropriate substituent prefix (acetyl, oxo, carbonyl, (thioxomethyl), etc.) of a heading parent.

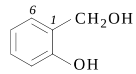
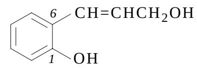
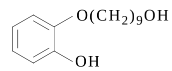
Examples:

AcN=NNH	**1-Triazene, 1-acetyl-** (not Ethanone,1-(1-triazenyl)-)
	**Phosphine, benzoyl-**
	**Piperidine, 1-(1*H*-pyrrol-1-ylcarbonyl)-** (an unexpressed amide (¶ 171))
$EtCOSiH_2OH$	**Silanol, (1-oxopropyl)-**
$H_2P(S)CSPh$	**Phosphine sulfide, (phenylthioxomethyl)-**

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 compond 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.

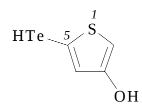
Examples:

EtOH	**Ethanol** (not Ethyl alcohol)
$H_2C{=}CHCH_2OH$	**2-Propen-1-ol** (not Allyl alcohol)
MeCH(OH)Me	**2-Propanol** (not Isopropyl alcohol)
$H_2C{=}CHCH_2CH(SH)CH_2Me$	**5-Hexene-3-thiol**
$MeSiH_2OH$	**Silanol, methyl-**
$Me(CH_2)_2CH_2TeH$	**1-Butanetellurol**
CH_2-$(CH_2)_{11}$-S-CH_2-CH_2-O-CH_2-CH_2-O-CH_2-CH_2-O-CH_2-CH_2-OH	**3,6,9-Trioxa-12-thiatetracosan-1-ol**
PhSeH	**Benzeneselenol**
	**1-Naphthalenol** (not 1-Naphthol)
CH_3-CH(SH)-CH(SH)-CH_3	**2,3-Butanedithiol**
HO-SiH_2-SiH_2-OH	**1,2-Disilanediol**
	**1,3-Benzenediol**

	**Benzenemethanol, 2-hydroxy-** (not Phenol, 2-(hydroxymethyl)-) (principle: largest parent)
	**Phenol, 2-(3-hydroxy-1-propenyl)-** (not 2-Propen-1-ol, 3-(2-hydroxyphenyl)-)
	**Phenol, 2-[(9-hydroxynonyl)oxy]-** (principle: a cyclic parent is preferred (¶ 138))
$HSCH_2CH_2OH$	**Ethanol, 2-mercapto-**

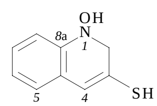
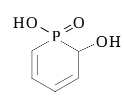
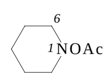
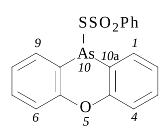
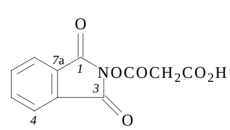
Hydroxy derivatives of thiophene, selenophene, and tellurophene are indexed at **Thiophene-ol,** etc., (the final "e" of the parents being left unelided to avoid confusion with chalcogen analogs of **Phenol**). The locant is placed immediately before the suffix.

Example:

	**Thiophene-3-ol, 5-telluryl-**

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:

H_2NNHSH	**Hydrazine, mercapto-**
Me_2BOH	**Borinic acid, dimethyl-**
	**3-Quinolinethiol, 1,2-dihydro-1-hydroxy-**
	**2-Phosphorinol, 1,2-dihydro-1-hydroxy- 1-oxide**
	**Piperidine, 1-(acetyloxy)-**
	**10*H*-Phenoxarsine, 10-[(phenylsulfonyl)thio]-**
	**Propanoic acid, 3-[(1,3-dihydro-1,3-dioxo-2*H*-isoindol-2-yl)oxy]-3-oxo-**

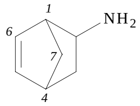
176. Amines are always named as primary amines, RNH_2, or their *N*-derivatives, by attaching the suffix "-amine" to the name of a molecular skeleton, cyclic or acyclic. Attachment may be at a carbon or hetero atom. Trivial names, e.g., Aniline, and radicofunctional names, e.g., Methylamine, are not used. Conjunctive names (¶ 124) are employed for monoamines where appropriate.

Examples:

$MeNH_2$	**Methanamine** (not Methylamine)
$MeCH(NH_2)Me$	**2-Propanamine** (not Isopropylamine)
$H_2C{=}CHCH(NH_2)Me$	**3-Buten-2-amine**
H_3PbNH_2	**Plumbanamine**

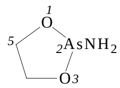
H_2PPHNH_2 — **Diphosphinamine**

$PhNH_2$ — **Benzenamine** (not Aniline)

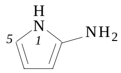


Bicyclo[2.2.1]hept-5-en-2-amine

$H_2NBiHNH_2$ — **Bismuthinediamine**



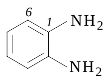
1,3,2-Dioxarsolan-2-amine



1*H*-Pyrrol-2-amine

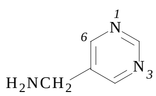
$H_2N\underset{2}{C}H_2\underset{1}{C}H_2NH_2$ — **1,2-Ethanediamine** (not Ethylenediamine)

$H_2N\underset{1}{C}H_2\underset{2}{C}H(NH_2)\underset{3}{Me}$ — **1,2-Propanediamine**



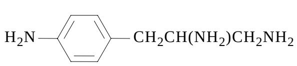
1,2-Benzenediamine (not 1,2-Phenylenediamine)

$Ph\underset{\beta}{C}H_2\underset{\alpha}{C}HMeNH_2$ — **Benzeneethanamine, α-methyl-**



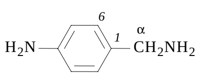
5-Pyrimidinemethanamine

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

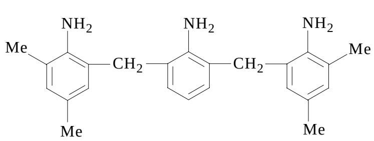


1,2-Propanediamine, 3-(4-aminophenyl)- (principle: maximum number of the principal group)

$H_2N(CH_2)_5SiH_2NH_2$ — **Silanamine, 1-(5-aminopentyl)-** (principle: hetero-atom parent preferred)



Benzenemethanamine, 4-amino- (principle: largest heading parent)

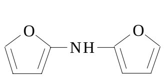


Benzenamine, 2,6-bis[(2-amino-3,5-dimethylphenyl)methyl]- (principle: centrality)

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:

$\underset{2}{Me}\underset{1}{C}H_2\underset{N}{N}HCH_2Me$ — **Ethanamine, *N*-ethyl-** (not Diethylamine)

$(Me_2CH)_3N$ — **2-Propanamine, *N*,*N*-bis(1-methylethyl)-** (not Triisopropylamine)

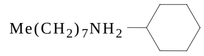


2-Furanamine, *N*-2-furanyl-

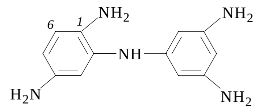
$H_2\underset{N'}{N}\text{-}\underset{3}{C}H_2\text{-}\underset{2}{C}H_2\text{-}\underset{1}{C}H_2\text{-}\underset{N}{N}H\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}NH_2$

1,3-Propanediamine, *N*-(3-aminopropyl)-

$H_3SiNHSnH_3$ — **Silanamine, *N*-stannyl-** (principle: preferred hetero atom)

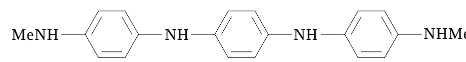


Cyclohexanamine, *N*-octyl- (principle: a cyclic parent is preferred)



1,2,4-Benzenetriamine, N^2-(3,5-diaminophenyl)- (principle: lowest locants for principal groups)

Me_2NONMe_2 — **Methanamine, *N*,*N*′-oxybis[*N*-methyl-** (principle: multiplication)



1,4-Benzenediamine, *N*,*N*′-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:

$Et\underset{N}{N}H\underset{1}{C}H_2CH_2\underset{3}{N}H[(CH_2)_2NH]_3\underset{13}{C}H_2\underset{14}{C}H_2\underset{N'}{N}HEt$

3,6,9,12-Tetraazatetradecane-1,14-diamine, *N*,*N*′-diethyl-

$CH_3\text{-}NH\text{-}CH_2\text{-}CH_2\text{-}\underset{N}{N}H\text{-}\underset{1}{C}H_2\text{-}\underset{2}{C}H_2\text{-}\underset{N'}{N}H\text{-}CH_2\text{-}CH_2\text{-}NH\text{-}CH_2\text{-}CH_2\text{-}NH\text{-}CH_3$

1,2-Ethanediamine, *N*-[2-(methylamino)ethyl]-*N*′-[2-[[2-(methylamino)ethyl]amino]ethyl]- (not 3,6,9-Triazaundecane-1,11-diamine, *N*,*N*′-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:

$PhN{=}CHPh$ — **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:

$PhNHOH$ — **Benzenamine, *N*-hydroxy-**

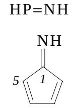
$EtN(O)Et_2$ — **Ethanamine, *N*,*N*-diethyl-*N*-oxide**

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:

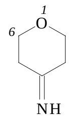
$\underset{2}{Me}\underset{1}{C}H{=}\underset{N}{N}H$ — **Ethanimine** (not Ethylideimine)

$\underset{1}{Me}\underset{2}{C}({=}NH)\underset{3}{Me}$ — **2-Propanimine**

$HP{=}NH$ — **Phosphinimine**



2,4-Cyclopentadien-1-imine



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

HN=C=NH

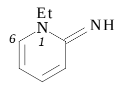
Methanediimine (not Carbodiimide)

$Me_2CHN{=}C{=}NCHMe_2$

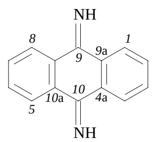
2-Propanamine, *N*,*N*′-methanetetraylbis- (not Methanediimine, bis(1-methylethyl)-)

$\underset{2}{Me}\underset{1}{C}H{=}\underset{N}{N}(O)Cl$

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



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



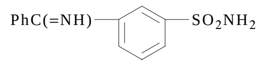
9,10-Anthracenediimine

$Ph_2C{=}NSSN{=}CPh_2$

Benzenemethanimine, *N*,*N*′-dithiobis[α-phenyl- (principle: multiplication 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.

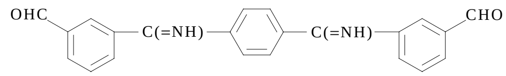
Examples:



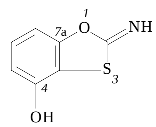
Benzenesulfonamide, 3-(iminophenylmethyl)-

$HN{=}\underset{3}{C}H\underset{2}{C}H_2\underset{1}{C}N$

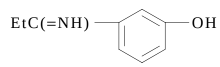
Propanenitrile, 3-imino-



Benzaldehyde, 3,3′-(1,4-phenylenedicarbonimidoyl)bis-



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



Phenol, 3-(1-iminopropyl)-

D. COMPOUND CLASSES

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178. Introduction. Previous sections have dealt with general principles and with the naming of specific compounds by combination of a molecular skeleton 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.

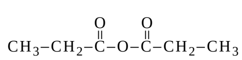
Example:

$HO_2\underset{1}{C}CH_2\underset{3}{C}O\underset{4}{O}\underset{5}{S}O_2CH_2\underset{7}{S}O_2\underset{8}{O}COCH_2\underset{11}{C}O_2H$

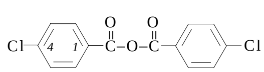
4,8-Dioxa-5,7-dithiaundecanedioic acid, 3,9-dioxo-5,5,7,7-tetraoxide

Symmetrical anhydrides of monobasic organic acids are indexed at the acid heading parent with the simple term "anhydride" in the modification. 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).

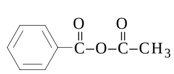
Examples:



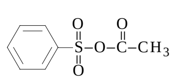
Propanoic acid anhydride



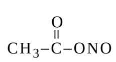
Benzoic acid, 4-chloro- anhydride



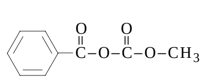
Benzoic acid anhydride with acetic acid



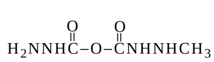
Acetic acid anhydride with benzenesulfonic acid



Acetic acid anhydride with nitrous acid



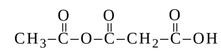
Benzoic acid anhydride with methyl hydrogen carbonate (the ester name is given in its uninverted form (¶ 185); not Benzoic acid, anhydride with methoxyformic acid)



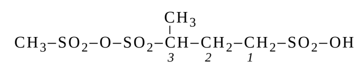
Dicarbonic dihydrazide, 2-methyl- (see also ¶ 183)

Anhydrides of monobasic organic acids with polybasic acids are indexed at the name of the preferred acid. The terms "mono," "di," etc., are used to indicate the number of molecules of water lost in anhydride formation, and locants must sometimes be cited. When three or more different acids are involved, the "anhydride with" term is repeated.

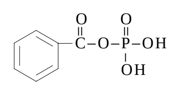
Examples:



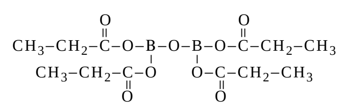
Propanedioic acid monoanhydride with acetic acid



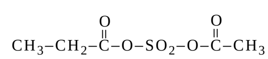
1,3-Butanedisulfonic acid 3-anhydride with methanesulfonic acid (not "3-monoanhydride with...")



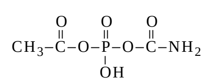
Benzoic acid monoanhydride with phosphoric acid



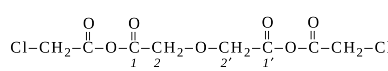
Propanoic acid tetraanhydride with boric acid ($H_4B_2O_5$)



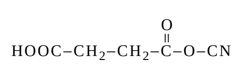
Propanoic acid monoanhydride with sulfuric acid, anhydride with acetic acid



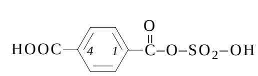
Acetic acid monoanhydride with phosphoric acid, monoanhydride with carbamic acid (repetition of "mono" is necessary here)



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



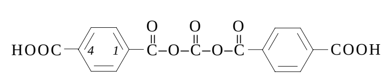
Butanedioic acid monoanhydride with cyanic acid



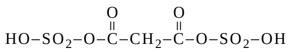
1,4-Benzenedicarboxylic acid monoanhydride with sulfuric acid

Acyclic anhydrides of different polybasic acids sometimes require ratios.

Examples:



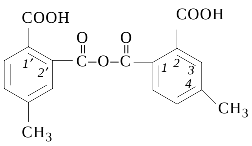
1,4-Benzenedicarboxylic acid anhydride with carbonic acid (2:1)



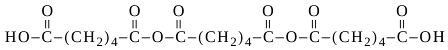
Propanedioic acid anhydride with sulfuric acid (1:2)

Anhydrides of a single polybasic organic acid have such terms as "bimol. monoanhydride" and "trimol. dianhydride" in the modification, with locants when necessary.

Examples:



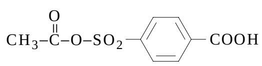
1,2-Benzenedicarboxylic acid, 4-methyl- bimol. 1,2′-monoanhydride



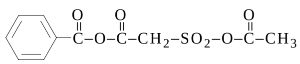
Hexanedioic acid trimol. dianhydride

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:



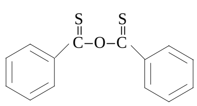
Benzoic acid, 4-[(acetyloxy)-sulfonyl]-



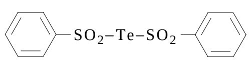
Benzoic acid anhydride with [(acetyloxy)-sulfonyl]acetic acid

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.

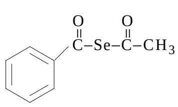
Examples:



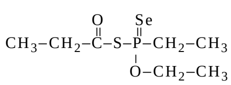
Benzenecarbothioic acid anhydride (not "anhydrosulfide")



Benzenesulfonotelluroic acid anhydrotelluride



Benzenecarboselenoic acid anhydroselenide with ethane-selenoic acid



Propanethioic acid anhydrosulfide with *O*-ethyl hydrogen ethylphosphonosel-enothioate

MeC(=NOH)SCN

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

Symmetrical anhydrides of the monobasic "oxo" acids F**ormic**, **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**, **Phosphonous**, and **Arsonous acids** and their substituted derivatives are indexed at Di-, Tri-, etc., acid headings.

Example:

MeAs(OH)OAs(OH)Me

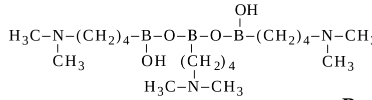
Diarsonous acid, dimethyl-

Anhydrides of **Borinic acid** are indexed at **Borane**. Symmetrical anhydrides of **Boronic acid** are indexed at the acid names with "bimol. monoanhydride," etc., in the modification.

Examples:

PhBMeOBMePh

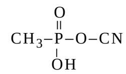
Borane, oxybis[methylphenyl-



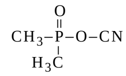
Boronic acid, [4-(dimethyl-amino)butyl]- trimol. dianhydride

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 "cyanatido" replacement affixes or by the class term "cyanate."

Examples:



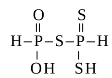
Phosphonocyanatidic acid, methyl-



Phosphinic cyanate, 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.

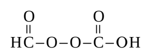
Example:



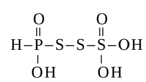
Thiodiphosphonic acid ((HO)HP(O)SHP(S)SH)

The peroxy analogs of this kind of "oxo" acid are indexed (with synonym line formulas) at such headings as **Thioperoxydiarsonic acid ([(HO)HAs(S)]$_2$S$_2$)**. Anhydrides of mononuclear peroxy "oxo" acids are generally named at **Peroxide**, **Disulfide**, etc.

Examples:



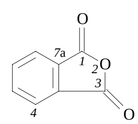
Peroxide, carboxy formyl



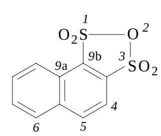
Disulfide, hydroxyphosphinyl sulfo

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

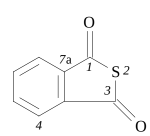
Examples:



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)



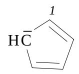
Benzo[*c*]thiophene-1,3-dione

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** (Si^{4-} only) and **Hydrazine** are named **Acetylide**, **Arsenide**, **Phosphide**, **Antimonide**, **Silicide**, and **Hydrazide**. Synonym line formulas are used, e.g., **Acetylide** (C_2^{2-}), except for **Hydrazide** (which is H_2NNH^-) 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.

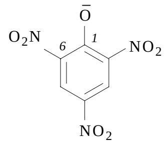
Examples:



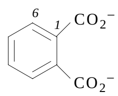
1,3-Cyclopentadiene ion(1–)

$MeCH_2CH_2O^-$

1-Propanol ion(1–) (not Propoxide)



Phenol, 2,4,6-trinitro- ion(1–)



1,2-Benzenedicarboxylic acid ion(2–)

Me_2As^-

Arsine, dimethyl- ion(1–)

$EtP(O)(OH)O^-$

Phosphonic acid, ethyl- ion(1–)

$PhOSO_3^-$

Sulfuric acid monophenyl ester, ion(1–)

$MeO_3SCH_2CH_2SO_3^-$

1,2-Ethanedisulfonic acid monomethyl ester, ion(1–)

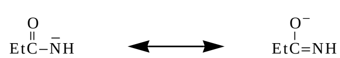
Certain resonance-stabilized anions and cations containing hetero atoms are indexed by *CA* at names corresponding to preferred canonical structures. In the same manner as the analogous tautomeric compounds (¶ 122), anions are normalized, i.e., recognized as equivalent, by machine programs, regardless of how the structures are shown in the original documents. Each ion is assigned a single CAS Registry Number (see Appendix II, ¶ 13) and a unique *CA* index name.

Resonance-stabilized anions of the general formula

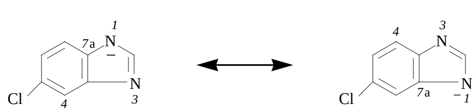
$$M{=}Q{-}Z^- \longleftrightarrow {}^-M{-}Q{=}Z$$

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 and nomenclature rules, and are identical except for addition of the index modification term "ion(1–)". Negative ions from tautomeric pyrazole and tropolone systems, though not normalized by the CAS Registry System, are handled like the uncharged tautomers.

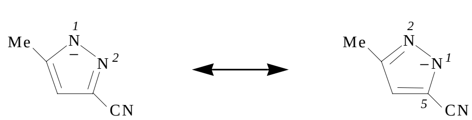
Examples:



Propanamide ion(1–) NOT **Propanimidic acid ion(1–)**



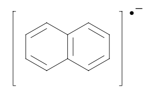
1*H*-Benzimidazole, 5-chloro- ion(1–) NOT **1*H*-Benzimidazole, 6-chloro- ion(1–)**



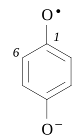
1*H*-Pyrazole-3-carbonitrile, 5-methyl- ion(1–) NOT **1*H*-Pyrazole-5-carbonitrile, 3-methyl- ion(1–)**

Radical ions are named at the neutral compound heading with "radical ion" terms in the modification.

Examples:



Naphthalene radical ion(1–)

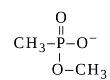


2,5-Cyclohexadiene-1,4-dione radical ion(1–)

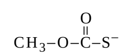
At cationic index headings, e.g., **Ethanaminium** (see ¶¶ 184, 198), anions are expressed by "-ide" or "-ate" terms, as described below, or by "salt with" phrases. The "salt with" phrase is followed by a ratio, e.g., (1:1).

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.

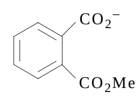
Examples:



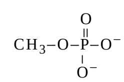
methyl methylphosphonate



***O*-methyl carbonothioate**



methyl 1,2-benzenedicarboxylate

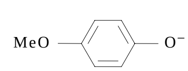


methyl phosphate

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.

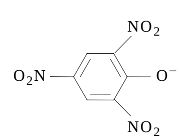
Examples:



salt with 4-methoxyphenol (not "4-methoxyphenoxide")

PhNH—

salt with benzenamine



salt with 2,4,6-trinitrophenol (not "picrate")

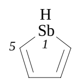
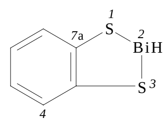
181. Antimony and Bismuth compounds, are conveniently discussed together because of the close similarity in the indexing treatment of their derivatives. Antimony and bismuth are metals (¶ 215), and their salts are named as such, not as cyclic or acyclic molecular skeletons. (Prior to *CA* Volume 95 (see ¶ 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 index 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:

Et_3Bi

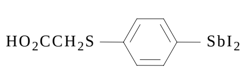
Bismuthine, triethyl-

$EtSbCl_2$	**Stibine, dichloroethyl-**
Ph_2BiI	**Bismuthine, iododiphenyl-**
$(F_3C)_2SbSbMe_2$ 2 1	**Distibine, 1,1-dimethyl-2,2-bis-(trifluoromethyl)-**
PhSb=SbPh	**Distibene, diphenyl-**
$Ph_2Sb(O)OH$	**Stibine oxide, hydroxydiphenyl-**
$H_2Sb(O)NH_2$ 1 N	**Stibinamine 1-oxide**
$EtBiH_2$=NMe 1 N	**Bismuthine imide, 1-ethyl-*N*-methyl-**
	**1*H*-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 (–SbO_2), stibinico (=Sb(O)OH), and stibono (–$Sb(O)(OH)_2$) were used prior to *CA* Volume 95 (see ¶ 101).)

	Substituent Prefix		*Substituent Prefix*
–SbH_2	stibino	–BiH_2	bismuthino
=SbH	stibylene	=BiH	bismuthylene
≡Sb	stibylidyne	≡Bi	bismuthylidyne
–Sb=Sb–	1,2-distibenediyl		

Examples:

	**Acetic acid, [[4-(diiodostibino)-phenyl]thio]-**
PhN=BiI N	**Benzenamine, *N*-(iodo-bismuthylene)-**

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:

$MeOSbCl_2$	**Stibine, dichloromethoxy-**
$(HO)_2Sb(O)NH_2$	**Stibinamine, 1,1-dihydroxy-1-oxide**

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)tetramine** and **1,2-Dicarbadodecaborane(12)-1,2-diethanol**.

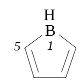
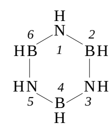
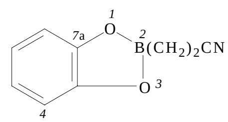
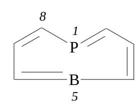
Acyclic carbon chains containing boron atoms are given "a" names if the requirements (¶ 127) are met.

Example:

$MeB(Me)CH_2O(CH_2)_2OCH_2B(Me)Me$ 1 2 4 7 9 10	**4,7-Dioxa-2,9-diboradecane, 2,9-dimethyl-**

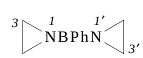
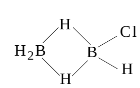
Heterocyclic boron compounds and their derivatives are named by the usual procedures (¶ 146). Intramolecular coordination bonds between boron atoms and other hetero atoms are ignored in naming; thus, a zwitterionic ring bond between boron and phosphorus in the last example below is disregarded, and the monocyclic system is named. (A monocycle entirely dependent on such a bond is named as an acyclic compound.)

Examples:

	**1*H*-Borole**
	**Borazine**
	**1,3,2-Benzodioxaborole-2-propanenitrile**
	**1,5-Phosphaborocine**

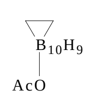
Boron molecular skeletons fall between nonfunctional bismuth and silicon compounds in the order of precedence of compound classes (¶ 106). Within the boron class, the descending order is carbapolyboranes, hetero polyboranes, polyboranes, heterocyclic boron compounds, and finally **Borane**. When more preferred groups or molecular skeletons are present, boron substituent prefixes (¶ 161) are used.

Examples:

Me_3B	**Borane, trimethyl-**
H_2SbBH_2	**Stibine, boryl-**
Me_2BNHMe 1 N	**Boranamine, *N*,1,1-trimethyl-** (principle: heteroatom molecular skeleton preferred)
	**Aziridine, 1,1′-(phenylborylene)bis-**
	**Diborane(6), chloro-**

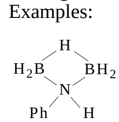
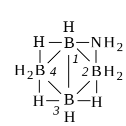
When the position of substituent suffixes or prefixes cannot be related to the accepted numbering of polyboranes and hetero polyboranes (as illustrated in the *Ring Systems Handbook* and current *Chemical Substance Index*), no numerical locants are used, but capital italic letters may be cited to denote substitution on a "hetero" atom in a hetero polyborane.

Examples:

	**1,2-Dicarbadodecaborane(12), (acetyloxy)-**
$B_{10}C_2Me_2H_{10}$	**Dicarbadodecaborane(12), *C*,*C*′-dimethyl-**

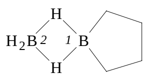
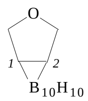
Substitution of *bridging hydrogen* of a polyborane or hetero polyborane is indicated by the prefix "μ" (mu); when necessary, the locants of the boron-atom bridgeheads are cited.

Examples:

	**Diborane(6), [μ-(phenylamino)]-**
	**Tetraborane(10), 1,2-μ-amino-**

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-Dicarbadodecaborane(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, salts, and hydrazides are named in the usual way, but their acid halides and amides are named as **Borane** and **Boranamine** derivatives, respectively. Chalcogen analogs are named by use of the detachable prefixes thio, seleno, and telluro.

Hydroxy derivatives of **Diborane(4)**, are now indexed at that index heading parent.

Examples:

MeB(OMe)OEt	**Boronic acid, methyl-** **ethyl methyl ester**
PhBMeOH	**Borinic acid, methylphenyl-**
$PhB(SH)_2$	**Boronic acid, phenyldithio-**
$AcOBMe_2$	**Acetic acid** **anhydride with dimethylborinic acid**
$PhB(NHNH_2)_2$	**Boronic acid, phenyl-** **dihydrazide**
$(HO)_2BB(OH)_2$	**Diborane(4), 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-**

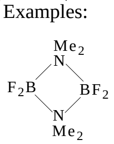
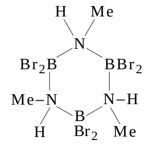
Addition compounds of neutral boranes are named as molecular coordination compounds (see ¶ 215). (Prior to *CA* Volume 95 (see ¶ 101), they were indexed at the component names (¶ 192).)

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-(dimethyl amino)]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-**, **dihydrogen** (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**, **oxo-)**, **Formamide**, **Formaldehyde**, **Hydrocyanic acid**, **Urea, Guanidine**, **Cyanic acid**, **Thiocyanic acid**, **Selenocyanic acid**, **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:

$H{-}\overset{O}{\overset{\|}{C}}{-}NCO$	**Formyl isocyanate**
$H{-}\overset{O}{\overset{\|}{C}}{-}OCN$	**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**.

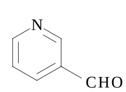
Examples:

$H{-}\overset{O}{\overset{\|}{C}}{-}O{-}OH$	**Methaneperoxoic acid**
$H{-}\overset{S}{\overset{\|}{C}}{-}SH$	**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**
$HO{-}\overset{S}{\overset{\|}{C}}{-}CO_2H$	**Formic acid, (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 hydrazino) are given functional replacement names. The replacement of one hydroxyl by amino leads formally to Carbonamidic 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 Carbonamidimidic acid) (**Urea** is preferred in indexing in the absence of a covalent acid derivative.)
$ClCO_2H$	**Carbonochloridic acid**
$NCCO_2H$	**Carbonocyanidic acid**
$(HOO)_2CO$	**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**, **oxo-**; the dicyanide is **Propanedinitrile**, **oxo-**; the trivial name **Guanidine** is employed for Carbonimidic diamide.

Examples:

$\underset{N'}{\mathrm{MeN}}\mathrm{HC}(=\underset{N''}{\mathrm{NH}})\underset{N}{\mathrm{N}}\mathrm{HEt}$	**Guanidine, *N*-ethyl-*N′*-methyl-**

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).

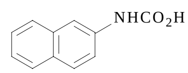
Examples:

$HO{-}\overset{\overset{O}{\Vert}}{C}{-}O{-}\overset{\overset{O}{\Vert}}{C}{-}OH$	**Dicarbonic acid**
$HO{-}\overset{\overset{NH}{\Vert}}{C}{-}O{-}\overset{\overset{NH}{\Vert}}{C}{-}O{-}\overset{\overset{NH}{\Vert}}{C}{-}OH$	**Tricarbonimidic acid**
$HO{-}O{-}\overset{\overset{O}{\Vert}}{C}{-}O{-}\overset{\overset{O}{\Vert}}{C}{-}O{-}OH$	**Dicarbonodiperoxoic acid**
HO_2COOCO_2H	**Peroxydicarbonic acid**
$HO{-}\overset{\overset{NH}{\Vert}}{C}{-}NH{-}\overset{\overset{NH}{\Vert}}{C}{-}NH{-}\overset{\overset{NH}{\Vert}}{C}{-}OH$	**Diimidotricarbonimidic acid**
$HO{-}\overset{\overset{S}{\Vert}}{C}{-}S{-}S{-}\overset{\overset{S}{\Vert}}{C}{-}OH$	**Thioperoxydicarbonic acid ($[(HO)C(S)]_2S_2$)**
$Cl{-}\overset{\overset{O}{\Vert}}{C}{-}O{-}\overset{\overset{O}{\Vert}}{C}{-}Cl$	**Dicarbonic dichloride**
$Cl{-}\overset{\overset{O}{\Vert}}{C}{-}NH{-}\overset{\overset{O}{\Vert}}{C}{-}Br$	**Imidodicarbonic bromide chloride**
$H_2NNHCONHCONHNH_2$	**Imidodicarbonic dihydrazide**
$ClCONHCO_2H$	**Carbamic acid, (chlorocarbonyl)-**
$NH_2{-}\underset{1}{\overset{\overset{O}{\Vert}}{C}}{-}\underset{2}{NH}{-}\underset{3}{\overset{\overset{O}{\Vert}}{C}}{-}\underset{4}{NH}{-}\underset{5}{\overset{\overset{O}{\Vert}}{C}}{-}\underset{6}{NH}{-}\underset{7}{\overset{\overset{O}{\Vert}}{C}}{-}\underset{8}{NH}{-}\underset{9}{\overset{\overset{O}{\Vert}}{C}}{-}NH_2$	**2,4,6,8-Tetraazanonanediamide, 3,5,7-trioxo-**

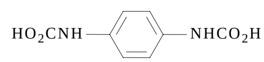
Carbonic acid and its relatives are placed in the order of precedence of compound classes just below acids expressed as suffixes attached to molecular skeleton names, e.g., sulfonic acids (¶ 106). Within this subclass of acids, they are ranked by the following criteria, applied successively until a decision 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**, **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:

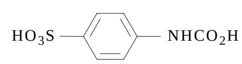


Carbamic acid, 2-naphthalenyl- (not 2-Naphthalenecarbamic acid)



Carbamic acid, 1,4-phenylenebis- (not Carbamic acid, *N,N′*-1,4-phenylenebis- (see ¶ 118))

Me_2NCS_2H	**Carbamodithioic acid, dimethyl-**
$PrNHC({=}NH)OEt$	**Carbamimidic acid, propyl- ethyl ester**

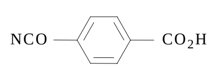


Benzenesulfonic acid, 4-(carboxyamino)-

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, phenyl-** (not Benzenecarbamonitrile)

Numerical and italic letter locants are used with carbonic acid relatives to place substituents. Unless a locant is expressed in the heading parent, none is cited for a substituent prefix unless needed to specify an isomer (¶ 117). Locants are not usually employed with monosubstituted **Guanidine** and **Carbamimidic acid**.

Examples:

$\underset{N}{\mathrm{MeN}}\mathrm{HCO}\underset{N'}{\mathrm{N}}\mathrm{H_2}$	**Urea, methyl-**
$\underset{N}{\mathrm{MeN}}\mathrm{HCS}\underset{N'}{\mathrm{N}}\mathrm{HMe}$	**Thiourea, *N,N′*-dimethyl-**
$H_2NNHC({=}NH)SEt$	**Hydrazinecarboximidothioic acid ethyl ester**

```
H2NNHCONHNH2
 2 1    1' 2'
```
Carbonic dihydrazide

```
H2NC(=NH)NH2
  N    N''  N'
```
Guanidine

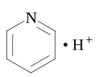
```
     N''     N'''
     NH      NH
     ||      ||
H2N-C-NH-C-NH2
 N   1  2   3  N'
```
Imidodicarbonimidic diamide

```
      N''     N'''     N''''
      NH      NH       NH
      ||      ||       ||
NH2-C-NH-C-NH-C-NH2
 N    1  2   3  4   5  N'
```
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" (if two or more heteroatoms are present) at the neutral component.

Examples:

MeOH • HF (not [MeOH$_2$] + F$^-$) — **Hydrofluoric acid**
compd. with methanol (1:1)
Methanol
compd. with hydrofluoric acid (1:1) (additional *Chemical Substance* and *Formula Index* entry)


Pyridine
conjugate acid

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 "monoprotonated".

Example:

$MeCH_4+$ — **Ethane**
monoprotonated

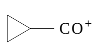
Orthodox carbonium compounds are named from the hydrocarbon (or other parent) *radical* by addition of "-ium."

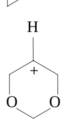
Examples:

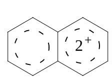
$MeCH_2+$ — **Ethylium**

Me_2CH^+ — **Ethylium, 1-methyl-** (not 2-Propylium

$MeCO^+$ (locants: Me 2, C 1) — **Ethylium, 1-oxo-** (not Acetylium)


Methylium, cyclopropyloxo- (not Cyclopropylcarbonylium)


1,3-Dioxan-5-ylium

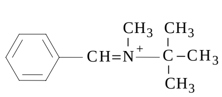

Naphthalenediylium, dihydro-

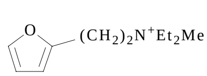
Acyclic *nitrogen cations* derived from amines attached to parent molecular skeletons are named by converting the preferred "-amine" name (¶ 176) to "-aminium" and expressing the remaining quaternizing groups as substituent prefixes.

Examples:

Me_4N^+ — **Methanaminium, *N*,*N*,*N*-trimethyl-**

Me_2N^+O — **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)

$Pr_3N^+(CH_2)_2N^+Pr_3$ — **1,2-Ethanediaminium, *N*,*N*,*N*,*N*′,*N*′,*N*′-hexapropyl-** (principle: maximum number of the preferred substituent suffix)

$MeC{\equiv}N^+Me$ — **Methanaminium, *N*-ethylidyne-**

Quaternary ammonium cations not included in the heading parent are expressed as substituted ammonio, $^+NH_3$–, iminio, $^+NH_2$=, and nitrilio, $^+NH{\equiv}$, radicals.

Example:

```
     CH3       CH3       CH3
      |+        |+        |+
H3C-N-(CH2)6-N-(CH2)3-N-(CH2)6-NH2
      |         |         |
     CH3       CH3       CH3
```

1,6-Hexanediaminium, *N*-[3-[(6-aminohexyl)dimethylammonio]propyl]-*N*,*N*,*N*′,*N*′,*N*′-pentamethyl- (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:

```
          CH3        CH3        CH3        CH3        CH3        CH3
           |+         |+         |+         |+         |+         |+
CH3-CH2-N-(CH2)6-N-(CH2)6-N-(CH2)6-N-(CH2)6-N-(CH2)6-N-CH2-CH3
          N|         7|         14|        21|        28|        N'|
          CH3        CH3        CH3        CH3        CH3        CH3
```

7,14,21,28-Tetraazoniatetratriacontane-1,34-diaminium, *N*,*N*′-diethyl-*N*,*N*,*N*′,*N*′,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).

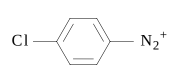
Example:

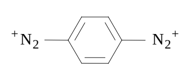
$Ph_2C{=}N^+{=}CPh_2$ — **Benzenemethaniminium, *N*-(diphenylmethylene)-α-phenyl-**

Diazonium compounds contain the $–N_2^+$ 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."

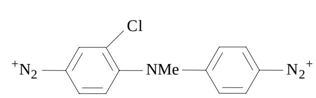
Examples:

$MeCOCH(N_2^+)COMe$ (locants: Me 1, CH 3, CO 4, Me 5) — **3-Pentanediazonium, 2,4-dioxo-**


Benzenediazonium, 4-chloro-


1,4-Benzenebis(diazonium)

$MeNHN_2^+$ — **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:

$PhN^+Me_2NH_2$ — **Hydrazinium, 1,1-dimethyl-1-phenyl-**

$H_2NN^+Me_2NH_2$ (locants: N 1, N 2, N 3) — **Triazanium, 2,2-dimethyl-**

$MeN{=}NN^+Me_3$ (locants: N 3, N 2, N 1) — **2-Triazenium, 1,1,1,3-tetramethyl-**

$Me_3N^+N^+Me_3$ — **Hydrazinium, hexamethyl-** (not Hydrazinium, 1,1,1,2,2,2-hexamethyl-)

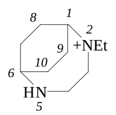
Acyclic cations from nonnitrogenous hetero atoms are indexed at **Phosphonium**, **Arsonium**, **Stibonium**, **Bismuthonium**, **Oxonium**, **Sulfonium**, **Iodonium**, etc. The corresponding substituent prefixes are phosphonio, arsonio, etc. **Diphosphine**, H_2P-PH_2, affords **Diphosphinium**.

Examples:

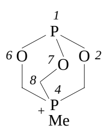
$Me_3P^+(CH_2)_2P^+Me_3$	**Phosphonium, 1,2-ethanediylbis-[trimethyl-** (analogous compounds with one or more noncarbon attachments to phosphorus are indexed at **Phosphorus(1+)** (see ¶ 215))
$Cl_2PP^+Me_3$	**Diphosphinium, 2,2-dichloro-1,1,1-trimethyl-**
Me_4As^+	**Arsonium, tetramethyl-**
Me_3S^+	**Sulfonium, trimethyl-** (the corresponding *S*-oxide is named **Sulfoxonium, trimethyl-)**
Ph_2I^+	**Iodonium, diphenyl-** (the corresponding *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.

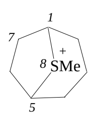
Examples:



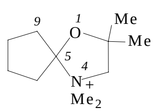
5-Aza-2-azoniabicyclo[4.2.2]decane, 2,2-diethyl-



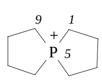
2,6,7-Trioxa-1-phospha-4-phosphoniabicyclo[2.2.2]octane, 4-methyl-



8-Thioniabicyclo[3.2.1]octane, 8-methyl-



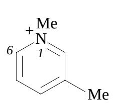
1-Oxa-4-azoniaspiro[4.4]nonane, 2,2,4,4-tetramethyl-



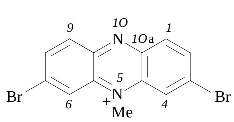
5-Phosphoniaspiro[4.4]nonane

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., **1*H*** (never **3*H***)-**Benzimidazolium**; a cationic center is numbered lower than a neutral hetero atom of the same element if a choice is available.

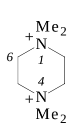
Examples:



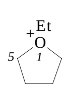
Pyridinium, 1,3-dimethyl-



Phenazinium, 3,7-dibromo-5-methyl- (not Phenazinium, 2,8-dibromo-10-methyl-)



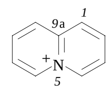
Piperazinium, 1,1,4,4-tetramethyl-



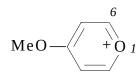
Furanium, 1-ethyltetrahydro-

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.

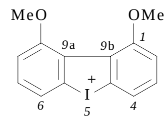
Examples:



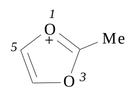
Quinolizinium



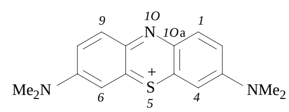
Pyrylium, 4-methoxy- (from **2*H*-** or **4*H*-Pyran**)



Dibenziodolium, 1,9-dimethoxy-



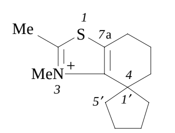
1,3-Dioxol-1-ium, 2-methyl-



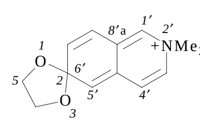
Phenothiazin-5-ium, 3,7-bis(dimethylamino)-

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.

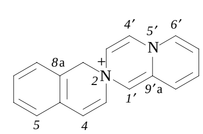
Examples:



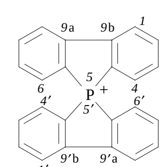
Spiro[benzothiazolium-4(5*H*),1′-cyclopentane], 6,7-dihydro-2,3-dimethyl-



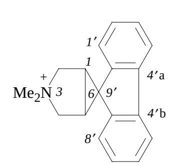
Spiro[1,3-dioxolane-2,6′(2′*H*)-isoquinolinium], 2′,2′-dimethyl-



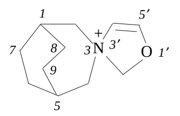
Spiro[isoquinoline-2(1*H*), 2′-[2*H*] pyrido[1,2-*a*]pyrazinium]



Spirobi[5*H*-dibenzophospholium]



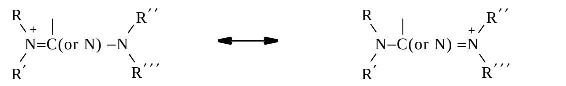
Spiro[3-azoniabicyclo[3.1.0]hexane-6,9′-[9*H*]fluorene], 3,3-dimethyl-



Spiro[3-azoniabicyclo[3.2.2]nonane-3,3′(2*H*)-oxazolium]

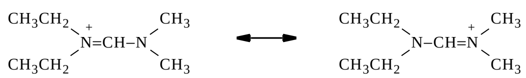
Dispiro compounds with other than “a”-named components and containing two cationic spiro atoms have the “ium” suffix appended to the terminal, i.e., the first and third, component names.

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). Normalized cations have the general structure:

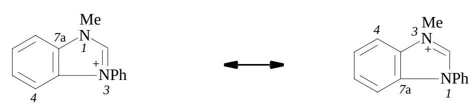


in which R, R′, R″, and R‴ represent any atom or group except hydrogen. The structure may be acyclic or wholly or partly within a ring system, and two or more structures may be linked through a common atom to permit further “migration” of the cationic center. The unique *CA Chemical Substance Index* name is derived in general by regular nomenclature rules (see ¶ 138).

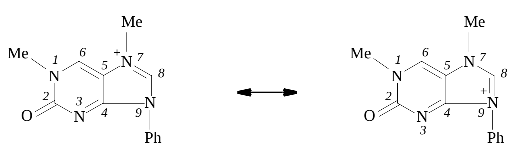
Examples:



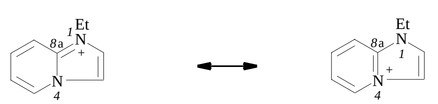
Ethanaminium, *N*-[(dimethylamino)methylene]-*N*-ethyl- (principle: preferred index parent) NOT **Methanaminium, *N*-[(diethylamino)methylene]-*N*-methyl-**



1*H*-Benzimidazolium, 1-methyl-3-phenyl- (principle: lowest locants for substituents) NOT **1*H*-Benzimidazolium, 3-methyl-1-phenyl-**



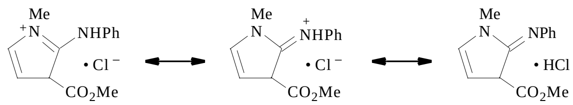
1*H*-Purinium, 2,9-dihydro-1,7-dimethyl-2-oxo-9-phenyl- (principle: lowest locant for indicated hydrogen, then for cationic center) NOT **1*H*-Purinium, 2,7-dihydro-1,7-dimethyl-2-oxo-9-phenyl-**



Imidazo[1,2-*a*]pyridinium, 1-ethyl- (principle: the neutral ring, quaternized by substitution, is preferred) NOT **1*H*-Imidazo[1,2-*a*]pyridin-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 monoacid” or (if the anion is known) as a salt such as “hydrochloride”.

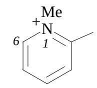
Example:



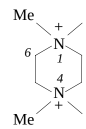
(The hydrochloride salt is the preferred structure.)

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, 2*H*-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.

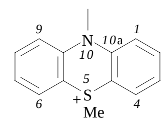
Examples:



(1-methylpyridinium-2-yl)



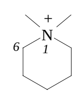
(1,4-dimethylpiperazinium-1,4-diyl)



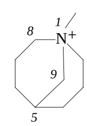
(5-methyl-10*H*-phenothiazinium-10-yl)

$Me_2\underset{4}{N}\underset{3}{N}{=}\underset{2}{N}\underset{1}{N}^{+}Me_2{}^{-}$

(1,1,4,4-tetramethyl-2-tetrazenium-1-yl)



piperidinium-1-ylidene



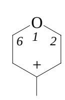
1-azoniabicyclo[3.3.1]non-1-yl

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.

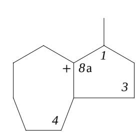
Examples:

H_2C^{+}— methyliumyl

$MeC^{+}H$ — 1-ethylium-1-yl



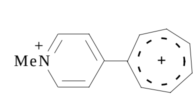
(tetrahydro-4*H*-pyran-4-ylium-4-yl)



(octahydro-8a(1*H*)-azulenylium-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.

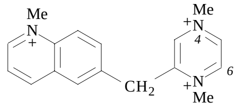
Examples:



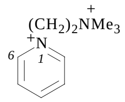
Cycloheptatrienylium, (1-methylpyridinium-4-yl)- (principle: carbon cation preferred)

$Me_3N^{+}(CH_2)_3S^{+}Me_2$

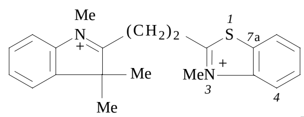
1-Propanaminium, 3-(dimethylsulfonio)-*N*,*N*,*N*-trimethyl- (principle: nitrogen cation preferred)



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)

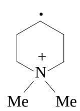


Benzothiazolium, 3-methyl-2-[2-(1,3,3-trimethyl-3*H*-indolium-2-yl)ethyl]- (principle: preferred ring)

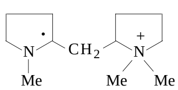
Cationic compounds of *indefinite structure* are named by use of alternative locants if possible, e.g., **Quinazolinium**, **1(***or* **3)-methyl-**, **iodide**; otherwise as molecular addition compounds of the neutral compounds with a term such as "compd. with iodomethane (1:1)" (not "monomethiodide") in the modification and additional *Chemical Substance* and *Formula Index* entries at the less preferred component, e.g., **Methane**, **iodo-**.

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:



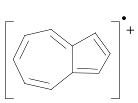
Piperidinium-4-yl, 1,1-dimethyl-



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 hetero atom of a molecular skeleton or of an isolated chalcogen atom are named similarly (¶ 270).

Example:

$Me_3N^{\bullet +}$ — **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:

EtOCN	**Cyanic acid** **ethyl ester**
$EtOClO_3$	**Perchloric acid** **ethyl ester**
EtN_3	**Ethane, azido-**
EtNCO	**Ethane, isocyanato-**
EtCl	**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 (H_3BO_3)**; **Carbamic acid**; **Carbamic acid**, **methyl-**; **Carbamic acid**, **phenyl-**; **Carbonic acid**; **Formic acid**; **Methanesulfonic acid**; **Nitric acid**; **Phosphoric acid**; **Phosphorodithioic acid**; **Phosphorothioic acid**; **Phosphorous acid**; **Propanoic acid**; **Sulfuric acid**; **Sul-furous acid**. All other acids, including isotopically labeled forms of "Class I" acids, belong to "Class II."

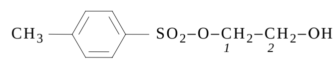
Esters of "Class I" monobasic acids with "Class II" alcohols and thiols are indexed at the latter. Esters of "Class I" acids with "Class I" alcohols and thiols are indexed at the acids. "Class I" alcohols are: **Benzeneethanol**; **Benzenemethanol**; **1-Butanol**; **1-Butanol**, **2-ethyl-**; **2-Butanol**; **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-**; **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., **Benzeneethanethiol**; **2-Propanethiol**, **2-methyl-**; except that the **Phenol** analog is **Benzenethiol**. All selenols and tellurols belong to "Class II."

Examples:

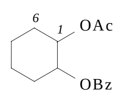
$AcO(CH_2)_2Ph$	**Acetic acid** **2-phenylethyl ester**
$MeOSO_3H$	**Sulfuric acid** **monomethyl ester** (the uninverted name is methyl hydrogen sulfate)
PhSP(S)(OMe)OH	**Phosphorodithioic acid** ***O*-methyl *S*-phenyl ester**

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.

Examples:



1,2-Ethanediol
mono(4-methylbenzenesulfonate)



1,2-Cyclohexanediol
acetate benzoate

$HCO_2CH_2CH_2O_2CH$ (1, 2)

1,2-Ethanediol
diformate (the uninverted name is 1,2-ethanediyl diformate)

$[Cl(CH_2)_2O]_3P(O)$

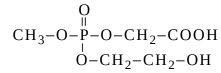
Ethanol, 2-chloro-
phosphate (3:1) (all the "Class II" alcoholic components are alike here; the ratio is necessary to indicate a neutral ester of known composition; the mono- and diesters are named with **"dihydrogen phosphate"** and **"hydrogen phosphate"**, respectively in the modification)

$HO(CH_2)_2OP(OMe)_2$

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.

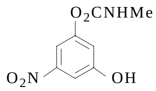
Example:



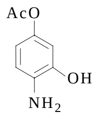
Acetic acid, [[(2-hydroxyethoxy)-methoxyphosphinyl]oxy]- (not Acetic acid, hydroxy-, 2-hydroxyethyl methyl phosphate)

If an "-ate" term in a modification could be interpreted to denote either an ester or a salt, the parenthetical expression "(ester)" is added. This is done whenever the index heading expresses any nitrogen atom or any trivalent phosphorus or arsenic atom. When a locant is needed in the modification, the "(ester)" term is dropped.

Examples:



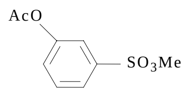
1,3-Benzenediol, 5-nitro- mono(methylcarbamate) (ester)



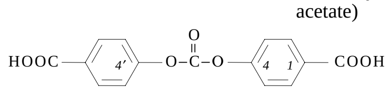
1,3-Benzenediol, 4-amino- 1-acetate

Esterified substituents of the index heading parent are expressed as substituents, not as modification phrases.

Examples:



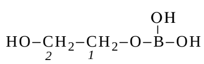
Benzenesulfonic acid, 3-(acetyloxy)-, methyl ester (not Benzenesulfonic acid, 3-hydroxy-, methyl ester acetate)



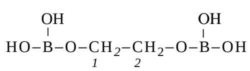
Benzoic acid, 4,4′-[carbonylbis(oxy)]bis- (not Benzoic acid, 4-hydroxy-, carbonate (2:1))

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 usually needed also unless "monoester with," "diester with," etc., phrases can be employed unambiguously.

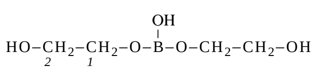
Examples:



1,2-Ethanediol monoester with boric acid (H_3BO_3)



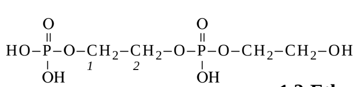
1,2-Ethanediol ester with boric acid (H_3BO_3) (1:2)



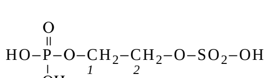
1,2-Ethanediol ester with boric acid (H_3BO_3) (2:1)

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.

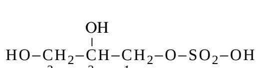
Examples:



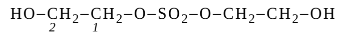
1,2-Ethanediol dihydrogen phosphate 2-hydroxyethyl hydrogen phosphate (principle: maximum number of functional derivatives)



1,2-Ethanediol dihydrogen phosphate hydrogen sulfate



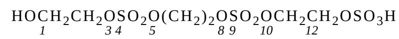
1,2,3-Propanetriol 1-(hydrogen sulfate)



1,2-Ethanediol sulfate (2:1)

Esters are named by replacement ("a") nomenclature if the requirements (¶ 127) are met.

Example:



3,5,8,10-Tetraoxa-4,9-dithiadodecane-1,12-diol mono(hydrogen sulfate), 4,4,9,9-tetraoxide

Multiplicative radicals in modifications are cited ahead of nonmultiplicative.

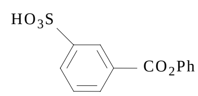
Example:

$(MeO)_2BO(CH_2)_3OB(OMe)_2$

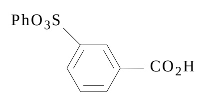
Boric acid (H_3BO_3) 1,3-propanediyl tetramethyl ester

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:



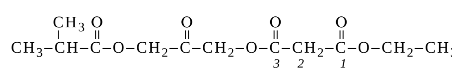
Benzoic acid, 3-sulfo- 1-phenyl ester



Benzoic acid, 3-(phenoxysulfonyl)-

Esterification of an alcoholic component cited in the index modification is expressed as a substituent of the esterifying radical.

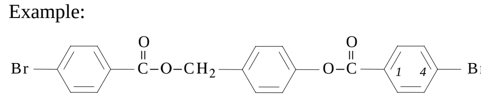
Example:



Propanedioic acid ethyl 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 (peroxoic, 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.

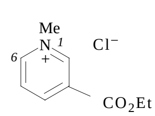
Example:



Benzoic acid, 4-bromo- 4-[[(4-bromobenzoyl)oxy]methyl]phenyl ester (not Benzoic acid, 4-bromo-, [4-[(4-bromobenzoyl)oxy]phenyl]methyl ester)

When functions higher in precedence than acids are present, all esters are expressed as substituents.

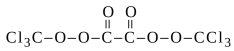
Example:



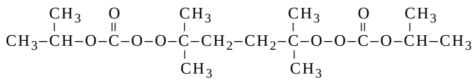
Pyridinium, 3-(ethoxycarbonyl)- 1-methyl- chloride

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.

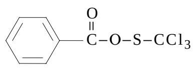
Examples:



Ethanediperoxoic acid bis(trichloromethyl) ester

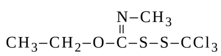


Carbonoperoxoic acid *OO,OO′*-(1,1,4,4-tetramethyl-1,4-butanediyl) *O,O′*-bis(1-methylethyl) ester



Benzenecarbo(thioperoxoic) acid *OS*-(trichloromethyl) ester

EtSSOMe — **Ethanesulfeno(thioperoxoic) acid *SO*-methyl ester**

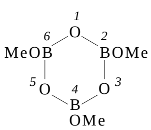


Carbono(dithioperox)imidic acid, methyl- *O*-ethyl *SS*-(trichloromethyl) ester

Esters of *boric acids* and their chalcogen analogs are indexed regularly, except for those of Hypoboric acid and cyclic metaboric acids, $(HBO_2)_n$, which are named as derivatives of the molecular skeletons.

Examples:

$(EtO)_2BB(OMe)_2$ — **Diborane(4), 1,1-diethoxy-2,2-dimethoxy-**



Boroxin, trimethoxy-

$(BuS)_2BOMe$ — **Thioboric acid ((HO)(HS)$_2$B) *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.

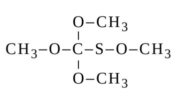
Examples:

$MeC(OMe)_3$ — **Ethane, 1,1,1-trimethoxy-** (not Orthoacetic acid, trimethyl ester)

$PhC(SMe)_3$ — **Benzene, [tris(methylthio)methyl]-**

$MeC(OEt)_2OH$ — **Ethanol, 1,1-diethoxy-**

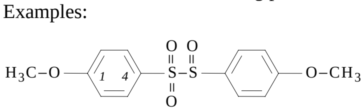
$MeC(OEt)_2OOCMe_3$ — **Peroxide, 1,1-diethoxyethyl 1,1-dimethylethyl**



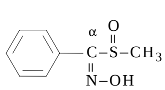
Methanesulfenic acid, trimethoxymethyl ester

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:



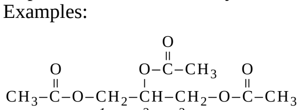
Benzene, 1-methoxy-4-[[(4-methoxyphenyl)sulfinyl]sulfonyl]-



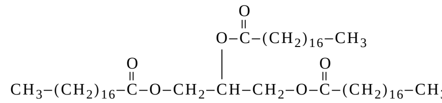
Benzenemethanimine, *N*-hydroxy-α-(methylsulfinyl)-

Glycerides, esters of **1,2,3-Propanetriol** (glycerol), are indexed at the name of the preferred acid unless only “Class I” acids are present.

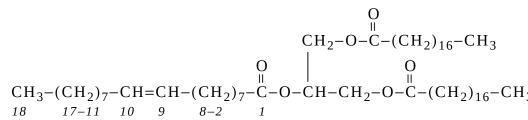
Examples:



1,2,3-Propanetriol triacetate



Octadecanoic acid 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**.

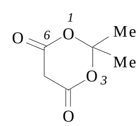
Examples:

$PhNHCO_2Et$ — **Carbamic acid, phenyl-ethyl ester**

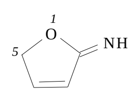
$PhOCS_2H$ — **Carbonodithioic acid *O*-phenyl ester**

Cyclic esters and lactones are indexed as heterocycles.

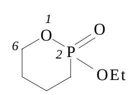
Examples:



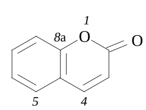
1,3-Dioxane-4,6-dione, 2,2-dimethyl- (not Propanedioic acid, cyclic 1-methylethylidene ester)



2(5*H*)-Furanimine (not 2-Butenimidic acid, 4-hydroxy-, γ-lactone)



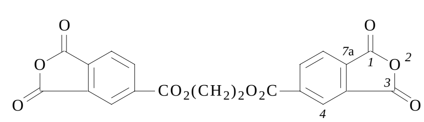
1,2-Oxaphosphorinane, 2-ethoxy-2-oxide (not Phosphonic acid, (4-hydroxybutyl)-, monoethyl ester, δ-lactone)



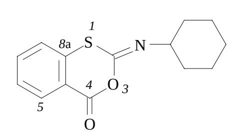
2*H*-1-Benzopyran-2-one (not Coumarin; not 2-Propenoic acid, 3-(2-hydroxyphenyl)-, δ-lactone)

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:

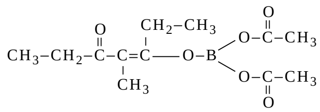


5-Isobenzofurancarboxylic acid, 1,3-dihydro-1,3-dioxo-1,2-ethanediyl ester

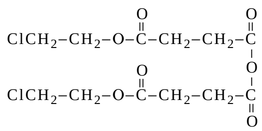


4*H*-3,1-Benzoxathiin-4-one, 2-(cyclohexylimino)- (not Carbonimidothioic acid, cyclohexyl-, anhydride with 2-mercaptobenzoic acid, cyclic ester)

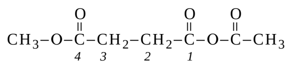
EtOP(OH)OAc — **Acetic acid**
monoanhydride with ethyl dihydrogen phosphite



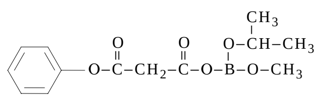
Acetic acid
dianhydride with boric acid (H_3BO_3) mono(1-ethyl-2-methyl-3-oxo-1-pentenyl) ester



Butanedioic acid
bimol. monoanhydride, bis(2-chloroethyl) ester

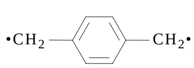


Butanedioic acid
monoanhydride with acetic acid, methyl ester



Propanedioic acid
monophenyl ester, anhydride with boric acid (H_3BO_3) monomethyl mono(1-methylethyl) ester (for the purposes of subdivision (see Appendix II, ¶10B), this compound is considered an anhydride, even though the ester term is cited first)

187. Free radicals are 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:

Et•	**Ethyl**
$PhCH_2$•	**Methyl, phenyl-**
	**Methyl, 1,4-phenylenebis-**
BrC⋮	**Methylidyne, bromo-**
EtO_2CCO• (2 1)	**Ethyl, 2-ethoxy-1,2-dioxo-** (not Acetyl, ethoxyoxo-)
H_2P•	**Phosphino**
F_2Si:	**Silylene, difluoro-**
$Ph_2NN(CHO)$• (2 1)	**Hydrazyl, 1-formyl-2,2-diphenyl-**

Free radicals that might be considered as derived from **Borane** are indexed at **Borane(1)** and **Borane(2)**.
Examples:

FHB•	**Borane(2), fluoro-** (not Boryl, fluoro-)
FB:	**Borane(1), fluoro-** (not Boron fluoride (BF))

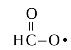
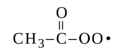
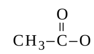
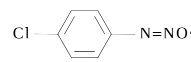
Free radicals from ammonia, amides, or amines are named as **Amidogen**, H_2N•, **Imidogen**, HN:, and their derivatives.

F_2N•	**Amidogen, difluoro-** (not Nitrogen fluoride (NF_2))
$PhCH(CO_2H)N$:	**Imidogen, (carboxyphenylmethyl)-**

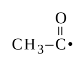
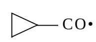
The heading parent **Nitroxide** is employed for the free radical H_2N-O•.
Example:

Me_2NO•	**Nitroxide, dimethyl**

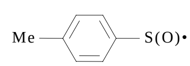
Free radicals from hydroxyl and hydroperoxy groups that are attached to a molecular skeleton, including (acyloxy) radicals (see below), are indexed at "-oxy" and "-dioxy" heading parents with systematically named nondetachable prefixes. Chalcogen analogs are named similarly at "-thio" and "-dithio" heading parents.
Examples:

MeO•	**Methoxy** (not Oxy, methyl-)
	**Methoxy, oxo-** (not Formyloxy)
	**Ethyldioxy, 1-oxo-**
	**Ethoxy, 1-oxo-** (not Acetyloxy)
	**Diazenyloxy, (4-chlorophenyl)-** (not (Phenylazo)oxy, 4-chloro-)
MeS•	**Methylthio**

Acyl free radicals (derived from aldehydes or acids) are named as α-oxo derivatives of the alkyl parents.
Examples:

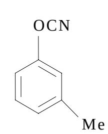
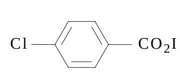
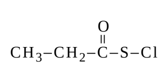
	**Ethyl, 1-oxo-** (not Acetyl)
	**Methyl, cyclopropyloxo-** (not Cyclopropylcarbonyl)
H_2NCO•	**Methyl, aminooxo-** (not Aminocarbonyl)

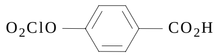
Free radicals from sulfonic and sulfinic acids are named as derivatives of alkyl and aryl sulfonyl and sulfinyl radicals and the analogous oxy radicals.
Examples:

CH_3-SO_2-O•	**(Methylsulfonyl)oxy**
	**Phenylsulfinyl, 4-methyl-**

The following chalcogen hydride free radicals are employed: **Hydroxyl**, HO•; **Hydroperoxo**, HOO•; **Mercapto**, HS•; **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; halic acids, $HOXO_2$; perhalic acids, $HOXO_3$; **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:

PhOF	**Hypofluorous acid** **phenyl ester**
$MeCO(CH_2)_2OBrO_2$	**Bromic acid** **3-oxobutyl ester**
	**Cyanic acid** **3-methylphenyl ester**
	**Benzoic acid, 4-chloro-** **anhydride with hypoiodous acid** (not Benzoyl hypoiodite, 4-chloro-)
	**Propanethioic acid** **anhydrosulfide with thiohypochlorous acid** (not Propanoyl thiohypochlorite)
$NCOCH_2CO_2H$	**Acetic acid, cyanato-**



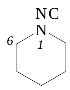
Benzoic acid, 4-(chloryloxy)-

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:

$CHCl_3$ **Methane, trichloro-** (not Chloroform)

$PhIO_2$ **Benzene, iodyl-**



Piperidine, 1-isocyano-

$Me_2Si(NCO)_2$ **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:

$PhI(OH)_2$ **Iodine, dihydroxyphenyl-**

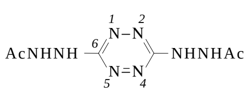
189. Hydrazides of principal acid groups are expressed by hydrazide terms in the index modification except for (*a*) sulfenic acid hydrazides, $R-S-NHNH_2$, which are indexed at **Hydrazine** with a "thio" substituent prefix; and (*b*) hydrazides of **Hydrazinecarboxylic acid**, for which the heading 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:

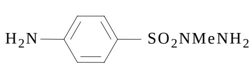
$PhCSNHNH_2$ **Benzenecarbothioic acid hydrazide**

AcNHNHAc **Acetic acid 2-acetylhydrazide** (not Hydrazine, 1,2-diacetyl-)

$HO_2CCH_2CONHNHPh$ **Propanedioic acid mono(2-phenylhydrazide)** (not Propanoic acid, 3-oxo-3-(2-phenylhydrazino)-)

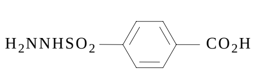


Acetic acid 2,2′-(1,2,4,5-tetrazine-3,6-diyl)dihydrazide

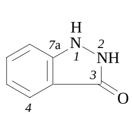


Benzenesulfonic acid, 4-amino-1-methylhydrazide

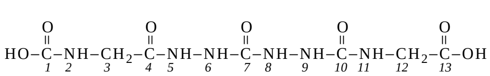
Diazenecarboxylic acid, (4-carboxyphenyl)-1-[2-(4-carboxyphenyl)hydrazide] (principle: hetero acyclic parent preferred)



Benzoic acid, 4-(hydrazinosulfonyl)-



3*H*-Indazol-3-one, 1,2-dihydro- (not Benzoic acid, 2-hydrazino-, cyclic hydrazide)

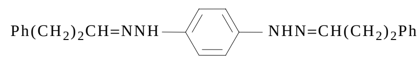


2,5,6,8,9,11-Hexaazatridecanedioic acid, 4,7,10-trioxo-

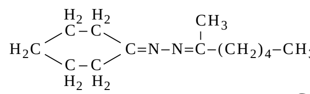
190. Hydrazones of ketone and aldehyde principal groups are expressed by hydrazone terms in the index modification except for hydrazones of carbonyl groups of acids, acid halides, and amides; these are usually indexed as hydrazonic acids (¶ 169) and their halides and amides. Azines are indexed as "-ylidene" hydrazones; osazones as dihydrazones (of adjacent carbonyl groups); cyclic hydrazones as heterocycles. In the presence of compound classes more preferred than the aldehyde or ketone bearing the hydrazone, a hydrazono substituent is cited.

Examples:

$Me_2C=NNH_2$ **2-Propanone hydrazone**



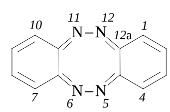
Benzenepropanal 1,4-phenylenedihydrazone



Cyclohexanone (1-methylhexylidene)hydrazone (not 2-Heptanone, azine with cyclohexanone) (principle: ring preferred to chain)

$PhNHN=CHSCH_2CO_2H$ **Acetic acid, [[(phenylhydrazono)methyl]thio]-** (not Acetic acid, mercapto-, formate, phenylhydrazone)

MeNHN=CPhCPh=NNHMe **Ethanedione, diphenyl-bis(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:

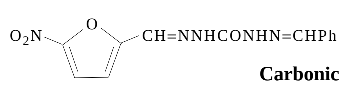
$MeCH=NN=PPh_3$ **Acetaldehyde (triphenylphosphoranylidene)hydrazone**

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:

$Me_2C=NNHCSNH_2$ (2 1) **Hydrazinecarbothioamide, 2-(1-methylethylidene)-** (not 2-Propanone, thiosemicarbazone)

PhCH=NNHCNHOEt **Hydrazinecarboximidic acid, (phenylmethylene)-ethyl ester** (not Benzaldehyde, 3-ethylisosemicarbazone)

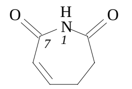


Carbonic dihydrazide, [(5-nitro-2-furanyl)methylene](phenylmethylene)- (not 2-Furancarboxaldehyde, 5-nitro, carbohydrazone with benzaldhyde)

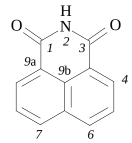
$PhCH=NNHCOCONH_2$ **Acetic acid, aminooxo-(phenylmethylene)hydrazide** (not Benzaldehyde, semioxamazone)

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, HN=C=NH (“carbodiimide”) is indexed at **Methanediimine**, and its derivatives are often to be found at amine or amide headings.

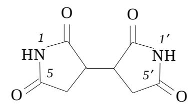
Examples:



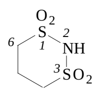
1*H*-**Azepine-2,7-dione, 3,4-dihydro-** (not 2-Hexenimide)



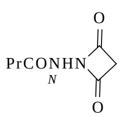
1*H*-Benz[*de*]isoquinoline-1,3-(2*H*)-dione (not 1,8-Naphthalenedicarboximide)



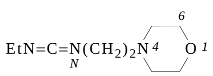
[3,3′-Bipyrrolidine]-2,2′,5,5′-tetrone (not 1,2,3,4-Butanetetracarboxylic 1,2:3,4-diimide



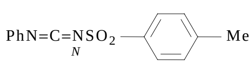
4*H*-1,3,2-Dithiazine, dihydro-1,1,3,3-tetraoxide (not 1,3-Propanedisulfonimide)



Butanamide, *N*-(2,4-dioxo-1-azetidinyl)-



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* at the name and formula of each component. (The formula headings used are those of the components.) 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, 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
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-
3*H*-Pyrazol-3-one, 2,4-dihydro-5-methyl-4-nitro-2-(4-nitrophenyl)-
Pyridine

In addition, compounds with *water* and *ammonia* are not indexed at these names; they are expressed as “hydrate” and “ammoniate,” with the prefixes mono, di, tri, etc. 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 (if known) in the modification. An additional entry appears at **Sulfurous acid**, **compounds**, **monosodium salt**, **compd**. **with**.... (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 stable anion of 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 (for molecular addition compounds that receive more than one) is that name to which cross-references in the *Index Guide* direct the reader from trivial names, 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*) a component other than a common component (see list above) selected according to the Order of Precedence of Compound Classes (¶ 106);

(*b*) a common component highest in the same order;

(*c*) 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):

1. (*a*) **2,5-Cyclohexadiene-1,4-dione, 2,3,5,6-tetrachloro-**
   compd. with coronene (no ratio cited because unknown; functional compound preferred to cyclic hydrocarbon)

   (*b*) **Coronene**
   compd. with 2,3,5,6-tetrachloro-2,5-cyclohexadiene-1,4-dione

2. (*a*) **Anthracene**
   compd. with 2,4,6-trinitrophenol (2:1) (only entry; the cyclic hydrocarbon is preferred to a common compound of higher rank)

3. (*a*) **Methane, 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)**” and an entry, in such a case, at **Chlorine**, **atomic**)

   (*b*) **Iodine**
   compd. with sulfinylbis[methane] (1:1) (note that multiplied heading parents are bracketed in the uninverted names)

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 isocyano, are always expressed as substituent prefixes (¶ 132). *aci*-Nitro, HON(O)=, is also a mandatory prefix, and it may be substituted; e.g., (propyl-*aci*-nitro) is $CH_3CH_2CH_2ON(O)=$; (benzoyl-*aci*-nitro) is $C_6H_5C(O)–ON(O)=$;

Diazene, HN=NH; **1-Triazene**, $NH=N–NH_2$; **Triazane**, $NH_2–NH–NH_2$, 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 Diazane and its derivatives. Except for hydrazides (¶ 189) and hydrazones (¶ 190), alkyl, aryl and acyl derivatives 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.

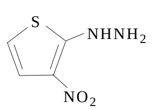
Examples (See also ¶ 161):

HN=N–	diazenyl (only when unsubstituted; otherwise azo is used)
–N=N–	azo (when attached to different atoms)
–N=N(O)–	azoxy (When used as a substituted monovalent radical, the position of the oxide (if known) is indicated by an *NNO*- or *ONN*-locant (see example below).)
H_2NNH–	hydrazino
H_2NN=	hydrazono
–NHNH–	hydrazo (when attached to different atoms)
–NHN=	1-hydrazinyl-2-ylidene
=NN=	azino
H_2NNHNH–	triazanyl
H_2NN=N–	1-triazenyl
HN=NNH–	2-triazenyl
–N=NNH–	1-triazene-1,3-diyl
$H_2NNHNHNH$–	tetrazanyl
=NNHNHN=	1,4-tetrazanediylidene

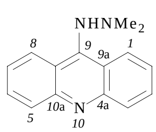
Hydrazides (¶ 189) and hydrazones (including azines) (¶ 190) are excluded from the following examples.

Examples:

H_2NNHCO_2H	**Hydrazinecarboxylic acid**
$HO_2CNHNHCO_2H$	**1,2-Hydrazinedicarboxylic acid**
$H_2NNHCONHMe$	**Hydrazinecarboxamide, *N*-methyl-**
Et_2NNHEt	**Hydrazine, triethyl-**
H_2NNHOH	**Hydrazine, hydroxy-**

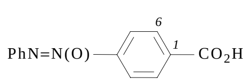


Hydrazine, (3-nitro-2-thienyl)- (principle: preferred hetero atom in heading parent (¶ 138))

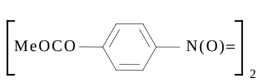


Acridine, 9-(2,2-dimethyl-hydrazino)- (principle: cyclic parent preferred (¶ 138))

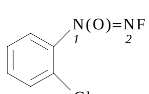
$PhN{=}NSO_3H$	**Diazenesulfonic acid, phenyl-**
$PhN{=}NCONH_2$	**Diazenecarboxamide, 2-phenyl-**



Benzoic acid, 4-(phenyl-*NNO*-azoxy)-

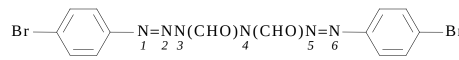


Benzoic acid, 4,4′-(dioxidoazo)bis-dimethyl ester

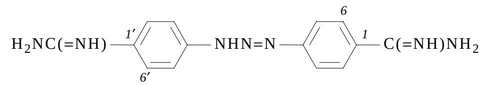


Diazene, (2-chlorophenyl)fluoro-1-oxide

$H_2NN{=}NAc$	**1-Triazene, 1-acetyl-**
$MeSO_2NHNHNHC({=}NH)Me$	**Triazane, 1-(1-iminoethyl)-3-(methylsulfonyl)-**



1,5-Hexazadiene-3,4-dicarboxaldehyde, 1,6-bis(4-bromophenyl)-

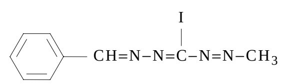


Benzenecarboximidamide, 4,4′-(1-triazene-1,3-diyl)bis-

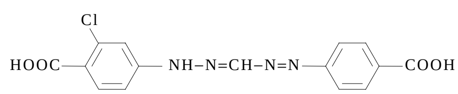
Formazan is a trivial name that describes the tautomeric compound H_2N–N=CH–N=NH. Beginning with the Thirteenth Collective period, the use of formazan and its associated prefixes, formazano and formazanyl, has been discontinued and compounds containing the formazan residue are named systematically.

Examples:

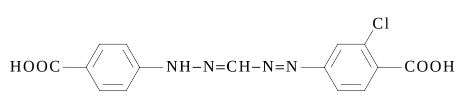
$H_2N{-}N{=}CH{-}N{=}NH$	**Diazenecarboxaldehyde, hydrazone** (formerly Formazan)
$H_2N{-}N{=}C(CH_3){-}N{=}N{-}CH_3$	**Diazene, (1-hydrazonoethyl)methyl-**
$H_2N{-}N{=}C(CH_2OH){-}N{=}N{-}CH_3$	**Ethanol, 2-hydrazono-2-(methylazo)-**



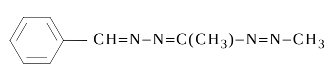
Diazenecarbohydrazonyl iodide, methyl(phenylmethylene)-



Benzoic acid, 4-[[[(4-carboxyphenyl)azo]methylene]hydrazino]-2-chloro-



Benzoic acid, 4-[[[(4-carboxyphenyl)hydrazono]methyl]azo]-2-chloro-



Benzaldehyde [1-(methylazo)ethylidene]hydrazone

Hydroxylamine, H_2NOH; **Thiohydroxylamine**, H_2NSH, 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; *S*-amino derivatives of **Thiohydroxylamine** are indexed as sulfenamides. When the nitrogen atom is unsubstituted, *O*-derivatives are usually indexed at **Hydroxylamine**, etc. The only suffixes employed are "sulfonic acid," "sulfonyl chloride," etc., when attached to the chalcogen atoms; the locant ("*O*" "*S*," etc.) is placed just ahead of the suffix.

Examples:

H_2NOSO_3H	**Hydroxylamine-*O*-sulfonic acid**
H_2NOAc	**Hydroxylamine, *O*-acetyl-**
H_2NOCO_2H	**Hydroxylamine, *O*-carboxy-**
$H_2NOCONH_2$	**Hydroxylamine, *O*-(aminocarbonyl)-**

$BuONH_2$	**Hydroxylamine, *O*-butyl-**
$H_2NO(CH_2)_2ONH_2$	**Hydroxylamine, *O*,*O*′-1,2-ethanediylbis-**
$EtSNH_2$	**Ethanesulfenamide**
PhNHOH	**Benzenamine, *N*-hydroxy-**
AcNHSH	**Acetamide, *N*-mercapto-**
$HONHCO_2H$	**Carbamic acid, hydroxy-**
$HONHCONH_2$	**Urea, hydroxy-**
$PhSO_2NHOH$	**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 (aminooxy), (aminothio), (hydroxyamino), etc., are employed.

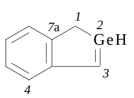
Examples:

$HONHCOCO_2H$	**Acetic acid, (hydroxyamino)oxo-**
$H_2NOCH_2NHNHNH_2$ (1 2 3)	**Triazane, 1-[(aminooxy)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:



1*H*-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:

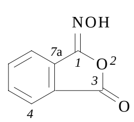
Li-Ph	**Lithium, phenyl-**
$Me_3P^+CH{=}CHCH_2HgBr \cdot Br^-$	**Phosphonium, [3-(bromomercurio)-1-propenyl]trimethyl-, bromide**

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), imidoyl halides (¶ 170), and imidamides (¶ 171). Cyclic oximes are indexed at heterocyclic parents, e.g., **Isoxazole**.

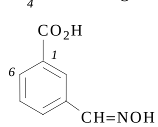
Acyclic oximes derived from aldehydes and ketones expressed as principal-group suffixes are expressed by "oxime" terms in the index modifications at the carbonyl-containing heading parents. When the carbonyl group is expressed as a substituent, it is replaced by the (hydroxyimino) radical, HO–N=. *O*-Alkyl, *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:

$H_2C{=}NOH$	**Formaldehyde, oxime**
$Ph_2C{=}NOH$	**Methanone, diphenyl-, oxime**

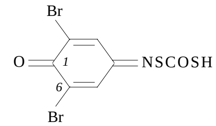


1,3-Isobenzofurandione, monooxime



Benzoic acid, 3-[(hydroxyimino)methyl]-

MeCH=NOMe	**Acetaldehyde, *O*-methyloxime**

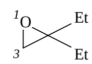


2,5-Cyclohexadiene-1,4-dione, 2,6-dibromo-, 4-[*S*-(thiocarboxy)thiooxime]

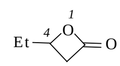
$MeCH{=}NOSO_3Me$	**Hydroxylamine-*O*-sulfonic acid, *N*-ethylidene-, methyl ester**

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.

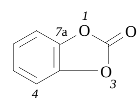
Examples:



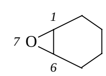
Oxirane, 2,2-diethyl- (not Butane, 1,2-epoxy-2-ethyl-)



2-Oxetanone, 4-ethyl- (not Pentanoic acid, 3-hydroxy-, β-lactone; see ¶ 185)



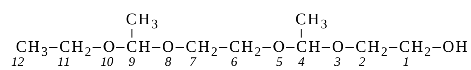
1,3-Benzodioxol-2-one (not Carbonic acid, cyclic 1,2-phenylene ester; see ¶ 185)



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:

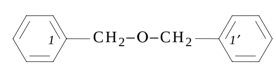


3,5,8,10-Tetraoxadodecan-1-ol, 4,9-dimethyl- (not Acetaldehyde, 1,2-ethanediyl ethyl 2-hydroxyethyl diacetal)

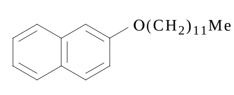
When "a" names are not permitted, acyclic ethers are indexed at heading parents (functional parent compounds, hydrocarbons, etc.) by use of "oxy" radicals, including the elided radicals (¶ 107) methoxy, ethoxy, propoxy, butoxy, and phenoxy.

Examples:

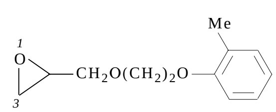
EtOMe	**Ethane, methoxy-** (not Ether, ethyl methyl)
Et_2O	**Ethane, 1,1′-oxybis-** (not Ethyl ether)



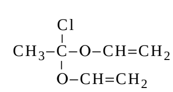
Benzene, 1,1′-[oxybis(methylene)]bis-



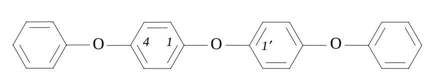
Naphthalene, 2-(dodecyloxy)- (principle: ring preferred to chain (¶ 138))



Oxirane, [[2-(2-methylphenoxy)ethoxy]methyl]- (principle: preferred ring)



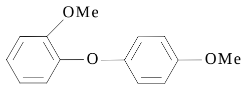
Ethene, 1,1′-[(1-chloroethylidene)bis(oxy)]bis- (principle: unsaturation)



Benzene, 1,1′-oxybis[4-phenoxy- (principles: centrality and multiplication)

$CH_3–CH_2–O–CH_2–CH_2–S–S–CH_2–CH_2–O–CH_2–CH_3$

Disulfide, bis(2-ethoxyethyl) (an "a" name cannot be used; only three hetero units (¶ 127) are present)



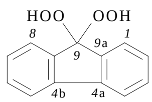
Benzene, 1-methoxy-2-(4-methoxyphenoxy)- principle: lowest locants for substituent prefixes)

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 sulfenothioic 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.

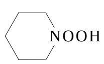
Examples:

EtOOH — **Hydroperoxide, ethyl** (the uninverted name is Ethyl hydroperoxide)

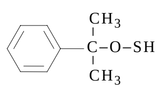


Hydroperoxide, 9*H*-fluoren-9-ylidenebis-

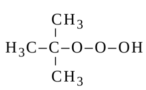
$HOOCH_2COPh$ — **Ethanone, 2-hydroperoxy-1-phenyl-**



Piperidine, 1-hydroperoxy-



Thiohydroperoxide, *O*-(1-methyl-1-phenylethyl)

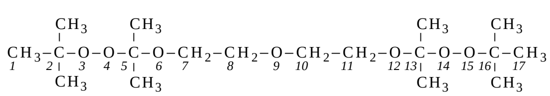


Hydrotrioxide, 1,1-dimethylethyl

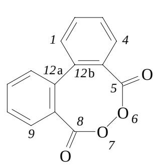
Acyl hydroperoxides are peroxy acids (¶ 165).

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:



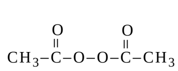
3,4,6,9,12,14,15-Heptaoxaheptadecane, 2,2,5,5,13,13,16,16-octamethyl-



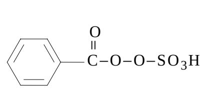
Dibenzo[*d*,*f*][1,2]dioxocin-5,8-dione

$Me_2CHOOCHMe_2$ — **Peroxide, bis(1-methylethyl)**

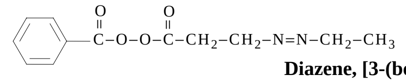
EtOOMe — **Peroxide, ethyl methyl** (the uninverted name is Ethyl methyl peroxide)



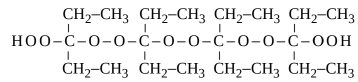
Peroxide, diacetyl



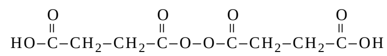
Peroxide, benzoyl sulfo



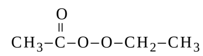
Diazene, [3-(benzoyldioxy)-3-oxopropyl]ethyl-



Hydroperoxide, [dioxybis[(1-ethylpropylidene)dioxy(1-ethylpropylidene)]]bis-

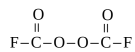


Butanoic acid, 4,4′-dioxybis[4-oxo-

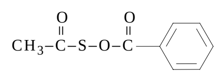


Ethaneperoxoic acid ethyl ester

MeOOF — **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), CH_3–O–O–O–, are used.

Example:

MeOOOMe — **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 **Phosphenous 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 (HO)P(O)(=NH) (or $(HO)_2P \equiv N$) and its chalcogen analogs.

TABLE VI
FUNDAMENTAL MONONUCLEAR PHOSPHORUS AND ARSENIC OXO ACIDS

	"Trivalent" acids		
$(HO)_3P$	**Phosphorous acid**	$(HO)_3As$	**Arsenous acid**
$(HO)_2HP$	**Phosphonous acid**	$(HO)_2HAs$	**Arsonous acid**
$(HO)H_2P$	**Phosphinous acid**	$(HO)H_2As$	**Arsinous acid**
HOPO	**Phosphenous acid** **Metaphosphorous acid (HPO_2)**	HOAsO	**Arsenenous acid**
	"Pentavalent" acids		
$(HO)_3PO$	**Phosphoric acid**	$(HO)_3AsO$	**Arsenic acid (H_3AsO_4)**
$(HO)_2HPO$	**Phosphonic acid**	$(HO)_2HAsO$	**Arsonic acid**
$(HO)H_2PO$	**Phosphinic acid**	$(HO)H_2AsO$	**Arsinic acid**
$HOPO_2$	**Phosphenic acid** **Metaphosphoric acid (HPO_3)**	$HOAsO_2$	**Arsenenic acid**

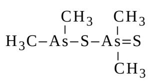
Examples:

$(PhNH)_2P(O)OH$ — **Phosphorodiamidic acid, *N*,*N*′-diphenyl-**

$Me_2\underset{2}{N}\underset{1}{N}HP(O)(OH)_2$	**Phosphorohydrazidic acid, 2,2-dimethyl-**
$Me\underset{N}{N}HP(OH)(=\underset{N''}{N}H)\underset{N'}{N}HMe$	**Phosphorodiamidimidic acid, *N*,-*N′*-dimethyl-**
Ph_2AsOH	**Arsinous acid, diphenyl-**
$EtNHAs(O)(OH)_2$	**Arsenamidic acid, 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:

$(EtO)_2PO(CH_2)_2NH_2$	**Phosphorous acid 2-aminoethyl diethyl ester**
$[Cl(CH_2)_2O]_3P$	**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**
	**Arsinodithioic acid, dimethyl- anhydrosulfide with dimethylarsinothious acid**

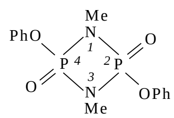
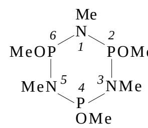
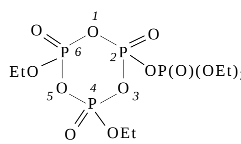
Nonacidic mononuclear arsenic and phosphorus names are derived from the acid names in the usual way by expressing the highest function as a class term, e.g., "amide," "chloride," and the other replacement terms in alphabetical order within the main part of the name. The descending order of precedence 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 ≡ N, are named at **Phosphonitrile** headings.

Examples:

$(H_2N)_3P{=}NH$	**Phosphorimidic triamide**
$Cl_3P{=}NH$	**Phosphorimidic trichloride**
$(H_2N)Cl_2PS$	**Phosphoramidothioic dichloride**
(H$_2$N)BrClPO	**Phosphoramidic bromide chloride**
(OCN)ClFPO	**Phosphorisocyanatidic chloride fluoride**
$(H_2N)_2(N_3)PO$	**Phosphorodiamidic azide**
$(H_2N)_2(NC)PO$	**Phosphorocyanidic diamide**
$(H_2NNH)F_2PO$	**Phosphorodifluoridic hydrazide**
$(H_2N)_3P$	**Phosphorous triamide**
Cl_3P	**Phosphorous trichloride**
ClF_2P	**Phosphorous chloride difluoride**
$(NC)H_2P$	**Phosphinous cyanide**
$(SCN)H_2P$	**Phosphinous isothiocyanate**
H_2NPS	**Phosphenothious amide**
ClP=NH	**Phosphenimidous chloride**
$(H_2N)ClHP{=}NH$	**Phosphonamidimidic chloride**
$Cl_2P{\equiv}N$	**Phosphonitrile chloride** (not Phosphoronitridic dichloride)
$(H_2N)_3AsO$	**Arsenic triamide**
$(H_2N)ClHAs{=}NH$	**Arsonamidimidic chloride**
$(NCS)_2HAsO$	**Arsonic dithiocyanate**
$(H_2N)H_2As{=}NH$	**Arsinimidic amide**
Cl_3As	**Arsenous trichloride**
Cl_2HAs	**Arsonous dichloride**
$(NC)H_2As$	**Arsinous cyanide**
ClAs=NH	**Arsenenimidous chloride**
BrAsO	**Arsenenous bromide**
Cl_3PO	**Phosphoric trichloride**
ClF_2PO	**Phosphoric chloride difluoride**
$(OCN)_3PO$	**Phosphoric triisocyanate**
Cl_3PS	**Phosphorothioic trichloride**
$OP{\equiv}N$	**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 at acyclic hydride names: **Phosphine**, PH_3; **Arsine**, AsH_3; **Phosphorane**, PH_5; **Arsorane** AsH_5; **Diphosphine**, $H_2P{-}PH_2$; **Triarsine**, $H_2As{-}AsH{-}AsH_2$; etc. Oxo, thio (etc.), and imino derivatives of **Phosphorane** and **Arsorane** are indexed at additive heading parents.

Examples:

H_3PO	**Phosphine oxide**
H_3AsSe	**Arsine selenide**
$H_3P{=}NH$	**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**
$Et_3P(Cl)P(O)Cl_2$	**Phosphonic dichloride, (chlorotriethylphosphoranyl)-**

Derivatives of **Phosphine** and other phosphorus and arsenic molecular skeleton parents are named substitutively by use of suffixes and prefixes.

Examples:

$(HO)_2P(O)CO_2H$	**Phosphinecarboxylic acid, dihydroxy- oxide**
F_4PNHMe	**Phosphoranamine, 1,1,1,1-tetrafluoro-*N*-methyl-**
Me_2AsCO_2H	**Arsinecarboxylic acid, dimethyl-**
$EtAsMe_2{=}NH$	**Arsine imide, *As*-ethyl-*As,As*-dimethyl-**

$(EtO)_5P$	**Phosphorane, pentaethoxy-**
$Ph_3As(OAc)_2$	**Arsorane, bis(acetyloxy)triphenyl-**
HPO	**Phosphine, oxo-**
MeAsS	**Arsine, methylthioxo-**
MePHPHMe	**Diphosphine, 1,2-dimethyl-**
(Me)(Ph)As–As(Ph)(Me)	**Diarsine, 1,2-dimethyl-1,2-diphenyl-**
MeAs=AsMe	**Diarsene, 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.)

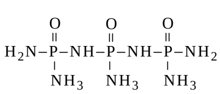
Examples:

$(HO)_2P(O)OP(O)(OH)_2$	**Diphosphoric acid**
$(HO)_2P(O)P(O)(OH)_2$	**Hypophosphoric acid**
$(HO)HP(O)OP(O)(OH)_2$	**Isohypophosphoric acid**
$(HO)_2POP(O)(OH)_2$	**Diphosphoric(III,V) acid**
$(HO)_2POP(OH)_2$	**Diphosphorous acid**
$(HO)_2P(O)NHP(O)(OH)_2$	**Imidodiphosphoric acid**
$(HO)_2P(O)OP(O)(OH)NHP(O)(OH)OP(O)(OH)_2$	*P′*-**Imidotetraphosphoric acid**
$(H_2N)_2P(O)NHP(O)(OH)_2$	*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 ($[(HO)_2P]_2S$)**; **Thiodiphosphoric(III,V) acid ($(HO)_2POP(S)(OH)_2$)**; **Thioperoxydiphosphoric acid ($[(HO)_2P(S)]_2S_2$)**; **Thioimidodiphosphoric acid ($[(HO)_2P(S)]_2NH$)**.

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:

$Cl_2P(O)OP(O)Cl_2$	**Diphosphoryl chloride** (the phosphorous analog is named **Diphosphorous tetrachloride**)
$(H_2N)_2POP(NH_2)_2$	**Diphosphorous tetraamide** (the phosphoric analog is named **Diphosphoramide**)
	**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**, see also 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_2P–	*phosphino	H_2As–	*arsino
$H_2P(O)$–	*phosphinyl	$H_2As(O)$–	*arsinyl
$H_2P(S)$–	phosphinothioyl	$H_2As(S)$–	arsinothioyl
$H_2P(=NH)$–	phosphinimyl	$H_2As(=NH)$–	arsinimyl
HP(≡N)–	phosphononitridyl	HAs(≡N)–	arsononitridyl
H_4P–	*phosphoranyl	H_4As–	*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)–	arsenoso
$P(O)_2$–	phospho	$As(O)_2$–	arso
$(HO)_2P(O)$–	phosphono	$(HO)_2As(O)$–	arsono
–P(O)(OH)–	phosphinico (multiplying radical only)	–As(O)(OH)–	arsinico (multiplying radical only)

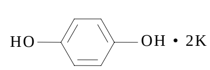
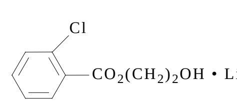
Radicals from polynuclear arsenic and phosphorus hydrides are formed like the carbon analogs.

Examples:

H_2PPH–	diphosphinyl
–PHPH–	1,2-diphosphinediyl
=PP=	1,2-diphosphinediylidene
–P=P–	1,2-diphosphenediyl
–As=As–	1,2-diarsenediyl
$–PH(PH)_2PH–$	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. The terms mono, di, and tri, Ewens-Bassett numbers (¶ 215), and ratios, are used as required (unless information is lacking), 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).

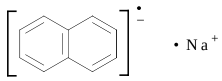
Examples:

AcOH • Na	**Acetic acid sodium salt**
	**1,4-Benzenediol dipotassium salt**
PhP(O)(OH)OEt • K	**Phosphonic acid, phenyl- monoethyl ester, potassium salt**
3 MeOH • Bi^{3+}	**Methanol bismuth(3+) salt**
	**Benzoic acid, 2-chloro- 2-hydroxyethyl ester, lithium salt**

When a metal (except Sb^{3+}, Bi^{3+}, Ge^{4+}, Sn^{4+}, or Pb^{4+}) 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**; **Acetamide**, **monosodium salt**; **Phosphine**, **cyclohexyl-**, **monolithium salt**; but unsubstituted **Hydrazine**, **Phosphine**, and **Arsine** afford the binary heading parents **Sodium hydrazide (NaN_2H_3)**; **Lithium arsenide (LiH_2As)**; **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.

Examples:



Naphthalene
radical ion(1–), sodium

$O_2N–\bar{C}H–NO_2 \cdot Na^+$

Methane, dinitro-
ion(1–), sodium

$CH_3–C(=O)–\bar{C}H–C(=O)–CH_3 \cdot K^+$

2,4-Pentanedione
ion(1–), potassium

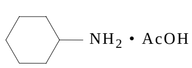
Uninverted names for metal salts of acids and esters are formed by citing first the metal, then the ester radical, then "hydrogen" (if any acidic group remains unaccounted for), and finally an "-ate" or "-ite" term. When the acid is one that requires a line formula, or has acidic sites, e.g., hydroxyl or amino substituents, elsewhere than in the principal chemical group, the acid name is placed first.

Examples:

sodium acetate
potassium hydrogen carbonate
calcium ethyl phosphate
zinc bis(methyl sulfate)
copper(2+) diacetate
boric acid (H_3BO_3) monopotassium salt
2-hydroxybenzoic acid monosodium salt
4-aminobenzoic acid calcium salt (2:1)

Amine, phosphine, etc., salts of acids, alcohols, thiols, etc., in general are indexed in the *Chemical Substance* and *Formula Indexes* at the names and formulas of both components. 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, 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 cyclohexanamine (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. Sometimes the designation "(salt)" must be added to an "-ate" term to differentiate it from an ester.

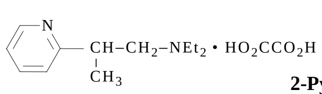
Examples:

$Me_2AsH \cdot HCl$

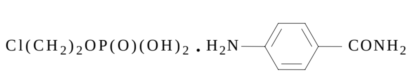
Arsine, dimethyl-
hydrochloride

$PhNH_2 \cdot H_3PO_4$

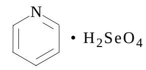
Benzenamine
phosphate (1:1)



2-Pyridineethanamine, ***N,N*-diethyl-β-methyl-**
ethanedioate (1:1)



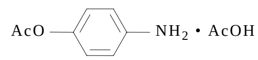
Benzamide, 4-amino-
compd. with 2-chloroethyl dihydrogen phosphate (1:1) (preferred index name)
Ethanol, 2-chloro-
dihydrogen phosphate, compd. with 4-aminobenzamide (1:1) (additional index name)



Selenic acid
compd. with pyridine (1:1) (only index name) (¶ 265A)

$MeCH_2CH(NH_2)CH_2OH \cdot HO_2CCO_2H$ (4 2 1)

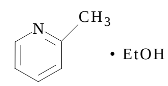
1-Butanol, 2-amino-
ethanedioate (1:1) (salt)



Phenol, 4-amino-
acetate (ester), acetate (salt)

For salts of amines, etc., with alcohols and thiols, a "compd. with" phrase and a ratio are used at both component headings.

Examples:



Ethanol
compd. with 2-methylpyridine (1:1) (preferred index name)
Pyridine, 2-methyl-
compd. with ethanol (1:1) (additional index name)

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). Both components are indexed in the *Chemical Substance* and *Formula Indexes* except for the following common anions:

(*a*) halide and halogenide simple anions, e.g., bromide, cyanide, thiocyanate, azide;
(*b*) chalcogenide anions, e.g., hydroxide, sulfide;
(*c*) anions derived from "Class I" acids, alcohols, and thiols (¶ 185), trifluoroacetic acid, trifluoromethanesulfonic acid, nitrous acid, perchloric acid, and 2,4,6-trinitrophenol;
(*d*) methyl sulfate ($MeOSO_3^-$), and ethyl sulfate ($EtOSO_3^-$);
(*e*) tetrafluoroborate(1–) (BF_4^-), tetraphenylborate(1–) (BPh_4^-), and hexafluorophosphate(1–) (PF_6^-).

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. In each example, below, the preferred index name is cited first; less preferred *Chemical Substance* and *Formula Index* names (if any) are then described.

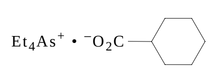
Examples:

$Me_4N^+ \cdot Br^-$

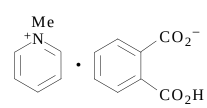
Methanaminium, *N,N,N*-trimethyl-
bromide

$Me_4N^+ \cdot MeCOS^-$

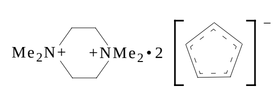
Methanaminium, *N,N,N*-trimethyl-
ethanethioate
Ethanethioic acid
ion(1–), *N,N,N*-trimethylmethanaminium



Arsonium, tetraethyl-
cyclohexanecarboxylate
Cyclohexanecarboxylic acid
ion(1–), tetraethylarsonium



Pyridinium, 1-methyl-
1,2-benzenedicarboxylate (1:1)
1,2-Benzenedicarboxylic acid,
ion(1–), 1-methylpyridinium



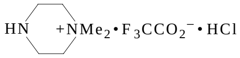
Piperazinium, 1,1,4,4-tetramethyl-
dicyclopentadienide
1,3-Cyclopentadiene
ion(1–), 1,1,4,4-tetramethylpiperazinium (2:1)

$Me_4N^+ \cdot {}^-NHPh$

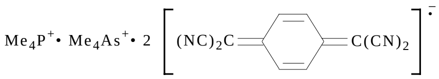
Methanaminium, *N,N,N*-trimethyl-
salt with benzenamine (1:1)
Benzenamine
ion(1–), *N,N,N*-trimethylmethanaminium

$Me_3N^+CH_2OH \cdot ClO_4^-$

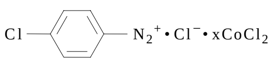
Methanaminium, 1-hydroxy-*N,N,N*-trimethyl-
perchlorate (salt) (note the use of the "(salt)" designation to resolve any ambiguity, even though the ester would have been named as a substituent)



Piperazinium, 1,1-dimethyl-
salt with trifluoroacetic acid (1:1), hydrochloride (¶ 281A)



Phosphonium, tetramethyl-
tetramethylarsonium, salt with 2,2′-(2,5-cyclohexadiene-1,4-diylidene)bis[propanedinitrile] (1:1:2)
Arsonium, tetramethyl-
tetramethylphosphonium, salt with 2,2′-(2,5-cyclohexadiene-1,4-diylidene)bis[propanedinitrile] (1:1:2)
Propanedinitrile, 2,2′-(2,5-cyclohexadiene-1,4-diylidene)bis-
radical ion(1−), tetramethylarsonium tetramethylphosphonium (2:1:1)

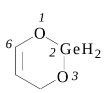


Benzenediazonium, 4-chloro-
chloride, compd. with cobalt chloride ($CoCl_2$)
Cobalt chloride ($CoCl_2$)
compd. with 4-chlorobenzenediazonium chloride
(Diazonium "double salts" of known ratio are indexed as "trichlorocobaltate(1−)," "tetrachlorocobaltate(2−)," etc.)

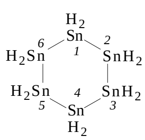
199. Silicon, **germanium**, **tin**, **and lead compounds** are indexed (*a*) as heterocyclic compounds, (*b*) as derivatives of acyclic hydride parents such as **Germane** or **Disilane**, (*c*) as special acyclic parents such as **Tristannathiane** or **Tetrasiloxane**, or (*d*) as silicic acids.

Heterocyclic compounds are indexed by the usual methods (¶¶ 146, 149).

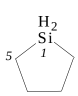
Examples:



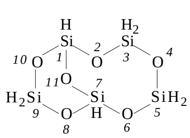
4*H*-1,3,2-Dioxagermin



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**, SiH_4; **Germane**, GeH_4; **Stannane**, SnH_4; **Plumbane**, PbH_4.

Examples:

H_3SiSiH_3	**Disilane**
$H_3GeGeH_2GeH_3$	**Trigermane**
$H_3Sn(SnH_2)_{11}SnH_3$	**Tridecastannane**
$H_3SiSiH_2SiH(SiH_3)SiH_2SiH_3$	**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:

$(H_3Si)_2O$	**Disiloxane**
$(H_3Si)_2S$	**Disilathiane**
$(H_3Ge)_2Se$	**Digermaselenane**
$(H_3Sn)_2Te$	**Distannatellurane**
$(H_3SnO)_2SnH_2$	**Tristannoxane**
$H_3Si(OSiH_2)_2OSiH_3$	**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, $H_3SiNHSiH_3$, 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.

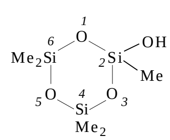
Example:

$\underset{1}{Me}\underset{2}{O}(CH_2)_2\underset{5}{O}CH_2\underset{7}{Si}Me_2\underset{8}{O}\underset{9}{Si}Me_2CH_2\underset{11}{O}(CH_2)_2\underset{14}{O}\underset{15}{Me}$

2,5,8,11,14-Pentaoxa-7,9-disilapentadecane, 7,7,9,9-tetramethyl-

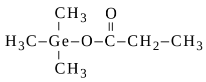
Derivatives of all these parents are named by the usual substitutive methods except for silicic acids and germanium, tin, and lead hydroxides and salts (see below). A hydroxyl group on a germanium, tin, or lead atom is expressed as a hydroxy prefix, but by the suffix "-ol" on a silicon atom when it is a principal group. *O*-Acyl silanols are named as esters.

Examples:

$SiCl_4$	**Silane, tetrachloro-**
Me_3SiCN	**Silanecarbonitrile, trimethyl-**
Me_3SnCN	**Stannanecarbonitrile, trimethyl-**
Me_3SiOH	**Silanol, trimethyl-**
$Et_3SiOSiEt_2OH$	**Disiloxanol, pentaethyl-**
H_3GeNH_2	**Germanamine**
$(HOSiMe_2)_2CH_2$	**Silanol, methylenebis[dimethyl-**
	**Cyclotrisiloxanol, pentamethyl-**
$\underset{1}{Cl}\underset{2}{Sn}Me_2\underset{3}{O}SnMe_2Cl$	**Distannoxane, 1,3-dichloro-1,1,3,3-tetramethyl-**
$Ph\underset{1}{Pb}(O)\underset{2}{O}\underset{3}{Pb}(O)Ph$	**Diplumboxane, 1,3-dioxo-1,3-diphenyl-**
$(Me_3Si)_2Se$	**Disilaselenane, hexamethyl-**
Me_2PbO	**Plumbane, dimethyloxo-**
$F_3\underset{1}{Si}\underset{2}{Si}H_3$	**Disilane, 1,1,1-trifluoro-**
$Et_3\underset{1}{Pb}\underset{2}{Pb}Et_3$	**Diplumbane, hexaethyl-**
$PhPb(O)OH$	**Plumbane, hydroxyoxophenyl-**
$HO\underset{1}{Ge}H_2\underset{2}{O}\underset{3}{Ge}H_2OH$	**Digermoxane, 1,3-dihydroxy-**

$(MeO)_3SiMe$ — **Silane, trimethoxymethyl-**

Me_3SiOAc — **Silanol, trimethyl-**
acetate



Germane, trimethyl(1-oxopropoxy)-

Substituent prefixes (radicals) from silicon, germanium, tin, and lead mononuclear hydrides are formed by adding the suffixes "-yl," "-ylene," and "-ylidyne" to the appropriate stem, or "-tetrayl" to the hydride name: silyl, H_3Si-; germylene, $H_2Ge=$; stannylidyne, HSn≡; plumbanetetrayl, =Pb=. Radicals from polynuclear hydrides and "oxanes," etc., are derived as for hydrocarbons.

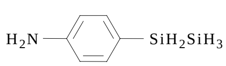
Examples:

H_3SiSiH_2-	disilanyl
$-GeH_2GeH_2-$ (1, 2)	1,2-digermanediyl (formerly digermanylene)
$H_3SnSnH_2SnH=$	tristannanylidene
≡SnSn≡ (1, 2)	1,2-distannanediylidyne
$H_3SiOSiH_2-$	disiloxanyl
$H_3SiNHSiH_2-$	disilazanyl
$-PbH_2OPbH_2-$ (1, 2 3)	1,3-diplumboxanediyl
$-SiH_2OSiHOSiH_2-$ (1, 3, 5; free valence on Si-3)	1,3,5-trisiloxanetriyl

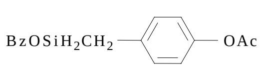
The nonfunctional silicon, germanium, tin, and lead hydrides fall (in that order) between boron and oxygen heading parents in order of precedence of compound classes (¶ 106). When a principal group is expressed as a suffix, the compound is classed accordingly. Thus **Silanol** is ranked with the alcohols, and the silicon "chain" places it above all carbon-chain monohydric alcohols, cyclic or acyclic (¶ 138).

Examples:

$Me_3SiOSiMe_2CH_2OH$ — **Methanol, (pentamethyldisiloxanyl)-** (not 3-Oxa-2,4-disilapentan-1-ol, 2,2,4,4-tetramethyl-)



Benzenamine, 4-disilanyl-



Silanol, [[4-(acetyloxy)phenyl]methyl]-
benzoate (not Phenol, 4-[[(benzoyloxy)silyl]methyl]]-, acetate)

$Et_3GeCH_2(CH_2)_4CH_2NH_2$ (6 … 1) — **1-Hexanamine, 6-(triethylgermyl)-**

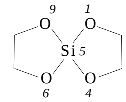
$H_3SiOSiH_2SSiH_3$ (3 2 1) — **Disiloxane, (silylthio)-**

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.

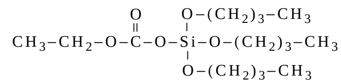
Examples:

$(EtO)_4Si$ — **Silicic acid (H_4SiO_4)**
tetraethyl ester

$(Me_2CHO)_3SiSH$ — **Thiosilicic acid (H_4SiO_3S)**
***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))



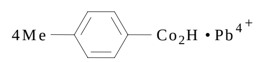
Carbonic acid
monoethyl ester, anhydride with silicic acid (H_4SiO_4) tributyl ester (see also ¶ 186)

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:

$Ge(OH)_4$ — **Germanium hydroxide ($Ge(OH)_4$)**

$SnO(OH)_2$ — **Tin hydroxide oxide ($Sn(OH)_2O$)**

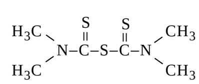


Benzoic acid, 4-methyl-
lead(4+) salt

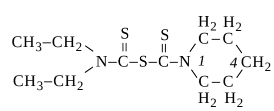
200. Sulfur, **selenium**, **and tellurium compounds** are often named similarly to oxygen compounds, but sometimes, e.g., in sulfonic and sulfenic acids (¶ 165), the sulfur, etc., acts as a nuclear atom in a functional group of which no oxygen analog is known. Because sulfur, selenium, and tellurium 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., **Thiodicarbonic acid**.

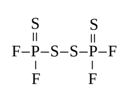
Examples:



Thiodicarbonic diamide ($[H_2NC(S)]_2S$), tetramethyl-



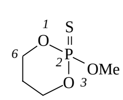
1-Piperidinecarbodithioic acid anhydrosulfide with diethylcarbamodithioic acid



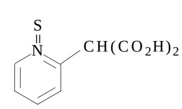
Thioperoxydiphosphoric tetrafluoride ($[F_2P(S)]_2S_2$)

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:

$MeC(=S=O)NH_2$ — **Ethanethioamide**
***S*-oxide**

$MeCH_2C(=S=O)CH_2(CH_2)_2Me$ (1, 3, 4, 7) — **3-Heptanethione**
***S*-oxide**

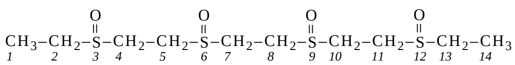
Phosphine sulfide, **Arsine sulfide**, and **Stibine sulfide** (¶¶ 181, 197) are substitutive parent compounds, but the sulfides of **Diphosphine**, **Triarsine**, etc., are named by modification terms.

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 (–S(O)–) and sulfonyl (–S(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."

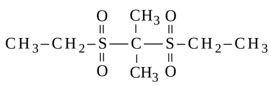
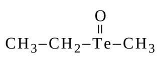
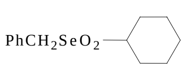
Examples:

$CH_3–S–CH_2–S–CH_2–S–CH_2–S–CH_3$ (numbered 1, 2, 3, 4, 5, 6, 7, 8, 9)

2,4,6,8-Tetrathianonane

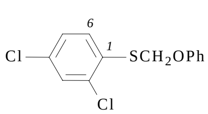


3,6,9,12-Tetrathiatetradecane 3,6,9,12-tetraoxide

$MeSeCH_2(CH_2)_2CO_2H$ (4 … 1)	**Butanoic acid, 4-(methylseleno)-**
$PhCOCH_2CH_2TePh$	**1-Propanone, 1-phenyl-3-(phenyltelluro)-**
$H_2NCH_2CH_2SeCH_2CH_2NH_2$ (1 2 2′ 1′)	**Ethanamine, 2,2′-selenobis-**
	**Propane, 2,2-bis(ethylsulfonyl)-** (principle: largest heading parent (¶ 138))
	**Ethane, (methyltellurinyl)-** (principle: largest heading parent)
$Me(CH_2)_6SO_2Ph$	**Benzene, (heptylsulfonyl)-** (principle: ring preferred over chain)
	**Benzene, [(cyclohexylselenonyl)-methyl]-** (principle: preferred ring system)
$H_2C{=}CHSCH_2SCH{=}CH_2$ (2 1 1′ 2′)	**Ethene, 1,1′-[methylenebis(thio)]-bis-** (principles: largest heading parent and multiplication)
$H_2C{=}CHSCHMeOEt$	**Ethene, [(1-ethoxyethyl)thio]-** (principle: maximum number of unsaturated bonds)

$Cl_2CHCH_2SCH_2CH_2SCH_2CH_2SCH_2CHCl_2$

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)
$Ph(CH_2)_2SPh$	**Benzene, [(2-phenylethyl)thio]-** (not Benzene, [2-(phenylthio)-ethyl]-) (principle: earliest index position)

Hydrodisulfides are named as dithioperoxoic acids, as sulfenothioic acids, or as thio analogs of mononuclear peroxy "oxo" acids. The oxides R–S(O)–SH and R–S(O)$_2$–SH are named as sulfinothioic and sulfonothioic acids.

Examples:

PhC(O)SSH	**Benzenecarbo(dithioperoxoic) acid**
EtSSH	**Ethanesulfenothioic acid**
$(HO)_2P(O)SSH$	**Phosphoro(dithioperoxoic) acid**
$HOSO_2SSH$	**Thioperoxymonosulfuric acid ((HO)(HSS)SO$_2$)**

The compounds R–S–S–SH, R–S(O)–S–SH, R–S(O)$_2$–S–SH, are named as sulfeno(dithioperoxoic) acids and their sulfino and sulfono analogs.

Example:

PhSSSH	**Benzenesulfeno(dithioperoxoic) acid**

Hydrotrisulfide is a radicofunctional heading parent for acyl derivatives, and **Hydrotetrasulfide**, etc., for alkyl, aryl, and acyl derivatives.

Example:

AcSSSH	**Hydrotrisulfide, acetyl**

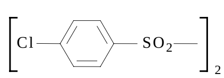
Cyclic polysulfides are named as heterocycles; acyclic sulfides fulfilling the requirements (¶ 127) of replacement nomenclature are indexed at "thia" names. Other acyclic disulfides, trisulfides, etc., are indexed at **Disulfide** and similar heading parents unless they are esters of dithioperoxoic acids 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 $HO_3S–S–S–SO_3H$.

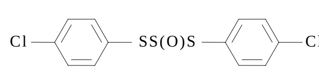
Examples:

$MeCH_2S(CH_2)_2OSSO(CH_2)_2SCH_2Me$ (1 3 6 7 8 9 12 14)	**6,9-Dioxa-3,7,8,12-tetrathiatetradecane**
$Me_2CHSSCHMe_2$	**Disulfide, bis(1-methylethyl)**
$PhCH_2SeSeCH_2Ph$	**Diselenide, bis(phenylmethyl)**
$(EtSSCH_2)_2$	**Disulfide, 1,2-ethanediylbis[ethyl**
PhSSSPh	**Trisulfide, diphenyl**
AcSSAc	**Disulfide, diacetyl**
$[Et_2P(Se)Se]_2Se$	**Triselenide, bis(diethylphosphinoselenoyl)**
EtOSSOEt	**Disulfide, diethoxy**
AcSSCl	**Disulfide, acetyl chloro**
$Cl(CH_2)_2SSSCl$	**Trisulfide, chloro 2-chloroethyl**
FC(O)SSCN	**Disulfide, cyano fluorocarbonyl** (not Formyl fluoride, (cyanodithio)-)

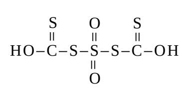
The heading parents **Disulfoxide**, **Trisulfone**, etc., are employed for chalcogen compounds in which the same number of oxygen atoms is attached to each skeletal atom. When all oxide atoms are on one sulfur, the compounds are named whenever possible as esters or anhydrides of thio analogs of sulfur 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.

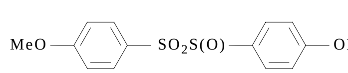
Examples:

$[MeS(O)]_2$	**Disulfoxide, dimethyl**
	**Disulfone, bis(4-chlorophenyl)**
$PhSO_2SPh$	**Benzenesulfonothioic acid *S*-phenyl ester**



Thiosulfurous acid (H$_2$S$_3$O) *S,S*-bis(4-chlorophenyl) ester

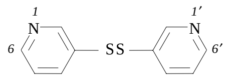
	**Carbonodithioic acid bis(anhydrosulfide) with thiosulfuric acid (H$_2$S$_3$O$_2$)**



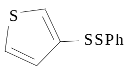
Benzene, 1-methoxy-4-[[(4-methoxyphenyl)sulfinyl]sulfonyl]- (not Benzene, 1-methoxy-4-[[(4-methoxyphenyl)sulfonyl]sulfinyl]-) (principle: earliest index position)

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)

$HO_3SCH_2CH_2SS(O)(CH_2)_2SO_3H$ (carbons numbered 1, 2)

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 dithioperoxoic acids or peroxy mononuclear "oxo" acids.

Examples:

$CH_3{-}C(=O){-}S{-}S{-}CH_3$

Ethane(dithioperoxoic) acid methyl ester

$PhSO_2SSPh$

Benzenesulfono(dithioperoxoic) acid phenyl ester

$HOSO_2SSMe$

Thioperoxymonosulfuric acid ((HO)(HSS)SO$_2$) ***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:

$HO{-}CH_2{-}CH_2{-}NH{-}C(=S){-}S{-}S{-}C(=S){-}NH{-}CH_2{-}CH_2{-}OH$

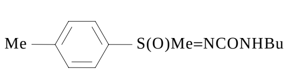
Thioperoxydicarbonic diamide ([(H$_2$N)C(S)]$_2$S$_2$), *N,N′*-bis(2-hydroxyethyl)-

Sulfilimine, $H_2S{=}NH$, and **Sulfoximine**, $H_2S(O){=}NH$, 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) but *N*-derivatives containing higher chemical functions must often be indexed at the chalcogen parents for lack of an acceptable name for the $H_2S{=}$, etc., radicals. However, higher functions in chalcogen-linked derivatives can be recognized by use of other chalcogen-nitrogen parents or by sulfonimidoyl, sulfinimidoyl, etc., radicals.

Examples:

$Et_2S{=}NSO_2Ph$

Sulfilimine, *S,S*-diethyl-*N*-(phenylsulfonyl)-



Sulfoximine, *N*-[(butylamino)carbonyl]-*S*-methyl-*S*-(4-methylphenyl)-

$PhS(OH){=}NPh$

Benzenesulfinimidic acid, *N*-phenyl-

$(MeO)_2S{=}NPh$

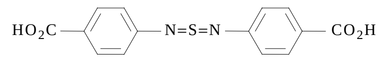
Imidosulfurous acid, phenyl-dimethyl ester

$MeS(O)({=}NH)CH_2CH_2CH(NH_2)CO_2H$ (carbons numbered 4, 2, 1)

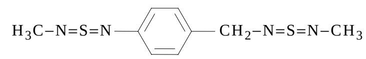
Butanoic acid, 2-amino-4-(*S*-methylsulfonimidoyl)-

Sulfur diimide, $HN{=}S{=}NH$, and **Sulfur triimide**, $HN{=}S({=}NH){=}NH$, are substitutive heading parents. All derivatives are, if possible, expressed as substituents.

Examples:



Sulfur diimide, bis(4-carboxyphenyl)-



Sulfur diimide, methyl[4-[[(methylsulfinimidoyl)amino]methyl]phenyl]-

Sulfimide, $O_2S{=}NH$, 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 ($O_2S{=}$) (sulfinylamino) ($OS{=}N{-}$), etc., radicals.

Examples:

$O_2S{=}NMe$ — **Methanamine, *N*-sulfonyl-**

$PhSO_2N{=}SO$ — **Benzenesulfonamide, *N*-sulfinyl-**

Amidosulfenyl chloride ($H_2N{-}S{-}Cl$) is ranked with mononuclear "oxo" acid halides and can be expressed by (chlorothio) and [(chlorothio)amino] radicals when necessary.

Example:

$PhSO_2NMeSCl$ — **Amidosulfenyl chloride, methyl-(phenylsulfonyl)-** (not Benzenesulfonamide, *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 sulfenic (etc.) acid analog.

Example:

PhSSePh — **Benzenesulfenoselenoic 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:

$PhSF_5$ — **Sulfur, pentafluorophenyl- (*OC*-6-21)-**

Ph_2TeCl_2 — **Tellurium, dichlorodiphenyl- (*T*-4)-**

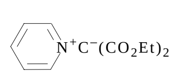
201. Zwitterionic compounds have internally compensating ionic centers. When the cationic center is known, the compound is named either as an "inner salt" or as an "ylide."

Ylides have a compensating carbanion *adjacent to* the cationic center. They are named at the "-ium" heading (except **Phosphonium**) with the suffix "-ide" added to the hydrocarbon radical to express the anion. Phosphonium ylides are indexed only as ylidene derivatives of **Phosphorane** (at this heading or by use of a phosphoranylidene radical).

Examples:

$Me_3N^+CH_2^-$ — **Methanaminium, *N,N*-dimethyl-methylide**

$PhCOC^-HS^+Me_2$ — **Sulfonium, dimethyl-2-oxo-2-phenylethylide**



Pyridinium 2-ethoxy-1-(ethoxycarbonyl)-2-oxoethylide

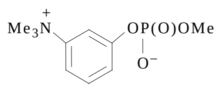
$Ph_3P{=}CHPh$ — **Phosphorane, triphenyl(phenylmethylene)-** (preferred index name)

Zwitterionic compounds other than ylides 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 "-diium" 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.

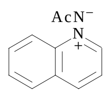
Examples:

$Me_3N^+CH_2CO_2^-$
N *1*

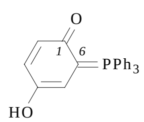
Methanaminium, 1-carboxy-*N*,*N*,*N*-trimethyl-
inner salt



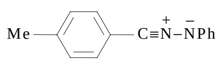
Benzenaminium, 3-[(hydroxymethoxyphosphinyl)oxy]-*N*,*N*,*N*-trimethyl-
inner salt



Quinolinium, 1-(acetylamino)-
inner salt



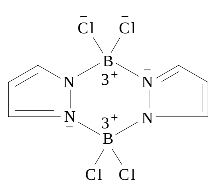
2,4-Cyclohexadien-1-one, 4-hydroxy-6-(triphenylphosphoranylidene)- (the alternative ionic structure is named **Phosphonium, (2,5-dihydroxyphenyl)triphenyl-, inner salt**)



Hydrazinium, [(4-methylphenyl)methylidyne]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:

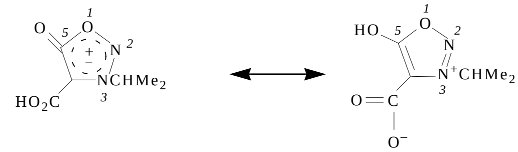


Boron, tetrachlorobis[μ-(1*H*-pyrazolato-*N*[1]:*N*[2])]di- (not 4*H*,4*H*,8*H*,8*H*-7a,8a-Diaza-3a,4a-diazonia-4,8-diborata-*s*-indacene, 4,4,8,8-tetrachloro-)

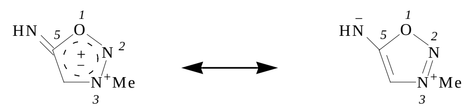
Meso-ionic compounds such as sydnone derivatives are named, if possible, at an "-ium" parent by use of the term "inner salt" in the modification.

Examples:

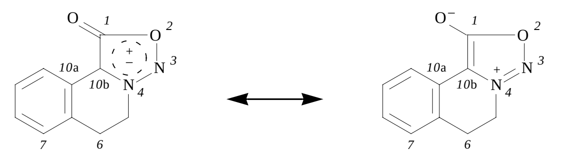
mesoionic form preferred structure



1,2,3-Oxadiazolium, 4-carboxy-5-hydroxy-3-(1-methylethyl)-
inner salt (formerly Sydnone, 4-carboxy-3-(1-methylethyl)-



1,2,3-Oxadiazolium, 5-amino-3-methyl-
inner salt (formerly Sydnone imine, 3-methyl-)



[1,2,3]Oxadiazolo[4,3-*a*]isoquinolin-4-ium, 5,6-dihydro-1-hydroxy-
inner salt

E. STEREOCHEMISTRY AND STEREOPARENTS

Introduction	¶ 202	Carbohydrates	¶ 208
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Peptides	206	Terpenes	212
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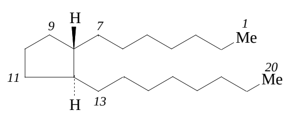
202. Introduction. A discussion of stereochemical descriptors for systematically named compounds, modified stereoparents, and coordination compounds follows this introduction. The remainder of Section E is directed to various classes of stereoparents. A stereoparent is an index heading parent the name 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.

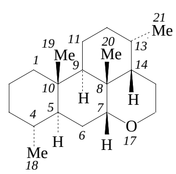
It is convenient to divide natural products into four classes according to the methods by which they are indexed. The classification has been most completely worked out for alkaloids, discussed more fully in ¶ 204, below.

Class A contains those substances, of little or no stereochemical complexity, which are indexed systematically rather than at 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 *((1S,2S)-1-heptyl-2-octylcyclopentane)*



Picrasane **(**(3*S*,3a*S*,6a*R*,7a*S*,8*R*,11a*S*,11b*R*,11c*S*)-*hexadecahydro-3,8,11a,11c-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, (5α,**17**β)- (not Butanoic acid, (5α,17β)-androstan-17-yl ester)
L-**Valine**
  2′-ester with adenosine

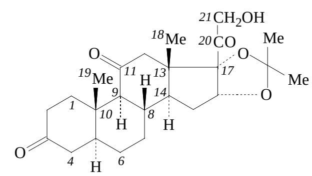
Molecular addition compounds and salts of stereoparents with nonstereoparents are indexed at the name and formula of each component. The preferred *CA* name is the one that employs the stereoparent in the index heading parent. Addition compounds and salts containing more than one stereoparent derivative are assigned preferred index names based on chemical functionality of the stereoparents.

Example:

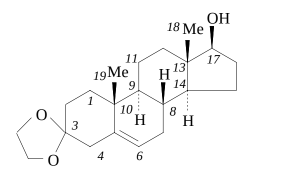
L-**Proline**
  compd. with (8α,9*R*)-cinchonan-9-ol (1:1) (preferred index name)
Cinchonan-9-ol
  (8α,9*R*)-, compd. with L-**proline (1:1)** (additional index name)

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)]-(5α,16α)-



Androst-5-en-3-one, 17-hydroxy-cyclic 1,2-ethanediyl acetal, (17β)-

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 names[1] 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

[1]For 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.

structures containing stereoparents. The new policy was expanded in June 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.

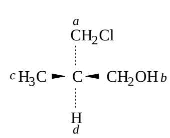
The terms *R* and *S* are employed for chiral elements possessing either absolute or relative stereochemistry. The term *rel* is used in conjunction with *R* and *S* for structures with only relative stereochemistry. *E* and *Z* are used primarily to describe geometrical isomerism about double bonds. 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 bromochlorofluoroiodomethane 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.

R *S*

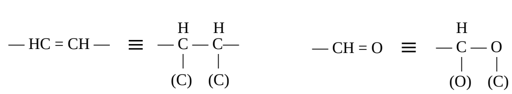
Alternative ways of drawing chiral diagrams are often more convenient: either (a) at most two bonds (as indicated by ordinary lines) are shown to be in the plane while one projects forward and one backward (as indicated by a wedge and a dotted line, respectively), or (b) two bonds are shown projecting 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.



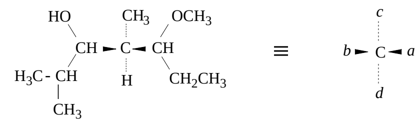
In the structure above, H clearly has the lowest priority, but it is necessary to establish the ranking of the three carbon groups. This is done by arranging the atomic numbers of *the most senior substituent* on each carbon in descending order: Cl, O, H. This elicits the absolute stereochemical descriptor *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.

The following groups are arranged in descending order of Sequence Rule priority: $-SCH_3$, -SH, $-OCOCH_3$, $-OCH_2CH_3$, $-OCH_3$, -OH, $-NO_2$, $-N(CH_3)_2$, $-NH_2$, -COOH, $-COCH_3$, -CHO, $-CH_2OH$, -C≡N, $-CH_2NH_2$, $-C_6H_5$, $-C(CH_3)_2CH_2CH_3$, $-C(CH_3)=CH_2$, $-CH(CH_3)CH_2CH_3$, $-CH_2CH_2CH_3$, $-CH_2CH_3$, $-CH_3$. 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 enter 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, $-OCH_2CH_3$ replaced $-OCH_3$ on the right.)

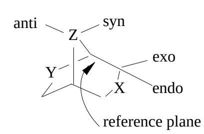
In complicated cases it is sometimes necessary to construct an exploration table or tree diagram in assigning *R* and *S* descriptors. A useful summary of Sequence Rule procedures is included in Section E of the IUPAC rules,[2] but consultation of the papers of Cahn, Ingold and Prelog, especially their 1966 paper,[3] may be necessary for resolution of the most difficult cases.

Relative descriptors of various kinds are used as follows:

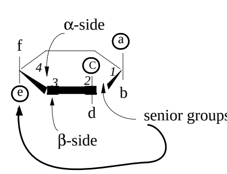
(*A*) *cis* and *trans* are restricted to cyclic structures with two achiral stereogenic atoms (an atom is stereogenic when interchange of two of the atoms or groups attached to it produces a nonidentical compound). An example is **1,3-Cyclobutanediol**. The *cis* isomer has the senior groups (as defined 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 ≥ 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).

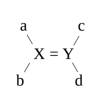
(*C*) *syn* and *anti* are restricted to achiral ring positions on the Z bridge of a bicyclo[X.Y.Z]ane in which X ≥ Y > Z > 0, and X + Y < 7. The *syn* isomer has the senior substituent oriented towards the X bridge.



(*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

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[2]International 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.

[3]R. 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.

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 (±) 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.

Treatment of categorized substance headings and structural repeating units is illustrated elsewhere in this appendix.

(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.

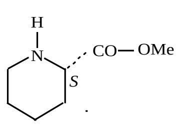
(11) Bicyclo[X.Y.Z]ane compounds in which X≥Y>Z>Ø, and X+Y<7, and which contain achiral stereogenic elements are the only structures for which *endo*, *exo*, *syn*, and *anti* are used. These terms are each preceded by a locant which is followed by a hyphen with the resulting stereochemical expression 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.

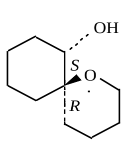
Examples:

$C_7H_{13}NO_2$
Stereo: absolute



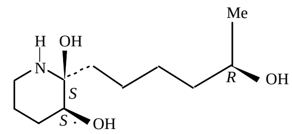
2-Piperidinecarboxylic acid, methyl ester, (2*S*)-

$C_{10}H_{18}O_2$
Stereo: relative



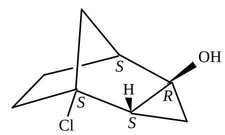
1-Oxaspiro[5.5]undecan-7-ol, (6*R*,7*S*)-*rel*-

$C_{11}H_{23}NO_3$
Stereo: absolute (-)



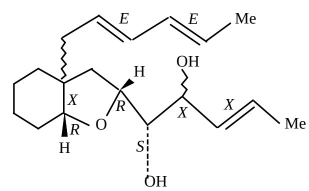
2, 3-Piperidinediol, 2-[(5*R*)-5-hydroxyhexyl]-, (2*S*,3*S*)-

$C_8H_{11}C10$
Stereo: relative



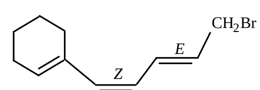
Tricyclo[3.2.1.0^{2,4}]octan-2-ol, 5-chloro-, (1*R*,2*S*,4*R*,5*R*)-*rel*-

$C_{19}H_{30}O_3$
Stereo: absolute partial



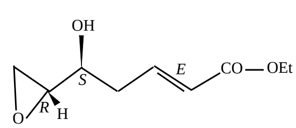
3-Pentene-1,2-diol, 1-[(2*R*,7a*R*)-3a-(2*E*,4*E*)-2,4-hexadienyloctahydro-2-benzofuranyl]-, (1*S*)-

$C_{11}H_{15}Br$
Stereo: relative



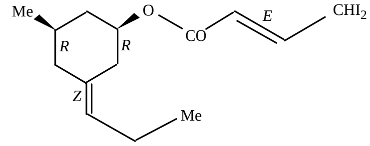
Cyclohexene, 1-[(1*Z*, 3*E*)-5-bromo-1,3-pentadienyl]-

$C_9H_{14}O_4$
Stereo: absolute



2-Pentenoic acid, 5-hydroxy-5-(2*R*)-oxiranyl-, (2*E*,5*S*)-

$C_{14}H_{20}I_2O_2$
Stereo: relative (+)

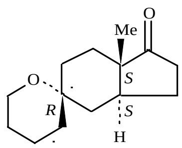


2-Butenoic acid, 4,4-diiodo-, (1*R*,3*R*,5*Z*)-3-methyl-5-propylidenecyclohexyl ester, (2*E*)-*rel*-(+)-

[The *Z* double bond is cited on the atom closer to the parent.]

[4] J. 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.

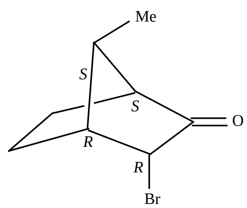
$C_{14}H_{22}O_2$
Stereo: absolute



Spiro[5*H*-indene-5,2´-[2*H*]pyran]-1(4*H*)-one, decahydro-7a-methyl-, (2´*R*,3a*S*,7a*S*)-

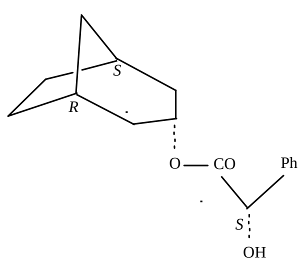
[The lower locant (2´) is used to cite the *R* center.]

$C_8H_{11}BrO$
Stereo: absolute



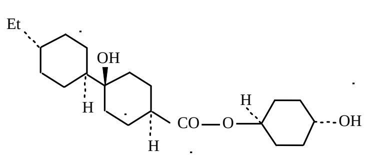
Bicyclo[2.2.1]heptan-2-one, 3-bromo-7-methyl-, (1*S*,3*R*,4*R*,7*S*)-

$C_{16}H_{20}O_3$
Stereo: absolute



Benzeneacetic acid, α-hydroxy-, (3-*endo*)-bicyclo[3.2.1]oct-3-yl ester, (α*S*)-

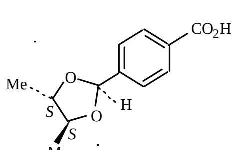
$C_{21}H_{36}O_4$
Stereo: relative



[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*.]

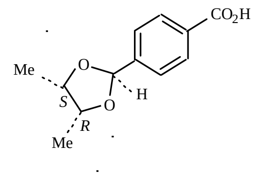
$C_{12}H_{14}O_4$
Stereo: absolute



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.]

$C_{12}H_{14}O_4$
Stereo: relative

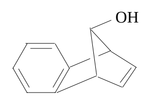


Benzoic acid, 4-[(2α,4β,5β)-4,5-dimethyl-1,3-dioxolan-2-yl]-

[The 2-position on the dioxolane ring is achiral stereogenic.]

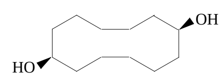
The stereochemistry of some compounds cannot be described completely by the rules above. The presence of stereochemical information in an original document is indicated in the index entries for such compounds by the modification term "stereoisomer."

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 (only the preferred index entry is shown here for each compound):

Cyclohexanol, 4-amino-
trans-, **acetate (salt)**

2-Furancarboxylic acid, tetrahydro-2-methoxy-
(2*R*)-, **compd. with** *rel*-**methyl (**1*R*,2*S***)-**
2-aminocyclobutanecarboxylate

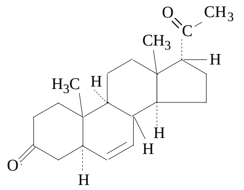
1,2-Cyclobutanedicarbonyl dichloride
*(*1*R*,2*R)-rel-*, **polymer with** *rel*-(2*R*,5*S*)-**2,5-dimethylpiperazine**

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.

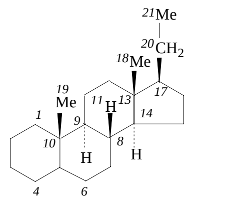
II. *Stereoparents* have been discussed in ¶ 202. Their use enables lengthy stereochemical descriptors to be dispensed with. Cross-references and synonyms relating stereoparents to the corresponding systematic names appear (as stereospecifically as possible) in the *Index Guide*, and author names for stereoparents and derivatives are also cross-referred.

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., [(5α,16*E*)-androstan-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]-,** (5α,6β)-.

Examples (the stereoparent diagram is compared with an author's diagram for a derivative in each case):

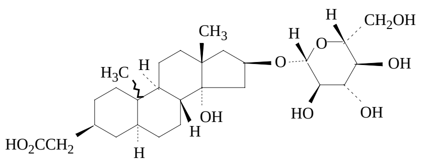


A pregnane derivative

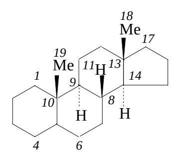


Pregnane (stereoparent)

[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 (5α,17α)-.]



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 (3β,5α,10ξ,16β)-. [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. Sloan[5] 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+}, $Pt2^{+}$, 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 ammines 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 complex-es 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.

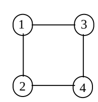
T-4	tetrahedral
SP-4	square planar
TB-5	trigonal bipyramidal
SP-5	square pyramidal
OC-6	octahedral
TP-6	trigonal prismatic
PB-7	pentagonal bipyramidal
OCF-7	octahedral faced monocapped
TPS-7	trigonal prismatic square faced monocapped
CU-8	cubic
SA-8	square antiprismatic
DD-8	dodecahedral
HB-8	hexagonal 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 $Ma_2b_2c_2$, 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:



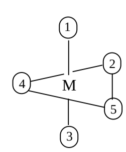
Configuration number = 4

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

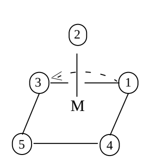
Chirality symbol = A

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*) S*quare 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

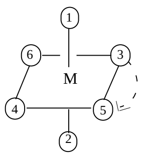
Stereochemical descriptor = (*SP*-5-25-*A*)-

(When all coordinating sites are unlike, 15 configurations are possible. Each is chiral, affording 30 possible stereoisomers.)

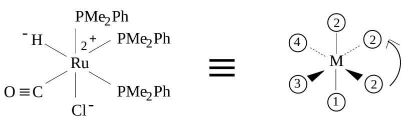
[5]T. E. Sloan in *Topics in Inorganic and Organometallic Stereochemistry*, G. Geoffroy, ed., John Wiley & Sons, Inc., New York, **1981**, 1-36.

(*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:



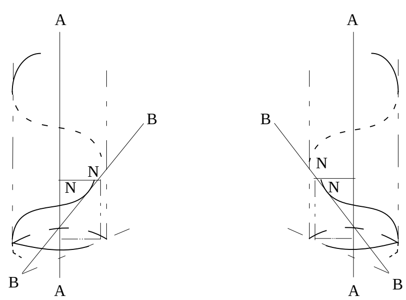
Configuration number	= 24
Chirality symbol	= C
Stereochemical descriptor	= (*OC*-6-24-*C*)-



(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:



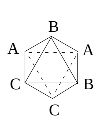
(*a*) Δ (*b*) Λ

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.

(*c*) (*d*)

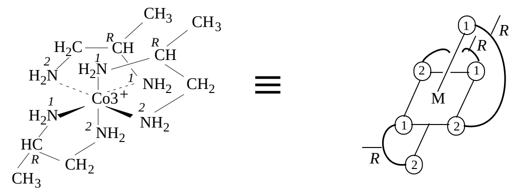
AA and BB have now lost their respective identities as axis and tangent and can be considered either as two tangents or as two segments of a double helix. BB is in front of AA in both diagrams; in (*c*), when AA is horizontal, BB descends to the right, in (*d*) to the left.

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.)



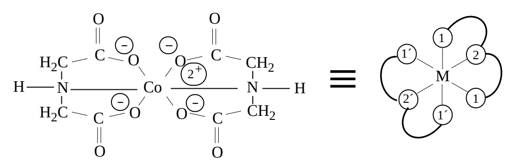
(*e*)

The helicity symbol replaces the chirality symbol in octahedral complexes of this type. In the complex named in abbreviated fashion as $[Co(1,2\text{-}pn)_3]^{3+}$ 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 CH_2). 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*)]-

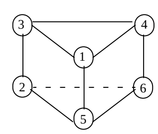
Octahedral complexes containing identical bis(tridentate) ligands are assigned geometric and chirality symbols in the same manner as normal octahedral complexes. However, in order to distinguish between enantiomers it is necessary to add primes to the donor atoms of one ligand. The primes are retained 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:

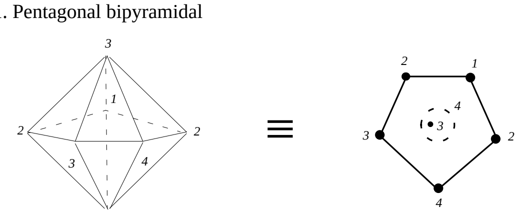


Configuration number	= 526
Chirality symbol	= A
Stereochemical descriptor	= (*TP*-6-526-*A*)

(g) Stereochemical descriptors were extended to 7-, 8-, and 9- coordinate complexes in *CA* indexes in 1977.[6]

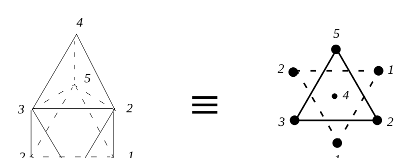
In the following table, all 12 model polyhedra for 7-, 8-, and 9-coordinate complexes are shown, with examples of priority numbers for ligands from which configuration numbers are derived.

1. Pentagonal bipyramidal



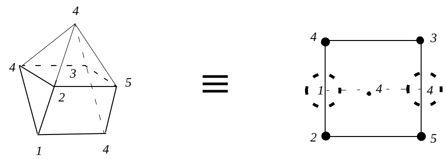
PB-7-34-12342

2. Octahedral faced monocapped



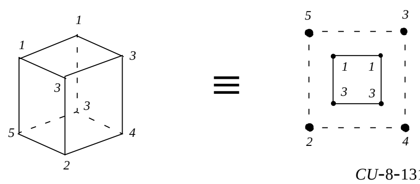
[6] M. F. Brown, B. R. Cook, and T. E. Sloan, *Inorg. Chem.* **1978**, 17, 1563-1568.

3. Trigonal prismatic square faced monocapped



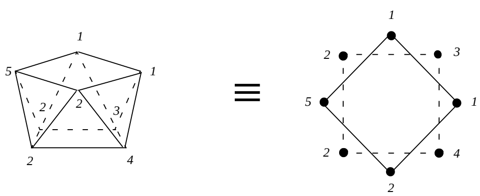
TPS-7-4-214345

4. Cubic



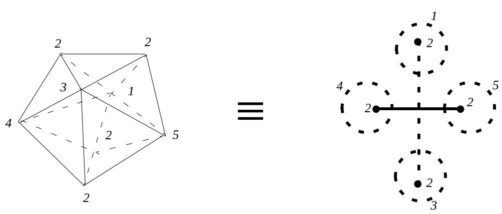
CU-8-13153234

5. Square antiprismatic



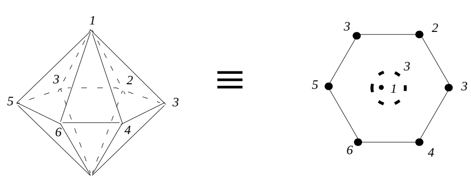
SA-8-12522413

6. Dodecahedral



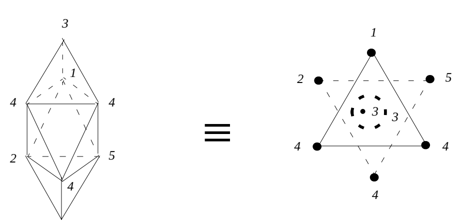
DD-8-24122532

7. Hexagonal bipyramidal



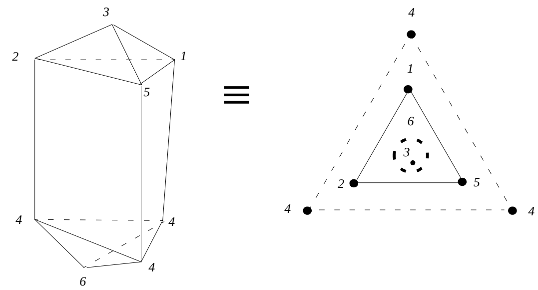
HB-8-13-234653

8. Octahedral trans-bicapped



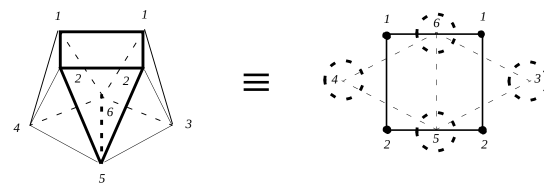
OCT-8-33-124445

9. Trigonal prismatic triangular faced bicapped



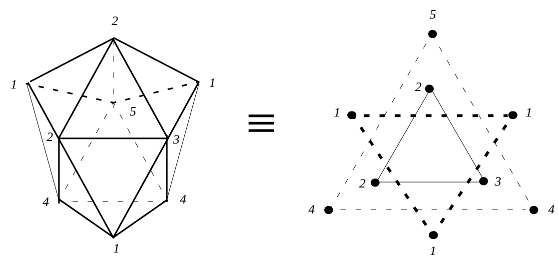
TPT-8-36-142454

10. Trigonal prismatic square faced bicapped



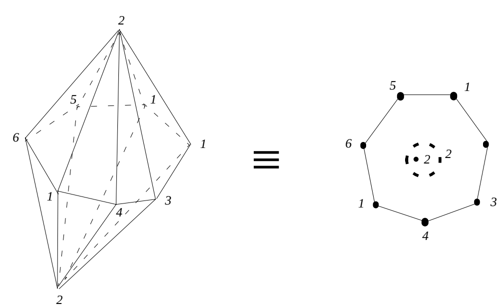
TPS-8-13252416

11. Trigonal prismatic square faced tricapped



TPS-9-241251341

12. Heptagonal bipyramidal



HB-9-22-1134165

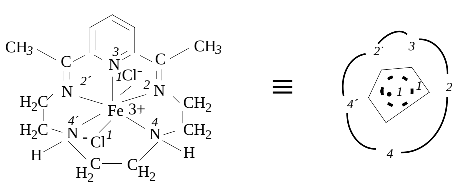
The configuration number is assigned by orienting the model structure with the highest-order axis in the vertical plane. The model structure is then viewed from the highest priority ligating atom on the highest-order axis or from a point on the highest-order axis above the most preferred end or terminal 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 anticlock-wise 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:

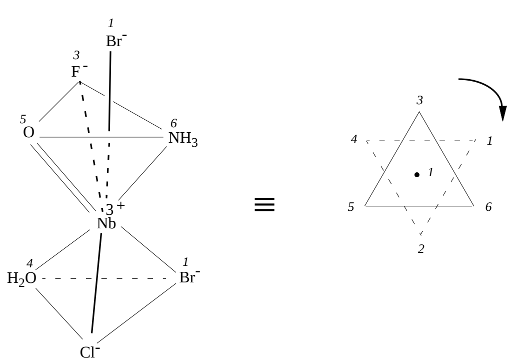
Pentagonal bipyramidal (PB-7)



(*PB*-7-11-232´4´4)-

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.

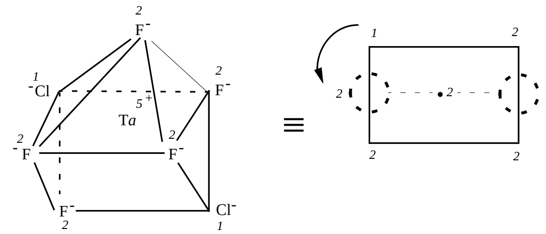
Octahedral faced monocapped (OCF-7)



(*OCF*-7-1-316254-*C*)-

[7]R. S. Cahn, C. K. Ingold, and V. Prelog, *Angew. Chem. Int. Ed. Engl.* **1966,** 5, 391-395.

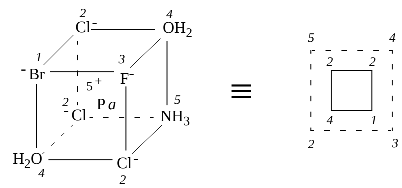
Trigonal prismatic square faced monocapped (TPS-7)



(*TPS*-7-2-122212-*A*)-

(The direction must be selected so as to cite the priority number of the atom in the next lower plane.)

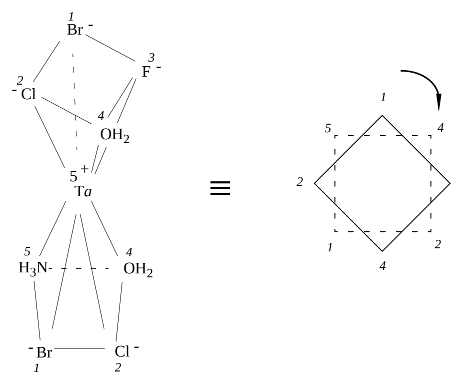
Cubic (CU-8)



(*CU*-8-13242542-*A*)-

(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.)

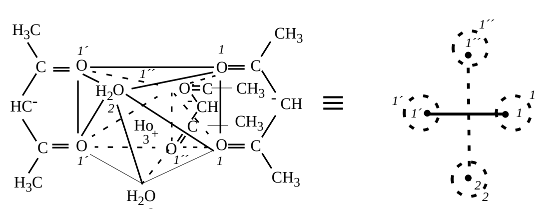
Square antiprismatic (SA-8)



(*SA*-8-14324125-*C*)-

(The preferred orientation must be determined before the descriptor assigned.)

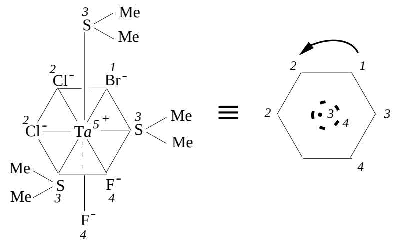
Dodecahedral (DD-8)



(*DD*-8-111´´1´´1´1´22)-

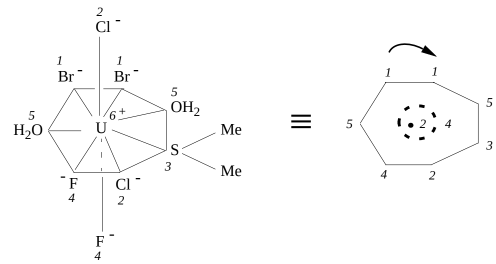
(The preferred orientation must be determined before the descriptor is assigned; also, the pathway is selected to pass through the atom of highest priority (lowest numerical value) in the next lower plane.)

Hexagonal bipyramidal (HB-8)



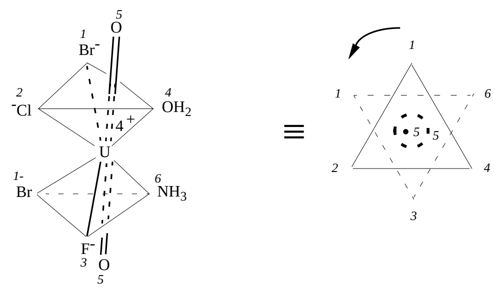
(HB-8-34-122343-A)-

Heptagonal bipyramidal (HB-9)



(HB-9-24-1153245-C)-

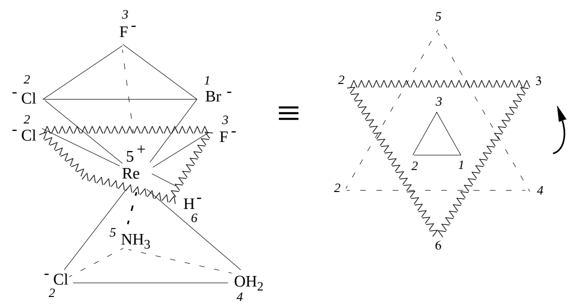
Octahedral trans-bicapped (OCT-8)



(OCT-8-55-112346-A)-

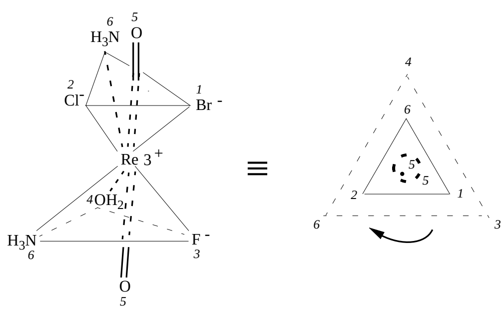
(The preferred orientation must be determined before the descriptor is assigned.)

Trigonal prismatic square faced tricapped (TPS-9)



(TPS-9-143352226-A)-

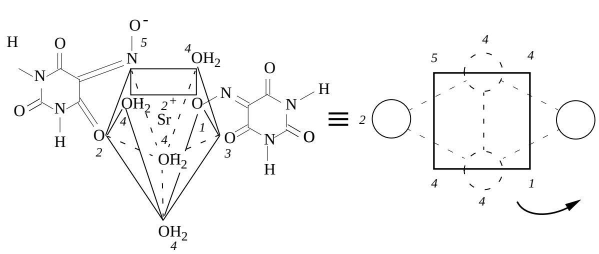
Trigonal prismatic triangular faced bicapped (TPT-8)



(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 **Vincaleukoblastine**, 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., **Vincaleukoblastine, 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 hydrazono 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 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), with an additional index entry at **Methane, iodo-**, compd. with alkaloid (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**

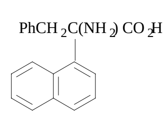
The following amino carboxylic, amino sulfonic, and amino arsonic acids, indexed prior to 1972 at their trivial names, are now named either systematically or as derivatives of an amino acid listed above:

Trivial name	*CA Index Name*
Allocystathionine	**Homocysteine,** ***S*-(2-amino-2-carboxyethyl)-**
Anthranilic acid	**Benzoic acid, 2-amino-**
Arsanilic acid (3 isomers)	**Arsonic acid, (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)-

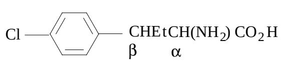
Radicals derived from the names of amino acid stereoparents, e.g., glycyl, L-alanyl, L-phenylalanyl, are employed only in naming peptides (¶ 206). In other situations, systematically named radicals are used; e.g., (aminoacetyl) instead of glycyl. The phenylalanyl radical is considered to be a specially 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:

$-COCH_2CH(NH_2)CO-$	aspartoyl
$HO_2CCH_2CH(NH_2)CO-$	α-aspartyl
$-COCH_2CH(NH_2)CO_2H$	β-aspartyl
$-CO(CH_2)_2CH(NH_2)CO-$	glutamoyl
$HO_2C(CH_2)_2CH(NH_2)CO-$	α-glutamyl
$-CO(CH_2)_2CH(NH_2)CO_2H$	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:

$\underset{N}{Bz}N\underset{2}{H}C\underset{1}{H_2}CO_2H$ — **Glycine, *N*-benzoyl-**



L-**Phenylalanine, 4-chloro-β-ethyl-**
(β*R*)- (not L-Norvaline, 3-(4-chlorophenyl)-,(3*R*)-)

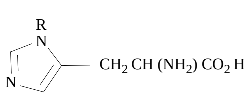
$Me(CH_2)_5CMe(NH_2)CO_2H$ — **Octanoic acid, 2-amino-2-methyl-** (not Alanine, α-hexyl-)

$PhCH(NH_2)CH_2CO_2H$ — **Benzenepropanoic acid, β-amino-** (β*R*)- (not β-Alanine, 3-phenyl-, (3*R*)-)

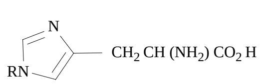
O-Substituted derivatives of the hydroxy amino acids (**Allothreonine**, **Homoserine, Serine, Threonine,** and **Tyrosine**) and *S*-derivatives of the mercapto amino acids (**Cysteine** and **Homocysteine**) are named at those stereoparents, the alkyl derivatives as substituents, e.g., **Serine**, ***O*-methyl-**, and the acyl derivatives as esters in the modification, e.g., L-**Cysteine, acetate (ester).** The stereoparent **Methionine**, $CH_3SCH_2CH_2CH(NH_2)COOH$, 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**, **Homocysteine**, and **Methionine** are indexed as sulfinyl and sulfonyl derivatives of simpler parents.

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**, $H_2NC(:NH)NH(CH_2)_3CH(NH_2)COOH$, substituted in the guanidino group are indexed as derivatives of **Ornithine**, $H_2N(CH_2)_3CH(NH_2)COOH$.

Histidine (R = H) is capable of existing in the following tautomeric forms:



(a)



(b)

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:

$EtO_2C(CH_2)_2CH(NH_2)CO_2Me$ — L-**Glutamic acid 5-ethyl 1-methyl ester**

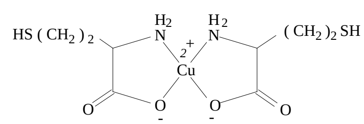
$HO_2CNHCHMeCO_2Et$ — L-**Alanine, *N*-carboxy- 1-ethyl ester** (the locant "l" is cited for clarity, even though the *N*-ethyl ester is indexed as L-**Alanine**, ***N*-(ethoxycarbonyl)-** (¶ 185))

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 headings 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 *Chemical Substance* and *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; L-**Phenylalanine**, methyl ester, hydrochloride.

Example:



Copper, bis (L-**homocysteinato-κ*N*, κ*O*)-**
(*T*-4)-

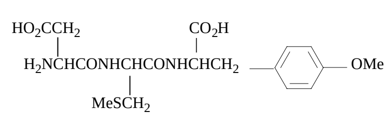
206. Peptides are generally named by use of amino acid stereoparents (¶ 205) and stereoparent radicals; the L-isomers are assumed for indexing purposes in the absence of contrary information. Trivial names of some peptides and all proteins are employed, and special "Cyclo" names are used for tri- and higher cyclic peptides. The systematic ring names are covered by cross-references in the *Index Guide.*

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 "N^6-" and "N^5-" 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 expressed by use of (*O*-acetyl-L-seryl), etc., radicals; when a hydroxyl- or mercapto-group-containing amino acid is the heading parent, the ester, e.g., "acetate," is cited in the modification.

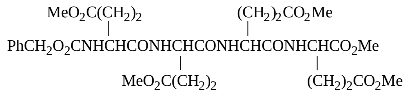
Examples:

H-L-Met-L-Asp(NH_2)-L-Pro-D-Phe-L-Phe-OH

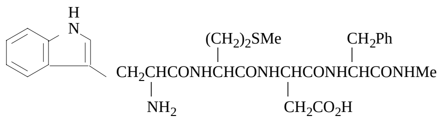
L-**Phenylalanine**, L-**methionyl**-L-**asparaginyl**-L-**prolyl**-D-**phenylalanyl-**



L-**Tyrosine**, L-**α-aspartyl-*S*-methyl**-L-**cysteinyl-*O*-methyl-**



L-**Glutamic acid**, *N*-**[(phenylmethoxy) carbonyl]**-L-α-**glutamyl**-L-α-**glutamyl**-L-α-**glutamyl-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**, $H_2NCOCH(NH_2)CH_2COOH$, and α-**Glutamine**, $H_2NCOCH(NH_2)(CH_2)_2COOH$. Peptides that do not meet this requirement are named systematically; e.g., **Butanoic acid, 4-amino-2-[(aminoacetyl)amino]-, (2*S*)-**.

When the above requirement is met, nonstandard α-amino acids are allowed 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-; 1*H*-Indole-2-carboxylic acid,** L-**seryl-**L-**methionyloctahydro-, (2*S*,3a*R*,7a*R*)-;** L-**Proline,** L-**histidyl-(3*R*)-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:

H-L-Ala-D-Gln-L-Lys-D-Ala-OH
H-L-Ala-D-Gln-L-Lys-D-Ala-L-Ala-L-Ala
H-L-Ala-L-Ala

D-**Alanine**,L-alanyl-D-glutaminyl-N^6-[L-alanyl-D-glutaminyl-N^6-(L-alanyl-L-alanyl)-L-lysyl-D-alanyl-L-alanyl-L-alanyl]-L-lysyl-

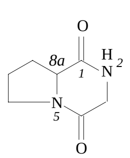
H-L-Leu-L-Ala-L-Phe
H-L-Pro-L-Met-L-Ser-L-Asp-OH

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.

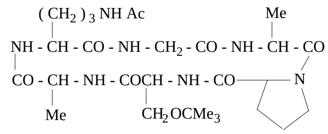
Cyclic dipeptides are indexed at systematic heterocycle names, with cross-references at "Cyclo" names (see below).

Example:



Pyrrolo[1,2-*a*]pyrazine-1,4-di-one, hexahydro- (cross-reference from Cyclo (glycylprolyl))

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).



Cyclo[L-**alanyl-*N*⁵-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 "cyclic (10→4)-peptide" 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 depsipeptide names (see below) are expressed by modification terms such as "(3→1)-lactone." Peptides containing disulfide linkages are indexed at the reduced (cysteinyl-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 heterocycle names.

Depsipeptides 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 "depsipeptide nomenclature"; otherwise a systematic name is employed. A depsipeptide name is based on the C-terminal 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 in this area.

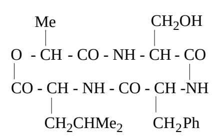
Example:

$HOCHMeCONHCHMeCO_2CHMeCONHCHMeCO_2H$

L-**Alanine,(2*R*)-2-hydroxypropanoyl-**L-**alanyl-(2*R*)-2-hydroxypropanoyl-**

Cyclic didepsipeptides are indexed as heterocycles. Cyclic tri- and higher depsipeptides are indexed at "Cyclo..." names analogous to those for cyclic peptides. Cyclic depsipeptides with one hydroxy acid are named as such, not as lactones.

Example:



Cyclo[L-**leucyl-(2*S*)-2-hydroxypropanoyl-**L-**seryl-**L-**phenylalanyl]** (the hydroxy acyl radical is alphabetized at "p," not "h")

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 ...-NH-CHR-X-X´-CHR´-CO-..., 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 ...-A-ψ(X-X´)-B-..., 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(CH_2-CH_2)-**L-**isoleucyl-**L-**alanyl-**.

Naturally occurring biologically active peptides with five or fewer amino acid residues are indexed as described above. Those with six to fifty residues are assigned the trivial names commonly used in the literature. Cross-references at peptide sequence names appear in the *Index Guide*, and illustrative diagrams appear for the more common natural peptides. For cysteine-containing natural peptides, only the reduced form is illustrated (**Oxytocin** and **Vasopressin**, below, are exceptions).

Examples:

H-L-Arg-L-Pro-L-Pro-Gly-L-Phe-L-Ser-L-Pro-L-Phe-L-Arg-OH
1 2 3 4 5 6 7 8 9

Bradykinin (cross-reference from L-Arginine,L-arginyl-L-prolyl-L-prolylglycyl-L-phenylalanyl-L-seryl-L-prolyl-L-phenylalanyl-)

→ L-Leu-D-Phe-L-Pro-L-Val-L-Orn
  1 2 3 4 5
L-Orn←L-Val←L-Pro←D-Phe←L-Leu ←
  10 9 8 7 6

Gramicidin S (cross-reference from Cyclo(L-leucyl-D-phenylalanyl-L-prolyl-L-valyl-L-ornithyl-L-leucyl-D-phenylalanyl-L-prolyl-L-valyl-L-ornithyl))

H-L-Cys-L-Asn-L-Cys-L-Lys-L-Ala-L-Pro-
  1 2 3 4 5 6

L-Glu-L-Thr-L-Ala-L-Leu-L-Cys-L-Ala-L-Arg-
  7 8 9 10 11 12 13

L-Arg-L-Cys-L-Gln-L-Gln-L-His-NH_2
  14 15 16 17 18

Apamin (reduced) (cross-reference from L-Histidinamide, L-cysteinyl-L-asparaginyl-L-cysteinyl-L-lysyl-L-alanyl-L-prolyl-L-a-glutamyl-L-threonyl-L-alanyl-L-leucyl-L-cysteinyl-L-alanyl-L-arginyl-L-arginyl-L-cysteinyl-L-glutaminyl-L-glutaminyl-)

Because the location of disulfide bonds in natural apamin has been determined, the following cross-reference appears in the *Index Guide*:

Apamin (reduced)
cyclic (1→11),(3→15)-bis(disulfide)-see *Apamin*

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 (swine 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., **1-34-Gastrin I (swine), 2-**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 a-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, N^2-L-**alanyl-** (N-terminal extension)

Glucagon (swine), *N*-**acetyl-** (N-terminal extension)

Bradykinin, 9a-L-**valine-9b-**L-**lysine-** (C-terminal extension)

Fibrinopeptide B (human), 14a-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 ...-A-$^{n}\psi^{n+1}$(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,** $^{7}\psi^{8}$**(CH=CH,*E*)-8-L-tyrosine-**. The formatting of the stereochemical data for X-X′ follows standard literature practice.

The prefix "*enantio*" denotes reversal of configuration of all amino acid residues; thus, *enantio*-**Bradykinin** contains only the D-forms of the amino acid residues, but in the same sequence as in **Bradykinin**. The new parent is used if more than half of the units have been replaced by their enantiomers; unchanged units are expressed by replacement nomenclature. The prefix "*retro*" denotes a reversal of the amino acid sequence; thus *retro*-**Gramicidin S** has the structure of **Gramicidin S** (see diagram above) but with the acid-amine linkages running from right to left. The combined prefix "*enantio-retro-*" indicates reversed configuration and reversed sequence.

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-**.

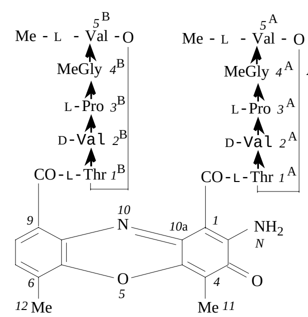
Oxytocin and **Vasopressin** derivatives in the disulfide form are named at these headings with replacement, etc., terms as usual, but reduced analogs are indexed at amino acid sequence names, not at **Oxytocin (reduced)** and **Vasopressin (reduced)**. The amino acid at position 8 of Vasopressin is always specified if known.

In α^{1-39}-**Corticotropin (swine)** "α" 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, but cross-references at the alternative names, e.g., α^{1-10}**Corticotropin**, appear in the *Index Guide*.

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. For each species, cross-references appear in the *Index Guide* at the amino acid sequence names of the two chains. 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., **Insulin (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 C_1) is one member of the actinomycin family.

Example:



Actinomycin D(cross-references from 3*H*-Phenoxazine-1,9-dicarboxamide,2-amino-*N*,*N*′-bis[hexadecahydro-2,5,9-trimethyl-6,13-bis(1-methylethyl)-1,4,7,11,14-pentaoxo-1*H*-pyrrolo[2,1-*i*][1,4,7,10,13]oxatetraazacyclohexadecin-10-yl]-4,6-dimethyl-3-oxo-; and 1*H*-Pyrrolo[2,1-*i*][1,4,7,10,13]oxatetraazacyclohexadecine)

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-**

Removal of a methyl group is indicated by "nor" or "dinor" prefixes, e.g., **11,12-Dinoractinomycin D**. When one or other or both of the peptide lactone rings are opened, the stereoparents **Actinomycin-5**^{A}**-oic D acid**, **Actinomycin-5**^{B}**-oic D acid**, and **Actinomycindioic D acid** are formed. Derivatives are named as for Actinomycin D.

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, for which 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. Carbohydrate stereoparents existing in the cyclic hemiacetal form must contain at least three asymmetric carbon atoms, including the anomeric carbon atom. 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:

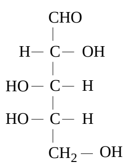
Pentoses:	**Arabinose, Lyxose, Ribose, Xylose.**
Hexoses:	**Allose, Altrose, Galactose, Glucose, Gulose, Idose, Mannose, Talose.**
2-Hexuloses:	**Fructose, Psicose, Sorbose, Tagatose.**
Acids:	**Ascorbic acid (¶ 224), Muramic acid, Neuraminic acid.**

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.

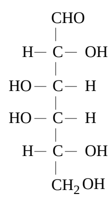
When a second stereoparent is represented in a structure, the parent of higher functionality is chosen in indexing.

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 "l" 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:



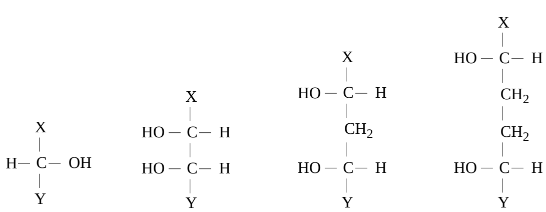
L-Arabinose



D-Galactose

Configurational prefixes, derived from trivial aldose names, are used in semisystematic carbohydrate nomenclature; for one asymmetric carbon atom, e.g., >CHOH, $>CHOCH_3$, $>CHNH_2$, *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):



D-*glycero*- L-*erythro*-

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-Hexodiulose**; 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)-**.

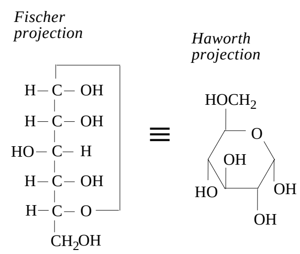
Oximes and hydrazones are expressed in the modification, osazones similarly as dihydrazones of osuloses. Hydrates, acetals, hemiacetals and esters are also named in the modification.

Examples:

D-**Xylose**
diethyl dithioacetal

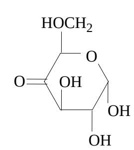
D-**Xylose**
2,3-diacetate 4,5-dibenzoate

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.

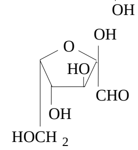


α-D-**Glucopyranose**

The following examples show the derivation of names for ketoaldoses when the ring closure involves (*a*) the aldehyde, and (*b*) the keto function.



(*a*) α-D-*xylo*-**Hexopyranos-4-ulose**



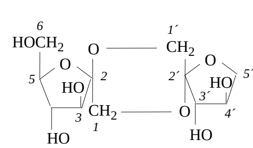
(*b*) α-L-*xylo*-**Hexos-2-ulo-2,5-furanose**

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.

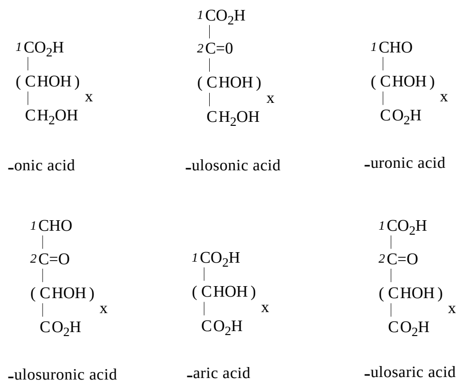
Intramolecular *anhydrides* are denoted by terms such as "1,5-anhydro" in which the locants define the pair of hydroxyl groups involved. The sulfur analogs are named with "dideoxy-epithio" terms. Intermolecular anhydrides are polysaccharides (below); intermolecular dianhydrides are named by citing the 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:



β-D-**Fructofuranose** β-D-*threo*-**2-pentulofuranose 1,2´:2,1´-dianhydride**

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).

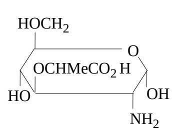
Examples:

D-**Gluconoyl chloride**

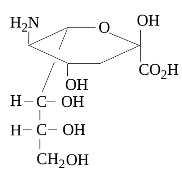
L-**Ribonic acid**
  γ-lactone

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:

FOR	ASSUME
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.

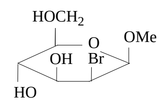
Examples:

α-D-**Glucopyranosylamine**

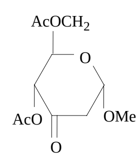
α-D-**Glucopyranuronamide, 1,1´-iminobis[1-deoxy-**

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-**Ribofura-noside**, 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 stereoparent 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**.

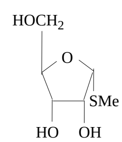
Examples:



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:

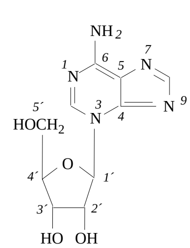
D-**Glucitol, 1,5-anhydro-1-*C*-phenyl-**
  (1*R*)-

4*H*-1-Benzopyran-4-one, 8-β-D-glucopyranosyl-2-phenyl-

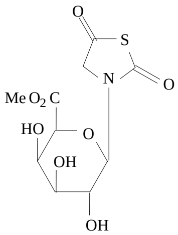
A naturally occurring glycoside is indexed at the systematic (or stereoparent) name if the structure, including the ring-size of the saccharide, is known, whether or not all the stereochemistry has been elucidated. (A "glucoside" is assumed to be the β-D-glucopyranoside, a "rhamnoside" the 6-deoxy-α-L-mannopyranoside.)

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:



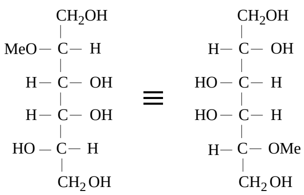
3*H*-Purin-6-amine, 3-β-D-ribo furanosyl-



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:

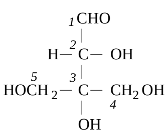


D-**Galactitol, 5-*O*-methyl-** (not L-Galactitol, 2-*O*-methyl-)

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:



D-**Apiose**

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-(acetylamino)-2,3-dideoxy-**
(2*Z*)-

9*H*-Purin-6-amine, 9-(2,3-dideoxy-β-D-*erythro*-hex-2-enopyranosyl)-

D-*xylo*-**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. Cross-references at oligosaccharide trivial names are found in the *Index Guide*.

Examples:

Lactose.	See D-*Glucose, 4-O-*β-D-*galactopyranosyl-*
Sucrose.	See α-D-*Glucopyranoside,* β-D-*fructofuranosyl*
Cellotriose.	See D-*Glucose, O-*β-D-*glucopyranosyl-(1→-4)-O-*β-D-*glucopyranosyl-(1→4)-*
Stachyose.	See α-D-*Glucopyranoside,* β-D-*fructofuranosyl O-*α-D-*galactopyranosyl-(1→6)-O-*α-D-*galactopyranosyl-(1→6)-*

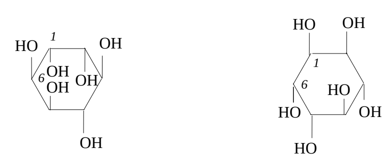
Polysaccharides are often indexed at common names, e.g., **Agar**, **Amylopectin**, **Cellulose**, **Starch**. Homoglycans (polysaccharides derived from one type of sugar residue) are named by converting the "-ose" suffix of an aldose or ketose, or the "-ic acid" of a glycuronic acid, to "-an," e.g., β-D-**Mannan**, (1→4)-; L-**Arabinan**; D-**Glucuronan**. Heteroglycans contain more than one kind of saccharide; the name, e.g., **Glucuronoarabinoxylan**, 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:

cis-**Inositol**	(1,2,3,4,5,6)
epi-**Inositol**	(1,2,3,4,5)
allo-**Inositol**	(1,2,3,4)
myo-**Inositol**	(1,2,3,5)
muco-**Inositol**	(1,2,4,5)
neo-**Inositol**	(1,2,3)
chiro-**Inositol**	(1,2,4)
scyllo-**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 counterclock-wise, 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 descrip-tors are used only when optical activity is present and can be determined from the original document.

Example:

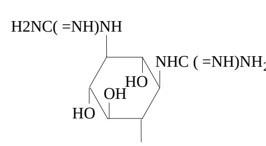


D-*chiro*-**Inositol** L-*chiro*-**Inositol**

Common names for inositols, e.g., **Scyllitol**, are cross-referred in the *Index Guide* to preferred index names. 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 configu-ration, 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.

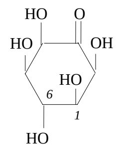
Example:



Streptamine, *N,N´*-bis(aminoiminomethyl)-

Inosose is the stereoparent for 2,3,4,5,6-pentahydroxycyclohexanone stereoisomers.

Example:



epi-**3-Inosose** (not *muco*-3-Inosose)

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).

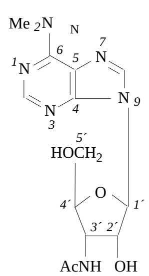
Trivial Name	*Index Name*
Adenine	**1*H*-Purin-6-amine**
Cytosine	**2(1*H*)-Pyrimidinone, 4-amino-**
Guanine	**6*H*-Purin-6-one, 2-amino-1,7-dihydro-**
Hypoxanthine	**6*H*-Purin-6-one, 1,7-dihydro-**
Thymine	**2,4(1*H*,3*H*)-Pyrimidinedione, 5-methyl-**
Uracil	**2,4(1*H*,3*H*)-Pyrimidinedione**
Xanthine	**1*H*-Purine-2,6-dione, 3,7-dihydro-**

Trivial names for seven common nucleosides and the related nucleotides are employed as stereoparents; these nucleosides are:

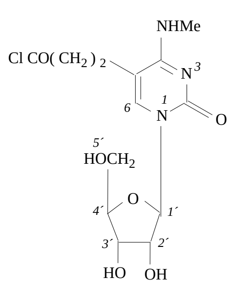
Purine derivatives	*Pyrimidine derivatives*
Adenosine	**Cytidine**
Guanosine	**Thymidine**
Inosine	**Uridine**
Xanthosine	

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-

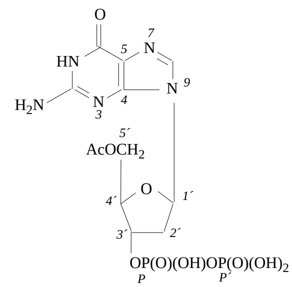


5-Pyrimidinepropanoyl chloride, 1,2-dihydro-4-(methylamino)-2-oxo-1-β-D-ribofuranosyl- (not Cytidine, 5-(3-chloro-3-oxopropyl)-*N*-methyl-)

Nucleotides are indexed at stereoparents descriptive of the type and position of the phosphate residue on the sugar moiety. Esters with phosphoric acid, H_3PO_4, 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.

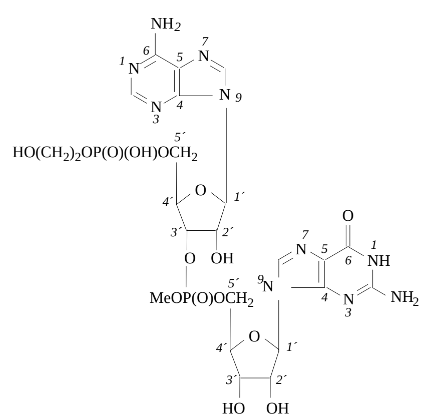
Example:

Inosine 5´-(trihydrogen diphosphate) 2´-(dihydrogen phosphate), *P*´ → 5´-ester with 3-(aminocarbonyl)-1-β-D-ribofuranosylpyridinium hydroxide, 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 "-ylyl" 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 "-ylyl" radicals are named as substituents without regard to higher functions. Nonnucleotidylyl 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´)-**.

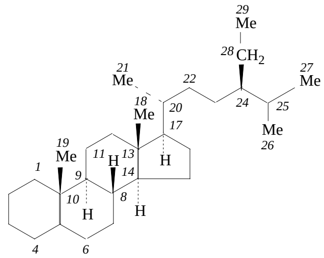
Example:



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_2Me	**Pregnane**
-CHMePr	**Cholane**
-CHMe$(CH_2)_3$CHMe_2	**Cholestane**
-CHMe$(CH_2)_2$CHMeCHMe_2	**Ergostane**
-CHMe$(CH_2)_2$CHEtCHMe_2	**Stigmastane**

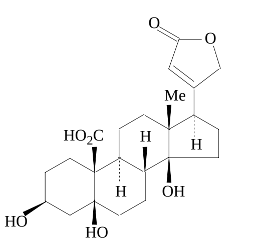
The implied configurations in all cases are **8β,9α,10β,13β,14α**. The configuration at the 5-position, when known, is cited as added stereochemistry in the modification. **Pregnane** is **17β**; **Cholane** and **Cholestane** are **17β,20*R***; **Ergostane** is **17β,20*R*,24*S***; **Stigmastane** is **17β,20*R*,24*R***. Illustrative diagrams appear for all these fundamental stereoparents to accompany the entries in the *Chemical Substance Index.*

Unsaturation in steroids is expressed by "en" and "yn" infixes, e.g., **Estra-1,3,5(10)-triene; Androst-1-en-16-ol, (5α)**-. 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**, for which diagrams showing the implied configurations are displayed in the *Chemical Substance Index* when required by current entries.

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 **14β** instead of **14α**. When a carboxylic acid or higher function is present the lactone ring is opened and named in the modification.

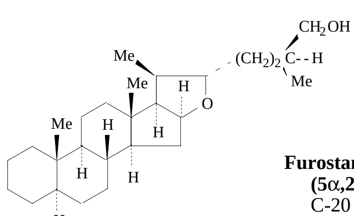
Example:



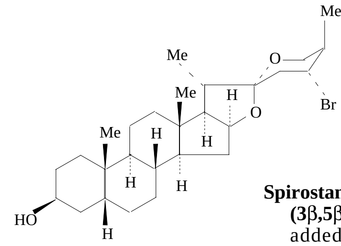
24-Norchol-20(22)-ene-19,23-dioic acid, 3,5,14,21-tetrahydroxy-γ-lactone, (3β,5β,14β)- (cross-reference from Card-20 (22)-enolid-19-oic acid)

Furostan is a stereoparent which represents 16β,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 (5α,20β,22α,25*S*)-(configuration at C-20 is reversed from that shown in the stereoparent diagram)



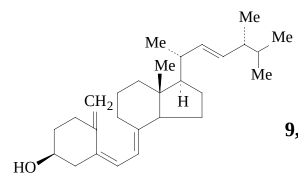
Spirostan-3-ol, 24-bromo-(3β,5β,24*R*,25*R*)-(configurations for added stereochemistry at C-3 and C-24 are indicated: there is no modified stereochemistry)

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 C_{27} 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-Dinorcholes-tane**; 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-).

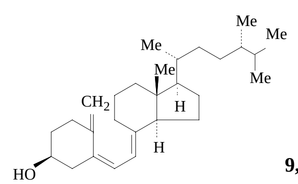
Ring contraction and expansion expressed by "nor" and "homo" prefixes are no longer permitted. Such substances are named systematically.

Ring scission is expressed by the "*seco*" prefix and two locants to indicate the positions between which the ring has been opened, is used only for 9,10-seco systems.

Examples:



9,10-Secoergosta-5,7,10(19),22-tetraen-3-ol (3β,5*Z*,7*E*,22*E*)-

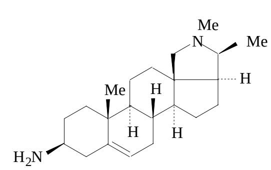


9,10-Secocholesta-5,7,10(19)-trien-3-ol (3β,5*Z*,7*E*)-

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)-,** (3β,20S)-. Kurchi alkaloids are named as derivatives of the stereoparent **Conanine**; implied configurations are the same as for **Pregnane**, with the addition of 20β.

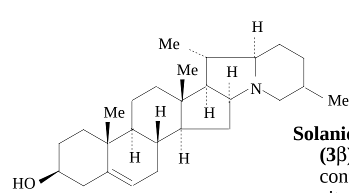
Example:



Con-5-enin-3-amine (3β)- (cross-reference from Conamine)

The solasodine-tomatidine and solanidine groups of *Solanum* alkaloids are indexed at **Spirosolane** and **Solanidane** stereoparents, respectively.

Example:



Solanid-5-en-3-ol (3β)-(When C-5 is asymmetric, its configuration, when known, is cited.)

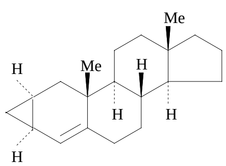
Veratrum alkaloids are indexed, according to type, at the stereoparents **Veratraman** and **Cevane**. Buxus alkaloids are indexed at such headings as **9,19-Cyclopregnane**. As usual, all these stereoparents are illustrated in the *Chemical Substance Index* when related entries appear there.

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., [(3β,5α)-3-hydroxyandrostan-5-yl]-. For acetals of steroids, see ¶ 202.

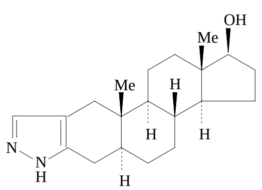
Steroids with -O- and -OO- bridges are indexed by use of "epoxy" and "epidioxy" substituents at the stereoparents. When the -NHNH- group is attached to a single skeletal atom, the "hydrazi" radical is employed. Steroid stereoparents may be adopted as components of spiro systems (¶ 156), e.g., **Spiro[androst-4-ene-2,1´-cyclopropan]-3-one.**

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:

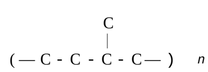


3´*H*-Cyclopropa[2,3]androsta-2,4-diene, 2,3-dihydro-(2α,3α)-



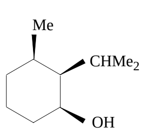
2´*H*-Androst-2-eno[3,2-*c*]pyrazol-17-ol (5α,17β)-

212. Terpenes contain repeating isopentane units:

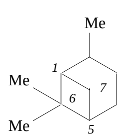


Mono-, sesqui-, di-, sester-, tri-, and tetraterpenes contain two, three, four, five, six, and eight such units; tetraterpenes are usually called carotenes (see below). Most mono-, sesqui-, and diterpenes are indexed by the principles of systematic substitutive nomenclature; stereoparents are employed 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. Illustrative diagrams for terpene stereoparents, exhibiting the numbering systems and partial or complete configurations, appear as needed in the *Chemical Substance Index*. Cross-references from trivially named terpenes, including all heading parents appearing in *CA* indexes prior to Volume 76, are supplied in the *Index Guide*, e.g., **Geraniol**. See *2,6-Octadien-1-ol, 3,7-dimethyl-, (E)-*.

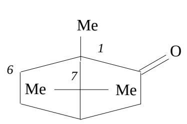
Examples:



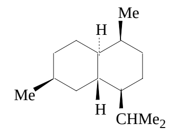
Cyclohexanol, 3-methyl-2-(1-methylethyl)-(1*S*,2*R*,3*R*)-(cross-reference from *o*-Neoisomenthol)



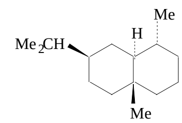
Bicyclo[3.1.1]heptane, 2,6,6-trimethyl- (cross-reference from Pinane)



Bicyclo[2.2.1]heptan-2-one, 1,7,7-trimethyl- (cross-reference from Camphor)



Naphthalene, decahydro-1,6-dimethyl-4-(1-methylethyl)-(1*S*,4*S*,4a*S*,6*S*,8a*S*)- (cross-reference from Cadinane)



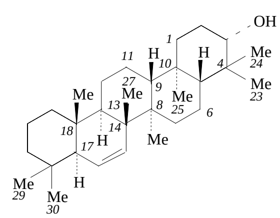
Naphthalene, decahydro-1,4a-dimethyl-7-(1-methylethyl)-(1*R*,4a*R*,7*R*,8a*S*) (cross-reference from Eudesmane)

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:

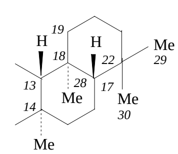


Gammacer-15-en-3-ol (3β)- (not Gammacer-6-en-21-ol, (21α)-)

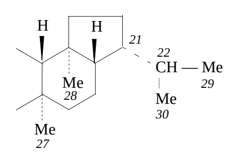
"Friedo," preceded by *D*, has been used to indicate *D:A*, *D:B*, or *D:C* as prefixed to pentacyclic triterpene stereoparents that angular methyl groups have shifted from their normal positions. These names are no longer used, and these substances are named as derivatives of other triterpenes.

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-

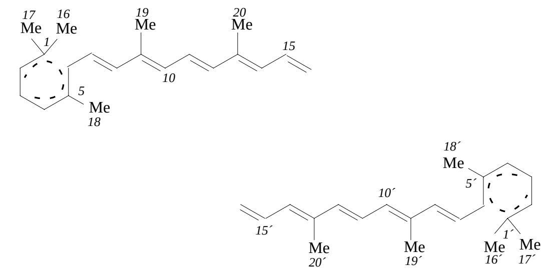
The prefix "cyclo" indicates a valence bond forming an extra ring, e.g., in **9,19-Cyclolanostane** a "fused" cyclopropane ring is formed.

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).

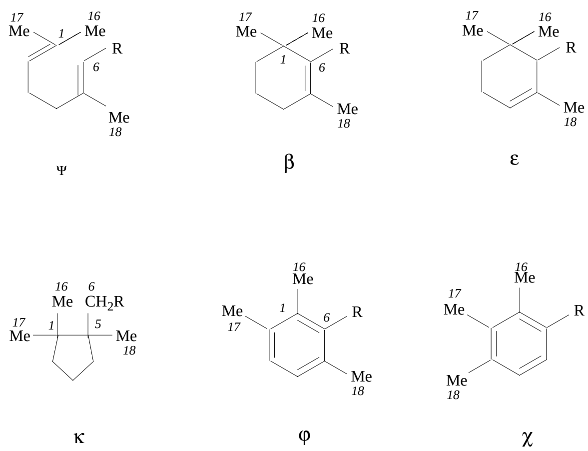
Lactones of triterpene acids are indexed at the acid names; cyclic acetals are likewise expressed in the modification at stereoparent headings.

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**:



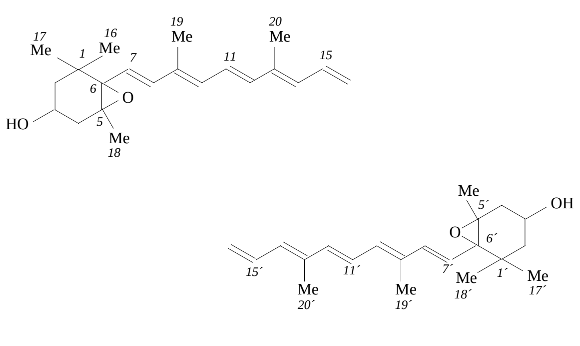
Each dotted curved line represents two double bonds or their equivalent; thus, individual compounds may have acyclic end groups with two double bonds, or terminal cyclohexenyl groups, or one of each. By extension, **Carotene** is used as the stereoparent representing dihydro and tetradehydro derivatives 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, OCH_3) 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.

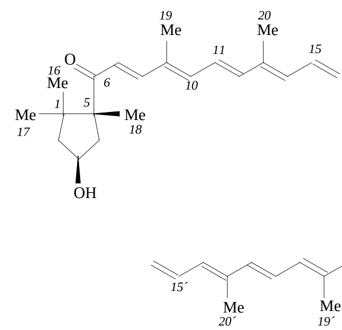
Carotenoids with diosphenol end-groups are indexed as the keto tautomers; e.g., β,β-**Carotene-3,3´,4,4´-tetrone**. For carotenoids with identical end groups, lowest locants are assigned to the principal groups, if present, and then to prefixes; e.g., ε,ε-**Carotene-2,3´-dione, 2´-methoxy-** (not ε,ε-Carotene-2´,3-dione, 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 at retinol, retinoic acid, etc., or systematically.

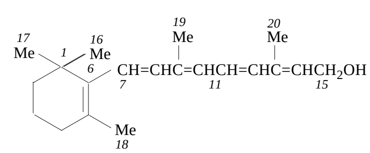
Stereochemistry of carotenoids is of two types. The geometrical configuration around double bonds is implied by the stereoparent stem **Carotene** to be *all-trans*. Abnormal configuration at one or more positions is indicated in the modification by terms such as "15-*cis*-." Absolute configuration at 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 the stereoparent:



Retinol (stereoparent)

Illustrative diagrams for **Retinol** and **Retinoic** acid appear in the *Chemical Substance Index.* Cross-references between retin names and Vitamin A terms are found in the *Index Guide*. Vitamin A_1 is indexed at **Retinol**; Vitamin A_2 at **Retinol, 3,4-didehydro-**. Hydrocarbon derivatives are indexed at systematic names. At **Retinol**, functions higher than the alcohol are expressed as substituents, e.g., **Retinol, 4-oxo-**. 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

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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 (Cunife 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, AISI, 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,^{235}U 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 named not as coordination compounds but 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 mononuclear carbonyls and nitrosyls are given binary salt names. Common oligomeric salts are named in the monomeric form, e.g., **Aluminum chloride ($AlCl_3$),** but studies of the dimers, etc., are indexed additionally at the oligomeric names, e.g., **Aluminum, di-μ-chlorotetrachlorodi-**.

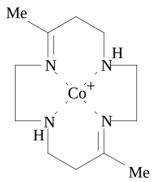
Coordination compounds may be anionic, neutral, or cationic, in accordance with the oxidation state of the central atom and the number and nature of the ligands; when the latter are derived from the molecular skeletons of substitutive nomenclature, including nonmetal hydrides, by loss of hydrogen, they are considered negative in computing the total charge of the complexes containing them. This charge is expressed by a 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 a 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 system[1]. The periodic table symbol of the ligated atom is stated as an italic capital-letter locant preceeded by the greek letter kappa, e. g. κ*N*, κO^1, κS^1. 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.

[1]IUPAC, *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-κN^1,κN^4,κN^8,κN^{11})-, (*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, sulfo. Among ligand names which differ are the following: superoxido (O_2–), amido (H_2N–), 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-κ*N*) (not nitro)
$^-$O=NO–	(nitrito-κ*O*) (not nitrito)
$^-$O–N=N–O$^-$	[hyponitrito(2–)]
OP(O$^-$)$_3$	[phosphato(3–)]

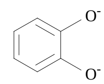
The following cyanato radicals are employed:

$^-$OCN–	(cyanato-κ*N*) (not isocyanato)
$^-$NCO–	(cyanato-κ*O*) (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 (phenylazo) 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 also methoxy through (dodecyloxy) radicals are used to express these ligands, but the chalcogen analogs and the substituted oxy radicals are named (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.

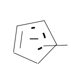
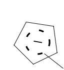
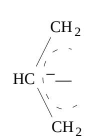
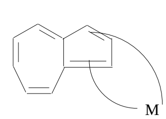
Examples (letter locants are added to many of these names in particular coordination names; e.g., (acetato-κ*O*,κ*O′*)):

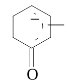
$^-O_2C^-$	(carboxylato) (this is an exception: not [carboxylato(2–)])
AcO$^-$	(acetato)
$^-CH_2CO_2^-$	[acetato(2–)]
Ph_2(O)P–	(diphenylphosphinyl)
Ph_2P(O)O$^-$	(diphenylphosphinito)
	[1,2-benzenediolato(2–)]
$^-O_2C(CH_2)_3CO_2^-$	[pentanedioato(2–)]
AcO$(CH_2)_2$O$^-$	(2-hydroxyethyl acetato) (an ester is named in its uninverted form)
MeO–S(O)$_2$–O$^-$	(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 H_2Al–.

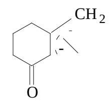
π*-bonded ligands*, and ligands attached to metal atoms by both π and σ bonds, are named by prefixing the Greek letter η (eta). (Delocalized bonds are "fixed" for the purpose of naming the ligand so that lowest locants are given first to the point of attachment, then for unsaturation, etc.) Locants (if 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:

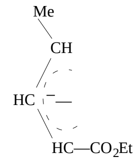
	[(1,2,3-η)-2,4-cyclopentadien-1-yl]
	($η^5$-2,4-cyclopentadien-1-yl)
	($η^3$-2-propenyl)
	[(1,2,3,3a-η)-azulene]



[(1,2,3-η)-4-oxo-2-cyclohexen-1-yl]-



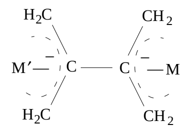
(η^3-2-methylene-6-oxocyclohexyl) (The choice is based on the preferred parent radical; the locants "α,1,2-" cannot be used because "α-" does not relate to the parent radical.)



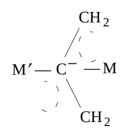
[(1,2,3-η)-4-ethoxy-1-methyl-4-oxo-2-butenyl]

In polynuclear compounds (see below) a colon partitions the locants into sets to indicate bonding to different metal atoms.

Examples:



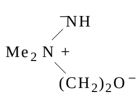
[μ-(η^3:η^3)-2,3-bis(methylene)-1,4-butanediyl)]



[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.

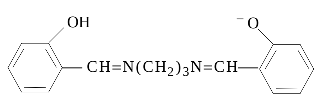
Example:



[1-(2-hydroxyethyl)-1,1-dimethylhydraziniumato(2−)]

Enclosing marks are used with all "ato" ligand names, and with ligands, like (cyano-*C*), 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:



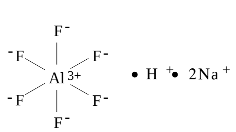
[[2,2′-[1,3-propanediylbis(nitrilomethylidyne)]bis[phenolato]](1−)]

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−)].

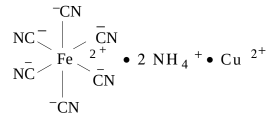
Neutral ligands are enclosed by parentheses or brackets (as required), except for ammine, aqua, carbonyl, and nitrosyl, e.g., (dinitrogen), (phosphine), (benzene); they are multiplied by "bis," "tris," etc.

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. Multiplicative terms are used with univalent cations if necessary, but when multivalent cations are present, ratios are employed for all. For metals of variable valency, Ewens-Bassett numbers are cited after their names.

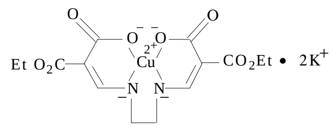
Examples:



Aluminate(3−), hexafluoro-disodium hydrogen, (*OC*-**6-11**)- (For the significance of the final term, see ¶ 203III.)



Ferrate(4−), hexakis(cyano-κ*C*)-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-κ*N* methylidyne)]]bis[propanedioato-κO^3]](4-)]-dipotassium (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:

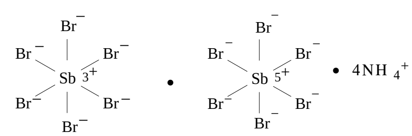
$Li_4[Co(NH_3)_6]_8[Fe(CN)_6]_7$

Cobalt(3+), hexaammine-(*OC*-6-11)-, lithium (*OC*-6-11)-hexakis(cyano-κ*C*)ferrate(4−) (8:4:7)

Ferrate(4−), hexakis(cyano-κ*C*)-(*OC*-6-11)-, (*OC*-6-11)-hexaamminecobalt(3+) lithium (7:8:4)

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−)** preferred over **Antimonate(1−)**; finally, by the earliest index position of the entire entry.

Example:

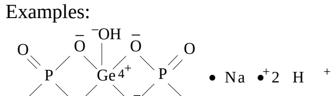


Antimonate(3−), hexabromo-(*OC*-6-11)-, ammonium (*OC*-6-11)-hexabromoantimonate(1−) (1:4:1)

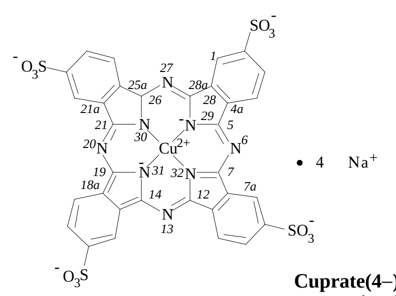
Antimonate(1−), hexabromo-(*OC*-6-11)-, ammonium (*OC*-6-11)-hexabromoantimonate(3−) (1:4:1)

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:



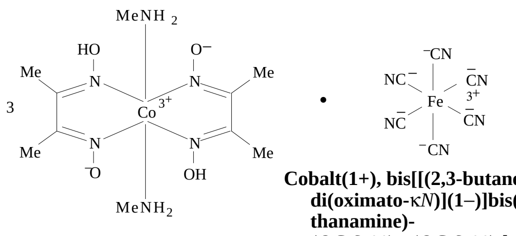
Germanate(3−), hydroxybis-[phosphato(3−)-κ*O*, κ*O′*]-sodium dihydrogen



Cuprate(4−), [29*H*,31*H*-phthalocyanine-2, 9,16,23-tetrasulfonato(6−)-κN^{29},κN^{30},κN^{31},κN^{32}]-tetrasodium, (*SP*-4-1)- (not Copper, [29*H*,31*H*-phthalocyanine-2,9,16,23-tetrasulfonato(2−)-κN^{29},κN^{30},κN^{31},κN^{32}]-, 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. Univalent anions are prefixed by "di," "tri," etc., if necessary; ratios are used with multivalent anions 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. Additional *Chemical Substance* and *Formula Index* entries will be found for the anions except for the common anions listed in ¶ 198.

Example:



Cobalt(1+), bis[[(2,3-butanedione di(oximato-κ*N*)](1–)]bis(methanamine)-(*OC*-6-11)-, (*OC*-6-11)-hexakis(cyano-κ*C*)ferrate(3–) (3:1)
Ferrate(3–), hexakis(cyano-κ*C*)-(*OC*-6-11)-, (*OC*-6-11)-tris[bis[[(2,3-butanedione di(oximato)-κ*N*)](1–)-*N*,*N*′]]bis(methanamine)cobalt(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.

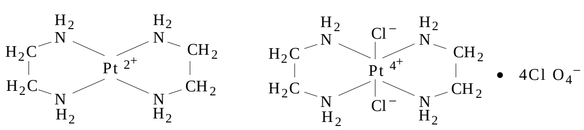
Example:

$Li_2H_2[Co(NH_3)_6]_8[Fe(CN)_6]_7$

Cobalt(3+), hexaammine-(*OC*-6-11)-, lithium hydrogen (*OC*-6-11)-hexakis(cyano-κ*C*)ferrate(4–) (8:2:2:7)
Ferrate(4–), hexakis(cyano-κ*C*)-(*OC*-6-11)-, (*OC*-6-11)-hexaamminecobalt(3+) lithium hydrogen (7:8:2:2)(additional *Chemical Substance* and *Formula Index* entry)

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. Additional entries for other complex cations, and for anions and ligands, appear as usual.

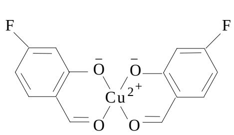
Example:



Platinum(2+), bis(1,2-ethanediamine-κ*N*,κ*N*′)-, (*SP*-4-1)-, dichlorobis(1,2-ethanediamine-κ*N*,κ*N*′)platinum(2+) perchlorate (1:1:4)
Platinum(2+), dichlorobis(1,2-ethanediamine-κ*N*,κ*N*′)-, (*SP*-4-1)-bis(1,2-ethanediamine-κ*N*,-κ*N*′)platinum(2+) perchlorate (1:1:4)

Neutral mononuclear coordination complexes are indexed at the central element names without a Ewens-Bassett number.

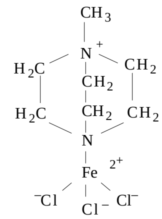
Example:



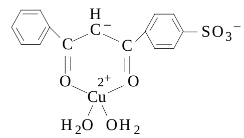
Copper,bis[4-fluoro-2-(hydroxy-κ*O*)benzaldehydato-κ*O*]-

Neutral complexes with internal charge compensation, e.g., with ligands which are ylides, inner salts, etc., are named according to structures provided in the original documents.

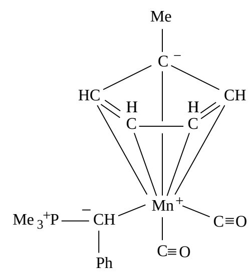
Example:



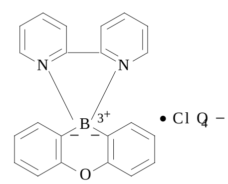
Iron, trichloro(1-methyl-4-aza-1-azoniabicyclo[2.2.2]octane-κN^4)-



Copper, diaqua[4-[1,3-dioxo-3-phenylpropyl]benzenesulfonato(2–)-O^4,$O^{4'}$]-



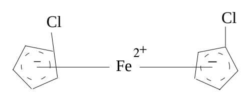
Manganese, dicarbonyl[(1,2,3,4,5-η)-1-methyl-2,4-cyclopentadien-1-yl][trimethylphosphonium (1-η)-phenylmethylide]-



Boron(1+), (2,2′-bipyridine-κN^1,κ$N^{1'}$)-(oxydi-2,1-phenylene)-*T*-4)-perchlorate

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.

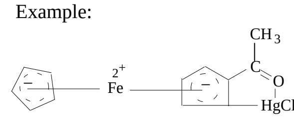
Example:



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.

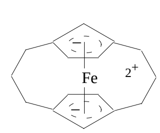
Example:



Mercury, [(2-(acetyl-κ*O*)ferrocenyl-κ*C*)chloro-

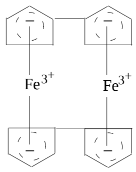
Suffixes are not attached to metallocene heading parents, and conjunctive names are not derived from them; thus, **Ferrocene, carboxy-** (not Ferrocenecarboyxlic acid); **Ferrocene, 1,1′-bis(carboxymethyl)-** (not 1,1′-Ferrocenediacetic acid). Bridged derivatives are named by use of bivalent substituent prefixes.

Example:



Ferrocene, 1,1′:3,3′-bis(1,3-propanediyl)-

The cationic analog of **Ferrocene** is named **Ferrocenium**.
Example:



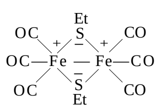
1,1′′:1′,1′′′-Biferrocenium(2+)

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., μ_3. 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-κ*O*:κ*O*′)]. 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-κ*O*:κ*O*′)]-(acetato-*O*). Colons within letter-locant sets indicate the distribution of bonds from a bridging ligand to individual metal atoms.

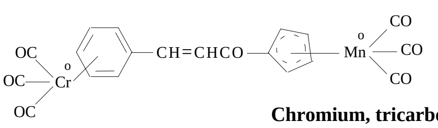
Bridging ligands are not treated as multiplying radicals; i.e., the total of nonbridging ligands on all nuclear atoms is indicated directly. The number of nuclear atoms is indicated, after citation of all ligands, by "di," "tri," etc. Letter-locant sets are partitioned by colons. The cyclic structure 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 "(3*Co-Co*)(3*Co-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:



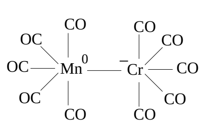
Iron, hexacarbonylbis[μ-(ethanethiolato)]di-
(*Fe-Fe*)



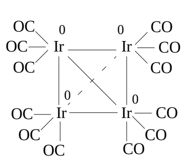
Chromium, tricarbonyl[μ-[η⁵:η⁶-1-(1-oxo-3-phenyl-2-propenyl)-2,4-cyclopentadien-1-yl]](tricarbonylmanganese)-

$(MeHg)_4S^{2+}$

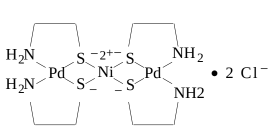
Mercury(2+), tetramethyl-μ₄-thioxotetra-



Chromate(1–), pentacarbonyl-(pentacarbonylmanganate)-
(*Cr-Mn*)
(Note: The "-ate" ending is used in all central atoms names in *anionic* complexes)



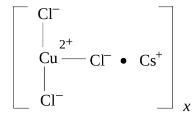
Iridium, dodecacarbonyltetra-,
tetrahedro



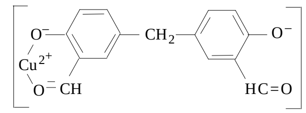
Palladium(2+), tetrakis[μ-[(2-(amino-κ*N*)ethanethiolato-κ*S*:κ*S*]] (nickel)di, dichloride

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 homopolymer



Copper, [S-[(3-formyl-4-hydroxyphenyl)methyl]-2-(hydroxy-κ*O*)-benzaldehydato(2-)-κ*O*]-homopolymer

Coordination compounds of indefinite structure are indexed (if the formula is unknown) at the organic ligand (if one is present) and at each metal "compounds" heading. These entries in the *Chemical Substance Index* are of a general nature and describe the entire series of complexes studied.

Example:

Pyridine, 2,6-dimethyl-
platinum complexes [if complexes with no other metal were studied]

Platinum, compounds
2,6-dimethylpyridine complexes [or "alkylpyridine complexes" or "nitrogen heterocycle complexes," etc., as appropriate]

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:

$AlTiCl_2Et_2(OH)_2$ — **Titanium, dichlorodiethyldihydroxy(aluminum)-**

$[AgAuCl_6]^{2-}$ — **Aurate(2–), hexachloroargentate-**

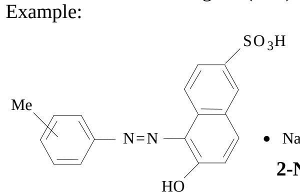
$[Nb_6O_3(SO_4)_{12}]^{8-}$ — **Niobate(8–), trioxododecakis[sulfato(2–)]hexa-**

$[Cu_4(OH)_5[N[(CH_2)_2OH]_3]_4]^{3+}$ — **Copper(3+), pentahydroxytetrakis[2,2′,2′′-nitrilotris[ethanol]]tetra-**

216. Dyes of established structure are indexed at their systematic names by the regular rules of substitutive nomenclature. For most classes of dyes a cross-reference will be found in the *Index Guide* at the *Colour Index* (C.I.) name, and the C.I. name is also used as a synonym (in the *Index Guide* and *Chemical Substance Index*) at the systematic name. 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-[(methylphenyl)azo]-monosodium salt (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.

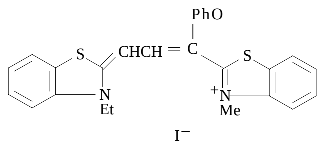
When an author supplies a structure for a trade-named dye which has been assigned a C.I. name but no constitution in the *Colour Index*, an entry will be found at the systematic name for the author's structures, and a separate entry,

[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.

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.

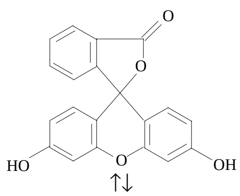
Example (name in original document: 3′-ethyl-3-methyl-8-phenoxythiacarbocyanine iodide):



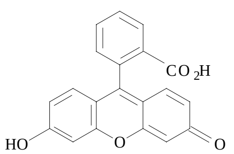
Benzothiazolium, 2-[3-(3-ethyl-2-(3*H*)-benzothiazolylidene)-1-phenoxy-1-propenyl]-3-methyl-iodide

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(3*H*),9′-[9*H*]xanthen]-3-one, 3′,6′-di hydroxy-



Benzoic acid, 2-(6-hydroxy-3-oxo-3*H*-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 *Spiro*[*isobenzofuran-1*(*3H*),*9′*-[*9H*]-*xanthen*]*-3-one, 3′,6′-dihydroxy-*
Phenolphthalein.	See *1(3H)-Isobenzofuranone, 3,3-bis(4-hydroxyphenyl)-*
Sulfonefluorescein.	See *Spiro*[*3H-2,1-benzoxathiole-3, 9′-[9H]-xanthene*]*-3′,6′-diol, 1,1-dioxide*
Phenolsulfonephthalein.	See *Phenol, 4,4′-(1,1-dioxido-3H-2,1-benzoxathiol-3-*ylidene)bis-

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, xanthene, 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 can be made both at the cationic heading, e.g., **Benzenediazonium**, and at the anion, e.g., **Zincate(1–), trichloro-,** or **Zincate(2–), tetrachloro-.** Otherwise it is indexed as a molecular addition compound (¶ 192) of the "-ium" chloride and **Zinc chloride ($ZnCl_2$)** with no ratio cited at either heading.

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 Λ(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*ππ; **Meson,** π, resonance *K*ππ.

(*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}In-(^{7}Li,3n)^{119m}*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}Cu-(^{12}C,α*p*)):

Carbon, reactions
ions of carbon-12, copper-63 bombardment by

Copper, reactions
isotope of mass 63, bombardment of, by carbon-12

[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, I.6-I.11).

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,** $\overline{\mathrm{He}}$, isotope of mass 4; **Antiproton,** $\overline{\mathrm{p}}$. 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,** μ^-(106).

(*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 (***K*Be**) (preferred index entry)

Beryllium, compounds
***K*-mesonic atom (*K*Be)** (additional entry)

2. The original document describes the exotic combination of muonium with chlorine:

Muon, μ
leptonic mol. with chlorine ($\mu^+e^-\mathbf{Cl}^0$) (preferred index entry)

Chlorine
leptonic mol. ($\mu^+e^-\mathbf{Cl}^0$) (additional entry)

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 $q^{((2-\frac{1}{3})\,\mathrm{He})}\ {}^{1}/_{3}{}^{+}$

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, and also in the *Index Guide* at **Enzyme Commission,** where E.C. designations are listed as part of cross-references leading to the preferred names. The E.C. designations are four-figure sets, e.g., E.C. 2.6.1.2 for Alanine aminotransferase, in which the first figure denotes one of the six main classes based on the type of reaction catalyzed by the enzyme, the second and third figures indicate further classification, and the final figure is a unique enzyme identification number. Whereas the E.C. cross-references lead directly from designation to enzyme name, the reverse route can also be taken by the user. At **Dehydrogenase** in the *Index Guide* appears the cross-reference “For related subclasses, see E.C. 1.” Such subclasses include **Reductase, Oxidase, Hydrogenase,** and **Hydroxylase,** all with E.C. 1 designations.

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 104-109, 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). For isotopically labeled inorganic compounds, see ¶ 220.

Elements of atomic number higher than 109, 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 (**$\mathbf{UuqF_4}$**) (formerly Element 114 fluoride (1:4))

These index headings are not subdivided into categories (see Appendix II, ¶ 10B) as is done for elements with established names (i.e., 1 through 109).

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. (S_8); **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, O_2^{2-}, F, N_3^{1-}, 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 ($\mathbf{Na_{0.37}WO_3}$)

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 ($SnCl_4$)); **Plumbane, diiodo-**. Hydrides, halides, etc., of most other elements are indexed at headings such as **Sodium hydride (NaH); Thorium hydride iodide ($\mathbf{ThHI_3}$).** The hydrides of nitrogen have trivial names: **Ammonia,** for NH_3; **Amidogen,** for NH_2; **Hydrazine,** for N_2H_4; and **Hydrazoic acid,** for HN_3. Some derivatives of ammonia also have trivial names: **Chloramine,** for NH_2Cl; **Fluorimide,** for NHF_2; **Hydroxylamine,** for $HONH_2$; **Sulfamide,** for $SO_2(NH_2)_2$; **Sulfimide,** for SO_2NH. 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 H_2O; **Hydrogen peroxide ($\mathbf{H_2O_2}$)**; **Hydrogen trioxide,** for H_2O_3; **Hydroxyl,** for HO; **Hydroperoxo,** for HO_2; **Hydrotrioxo,** for HO_3; **Selenyl,** for HSe; and **Hydrogen sulfide ($\mathbf{H_2S}$).**

[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.

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 ((NH_4)Cl)

Phosphonium cyanide ((PH_4)CN)

Oxonium chloride ((OH_3)Cl)

Perchloric acid, compounds
ammonium salt (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 (Na_2O), Iron oxide** (with a synonym line formula, if known), **Chlorine oxide (ClO_2).** Uninverted peroxide, superoxide, and ozonide headings are also employed, e.g., **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 ($Cr(OH)_3$).** 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 ($Sn(OH)_6{}^{2-}$), dipotassium,** (*OC*-**6-11**)-; **Tantalate(Ta_6(OH)-$O_{18}{}^{7-}$), heptapotassium; Molybdate(2−), tetra-μ-oxotetraoxoferratedi-, disodium**. Hydroxide-oxides that contain no Group IA or IIA metals are indexed at such headings as **Manganese hydroxide oxide (Mn(OH)O).** The index heading parents **Chromic acid (H_2CrO_4), Chromic acid ($H_2Cr_2O_7$), 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 (Na(HO_2)),** for Na(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 ($H_3N_2{}^{1-}$) and ($H_2N_2{}^{2-}$); 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 (K(I_3)), Calcium niobium fluoride** [formula unknown]. **Sodium phosphide (Na(H_2P)), Cyanogen chloride ((CN)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 ((Al,Ga)As)

Cadmium silicon phosphide ($CdSiP_2$) (not Cadmium phosphide silicide)

Thallium phosphide selenide (TIPSe) (not Thallium selenium phosphide)

Mercury iodide phosphide ($Hg_3I_4P_2$)

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 ($Al_{0.5}Ga_{0.5}As$)

Cadmium mercury telluride ((Cd,Hg)Te)

Copper platinum sulfide ($Cu_{1.7\text{-}1.8}Pt_{3\text{-}3.2}S_6$)

Iron manganese zinc oxide ($Fe_{2.3}Mn_{0.5}Zn_{0.2}O_{3.9}$)

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 Na[ICl_2]. Acetylides are indexed at names such as **Sodium acetylide (Na(C_2H)).** The common name **Calcium carbide (Ca(C_2))** is the single exception. Metal derivatives of *substituted* **Ethyne** and of other alkynes are indexed by organometallic nomenclature (¶ 194).

Examples:

BrC≡CAg	**Silver, (bromoethynyl)-**
EtC≡CNa	**Sodium, 1-butynyl-**

Graphite compounds are indexed at the **Graphite** index heading parent and at the name of the other component(s) as molecular addition compounds. Prior to *CA* Volume 95 (see ¶ 101), binary headings such as **Graphitic acid, Graphite nitrate,** etc., were employed.

Example:

C • 1/10 HNO_3	**Nitric acid, compd. with graphite (1:10)** **Graphite, compd. with nitric acid (10:1)**

The following metal-oxide radical names are sometimes used: americyl (O_2Am− and O_2Am=), chromyl (O_2Cr=), neptunyl (O_2Np− and O_2Np=), permanganyl (O_3Mn−), perrhenyl (O_3Re−), pertechnetyl (O_3Tc−), plutonyl (O_2Pu− and O_2Pu=), titanyl (O_2Ti=), uranyl (O_2U− and O_2U=), vanadyl, (OV−, OV=, and OV≡), and zirconyl (OZr=). 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-**
$K_2UO_2(SO_4)_2$	**Uranate(2−), dioxobis[sulfato-(2−)-κ*O*]-dipotassium**

The following nonmetal oxide radicals and their chalcogen analogs are employed: nitrosyl (ON-), nitryl (O_2N-), sulfinyl (OS=) (thionyl is limited to halides and halogenides), sulfonyl (O_2S=) (sulfuryl is limited to halides and halogenides), thiotrithiazyl (N_3S_4-), diphosphoryl (O_3P_2),disulfonyl (O_5S_2-), chlorosyl (OCl-), chloryl (O_2Cl-), perchloryl (O_3Cl-) (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:

Cl-S(O_2)-S(O_2)-Cl	**Disulfonyl chloride**
(SO)Br_2	**Thionyl bromide**
NOH(S_2O_7)	**Nitrosyl (disulfate) ((NO)H(S_2O_7))**
(SeO_2)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 ($Cr(CO)_6$),** (*OC*-6-11)-. Polynuclear carbonyls and nitrosyls of known structures are named as coordination complexes. (Simple metal nitrosyl dimers may be hyponitrites, e.g., $Na_2N_2O_2$, **Hyponitrous acid,** disodium salt.) Polynuclear carbonyls and nitrosyls of known composition are indexed as coordination compounds (¶ 215); cross-references will be found at the metal carbonyl headings in the *Index Guide*.

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 (KrF_2)**
XeO_4	**Xenon oxide (XeO_4)**
$K_2[XeF_8]$	**Xenonate(2−), octafluoro-dipotassium**
$Xe(ClO_4)_2$	**Xenon perchlorate ($Xe(ClO_4)_2$)** (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 with an additional entry at the more structurally descriptive oligomer. Clusters with unspecified oligomeric bonding are not reduced to their empirical formulas.

Examples:

Al_2Cl_6	**Aluminum, di-μ-chlorotetra-chlorodi-** (preferred index name) **Aluminum chloride ($AlCl_3$)** (additional index name)
Be_3Cl_6	**Beryllium, hexa-μ-chlorotri-,** *triangulo* (preferred index name) **Beryllium chloride ($BeCl_2$)** (additional index name)

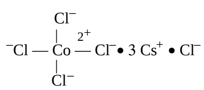
Metal-containing inorganic clusters receive standard nomenclature for inorganic compounds, e.g., **Sodium fluoride (Na_7F_7), Lithium potassium chloride ($Li_6K_4Cl_{10}$).** Nonmetallic inorganic clusters receive oligomeric names when the monomeric form does not receive a line formula. All other nonmetallic 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 (S_7F_{42})**

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.

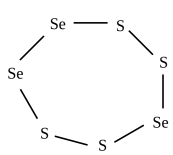
Examples:



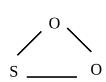
Cobaltate(2–), tetrachloro- cesium chloride (1:3:1), (*T*-4)-

$UOCl_2$	**Uranium chloride oxide (UCl_2O)**
$Co_5(NO_3)_2(SO_4)_4$	**Cobalt nitrate sulfate ($Co_5(NO_3)_2(SO_4)_4$)**
$H_2O_3S{\cdot}1/2Fe{\cdot}NH_3{\cdot}3H_2O$	**Sulfuric acid ammonium iron(2+) salt (2:2:1), hexahydrate**
$2NaCl{\cdot}Na_2SO_4$	**Sodium chloride sulfate ($Na_4Cl_2(SO_4)$)**
$B_2O_3{\cdot}P_2O_5$	**Boron phosphate ($B(PO_4)$)**

Cyclic inorganic substances composed of two or more elements and containing no metals of Groups 1-13 are named as ring systems.

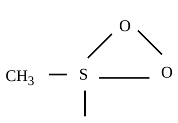


1,2,4,5,3,6,7- Tetrathiatriselenepane



Dioxathiirane

Organic derivatives of these substances may also be named as rings when there is no coordinate bonding.



Dioxathiirane, 3,3-dihydro- 3-mereapto-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- dichloride, (*OC*-6-11)-**
$NiCl_2.6H_2O$	**Nickel chloride ($NiCl_2$) hexahydrate** (additional *Chemical Substance* and *Formula Index* entry)
$Ca_3(PO_4)_2.3/2H_2O$	**Phosphoric acid calcium salt, hydrate (4:6:3)**

Binary and pseudobinary inorganic acids are restricted to **Hydrofluoric, Hydrochloric, Hydrobromic, Hydriodic, Hydrocyanic**, **Hydrazoic** (HN_3), **Fulminic** (HONC), **Cyanic,** and **Thiocyanic acid,** together with **Hydrogen triiodide** (HI_3) 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 in general indexed at metal oxide and hydroxide headings, e.g., **Antimony hydroxide ($Sb(OH)_3$)**; however, the metal acid names **Chromic acid (H_2CrO_4), Chromic acid ($H_2Cr_2O_7$), Manganic acid (H_2MnO_4),** and **Permanganic acid ($HMnO_4$)** 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 **Carbonoperoxoic acids,** see ¶ 183. Other peroxy acid names include **Peroxychromic acid ($H_2CrO_2(O_2)_2$),** etc. The two mononuclear **Boric acid** headings are differentiated by the synonym line formulas **HBO_2** and **H_3BO_3**. 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 (H_3BS_3).** Isopoly acids can be considered to arise formally by condensation of a mononuclear acid, thus, $2H_3BO_3 \rightarrow H_4B_2O_5 + H_2O$. The names used in indexing isopoly acids are the same as those of the mononuclear precursors, e.g., **Boric acid ($H_4B_2O_5$).** The synonym line formulas are usually empirical, but molecular formulas are shown for cyclic "meta" acids. Thus, **Boric acid ($H_3B_3O_3$).** 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 ($H_2B_2S_4$), Thiosilicic acid ($H_4Si_3O_4S_3$), Selenotellurodiarsenous acid ($H_4As_2Se_3Te_2$).**

The single name **Telluric acid** is used in association with the following synonym line formulas: **H_2TeO_3, H_2TeO_4, $H_2Te_2O_5$, $H_2Te_2O_7$, H_6TeO_6, $H_8Te_2O_{10}$.**

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 ($HSeFO_2$), Amidoselenic acid ($Se(NH_2)(OH)O_2$).** Replacement of both groups leads to a nonacid heading, e.g., **Selenic diamide ($Se(NH_2)_2O_2$), Amidoselenonyl fluoride ($(SeO_2)(NH_2)F$)** (acid halides rank higher than amides (¶ 106)). An example of a polyselenic acid derivative is **Imidodiselenic diamide ($NH[Se(NH_2)O_2]_2$).**

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:

$(HO)_2S$	**Sulfoxylic acid**
$(HO)_2SO$	**Sulfurous acid** (the selenium analog is **Selenious acid**.)
$(HO)_2SO_2$	**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 (SCl_2).** Monohydrazides are indexed at hydrazine headings, e.g., **Hydrazinesulfonyl chloride** for **H_2NNHSO_2Cl**. Some trivial names are employed. For **Sulfur diimide**, see ¶ 200.

Examples:

$H_2N(HO)S$	**Amidosulfoxylic acid**
H_2NSCl	**Amidosulfenyl chloride**
$HO(NC)SO$	**Cyanosulfurous acid**
$Cl(NC)SO$	**Thionyl chloride cyanide**
$(HO)_2S(S)$ (or $HO(HS)S(O)$)	**Thiosulfurous acid ($H_2S_2O_2$)**
$Cl(H_2N)S{=}NH$	**Amidoimidosulfurous chloride**
$HO(N_3)SO_2$	**Azidosulfuric acid**
$Cl(HO)SO_2$	**Chlorosulfuric acid**
$HO(H_2N)SO_2$	**Sulfamic acid**
Cl_2SO_2	**Sulfuryl chloride**
$F(ON)SO_2$	**Nitrososulfonyl fluoride**
$HO(H_2N)S(O){=}NH$	**Imidosulfamic acid**
$F_2N(H_2N)SO_2$	**Sulfamide, *N*,*N*-difluoro-**
$Cl(HO)S(O){=}NH$	**Chloroimidosulfuric acid**
$Cl_2S(O)S$	**Thiosulfuryl chloride ($(S_2O)Cl_2$)**
$(H_2N)_2S(O){=}NH$	**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 $(HO)S(O_2)O(O_2)S(OH)$), **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:

$(N_3)SO_2OSO_3H$	**Azidodisulfuric acid**
$HO(SO_2NH)_2SO_3H$	**Diimidotrisulfuric acid**
$H_2NSO_2NHSO_3H$	**Amidoimidodisulfuric acid**
HO_3SOOSO_3H	**Peroxydisulfuric acid ($[(HO)S(O)_2]_2(O)_2$)**
$ClSO_2OSO_2OSO_2Cl$	**Trisulfuryl chloride**
$H_2NSO_2OSO_2NH_2$	**Disulfamide**
$(ClSO_2)_2NNH_2$	**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** ($H_3P_3O_9$) are indexed at the heterocyclic parent **1,3,5,2,4,6-Trioxatriphosphorinane** (¶ 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 $[(H_2N)_2P]_2O$, and **Peroxydiphosphoramide,** for $[(H_2N)_2P(O)]_2O_2$. 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:

$(HO)_2P(O)OP(O)(OH)_2$	**Diphosphoric acid**
$(HO)_2P(O)OP(O)(OH)OP(O)(OH)_2$	**Triphosphoric acid**
$(HO)_2P(O)P(O)(OH)_2$	**Hypophosphoric acid**
$(HO)HP(O)P(O)(OH)_2$	**Isohypophosphoric acid**
$(HO)_2POP(OH)_2$	**Diphosphorous acid**
$(HO)_2POP(O)(OH)_2$	**Diphosphoric(III,V) acid**
$(HO)_2POP(O)(OH)OP(OH)$-$OP(O)(OH)_2$	**Tetraphosphoric(III,V,III,V) acid**
$(HO)_2P(O)NHP(O)(OH)_2$	**Imidodiphosphoric acid**
$[(HO)_2P(O)OP(O)(OH)]_2NH$	***P*′-Imidotetraphosphoric acid**
$Cl_2P(O)OP(O)(OH)Cl$	**Trichlorodiphosphoric acid**
$H_2N(HO)P(O)OP(O)(OH)_2$	**Amidodiphosphoric acid**
$(HO)_2POP(O)(OH)NH_2$	***P*′-Amidodiphosphoric(III,V) acid**
$HO(HS)P(O)SP(O)(OH)SH$	**Thiodiphophoric acid ($[(HO)(HS)P(O)]_2S$)**
$(HO)_2P(S)SSP(S)(OH)_2$	**Thioperoxydiphosphoric acid ($[(HO)_2P(S)]_2S_2$)**
$H_2N(HO)POP(S)(OH)_2$	***P*-Amido-*P*′-thiodiphosphoric (III,V) acid**
$Cl(H_2N)P(O)OP(O)Cl_2$	**Amidodiphosphoryl chloride**
$Cl_2P(O)OP(O)(Cl)F$	**Diphosphoryl chloride fluoride ($Cl_2P(O)OP(O)ClF$)**
$[(HO)_2P(O)]_3N$	**Nitridotriphosphoric acid**
$[(H_2N)_2P(O)NH]_2P({=}NH)NH_2$	***P*′-Iminodiimidotriphosphoramide**

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 nitryl 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 (HIO_3)**
$(HO)_2IO_2$	**Iodic acid (H_2IO_4)**
$HOClO_3$	**Perchloric acid**
$HOIO_3$	**Periodic acid (HIO_4)**
$(HO)_5IO$	**Periodic acid (H_5IO_6)**

Mixed halides are indexed at such names as **Chloryl fluoride ($(ClO_2)F$).**

Silicon oxo acids in *CA* indexing are named as **Silicic acid** with one of the following synonym line formulas: **H_2SiO_3, H_4SiO_4, $H_2Si_2O_5$, $H_6Si_2O_7$.** 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 ($Cl(NO_3)$)**
$B(OPO_2)_3$	**Boron metaphosphate ($B(PO_3)_3$)**

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:

$EtOSO_2OClO_3$	**Perchloric acid anhydride with ethyl hydrogen sulfate**
$HOSO_2OSi(OH)_2OSO_2OH$	**Sulfuric acid anhydride with silicic acid (H_4SiO_4) (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:

$HO_3SSSP(O)(OH)_2$	**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 ($K_2H_3(PO_4)(SO_4)$)).** 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:

$3\ HClO_3 \cdot Al$	**Chloric acid aluminum salt**
$3\ HNO_3 \cdot Ag$	**Nitric acid silver(1+) salt (3:1)**
$H_2SO_4 \cdot Ca$	**Sulfuric acid calcium salt (1:1)**
$HOSO_2OSO_2OH \cdot Na$	**Disulfuric acid monosodium salt**
$2\ H_2NSO_2OH \cdot Sn$	**Sulfamic acid tin(2+) salt (2:1)**
$HN(SO_2F)_2 \cdot Ag$	**Imidodisulfuryl fluoride silver(1+) salt**
$H_3PO_4 \cdot NH_3 \cdot Mg$	**Phosphoric acid ammonium magnesium salt (1:1:1)**
$2\ HClO_4 \cdot Xe$	**Xenon perchlorate ($Xe(ClO_4)_2$)**

Alums, chrome alums, etc., are indexed (*a*) at oxo acid names, e.g., **Sulfuric acid, compounds, aluminum potassium salt (2:1:1), dodecahydrate**, (*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 (2:1), compd. with guanidine (1:1)**, with an additional entry at **Guanidine, compd. with aluminum sulfate (1:1:2).**

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 ($H_3N_2^{1-}$).** 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 dihydrogen**
$EtSO_4^-$	**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:

(*a*) American Geological Institute, *Glossary of Geology*, Washington, D.C., 1972, 857 pp.
(*b*) 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.
(*c*) 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.
(*d*) 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.
(*e*) M. Fleischer, *Glossary of Mineral Species*, Mineralogical Record, Tucson, Arizona, 1980, 192 pp.
(*f*) 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.
(*g*) C. Hintze, *Handbuch der Mineralogie*, Supplement 2, *Neue Mineralien und Neue Mineralnamen*, Walter de Gruyter, Berlin, 1960, 958 pp.
(*h*) C. M. Rice, *Dictionary of Geological Terms*, Edwards Brothers, Ann Arbor, Mich., 1961, 465 pp.
(*i*) H. Strunz, *Mineralogische Tabellen*, 4th rev. ed., Akademische Verlagsgesellschaft Geest und Portig K.-G., Leipzig, 1966, 560 pp.
(*j*) 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. Cross-references from less preferred to more preferred index names appear in the *Index Guide*. 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 adjectival 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:

Chloride ($^{38}Cl^{1-}$)
Hydride-*d* (not Deuteride)
Tin
  isotope of mass 120 (^{120}**Sn**$^{1-}$)
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:

Iodide ($^{131}I_3{}^{1-}$)

Nitrogen
mol. ($N^{15}N$) (a labeled atom is cited *after* an unlabeled atom of the same element)

Helium
mol. ($^3He_2$)

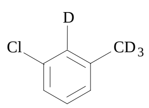
Deuterium
ion ($D_2{}^{1+}$)

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; in either case, locants are cited if necessary. 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*.)

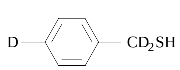
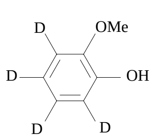
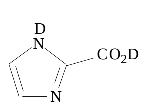
In labeled heading parents with single-word names and no hydrogen-containing principal group, the *d* is placed after the parent. No locant is needed if the positions are equivalent or are fully deuterated.

Examples:

MeD	**Methane**-*d*
CD_4	**Methane**-d_4
F_3CCH_2D	**Ethane**-*d*, **2,2,2-trifluoro-** (not Ethane-2-*d*, 1,1,1-trifluoro-)
	**Benzene**-*d*, **2-chloro-6-(methyl-**d_3**)-** (not Benzene-*2-d*, 1-chloro-3-(methyl-d_3)-)
$MePD_2$	**Phosphine**-d_2, **methyl-**
$(D_2N)_2CO$	**Urea**-d_4

Fully deuterated alcohols, amines, or imines are indexed similarly, but partially deuterated compounds of these classes have the "*d*" symbol placed after the appropriate part(s) of the name, with locants if necessary.

Examples:

$DOND_2$	**Hydroxylamine**-d_3
D_3CCD_2OD	**Ethanol**-d_6
$(D_3C)_2NH$	**Methan**-d_3-**amine**, *N*-(**methyl**-d_3)-
H_3SiND_2	**Silanamine**-d_2
DNHOD	**Hydroxyl**-*d*-**amine**-*d*
$D(CH_2)_2NH_2$	**Ethan**-*2-d*-**amine**
MeOD	**Methanol**-*d*
$MeSO_3CH_2D$	**Methan**-*d*-**ol 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-)
$MeCH(ND_2)CO_2D$	DL-**Alanine**-*N,N,1*-d_3
	1*H*-**Imidazole**-*1-d*-**2-carboxylic acid**-*d*

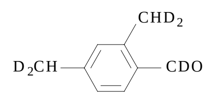
When a heading parent contains locants the labeling of each part is expressed separately and locants for the labeling are cited.

Example:

$DOCD_2CD_2OD$	**1,2-Ethane**-*1,1,2,2*-d_4-**diol**-d_2

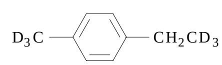
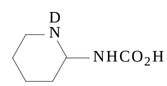
The "*d*" symbol is placed after the appropriate word in multiword headings for classes not yet discussed, e.g., **Acetic**-d_3 **acid**-*d*; **Acetyl**-d_3 **chloride**. In most other cases the "*d*" is cited after the complete heading parent, and conventional locants or italicized words are often necessary to denote the labeled position.

Examples:

DCH_2CDO	**Acetaldehyde**-*1,2*-d_2
$D(CH_2)_2CONHD$	**Propanamide**-*N,3*-d_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)

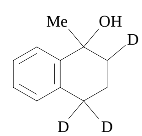
Enclosing marks are used with a labeled radical if it is preceded by a locant which expresses its attachment to a heading parent or parent radical, but not if such a locant belongs to the radical itself.

Examples:

	**Benzene, 1-(ethyl**-*2,2,2*-d_3**)-4-(methyl**-d_3**)-**
	**Carbamic acid, 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 monoacid-*d*" 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:

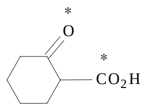
$(D_3C)_2CO$	2-**Propanone**-*1,1,1,3,3,3*-d_6

Exceptions are "*d*" and "*t*" terms placed after the word "acid" and after the suffixes of amines, imines, alcohols, etc. (see above), for which locants are seldom employed.

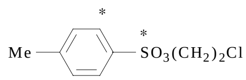
The examples above have dealt with organic compounds labeled with deuterium (tritium-labeling is handled similarly). Isotopes of elements other than hydrogen in organic compounds are expressed by the appropriate symbols. Nomenclature is similar, except that the instances in which the isotopic symbol 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):

$MeC(\overset{*}{O})\overset{*}{O}H$	**Acetic**-$^{17}O_2$ **acid**
$PhC(\overset{*}{O})OMe$	**Benzoic**-^{18}O **acid** ^{16}O-**methyl ester**
$Ph\overset{*}{C}H_2\overset{*}{C}O_2H$	**Benzeneacetic**-*carboxy*,α-$^{14}C_2$ **acid**
$MeC\overset{*}{O}F$	**Acetyl**-^{17}O **fluoride**
$\overset{*}{O}=C=\overset{*}{O}$	**Carbon dioxide**-$^{18}O_2$
$H_3\overset{*}{Ge}C\overset{*}{N}$	**Germane**-^{74}Ge-**carbonitrile**-^{15}N



Cyclohexanecarboxylic-^{14}*C* **acid, 2-(oxo-**^{17}*O*)-

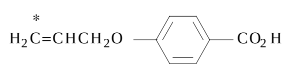


Benzene-2-^{14}*C*-**sulfonic-**^{35}*S* **acid 2-chloroethyl ester** (labeled "Class I" acids (¶ 185) belong to "Class II")

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 "*t*") 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_2CH_2OH	**Ethan**-*2*-*d*-**ol**-*1*-^{14}*C*
$MeCONH_2$	**Acetamide**-*1*-^{13}*C*-^{15}*N*
$MeCONDCH_2CHDMe$	**Acetamide**-*N*-*d*-^{15}*N*, *N*-(**propyl**-*2*-*d*)-



Benzoic acid, 4-(**2-propenyl**-*3*-^{14}*C*-**oxy**)-

Apart from isotopes of "hydro" (see above), a multiplicity of substituents which 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:

$(H_3C)_2SiMe_2$	**Silane, dimethyldi**(**methyl**-^{13}*C*)-
Cl_2C:	**Methylene, chloro-**^{35}*Cl*-**chloro-**^{37}*Cl*-
$Me_2CHNHCDMe_2$	**2-Propanamine**-*2*-^{14}*C*, *N*-(**1-methylethyl**-*1*-*d*)- (not **2-Propan**-*2*-*d*-**amine**, *N*-(**1-methylethyl**-*1*-^{14}*C*)-)

For derivatives named in modifications, labeling is expressed by such terms as "oxime-^{15}*N*," "calcium-^{44}*Ca* salt," "di(hydrate-d_2)." For labeled hydrates and ammoniates, additional index entries will be found at **Water**-d_2, **Ammonia**-^{15}*N*, etc. 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-$^{14}C_2$, **2-methoxy-**

Benzoic acid, 4-(**ethyl-**^{14}*C*)-

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**-*d*-*t*
$P(SiD_3)_3$	**Phosphine, tri(silyl-**d_3**)-**
$DP(O)(O^-)_2$	**Phosphonic**-*d* **acid ion(2−)**
$H_3{}^{32}PO_4$	**Phosphoric-**^{32}*P* **acid**
$H_3PO_4 \cdot 3\ {}^{22}Na$	**Phosphoric acid tri(sodium-**^{22}*Na*) **salt**
$HDSO_4$	**Sulfuric acid**-*d*
^{35}ClT	**Hydrochloric-**^{35}*Cl* **acid**-*t*
^{18}OSO	**Sulfur dioxide-**^{18}*O*
$D_2{}^{18}O$	**Water**-d_2-^{18}*O*

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 (D_2S)

Cobalt iron oxide ($CoFe_2O_3{}^{18}O$)

Molybdenum carbonyl ($Mo(CO)_4({}^{13}CO)_2$)

Nitrogen fluoride ($N^{15}NF_2$)

Sodium chloride ($^{24}NaCl$)

Sodium sulfide ($Na_2{}^{35}S$)

Uranium chloride ($^{213}UCl_3$)

Salts of inorganic oxo acids with labeled *cations* are named in the modification by such terms as "strontium-^{90}*Sr* salt," "ammonium-d_4 salt," if no ratio is employed for the unlabeled salt; otherwise the ratio is replaced by a labeled synonym line formula. Such formulas are also needed to indicate unsymmetrical labeling of anions.

Examples:

Phosphoric acid
calcium salt (**$Ca_2{}^{44}Ca(PO_4)_2$**)

Phosphoric-^{32}*P* **acid**
calcium salt (**$Ca_3(PO_4)({}^{32}PO_4)$**) (the unlabeled acid is not indexed)

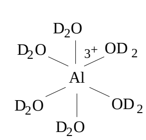
Compounds with indefinite labeled structures are indexed at the unlabeled headings with "labeled with" modification phrases.

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, ^{233}U 5.** For intermetallic compounds, synonym line formulas are cited in the modification instead of a ratio, e.g., **Iron, compound with uranium ($Fe_2{}^{235}U$).**

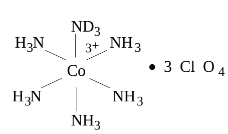
Labeled *minerals* are indexed at the systematic and mineral names, as well as at the name of the unlabeled mineral if it is studied. Labeling is indicated at the mineral name by synonym line formulas which contain isotope symbols or by modification phrases such as "labeled with boron-10" or "deuterated hydrate."

Coordination compounds (¶ 215) containing isotopic nuclear atoms are indexed at the labeled element or "ate" term, e.g., **Copper-**^{64}*Cu*, **Borate**(1−)-^{10}*B*. Labeled ligands have the isotopic symbols appended; the ligand names are enclosed in parentheses if multiplicative prefixes are needed.

Examples:



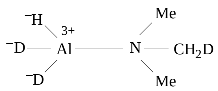
Aluminum(3+), hexa(aqua-d_2)-(*OC*-**6-11**)- (see also ¶ 203 III)



Cobalt(3+), pentaammineammine-d_3-, (*OC*-**6-22**)-, **triperchlorate**

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*-**dimethyl methan**-*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 involve components 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 nonstereoparents depend on functionality, as for molecular addition compounds (¶ 192) and polymers (¶ 222). Components are cited in each modification in alphabetical order, esters and salts being expressed in their uninverted format. Mixtures containing ill-defined, nonregistrable substances such as egg white are indexed as usual, with the **Egg white** entry appearing in the *General Subject Index*. The "compounds" functional subdivision (Appendix II, ¶ 10B) is used for components that have subdivided headings.

Example:

Glycine, compounds
  mixt. with egg white and sodium chloride (NaCl)
  (preferred *Chemical Substance Index* entry; cross-reference at Yumol)
Egg white
  mixt. contg. (*General Subject Index* entry)

Mixtures of ten or more indexable components are registered as usual, but, because of the excessive length of index entries which list the components, they are indexed only at the mixture name. "See also" cross-references at the component names in the *Index Guide* lead the index user to the entries at the mixture heading.

A mixture of salts of a single parent is indexed only once, although all salts are registered.

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. (Cross-references at the monomer names appear in the *Index Guide*). 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 Society[5]. 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.

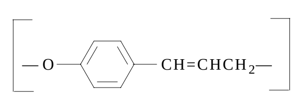
Polymers of unspecified length and chains of reported "average" length, are named by the methods described above. The prefix "oligo-" is not used to differentiate polymers of relatively low molecular weight from high polymers. When, however, the number of structural repeating units is exactly specified, the oligomer is usually named according to the principles of substitutive nomenclature.

Examples:

$(-CH_2-)_n$	**Poly(methylene)**
$(-CHMeCH_2-)_n$	**Poly(1-methyl-1,2-ethanediyl)**
$(-CH{=}CH-)_n$ (not $(=CHCH=)_n$)	**Poly(1,2-ethenediyl)** (not Poly(1,2-ethanediylidene))
$[-(CO)_2(CH_2)_2-]_n$	**Poly(1,2-dioxo-1,4-butanediyl)** (not Poly(1,4-dioxo-1,4-butanediyl))
$(-CH{=}CHCHMeCH_2-)_n$	**Poly(3-methyl-1-butene-1,4-diyl)**

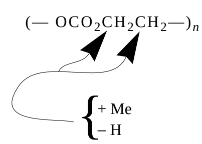
For more complex examples, further criteria for arranging the components of an SRU are required. The descending order of priority of citation (and of structuring of the SRU) is (*a*) heterocyclic rings, (*b*) acyclic hetero atoms in the order: O, S, Se, Te, N, P, As, Sb, Bi, Si, Ge, Sn, Pb, B, Hg, (*c*) 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:



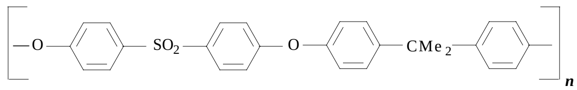
Poly(oxy-1,4-phenylene-1-propene-1,3-diyl)

$[-NHCO(CH_2)_2-]_n$	**Poly[imino(1-oxo-1,3-propanediyl)]**
$[-(SO_2)_2(CH_2)_2-]_n$	**Poly(disulfonyl-1,2-ethanediyl)**



Poly[oxycarbonyloxy(methyl-1,2-ethanediyl)] (The position of the methyl group is not assumed in this polyester from carbonic acid and 1,2-propanediol.)

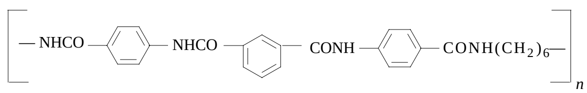
[5]"A Structure-based Nomenclature for Linear Polymers", *Macromolecules* **1968**, 1(3), 193-198. The IUPAC recommendations (*Pure Appl. Chem*. **1976**, 48, 373-385; **1993**, 65 (7), 1561-1580) are in full agreement with CAS practice. The IUPAC term "constitutional repeating unit" (CRU) corresponds to *CA*'s SRU.



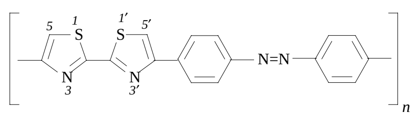
Poly[oxy-1,4-phenylenesulfonyl-1,4-phenyleneoxy-1,4-phenylene(1-methylethylidene)-1,4-phenylene] (With equal numbers of atoms between the oxygen atoms in two possible arrangements, the preferred path includes the other hetero atom, sulfur, as early as possible.)

$[-OCH_2SNH(CH_2)_2OCH_2SCH_2NHCH_2-]_n$

Poly(oxymethylenethioimino-1,2-ethanediyloxymethylenethiomethyleneiminomethylene) (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-phenyleneiminocarbonyl-1,3-phenylenecarbonylimino-1,4-phenylenecarbonylimino-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-phenyleneazo-1,4-phenylene)

$[-NHCOCH(CO_2Pr)-]_n$

Poly[imino[1-oxo-2-(propoxycarbonyl)-1,2-ethanediyl]] (not Poly[imino(1-carboxy-2-oxo-1,2-ethanediyl)], propyl ester)

$\left[\begin{array}{c} -N^+Me_2(CH_2)_2- \\ \cdot\ Br^- \end{array} \right]_n$

Poly[(dimethyliminio)-1,2-ethanediyl bromide] (the ionic derivative term is included in the 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.

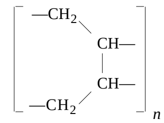
Examples:

$Cl-(CH_2)_n-CCl_3$ **Poly(methylene) α-chloro-ω-(trichloromethyl)-**

$Cl_3C-(CF_2-CH_2-)_nCl$ **Poly(1,1-difluoro-1,2-ethanediyl) α-(trichloromethyl)-ω-chloro-**

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.

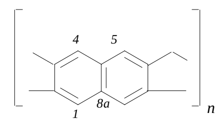
Example:



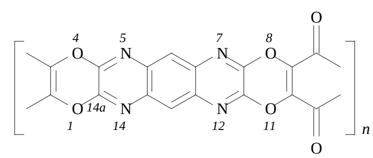
Poly(1,4:2,3-butanetetrayl)

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-.

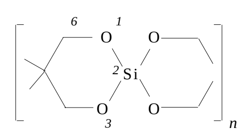
Examples:



Poly(2,3:6,7-naphthalenetetrayl-6-methylene)



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.)



Poly[1,3-dioxa-2-silacyclohexane-5,2-diylidene-2,2-bis(oxymethylene)] (not Poly[1,3-dioxa-2-silacyclohexane-2,5-diylidene-5,5-bis(methyleneoxy)] (The direction is determined by the shortest path from the hetero atom in the ring to the acyclic hetero atom.)

Linear polymers composed of SRUs within SRUs, e.g.,

$[-[O(CH_2)_2]_m-O_2C(CH_2)_4CO_2-]_n$

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, are cross-referred in the *Index Guide* from monomer names to 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-ethanediyloxycarbonyl-1,4-phenylenecarbonyl)*

A cross-reference appears also at **1,4-Benzenedicarboxylic acid, esters, 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:

$(BuCH{=}CH_2)_n$	**1-Hexene** **homopolymer** (only index entry)
$[H_2C{=}CMeCO_2(CH_2)_{12}Me]_n$	**2-Propenoic acid, 2-methyl-** **tridecyl ester, homopolymer** (only index entry)
$[H_2N(CH_2)_{10}CO_2H]_n$	**Undecanoic acid, 11-amino-** **homopolymer** (the *Formula Index* entry appears at $C_{11}H_{23}NO_2$; a systematic entry is also made at the assumed SRU name: **Poly[imino-(1-oxo-1,11-undecanediyl)],** $(C_{11}H_{21}NO)_n$)

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. The preferred index name is determined by the usual rules for selection of a heading parent (¶ 138) but a stereoparent is preferred over a nonstereoparent, 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 (Appendix II, ¶ 10B) 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:

1(*a*) **1-Heptene**
polymer with 1-hexene (preferred index entry)

2(*a*) **2-Propenoic acid**
butyl ester, polymer with 1-ethenyl-4-methylbenzene and 2,5-furandione (preferred index entry)

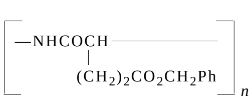
Peptides of established structure are indexed at systematic peptide names such as **Glycine**, **glycylglycyl-** (see ¶ 206). Peptides of unknown structure are indexed as polymers.

Example:

$[HO_2CCH(NH_2)(CH_2)_2CO_2CH_2Ph]_n$

L-**Glutamic acid**
5-(phenylmethyl) ester, homopolymer

and the assumed structural repeating unit:



Poly[imino[(2*S*)-1-oxo-2-[3-oxo-3-(phenylmethoxy)propyl]-1,2-ethanediyl]]

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. 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 preferred index entry is at **1-Heptene**, polymer with 1-hexene, graft, with an additional entry at **1-Hexene**, polymer with 1-heptene, 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:

Silane, dichlorodimethyl-
polymer with dichlorodiphenylsilane, 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 unsatd. nitriles
Nitriles
unsatd.; 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** which are cross-referred in the *Index Guide*).

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:

$Cl\text{-}(CH_2)_6\text{-}CCl_3$	**Heptane, 1,1,1,7-tetrachloro-**
$Cl\text{-}(CF_2\text{-}CH_2)_n\text{-}CHCl_2$	**Poly(1,1-difluoro-1,2-ethanediyl) 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
Methane, tetrachloro-
telomer with 1-hexene

Post-treated polymers are described by modification terms after the polymer has been described.

Examples:

2-Propenoic acid
homopolymer, sodium salt

Benzenamine, 4-ethenyl-
polymer with ethenylbenzene, hydrochloride

2-Propenoic acid, 2-methyl-
decyl ester, homopolymer, hydrolyzed

Poly[1-(4-sulfophenyl)-1,2-ethanediyl]
propyl ester

Ethenol (vinyl alcohol) polymers that are indexed at that heading are exceptions (they are prepared by hydrolysis of ethenol ester polymers). Also, acetals of ethenol polymers are entered in the *General Subject Index* at the trivially named class terms **Polyvinyl acetals** and **Polyvinyl butyrals** with a modification, e.g., "chlorobenzals," to indicate the type of acetal when appropriate. Cross-references or additional entries (in the *Chemical Substance Index*) are found at the aldehyde names.

Molecular addition compounds of polymers are indexed in the usual way (¶ 192), e.g., **Ethenesulfonic acid,** homopolymer, compd. with 4-ethenylpyridine homopolymer, with an additional entry for the other component.

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-** (a cross-reference will be found in the *Index Guide* at **Hexapropylene glycol**). 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-ethanediyl), α-hydro-ω-hydroxy-**, and **Poly[oxy(methyl-1,2-ethanediyl)], 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 ethanediyl 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, methyl-**, polymer with oxirane, with an additional *Chemical Substance* and *Formula Index* entry at **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 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:

$Me(CH_2)_{16}CO\left[O(CH_2)_2\right]_nOH$

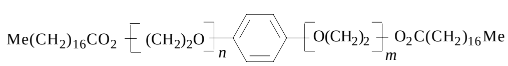
Poly(oxy-1,2-ethanediyl)
α-(1-oxooctadecyl)-ω-hydroxy-

$Ac\left[O(CH_2)_2\right]_nO_2CCMe=CH_2$

Poly[oxy-1,2-ethanediyl]
α-acetyl-ω-[(2-methyl-1-oxo-2-propenyl)oxy]-

$H_2C=CHCO\left[O(CH_2)_2\right]_nO(CH_2)_{11}Me$

Poly(oxy-1,2-ethanediyl)
α-(1-oxo-2-propenyl)-ω-(dodecyloxy)-



Poly(oxy-1,2-ethanediyl)
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

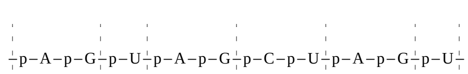
Cytidine, 5′-*O*-phosphonoadenylyl-(3′→5′)-
homopolymer

5′-Guanylic acid
polymer with 5′-adenylic acid and 5′-cytidylic acid (additional *Chemical Substance* and *Formula Index* entries at 5′-**Adenylic acid** and **5′-Cytidylic acid**

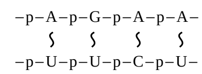
Polynucleotides in which different primary chains are associated intermolecularly by hydrogen bonds are indexed as molecular addition compounds at each component (the modification term "complex" is used in this special case); e.g., **5′-Adenylic acid, homopolymer, complex with 5′-uridylic acid homopolymer (1:1).**

In more complicated cases, a combination of policies is applied.

Examples:



Guanosine, 5′-*O*-phosphonoadenylyl-(3′→5′)- polymer with 5′-cytidylic acid and 5′-uridylic acid (additional *Chemical Substance* and *Formula Index* entries at **5′-Cytidylic acid** and **5′-Uridylic acid)**



5′-Guanylic acid
polymer with 5′-adenylic acid, complex with 5′-uridylic acid, polymer with 5′-cytidylic acid (1:1) (three additional *Chemical Substance* and *Formula Index* entries at the names of the other components)

Trade names are frequently used for polymers and are cross-referred to specific polymers if the components can be structurally defined. If the polymer components are unknown, or only partially known, or cannot structurally be defined, an index citation is made at the trade name and at the appropriate polymer class name.

Natural *rubber* is indexed at the *General Subject Index* heading **Natural rubber** and chlorine-treated rubber at **Chlorinated natural rubber**. When a synthetic rubber is indexed at **Butadiene rubber, Isoprene rubber,** etc., no additional entry will be found in the printed *Chemical Substance Index*, but for studies indexed at **Synthetic rubber, Urethane rubber,** or at **Polysulfide rubber,** information will also be found, when available, at the appropriate printed chemical compound or polymer heading, with "rubber" cited in the index modification.

Examples:

Synthetic rubber
styrene-vinyl bromide
(*General Subject Index* entry)
Benzene, ethenyl-
polymer with bromoethene, rubber
(preferred *Chemical Substance Index* entry)
Ethene, bromo-
polymer with ethenylbenzene, rubber
(additional *Chemical Substance Index* entry)

General subject headings for fibers are presented under the Top Term Fibers in Appendix I. For studies indexed at **Rayon, Acetate fibers,** etc., no additional index entries will be found, but for studies of fibers of specific chemical composition entered at **Polyamide fibers, Synthetic polymeric fibers,** etc., additional information is entered at the appropriate chemical substance name, except where a cross-reference to the fiber class appears.

Example:

Synthetic polymeric fibers
adipic acid-butanediol (*General Subject Index* entry)

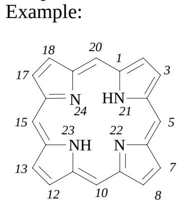
Hexanedioic acid
polymer with 1,4-butanediol, fiber (additional *Chemical Substance Index* entries at **1,4-Butanediol** and at the SRU name)

Stereochemistry of polymers is expressed by special modification terms when the necessary information is reported; such terms include isotactic, syndiotactic, threo-diisotactic, erythro-diisotactic, and disyndiotactic. The term "atactic" (for a random configuration) is not employed by *CA* in indexing specific polymers.

In addition to the special terms above, polymer stereochemistry is defined, when appropriate, by the regular descriptors *E*, *Z*, *R*, *S*, *R**, and *S** (¶ 203 I). For commercial elastomeric polymers, which cannot generally be assumed to be stereochemically homogeneous, terms such as "1,2-configuration," and "cis-1,4-configuration" are included in the descriptive portions of index modifications, but are not made part of the unique preferred *CA* index names.

223. Porphyrins and **Bile pigments.** The porphyrins embrace all cyclic tetrapyrroles in which single methene groups link pairs of pyrrole rings. The parent **21*H*,23*H*-Porphine** is used, with a suffix to express principal groups if present, for all derivatives, including hydrogenated derivatives, unless an author emphasizes the absence of hydrogen at the 21- and 23-positions.

Example:

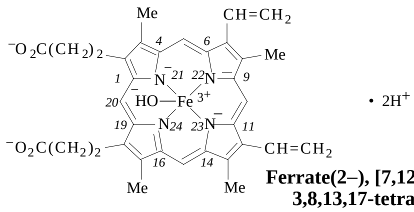


21*H*,23*H*-Porphine

Porphyrin analogs containing additional hetero atoms are indexed by organic replacement nomenclature (¶ 127) at such names as **21*H*-5-Thiaporphine** and **21*H*,23*H*-5,15-Diazaporphine.** The trivial name **21*H*,23*H*-Porphyrazine** is employed instead of 21*H*,23*H*-5,10,15,20-Tetraazaporphine, and its fused tetrabenzo derivative is **29*H*,31*H*-Phthalocyanine**. Radicals are formed in the regular way; e.g., 21*H*,23*H*-porphin-2-yl, 29*H*,31*H*-phthalocyanine-2,9,17,24-tetrayl.

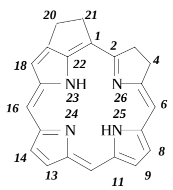
The metal complexes, including the biologically important porphyrin iron and magnesium complexes (hemes and chlorophylls) are indexed as coordination compounds (¶ 215) with italic letter locants to indicate coordinating atoms.

Example:



Ferrate(2–), [7,12-diethenyl-3,8,13,17-tetramethyl-21*H*,23*H*-porphine-2,18-dipropanoato(4–)-*N*^{21},*N*^{22},*N*^{23},*N*^{24}]hydroxy-, dihydrogen, (*SP*-**5-13**)-
(cross-reference from Hematin)

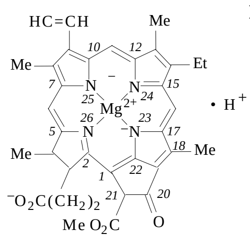
Phorbine is a cyclopentaporphine derivative:



Phorbine

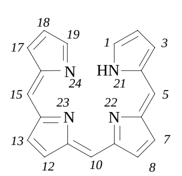
Indicated hydrogen is not expressed with Phorbine, which contains six saturated centers. Removal of hydrogen is indicated by dehydro terms, e.g., **Phorbine, 3,4-didehydro-**. Metal complexes, radicals, etc., are named as for the analogous porphine derivatives.

Example:



Magnesate(1-), [(3*S*,4*S*,21*R*)-9-ethenyl-14-ethyl-21-(methoxycarbonyl)-4,8,13,18-tetramethyl-20-oxo-3-phorbinepropanoato(3-)-κ*N*^{23},κ*N*^{24},κ*N*^{25},κ*N*^{26}]-, hydrogen, (*SP*-4-2)-
(cross-reference from Chlorophyllide a)

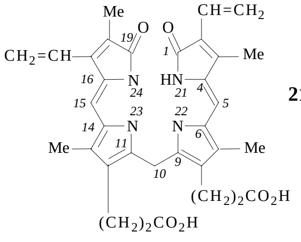
Bile pigments are indexed at **21*H*-Biline,** the numbering system of which derives from that of porphyrin (the carbon atom involved in ring closure, C-20, is omitted from the numbering system).



21*H*-Biline

All derivatives, including hydrogenated derivatives, are indexed at **21*H*-Biline** unless hydrogen is absent at the 21-position, in which case the 22*H*-parent is preferred over lower positions. The (*all-Z*) stereochemistry shown in the diagram above is assumed. The 1,19-dihydroxy derivatives are tautomeric with the dioxo compounds, which are preferred in indexing.

Example:



21*H*-Biline-8,12-dipropanoic acid, 2,17-diethenyl-1,10,19,22,23,24-hexahydro-3,7,13,18-tetramethyl-1,19-dioxo-
(cross-reference from Bilirubin)

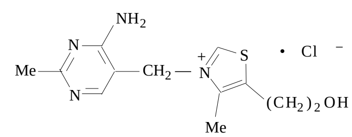
For derivatives of **Corrin,** see **Vitamin B$_{12}$** (¶ 224).

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 B$_4$, Vitamin B$_6$, 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, but "see also" cross-references in the *Index Guide* lead from these names to more specific related headings whenever possible. Vitamin names occasionally still encountered, e.g., **Vitamin P$_4$, Vitamin U,** but not discussed in the present account will usually be found cross-referred in the *Index Guide* to the preferred index names.

Vitamin A is a heading parent employed for the group of A vitamins and for vitamin A activity in general. Vitamin A$_1$ is indexed at the carotenoid heading **Retinol** (¶ 212); Vitamin A$_2$ 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.

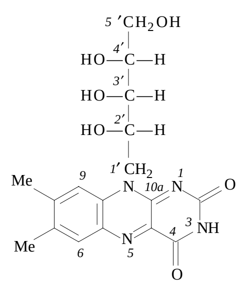
Vitamin B is a heading parent employed for the B-complex and vitamin B activity in general. **Vitamin B$_1$** and related compounds are indexed at the systematic names. (The trivial name Thiamine, not used as a *CA* index heading, implies presence of a chloride anion.)

Example:



Thiazolium, 3-[(4-amino-2-methyl-5-pyrimidinyl)methyl]-5-(2-hydroxyethyl)-4-methyl-chloride
(cross-references from Aneurine; Thiamine; and Vitamin B$_1$)

The diphosphoric (pyrophosphoric) acid ester of Vitamin B$_1$ (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-dioxa-4,6-diphosphahex-1-yl)-. Vitamin B$_2$ contains a ribitol residue and is indexed at the stereoparent
Riboflavin:



Riboflavin
(cross-references from Benzo[*g*]pteridine-2,4(3*H*,10*H*)-dione, 7,8-dimethyl-10-(D-*ribo*-2,3,4,5-tetrahydroxypentyl)-; Lactoflavin; D-Ribitol, 1-deoxy-1-(3,4-dihydro-7,8-dimethyl-2,4-dioxobenzo[*g*]pteridin-10(2*H*)-yl)-; Vitamin B$_2$; Vitamin G)

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)-** (cross-reference in the *Index Guide* at Galactoflavin).

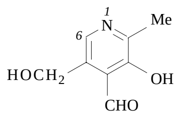
Vitamin B$_3$ is indexed at **3-Pyridinecarboxamide**; Vitamin B$_5$ is a little-used term for Pantothenic acid, which is indexed at β-**Alanine:**

$HOCH_2CMe_2CH(OH)CONH(CH_2)_2CO_2H$

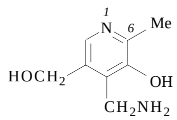
β-**Alanine, N-[(2*R*)-2,4-dihydroxy-3,3-dimethyl-1-oxobutyl)-**] (cross-reference from Pantothenic acid) (The (*R*)-isomer is assumed unless otherwise stated in the original document.)

Vitamin B_6 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.

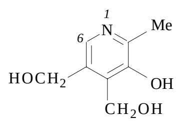
Examples:



4-Pyridinecarboxaldehyde, 3-hydroxy-5-(hydroxymethyl)-2-methyl-
(cross-reference from Pyridoxal)

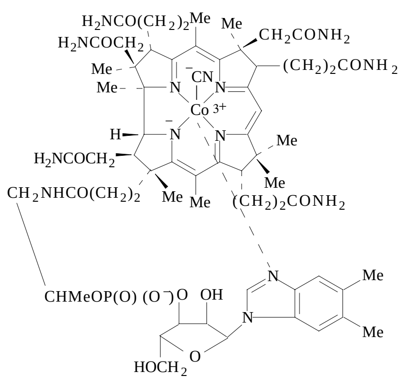


3-Pyridinemethanol, 4-(aminomethyl)-5-hydroxy-6-methyl-
(cross-reference from Pyridoxamine)



3,4-Pyridinedimethanol, 5-hydroxy-6-methyl-
(cross-references from Pyridoxine; Pyridoxol)

Vitamin B_{12} is an index heading used for the vitamin itself:

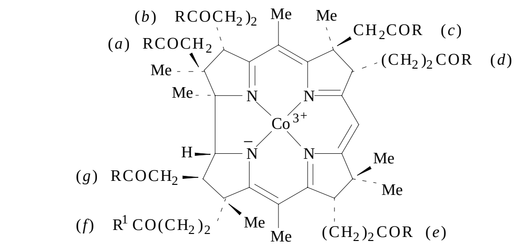


Vitamin B_{12}
(cross-references from Cobalamin, cyano-; Cobamin; Cobinamide, cyanide, dihydrogen phosphate (ester), inner salt, 3′-ester with 5,6-dimethyl-1-α-D-ribofuranosyl-1*H*-benzimidazole; and Cyanocobalamin)

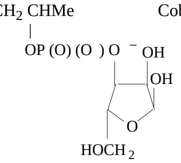
The terms Cyanocobalamin and Cobalamin are not used in index names. Derivatives, other than functional derivatives, of Vitamin B_{12} are indexed largely in accordance with rules of the International Union of Pure and Applied Chemistry,[6] which should be consulted for details.

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: **Cobyrinic acid, Cobinic acid, Cobamic acid,** or the corresponding amides.

[6]IUPAC, “Nomenclature of Corrinoids (Rules approved 1975)”, *Pure Appl. Chem.* **1976**, 48, 495-502; *Biochemistry* **1974**, 13, 1555-60.



R= R^1 = OH	Cobyrinic acid
R= R1 = NH2	Cobyrinamide acid
R= OH; R^1= $NHCH_2CHMeOH$	Cobinic acid (in Cabinamide, R= NH_2)
R= OH; R^1= $NHCH_2$ CHMe	Cobamic acid (in Cobamide, R= NH_2)

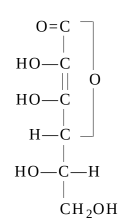


In **Cobamic acid** and **Cobamide,** the structures (above) have been shown as inner salts; the cobalt(3+) nucleus is also coordinated with the nitrogen atoms with loss of one proton overall. The compound therefore still possesses a 1+ charge. Similarly, **Cobyrinic** and **Cobinic acids** (and their amides), which lack the phosphate group, have a 2+ charge, and can form dihydroxides, cyanide hydroxides, etc. Partial amides of **Cobyrinic acid** are designated by use of the small italic locants shown in the diagram above; e.g., **Cobyrinic acid-*abcdeg*-hexamide,** dicyanide. Substitution on amide groups is indicated by *N* with a superscript, e.g., N^f-(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*-ammine, *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-Bassett numbers (¶ 215) or Stock numbers are cited in the heading; e.g., **Cobinamide-*Co*(*1+*)**, ***Co*-ethyl deriv., monohydrate** (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 **Cobyrinic 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 cobyrinic acid are named **Ferrobyrinic acid** and **Nickelibyrinic acid,** respectively. The hydrogen analog is **Hydrogenobyrinic acid.**

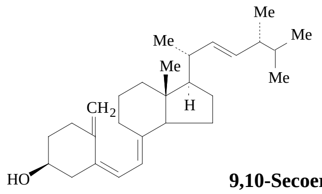
Vitamin C is indexed at L-**Ascorbic acid:**



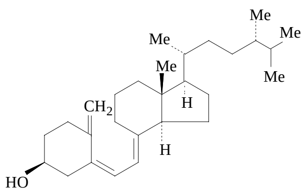
L-**Ascorbic acid**
(cross-references from L-*threo*-Hex-2-enonic acid, γ-lactone; Vitamin C)

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 D_1 is a molecular addition compound of Vitamin D_2 and (3β,9β,10α)-ergosta-5,7,22-trien-3-ol (lumisterol). Vitamins D_2 and D_3 are indexed in accordance with the rules for secosteroids (¶ 211).

Examples:

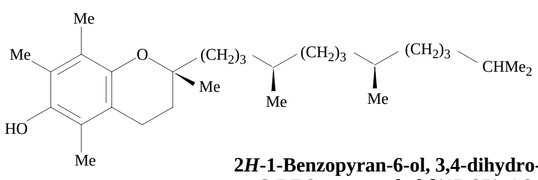


9,10-Secoergosta-5,7,10(19),22-tetraen-3-ol
(**3β,5*Z*,7*E*,22*E***)- (cross-references from Calciferol, Ergocalciferol, and Vitamin D_2)



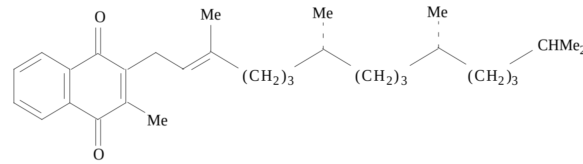
9,10-Secocholesta-5,7,10(19)-trien-3-ol
(**3β,5*Z*,7*E***)- (cross-references from Cholecalciferol and Vitamin D_3)

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:

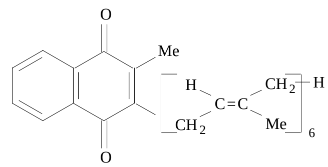


2*H*-1-Benzopyran-6-ol, 3,4-dihydro-2,5,7,8-tetramethyl-[(4*R*,8*R*)-4,8,12-trimethyltridecyl]-, (2*R*-)
(cross-reference from α-Tocopherol; "see also" cross-reference at Vitamin E)

Vitamin K is used as a group heading; the specific compounds are named systematically.
Examples:



1,4-Naphthalenedione, 2-methyl-3-[(2*E*,7*R*,11*R*)-3,7,11,15-tetramethyl-2-hexadecenyl]-
(cross-references from Phylloquinone and Vitamin $K_{1(20)}$)



1,4-Naphthalenedione, 2-[(2*E*,6*E*,10*E*,14*E*,18*E*)-3,7,11,15,19,23-hexamethyl-2,6,10,14,18,22-tetracosahexaenyl]-3-methyl-
(cross-references from Farnoquinone, and Vitamin $K_{2(30)}$)

G. CHEMICAL SUBSTANCE NAMES FOR RETROSPECTIVE SEARCHES

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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 peroxoic 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, sydnones). 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)
Butanethioyl 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** (*E*)- (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-Propanesulfeno(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)-	(Succinanilic acid)
Acetamide, *N*-hydroxy-	(Acetohydroxamic acid)
Acetaldehyde, 1-nitro-oxime	(Acetonitrolic acid)

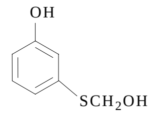
See also **Oxo acids** (¶ 273).

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.

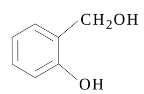
Effective with Volume 124, oxides, etc. attached to the parent portion of the name continue to be cited as oxide, sulfide, etc., with an appropriate locant in the modification portion of the name, however, if the attachment is not to the parent, terms such as oxido, sulfido, selenido, or tellurido will 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*-hydroxyphenyl)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 polyhydric 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-hydroxy-3-methyl-	(2,3-Cresotaldehyde)
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 **Ethanethio**a**mide**. Anilides are now indexed as *N*-phenyl amides. Secondary and tertiary amides are named at the preferred primary amide name. Thio analogs of sulfonamides are named as sulfonothioamides and sulfonodithioamides. 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).

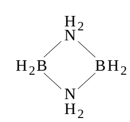
Beginning in 1992, primed locants are assigned to the side-chain methyl group of isoleucine, alloisoleucine, leucine, valine, and isovaline. Such branched-chained derivatives of these acids are no longer named as derivatives of the linear acid (Butanoic acid or Norvaline).

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 **Tricarbon**i**c acid** are used for carbonic acid anhydrides and their analogs (¶ 183). Anhydrides of phosphonic, phosphorous, arsonic, 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 polyhydric 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 alditols.

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, $H_2NN{:}C(Cl)SH$, became **Carbonochloridohydrazonothioic acid**. **Cyanic acid, Thiocyanic**

acid, etc., were retained. **Carbamic acid** was kept as an acceptable abbreviated version of Carbonamidic acid; the abbreviation is also employed when other affixes are present, as indicated in the following list of revised names.

Carbamic acid	H_2NCO_2H
Carbamohydrazonic acid	$H_2NC(=NNH_2)OH$
Carbamimidic acid	$H_2NC(=NH)OH$
Carbamothioic acid *S*-**ethyl ester**	$H_2NC(O)SEt$
Carbamo(dithioperox)imidic acid	$H_2NC(=NH)SSH$

Carbonic acids with a single hydrazide residue replacing an acid group are indexed, not as Carbonohydrazidic acid derivatives, but at **Hydrazine** index heading parents such as **Hydrazinecarboxylic acid**. The dihydrazide is named **Carbonic dihydrazide**. Phosgene, $C(:O)Cl_2$, is indexed at **Carbonic dichloride**.

Carbonic acid is now a “Class I” acid in the naming of esters (¶¶ 185, 247) as are **Formic acid, Carbamic acid, Carbamic acid, methyl-,** and **Carbamic acid, phenyl-**.

242. Coordination compounds (¶ 215). Beginning in Volume 76 (1972), the stereochemistry (when known) of mononuclear coordination complexes has been described in the index name modification by capital italic letter symbols (¶ 203 III).

The ligating atoms of ligands, with certain limitations, are denoted by capital italic element-symbol locants for mononuclear complexes and for non-bridging ligands of polynuclear complexes. Use of these locants has resulted in a change in some simple inorganic ligand names; thus nitrito became (nitrito-*O*) and nitro became (nitrito-*N*).

Delocalized ligands are now denoted by the “hapto” convention, in which the Greek letter eta (η) is employed, along with locants to indicate the particular ligand atoms involved, or else a superscript indicating the total number of such atoms (when all are involved).

Compounds containing more than one complex anion are indexed at the preferred anion while other anions are cited with (simple) cations in the modification.

Ligands containing ester groups now normally include the esters in the ligand names. The rules for choice of a radical name for a ligand, rather than a name ending in “-ato,” underwent some modification. Enclosing marks are employed around all “-ato” ligand names, and additional enclosing marks are added for bridging ligands when the ligand name itself requires enclosing marks; e.g., [μ-(acetato-*O*:*O*′)].

Beginning in Volume 106 (1987) salts of dithio(seleno, telluro) organic acids and polythio(seleno, telluro) arsenic and phosphorus acids with coordination metals are structured and named at the chelated forms.

Metal “radical” names, e.g., “aluminio,” are no longer employed for attachment of one metal to another in a binuclear complex, or as multiplicative radicals (¶ 194).

Numerical prefixes gave way to numerical ratios when mixed cations and anions (or at least one multivalent ion) are expressed in the modification. The terms “ion(1+),” “ion(2+),” etc., are not cited in modifications.

Chemical Substance Index entries at the names of the ligands, with certain exceptions such as uncommon stereoparents, rings, and heterocyclic parents (¶ 215), were discontinued for the Twelfth Collective Index period.

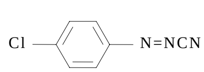
Beginning in Volume 126 (1997), the Kappa system replaces the donor atom system for describing the position of ligand attachment to a coordination center. In the Kappa system, when it is necessary to indicate the attachment of a ligand to a coordination center, the ligating atom(s) are indicated by the italic element symbol of the atom(s) preceded by a Greek Kappa (κ). This combination of italic element symbol and Greek Kappa is placed after that portion of the index name to which it directly applies; e.g., (2-aminoethanolato-κ*O*).

Beginning with Volume 129, some substances which have had coordination names will receive ring names. These are heteroatom rings that have no coordinate bonds and that meet the criteria for rings as outlined in Section B of *Index Guide* Appendix IV.

Old Name Sulfur, mercaptomethylperoxy-, (T-4)-
New Name Dioxathiirane, 3,3-dihydro-3-mercapto-3-methyl-

243. Diazo compounds, including diazohydroxides, etc., are now often named at **Diazene** headings (¶ 193).

Example:



Diazenecarbonitrile, (4-chlorophenyl)- (formerly Benzenediazocyanide, *p*-chloro-)

The unsubstituted radical HN=N– is now named diazenyl (formerly diazeno).

244. Dyes (¶ 216) of known constitution are now always indexed at their systematic names. Previously, azo dyes and a few other classes were given C.I. (*Colour Index*) names for indexing purposes. Mixed dyes are indexed (like other mixtures, ¶ 221) at the names of their components when these are known. C.I. names are employed, when available, for dyes of unknown composition.

245. Elementary particles (¶ 217) are now indexed and registered as chemical substances.

Examples:

Lepton
Meson, π^- (140)
Muon, μ^+ (106)
Nucleon
  resonance N*(2040)
Positron
  leptonic mol. with chlorine ($e^+e^-Cl^0$)
Proton

246. Enzymes (¶ 218) are now indexed as chemical substances to which CAS Registry Numbers are assigned. At the index heading **Enzyme Commission** in the *Index Guide*, a list of E.C. numbers will be found from which cross-references lead to the *CA* index names. These are inverted if they consist of more than one word.

Examples:

Dehydrogenase, lactate
Phosphatase, adenosine tri-
Asparaginase
Papain

The heading may contain further information regarding secondary activities, etc.; thus: **Dehydrogenase, malate** (**decarboxylating**).

247. Esters (¶ 185). Some changes were made in the list of “Class I” (i.e., common) acids. The following acids were added:

Benzoic acid, amino- (all isomers)
Carbamic acid, methyl-
Carbonic acid
Phosphorodithioic acid
Phosphorothioic acid

Inorganic oxo acids other than **Boric acid** (**H_3BO_3**)**, Nitric, Phosphoric, Phosphorous, Sulfuric,** and **Sulfurous acids** were removed from the Class I list and therefore are now preferred as the heading parents for esters with Class I and Class II alcohols. (Additional entries for esters were discontinued.)

Cyclic esters are named as heterocycles. Esters of stereoparents with systematically named acids are indexed at the stereoparents (¶ 202).

The use of a radical term ending in “-yl ester” is now preferred to “ester with...,” even when the alcoholic component contains a chemical function higher than alcohol (see ¶ 250), unless the latter phrase is followed by a stereoparent, as in “5′-ester with adenosine,” or by an acid requiring a synonym line formula, as in “triester with boric acid (H_3BO_3).” When the “-ate” form of a polybasic acid name is cited in the modification at an alcohol heading, all free acid groups are denoted by the word “hydrogen,” e.g., **Cyclohexanol, 4-bromo-, dihydrogen phosphate**.

Esters of substituents of index heading parents are expressed as substituents. Thus, the acetate of **Benzenesulfonic acid, 4-hydroxy**- is named **Benzenesulfonic acid, 4-**(**acetyloxy**)-, and the methyl ester of **Pyridinium**, **3-carboxy-1-methyl-, chloride**, is indexed at **Pyridinium, 3-**(**methoxycarbonyl**)**-1-methyl-, chloride**.

Ortho esters are named as ethers, i.e., as alkyloxy and aryloxy substituents. Organic replacement “a” names are used for esters where appropriate (¶ 127).

248. Ethers (¶ 196) are named as substituents of hydrocarbons and other index heading parents; Ether as a heading parent was discontinued. Thus, Ethyl ether became **Ethane, 1,1′-oxybis-**. Polyethers may often be named by organic replacement nomenclature (“a” names) (¶ 127). Methylenedioxy derivatives of benzene and its hydrogenated derivatives are named at **1,3-Benzodioxole**.

249. Formazan (¶ 193) was retained in 1972, but was ranked just below imines as the highest of the nitrogen compound classes lacking functional suffixes. Formazan radicals were also retained. However, beginning with the Thirteenth Collective period formazan, in all its aspects, is named systematically (¶ 193).

250. Functional derivatives (¶ 112) (now restricted to acyclic anhydrides, esters, hydrazides, hydrazones, and oximes) of principal chemical functions have continued to be expressed in the index modifications at boldface index headings, but derivatives of subsidiary functions are usually included in the substituent prefixes which follow the comma of inversion in an inverted heading. Hence Benzoic acid, *p*-hydroxy-, ethyl ester, acetate, is now named **Benzoic acid, 4-(acetyloxy)-, ethyl ester** (¶ 185). Esters are always expressed by use of an “-yl ester” phrase when possible, not by an “ester with” phrase, unless a stereoparent or an acid which requires a synonym line formula is being cited in a modification. Prior to Volume 76, “ester with” was used when the alcoholic component contained a higher functon; now, “ester with glycolic acid” becomes “carboxymethyl ester.”

251. Guanidine and relatives. Guanidine (¶ 183) was retained as an index heading parent for Carbonimidic diamide with the locants shown (numerical locants were formerly employed):

$$H_2\underset{N}{N}C(=\underset{N''}{N}H)\underset{N'}{N}H_2$$

It is ranked below **Urea** (carbonic diamide).

Biguanidine is now named **1,2-Hydrazinedicarboximidamide** with the locants shown:

$$H_2\underset{N}{N}C(=\underset{N'}{N}H)\underset{1}{N}H\underset{2}{N}HC(=\underset{N'''}{N}H)\underset{N''}{N}H_2$$

It ranks as the amide of a diimidic acid of a nitrogen acyclic parent, e.g., above **Benzenedicarboximidamide** but below **Benzamide**.

Biguanide and Triguanide are now named systematically as **Imidodicarbonimidic diamide** and **Diimidotricarbonimidic 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 hydrazino and hydrazono 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. Semioxamazones are treated as alkylidene hydrazides of **Acetic acid, aminooxo-**, 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 imidoyl radicals; hence, formimidoyl has become (iminomethyl), and propionimidoyl is indexed as (1-iminopropyl).

255. Index name selection policies for chemical substances (¶ 138) were revised for Volume 76 and subsequent volumes as follows:

(*a*) "Like treatment of like things" was abandoned.

(*b*) The principle of "complexity" (a measure of the number of parentheses and brackets in a name) is no longer employed.

(*c*) The principle of "lowest locants" of substituents on an index heading parent (¶¶ 137, 138) was introduced on a regular basis.

(*d*) The principle of "centrality" is now applied when a compound contains a sequence of three or more occurrences of the same heading parent.

(*e*) Conjunctive nomenclature (¶ 124) was extended for the first time to benzene with a *single* acyclic functional substituent, as in **Benzenemethanol** (names such as **Benzenediacetic 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.

(*f*) Multiplicative nomenclature (¶ 125) based on hydrocarbons is now permitted, as in **Ethane, 1,1′-oxybis-**, and **Benzene, 1,1′-[1,2-ethanediylbis(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 $-CH(CH_3)-SiH_2-$. 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**, $(H_2N)FP(O)O$-$P(O)F(NH_2)$; ***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).

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 substitutively; acid isocyanides are treated like acid halides. For example, Isopropyl isocyanide became **Propane, 2-isocyano-**; **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 now cited to indicate positions of attachment of the multiplying radical to the heading parent, unless such a parent (*a*) contains only one skeletal atom, e.g., **Methanone, Silane**; (*b*) is a functional parent compound (¶ 130) possessing replaceable hydrogen at only one position, e.g., **Carbamic acid**, **Formic acid**, **Phosphonic acid**; or (*c*) is a radicofunctional heading parent, e.g., **Disulfide**.

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 conjuctive 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; an index entry appears also at **Benzene, pentachloronitro-**, mixt. contg.

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; Ethanamine, *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.

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, Triguanide, 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 ($RC{\equiv}N-\overset{+}{N}-\overset{-}{R'}$) are named as substituted hydrazinium hydroxide inner salts (¶ 201) beginning in the Twelfth Collective period.

268. Nitrone, $H_2C{=}NH{=}O$, 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 (formerly Ammonium, diethyldimethyl-, 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*) 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).

(*b*) **Ferrocene** and other metallocenes are ranked with neutral coordination complexes.

(*c*) 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, Benzenearsonic 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.

(*d*) Alcohols and phenols now rank as equal in precedence.

(*e*) 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.

(*f*) 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.

(*g*) 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_5, **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:

Arsenic acid (H_3AsO_4)	$(HO)_3AsO$
Arsonic acid	$(HO)_2HAsO$
Arsinic acid	$(HO)H_2AsO$
Arsenenic 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^5-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 depsipeptides are now usually indexed at the *C*-terminal *amino*-acid names; terminal hydroxy acids are expressed as carboxyalkyl esters. Cyclic depsipeptides are indexed at ring names or "Cyclo" names in analogy with peptides.

Effective with Volume 129, the rules for naming peptites have been revised as follows: (1) In depsipeptide 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 depsipeptides 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*, *N^2-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**); cross-references in the *Index Guide* show the species relationships; thus, **Insulin (human-B reduced)**. See *Insulin* (*ox-B reduced*), *30-L-threonine-*. **Actinomycin D** is the reference stereoparent 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 (ethyldioxy) 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, H_2P–PH–, was renamed diphosphinyl, and diphosphinetetrayl became 1,2-diphosphinediylidene. **Phosphorothioic** and **Phosphorodithioic 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 ylidene 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 ($POCl_3$) is now phosphoric trichloride.

277. Polymers (¶ 222). Polymers whose component monomers are known are now indexed at the names of each of the component monomers as actually reported in the original document. 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-hexanediyl*)]. 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.

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".

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. **21*H*,23*H*-Porphine** and **21*H*,23*H*-Porphyrazine** are the forms preferred for these and related substances unless an original document emphasizes the absence of hydrogen at these positions. The **29*H*,31*H*-form** of **Phthalocyanine** is preferred; the heading **21*H*-Biline** is employed unless hydrogen is absent from that position, in which case **22*H*-Biline** is indexed. (An (*all-Z*) form is now assumed for Biline.)

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 disiloxanediyl) 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	(Formamidine)
Imidodicarbonic acid	(Imidodicarboxylic acid)
Diimidotricarbonimidic diamide	(Triguanide)
1,3-Benzenedisulfonothioic acid	(*m*-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-Thiatricyclo[3.3.1.1^{3,7}] decane**, etc. (¶ 155). The locants *o*-, *m*-, *p*-, and ν- in ring names were replaced by numerals; *as*- and *s*- 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 **1*H*-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. 1λ^4,3λ^4,5λ^4,7λ^4-**1,3,5,7,2,4,6,8-Tetrathiatetrazocine** (formerly 1*H*,3*H*,5*H*,7*H*-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. **2*H*-1,4-Selenazin-2-one, 1,1-dihydro-1,1-dimethyl-**(formerly 2*H*-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, trifluoro-, ion(1-); Borate(1-), tetrafluoro-; Borate(1-), tetraphenyl-; Methanesulfonic acid, 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 ($SiCl_4$), 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 silathianes; 1,3-disiloxanediyl, 1,5-trisilathianediyl, 1,7-tetrasilazanediyl, 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-methylethoxy). 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 (±)- 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 ther 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-alanylglycyl-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(CH_2-NH)-L-tyrosyl-.

286. Steroids (¶ 211). Stereochemical descriptors, e.g., "5α-," 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;* they are now cross-referred to systematic ring names. Cyclogonane *stereoparents* are retained, with stereochemistry defined by illustrative diagrams in the *Chemical Substance Index* and the *Index Guide.*

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 isocyano, 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 –IO_2. 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.; ν-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)–; carbonohydrazonoyl, –C(:NNH_2)–, 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-dioxa-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-Episulfides are named as **Thiirane** or **Thiirene** derivatives; 1,3-episulfides as **Thietane** or **Thiete** derivatives. Acyclic mercaptals and mercaptoles 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 SO_2 groups, e.g., **Butane**, **1-chloro-3-(methyl-sulfonyl)-** (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 a 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. Cross-references in the *Index Guide* reflect these policies; thus, Uracil is cross-referred to **2,4(1*H*,3*H*)-Pyrimidinedione**, not to 2,4-Pyrimidinediol.

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*,4a*R*,7*R*,8a*S*)-.

Illustrative diagrams for terpene stereoparents, e.g., **Gammacerane, Lanostane,** showing the stereochemistry for each, are provided in the *Chemical Substance Index* and the *Index Guide*. 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 **Benzeneethanethiol**, 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, *N′*-ethyl-*N*,*N*-dimethyl-	(Urea, 3-ethyl-1,1-dimethyl-)
Acetamide, *N*-(aminocarbonyl)-	(Urea, acetyl-)
Ethanethioamide, *N*-(aminocarbonyl)-	(Urea, (thioacetyl)-)
Urea, (aminoiminomethyl)-	(Urea, amidino-)
1,2-Hydrazinedicarboxamide	(Biurea)
Imidodicarbonic diamide	(Biuret)
Urea, *N*,*N′*-diphenyl-	(Carbanilide)
Diimidotricarbonic diamide	(Triuret)
Carbamimidothioic acid, 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 A_1 (Vitamin A_2 is indexed at **Retinol, 3,4-didehydro-**); **Riboflavine** (**Riboflavin** beginning in Volume 86) for Vitamin B_2; and L-**Ascorbic acid** for Vitamin C. **Vitamin B_{12}** 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.

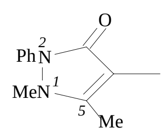
H. ILLUSTRATIVE LIST OF SUBSTITUENT PREFIXES

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.)

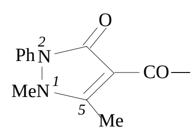
abietamido = [[[1,2,3,4,4a,4b,5,6,10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-1-phenanthrenyl]carbonyl]amino] $C_{19}H_{29}CONH$–
acenaphthenyl = (1,2-dihydroacenaphthylenyl) $(C_{12}H_9)$–
1,2-acenaphthenylene = (1,2-dihydro-1,2-acenaphthylenediyl) –$(C_{12}H_8)$–
1-acenaphthenylidene = 1(2*H*)-acenaphthylenylidene $(C_{12}H_8)$=
acetamido = (acetylamino) AcNH–
acetenyl = ethynyl HC≡C–
acetimido = (acetylimino) or (1-iminoethyl) AcN= or MeC(=NH)–
acetimidoyl = (1-iminoethyl) MeC(=NH)–
acetoacetamido = [(1,3-dioxobutyl)amino] $MeCOCH_2CONH$–
acetoacetyl = (1,3-dioxobutyl) $MeCOCH_2CO$–
acetohydroximoyl = [1-(hydroxyimino)ethyl] MeC(=NOH)–
acetonyl = (2-oxopropyl) $MeCOCH_2$–
acetonylidene = (2-oxopropylidene) MeCOCH=
acetoxy = (acetyloxy) AcO–
acetyl Ac (MeCO–)
acetylene = 1,2-ethanediylidene =CHCH=
acridanyl = (9,10-dihydroacridinyl) $(C_{13}H_{10}N)$–
acryloyl = (1-oxo-2-propenyl) H_2C=CHCO–
acrylyl = (1-oxo-2-propenyl) H_2C=CHCO–
adamantyl = tricyclo[3.3.1.$1^{3,7}$]decyl $(C_{10}H_{15})$–
adamantylene = tricyclo[3.3.1.$1^{3,7}$]decanediyl –$(C_{10}H_{14})$–
adipaldehydoyl = (1,6-dioxohexyl) $HCO(CH_2)_4CO$–
adipamoyl = (6-amino-1,6-dioxohexyl) $H_2NCO(CH_2)_4CO$–
adipaniloyl = [1,6-dioxo-6-(phenylamino)hexyl] $PhNHCO(CH_2)_4CO$–
adipoyl = (1,6-dioxo-1,6-hexanediyl) –$CO(CH_2)_4CO$–
adipyl = (1,6-dioxo-1,6-hexanediyl) –$CO(CH_2)_4CO$–
alaninamido = [(2-amino-1-oxopropyl)amino] $MeCH(NH_2)CONH$–
alanyl[1] = (2-amino-1-oxopropyl) $MeCH(NH_2)CO$–
β-**alanyl**[1] = (3-amino-1-oxopropyl) $H_2N(CH_2)_2CO$–
aldo[2] = oxo O=
alloisoleucyl[1] = (2-amino-1-methyl-1-oxopentyl) $EtCHMeCH(NH_2)CO$–
allophanamido = [[[(aminocarbonyl)amino]carbonyl]amino] $H_2N(CONH)_2$–
allophanoyl = [[(aminocarbonyl)amino]carbonyl] $H_2NCONHCO$–
allothreonyl[1] = (2-amino-3-hydroxy-1-oxobutyl) $MeCH(OH)CH(NH_2)CO$–
allyl = 2-propenyl $H_2C=CHCH_2$–
β-**allyl** = (1-methylethenyl) H_2C=CMe–
π-**allyl** = (η^3-2-propenyl)

$$[CH_2\!\equiv\!CH\!\equiv\!CH_2]-$$

allylidene = 2-propenylidene H_2C=CHCH=
ambrosan-6-yl = [decahydro-3a,8-dimethyl-5-(1-methylethyl)-4-azulenyl] $(C_{15}H_{27})$–
amidino = (aminoiminomethyl) $H_2NC(=NH)$–
amidoxalyl = (aminooxoacetyl) H_2NCOCO–
amino H_2N–
(**aminoamidino**) = (aminohydrazonomethyl) or (hydrazinoiminomethyl) $H_2NC(=NNH_2)$– or $H_2NNHC(=NH)$–
(**aminoiminophosphoranyl**) = (*P*-aminophosphinimyl) $H_2NPH(=NH)$–
ammonio H_3N^+–
amoxy = (pentyloxy) $Me(CH_2)_4O$–
amyl = pentyl $Me(CH_2)_4$–
tert-**amyl** = (1,1-dimethylpropyl) $EtCMe_2$–
amylidene = pentylidene BuCH=
anilino = (phenylamino) PhNH–
anisal = [(methoxypheny])methylene] $MeOC_6H_4CH$=
anisidino = [(methoxyphenyl)amino] $MeOC_6H_4NH$–
anisoyl = (methoxybenzoyl) $MeOC_6H_4CO$–
anisyl = (methoxyphenyl) or [(methoxyphenyl)methyl] $MeOC_6H_4$– or $MeOC_6H_4CH_2$–
anisylidene = [(methoxyphenyl)methylene] $MeOC_6H_4CH$=
anthranilamido = [(2-aminobenzoyl)amino] 2–$H_2NC_6H_4CONH$–
anthraniloyl = (2-aminobenzoyl) 2–$H_2NC_6H_4CO$–
anthranoyl = (2-aminobenzoyl) 2–$H_2NC_6H_4CO$–
anthraquinonyl = (9,10-dihydro-9,10-dioxoanthracenyl) $(C_{14}H_7O_2)$–
anthraquinonylene = (9,10-dihydro-9,10-dioxoanthracenediyl) –$(C_{14}H_6O_2)$–
anthroyl = (anthracenylcarbonyl) $(C_{14}H_9)CO$–
anthryl = anthracenyl $(C_{14}H_9)$–
anthrylene = anthracenediyl –$(C_{14}H_8)$–
antimono = 1,2-distibenediyl –Sb=Sb–
antipyrinyl (**antipyryl**) = (2,3-dihydro-1,5-dimethyl-3-oxo-2-phenyl-1*H*-pyrazol-4-yl)



antipyroyl = [(2,3-dihydro-1,5-dimethyl-3-oxo-2-phenyl-1*H*-pyrazol-4-yl)carbonyl]

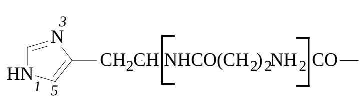


apocamphanyl = (7,7-dimethylbicyclo[2.2.1]heptyl) (C_9H_{15})–
apotrichothecanyl = (decahydro-3a,6,8a,8b-tetramethyl-1*H*-cyclopenta[*b*]benzofuranyl) $(C_{15}H_{25}O)$–
arginyl[1] = [2-amino-5-[(aminoiminomethyl)amino]-1-oxopentyl] $H_2NC(=NH)NH(CH_2)_3CH(NH_2)CO$–
arseno = 1,2-diarsenediyl –As=As–
arsenoso OAs–
arsinico[3,4] HOAs(O)=
arsinidenio H_2As^+=
arsinimyl AsH_2(=NH)–
arsino AsH_2–
arsinothioyl AsH_2(S)–
arsinyl AsH_2(O)–
arsinylidene AsH(O)=
arso O_2As–
arsonio H_3As^+–
arsono[4] $(HO)_2As(O)$–
arsononitridyl AsH(≡N)–
arsoranyl AsH_4–
arsoranylidene H_3As=
arsoranylidyne AsH_2≡
arsylene = arsinidene AsH=
arsylidyne = arsinidyne As≡
asaryl = (2,4,5-trimethoxyphenyl) 2,4,5–$(MeO)_3C_6H_2$–
asparaginyl[1] = (2,4-diamino-1,4-dioxobutyl) $H_2NCOCH_2CH(NH_2)CO$–
α-**asparaginyl**[1] = (3,4-diamino-1,4-dioxobutyl) $H_2NCOCH(NH_2)CH_2CO$–
asparagyl = asparaginyl
aspartoyl[1] = (2-amino-1,4-dioxo-1,4-butanediyl) –$COCH_2CH(NH_2)CO$–
aspartyl = aspartoyl or unspecified aspartyl (see below)
α-**aspartyl**[1] = (2-amino-3-carboxy-1-oxopropyl) $HO_2CCH_2CH(NH_2)CO$–
β-**aspartyl**[1] = (3-amino-3-carboxy-1-oxopropyl) $HO_2CCH(NH_2)CH_2CO$–
astato At–
astatoxy = astatyl O_2At–
atisanyl (from atisane) $(C_{20}H_{33})$–
atropoyl = (1-oxo-2-phenyl-2-propenyl) H_2C=CPhCO–
azelaoyl = (1,9-dioxo-1,9-nonanediyl) –$CO(CH_2)_7CO$–
azelaaldehydoyl = (1,9-dioxononyl) $HCO(CH_2)_7CO$–
azi[5] (see also azo) –N=N–
azido N_3–
(**azidoformyl**) = (azidocarbonyl) N_3CO–
azino =NN=
azo[6] (see also azi) –N=N–
azoxy –N(O)=N–

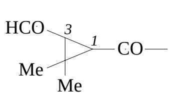
benzal = (phenylmethylene) PhCH=
benzamido = (benzoylamino) BzNH–
benzenesulfenamido = [(phenylthio)amino] PhSNH–
benzenesulfonamido = [(phenylsulfonyl)amino] $PhSO_2NH$–
benzenetriyl C_6H_3≡
benzenyl = (phenylmethylidyne) PhC≡
benzhydryl = (diphenylmethyl) Ph_2CH–
benzhydrylidene = (diphenylmethylene) Ph_2C=
benzidino = [(4′-amino[1,1′-biphenyl]-4-yl)amino] 4–$(4–H_2NC_6H_4)C_6H_4NH$–
benziloyl = (hydroxydiphenylacetyl) $Ph_2C(OH)CO$–
(**3-benziloylpropyl**) = (5-hydroxy-4-oxo-5,5-diphenylpentyl) $Ph_2C(OH)CO(CH_2)_3$–
benzimidazolinyl = (2,3-dihydro-1*H*-benzimidazolyl) $(C_7H_7N_2)$–
2-benzimidazolyl = 1*H*-benzimidazol-2-yl $(C_7H_5N_2)$–
benzimido = (benzoylimino) or (iminophenylmethyl) BzN= or PhC(=NH)–
benzimidoyl = (iminophenylmethyl) PhC(=NH)–
benzofuryl = benzofuranyl (C_8H_5O)–
benzohydroximoyl = [(hydroxyimino)phenylmethyl] PhC(=NOH)–
o-**benzoquinon-3-yl** = (5,6-dioxo-1,3-cyclohexadien-1-yl) $(C_6H_3O_2)$–
p-**benzoquinon-2,5-ylene** = (3,6-dioxo-1,4-cyclohexadiene-1,4-diyl) –$(C_6H_2O_2)$–
benzoselenophene-yl C_8H_5Se–
benzoxy = (benzoyloxy) BzO–
benzoyl Bz (PhCO–)
(**benzoylacetyl**) = (1,3-dioxo-3-phenylpropyl) $PhCOCH_2CO$–
(**benzoylformyl**) = (oxophenylacetyl) PhCOCO–
benzyl = (phenylmethyl) $PhCH_2$–
benzylidene = (phenylmethylene) PhCH=
benzylidyne = (phenylmethylidyne) PhC≡
(**benzyloxy**) = (phenylmethoxy) $PhCH_2O$–
(**benzylselenyl**) = [(phenylmethyl)seleno] $PhCH_2Se$–
bicarbamoyl = (hydrazodicarbonyl) –CONHNHCO–
bicyclo[1.1.0]butylene = bicyclo[1.1.0]butanediyl –(C_4H_4)–
biphenylyl = [1,1′-biphenyl]yl PhC_6H_4–
biphenylene = [1,1′-biphenyl]diyl –$(C_{12}H_8)$–
biphenylylene = [1,1′-biphenyl]diyl –$(C_{12}H_8)$–
bismuthino BiH_2–
bismuthylene BiH=
bismuthylidyne Bi≡
[**2,2′-bithiophen**]**-5-yl** $C_8H_5S_2$–
2-bornyl = (1,7,7-trimethylbicyclo[2.2.1]hept-2-yl) $(C_{10}H_{17})$–
3-bornylidene = (4,7,7-trimethylbicyclo[2.2.1]-hept-2-ylidene) $(C_{10}H_{16})$=
borono[4] $(HO)_2B$–
boryl BH_2–
borylene BH=
borylidyne B≡
bromo Br–
1,3-butadienediylidene = 1,3-butadiene-1,4-diylidene =C=CHCH=C=
butadiynylene = 1,3-butadiyne-1,4-diyl –C≡CC≡C–
2-butenylene = 2-butene-1,4-diyl –$CH_2CH=CHCH_2$–
butoxy BuO–
sec-**butoxy** = (1-methylpropoxy) EtCHMeO–
tert-**butoxy** = (1,1-dimethylethoxy) Me_3CO
butyl Bu ($Me(CH_2)_3$–)

butyl$^{\beta}$ = (2-methylpropyl) Me_2CHCH_2–
butyl$^{\gamma}$ = (1,1-dimethylethyl) Me_3C–
sec-**butyl** = (1-methylpropyl) EtCHMe–
tert-**butyl** = (1,1-dimethylethyl) Me_3C–
1,4-butylene = 1,4-butanediyl –$(CH_2)_4$–
sec-**butylidene** = (1-methylpropylidene) EtCMe=
(**butyloxy**) = butoxy BuO–
butynedioyl = (1,4-dioxo-2-butyne-1,4-diyl) –COC≡CCO–
butyryl = (1-oxobutyl) PrCO–

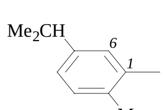
cacodyl = (dimethylarsino) Me_2As–
cadinan-1-yl = [octahydro-4,7-dimethyl-1-(1-methylethyl)-4a(2*H*)-naphthalenyl] $(C_{15}H_{29})$–
2-camphanyl = (4,7,7-trimethylbicyclo[2.2.1]hept-2-yl) $(C_{10}H_{17})$–
camphoroyl (from camphoric acid) = [(1,2,2-trimethyl-1,3-cyclopentanediyl)dicarbonyl] –$CO(C_8H_{14})CO$–
5-camphoryl (from camphor) = (4,7,7-trimethyl-5-oxobicyclo[2.2.1]hept-2-yl) $(C_{10}H_{15}O)$–
canavanyl = [*O*-[(aminoiminomethyl)amino]-homoseryl][1] or [2-amino-4-[[(aminoiminomethyl)amino]oxy]-1-oxobutyl] $H_2NC(=NH)NHO(CH_2)_2CH(NH_2)CO$–
caprinoyl = (1-oxodecyl) $Me(CH_2)_8CO$–
caproyl (from caproic acid) = (1-oxohexyl) $Me(CH_2)_4CO$–
capryl (from capric acid) = (1-oxodecyl) $Me(CH_2)_8CO$–
capryloyl (from caprylic acid) = (1-oxooctyl) $Me(CH_2)_6CO$–
caprylyl (from caprylic acid) = (1-oxooctyl) $Me(CH_2)_6CO$–
carbamido = [(aminocarbonyl)amino] H_2NCONH–
carbamoyl = (aminocarbonyl) H_2NCO–
carbamyl = (aminocarbonyl) H_2NCO–
carbanilino = [(phenylamino)carbonyl] PhNHCO–
carbaniloyl = [(phenylamino)carbonyl] PhNHCO–
carbazimidoyl = (hydrazinoiminomethyl) $H_2NNHC(=NH)$–
carbazol-9-yl = 9*H*-carbazol-9-yl $(C_{12}H_8N)$–
carbazoyl = (hydrazinocarbonyl) H_2NNHCO–
carbethoxy = (ethoxycarbonyl) EtO_2C–
carbobenzoxy = [(phenylmethoxy)carbonyl] $PhCH_2O_2C$–
carbonimidoyl[7] (see also (iminomethyl)) –C(=NH)–
carbonothioyl[7] (see also (thioxomethyl)) –CS–
carbonyl –CO–
(**carbonyldioxy**) = [carbonylbis(oxy)] –OCO_2–
(**1-carbonylethyl**) = (methyloxoethenyl) O=C=CMe–
(**carbonylmethyl**) = (oxoethenyl) O=C=CH–
(**carbonylmethylene**) = (1-oxo-1,2-ethanediyl) –$COCH_2$– or (oxoethenylidene) O=C=C=
carboxy[4] HO_2C–
(**carboxyformyl**) = (carboxycarbonyl) HO_2CCO–
(**5-carboxyvaleryl**) = (5-carboxy-1-oxopentyl) $HO_2C(CH_2)_4CO$–
carnosyl = (*N*-β-alanylhistidyl)[1] or [2-[(3-amino-1-oxopropyl)amino]-3-(1*H*-imidazol-4-yl)-1-oxopropyl]



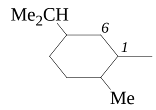
caronaldehydoyl = [(3-formyl-2,2-dimethylcyclopropyl)carbonyl]



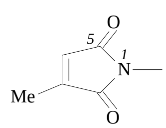
carvacryl = [2-methyl-5-(1-methylethyl)phenyl]



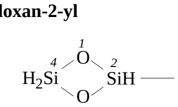
carvomenthyl = [2-methyl-5-(1-methylethyl)-cyclohexyl]



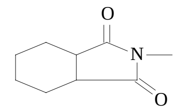
10-caryl = [(7,7-dimethylbicyclo[4.1.0]hept-3-yl)-methyl] $(C_9H_{15})CH_2$–
cathyl = [(ethoxycarbonyl)oxy] $EtOCO_2$–
cedranyl = (octahydro-3a,6,8,8-tetramethyl-1*H*-3a,7-methanoazulenyl) $(C_{15}H_{25})$–
cetyl = hexadecyl $Me(CH_2)_{15}$–
chaulmoogroyl (from chaulmoogric acid) = [13-(2-cyclopenten-1-yl)-1-oxotridecyl] $C_5H_7(CH_2)_{12}CO$–
chaulmoogryl (from chaulmoogryl alcohol) = [13-(2-cyclopenten-1-yl)tridecyl] $C_5H_7(CH_2)_{13}$–
chloro Cl–
(**chloroformyl**) = (chlorocarbonyl) ClCO–
(**chloroglyoxyloyl**) = (chlorooxoacetyl) ClCOCO–
(**chlorooxalyl**) = (chlorooxoacetyl) ClCOCO–
chlorosyl OCl–
chloryl O_2Cl–
cholesteryl (from cholesterol) = cholest-5-en-3-yl (from cholestene) $(C_{27}H_{45})$–
choloyl (from cholic acid) = (3,7,12-trihydroxy-24-oxocholan-24-yl) $(HO)_3(C_{23}H_{36})CO$–
chromanyl = (3,4-dihydro-2*H*-1-benzopyranyl) (C_9H_9O)–
cinchoninoyl (from cinchoninic acid) = (4-quinolinylcarbonyl) $(4–C_9H_6N)CO$–
cinnamal = (3-phenyl-2-propenylidene) PhCH=CHCH=
cinnamenyl = (2-phenylethenyl) PhCH=CH–
cinnamoyl = (1-oxo-3-phenyl-2-propenyl) PhCH=CHCO–
cinnamyl = (3-phenyl-2-propenyl) $PhCH=CHCH_2$–
cinnamylidene = (3-phenyl-2-propenylidene) PhCH=CHCH=
citraconimido = (2,5-dihydro-3-methyl-2,5-dioxo-1*H*-pyrrol-1-yl)



citraconoyl = (2-methyl-1,4-dioxo-2-butene-1,4-diyl) –COCMe=CHCO–
conaninyl (from conanine) $(C_{22}H_{36}N)$–
cresotoyl (from cresotic acid) = (hydroxymethylbenzoyl) $HO(Me)C_6H_3CO$–
cresoxy = (methylphenoxy) MeC_6H_4O–
cresyl = (hydroxymethylphenyl) $HO(Me)C_6H_3$– or (methylphenyl) MeC_6H_4–
cresylene = (methylphenylene) –(MeC_6H_3)–
crotonoyl = (1-oxo-2-butenyl) MeCH=CHCO–
crotonyl = (1-oxo-2-butenyl) MeCH=CHCO–
crotyl = 2-butenyl $MeCH=CHCH_2$–
cumal = [[4-(1-methylethyl)phenyl]methylene] $4–(Me_2CH)C_6H_4CH$=
cumenyl = [(1-methylethyl)phenyl] $Me_2CHC_6H_4$–
cumidino = [[4-(1-methylethyl)phenyl]amino]-4-$(Me_2CH)C_6H_4NH$–
cuminal = [[4-(1-methylethyl)phenyl]methylene] $4–(Me_2CH)C_6H_4CH$=
cuminyl = [[4-(1-methylethyl)phenyl]methyl] $4–(Me_2CH)C_6H_4CH_2$–
cuminylidene = [[4-(1-methylethyl)phenyl]methylene] $4–(Me_2CH)C_6H_4CH$=
cumoyl = [4-(1-methylethyl)benzoyl] $4–(Me_2CH)C_6H_4CO$–
cumyl[8] = [(1-methylethyl)phenyl] $(Me_2CH)C_6H_4$–
α-**cumyl** = (1-methyl-1-phenylethyl) –$PhCMe_2$–
cyanamido = (cyanoamino) NCNH–
cyanato NCO–
cyano NC–
cyclodisiloxan-2-yl

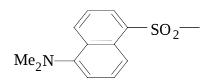


cyclohexadienylene = cyclohexadienediyl –C_6H_6–
cyclohexanecarboxamido = [(cyclohexylcarbonyl)amino] $C_6H_{11}CONH$–
1,2-cyclohexanedicarboximido = (octahydro-1,3-dioxo-2*H*-isoindol-2-yl)



cymyl = [methyl(1-methylethyl)phenyl] $Me(Me_2CH)C_6H_3$–
cysteinyl[1] = (2-amino-3-mercapto-1-oxopropyl) $HSCH_2CH(NH_2)CO$–
cysteyl = (3-sulfoalanyl)[1] or (2-amino-1-oxo-3-sulfopropyl) $HO_3SCH_2CH(NH_2)CO$–

dansyl = [[5-(dimethylamino)-1-naphthalenyl]sulfonyl]



decanedioyl = (1,10-dioxo-1,10-decanediyl) –$CO(CH_2)_8CO$–
decanoyl = (1-oxodecyl) $CH_3(CH_2)_8CO$–
decasiloxanylene = 1,19-decasiloxanediyl –$SiH_2(OSiH_2)_8OSiH_2$–
desyl = (2-oxo-1,2-diphenylethyl) PhCOCHPh–
diarsenyl HAs=As–
diarsinetetrayl = 1,2-diarsinediylidene =AsAs=
diarsinyl H_2AsAsH–
1,2-diazenediyl = azi or azo –N=N–
diazeno = diazenyl[4] (see also azo) HN=N–
diazo[5] N_2=
diazoamino = 1-triazene-1,3-diyl –NHN=N–
diazonio N_2^+–
dibenzothiophene-yl = dibenzothienyl $(C_{12}H_7S)$–
diborane(4)tetrayl = 1,2-diborane(4)diylidene =BB=
1,2-dicarbadodecaboran(12)-1-yl $(C_2H_{11}B_{10})$–
digermanylene = 1,2-digermanediyl –GeH_2GeH_2–
digermthianyl = digermathianyl $H_3GeSGeH_2$–
diglycoloyl = [oxybis(1-oxo-2,1-ethanediyl)] –$COCH_2OCH_2CO$–
(**dimethyliminio**) Me_2N^+=
dioxy[9] (see also epidioxy) –OO–
1,2-diphosphinediyl –PHPH–
diphosphinetetrayl = 1,2-diphosphinediylidene =PP=
diphosphino = diphosphinyl H_2PPH–
diphosphinylidene H_2P–P=
diseleno[9] (see also epidiseleno and seleninoselenoyl) –SeSe–
disilanoxy = (disilanyloxy) H_3SiSiH_2O–
disilanyl H_3SiSiH_2–
disilanylene = 1,2-disilanediyl –SiH_2SiH_2–
disilazanoxy = (disilazanyloxy) $H_3SiNHSiH_2O$–
disilazanyl $H_3SiNHSiH_2$–
2-disilazanyl = (disilylamino) $(H_3Si)_2N$–
disiloxanediylidene = 1,3-disiloxanediylidene =SiHOSiH=
disiloxanoxy = (disiloxanyloxy) $H_3SiOSiH_2O$–
disiloxanylene = 1,3-disiloxanediyl –SiH_2OSiH_2–
disilthianoxy = (disilathianyloxy) $H_3SiSSiH_2O$–
distannanylene = 1,2-distannanediyl –SnH_2SnH_2–
distannthianediylidene = 1,3-distannathianediylidene =SnHSSnH=
disulfinyl[6] –S(O)S(O)–
disulfonyl –SO_2SO_2–
dithio[9] (see also epidithio and sulfinothioyl) –SS–
(**dithiobicarbamoyl**) = (hydrazodicarbonothioyl) –CSNHNHCS–
(**dithiocarboxy**) HS_2C–
(**dithiohydroperoxy**) = (thiosulfeno)[4] HSS–
dodecanoyl = (1-oxododecyl) $Me(CH_2)_{10}CO$–
duryl = (2,3,5,6-tetramethylphenyl) 2,3,5,6-Me_4C_6H–
durylene = (2,3,5,6-tetramethyl-1,4-phenylene) –$(2,3,5,6–Me_4C_6)$–

enanthoyl = (1-oxoheptyl) $Me(CH_2)_5CO–$

enanthyl = (1-oxoheptyl) $Me(CH_2)_5CO–$

epidioxy[10] (see also dioxy) –OO–

epidiseleno[10] (See also diseleno and seleninoselenoyl) –SeSe–

epidithio[10] (see also dithio and sulfinothioyl) –SS–

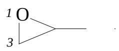
epioxy = epoxy (see also oxy and oxo) –O–

episeleno[10] (see also seleno and selenoxo) –Se–

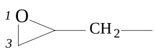
epithio[10] (see also thio and thioxo) –S–

epoxy[10] (See also oxy and oxo) –O–

(**epoxyethyl**) = oxiranyl



(**2,3-epoxypropyl**) = (oxiranylmethyl)



eremophilan-1-yl = [decahydro-4,4a-dimethyl-5-(1-methylethyl)-1-naphthalenyl] $(C_{15}H_{27})–$

ethanediylidene = 1,2-ethanediylidene =CHCH=

1,2-ethenediyl –CH=CH–

ethinyl = ethynyl HC≡C–

ethoxalyl = (ethoxyoxoacetyl) $EtO_2CCO–$

ethoxy EtO–

(**ethoxycarbonyl**) $EtO_2C–$

(**1-ethoxyformimidoyl**) = (ethoxyiminomethyl) EtOCH(=NH)–

(**ethoxyphosphinyl**) EtOPH(O)–

ethyl Et $(MeCH_2–)$

ethylene = 1,2-ethanediyl $–CH_2CH_2–$

[**ethylenebis**(**nitrilodimethylene**)] = [1,2-ethanediylbis[nitrilobis(methylene)] $(–CH_2)_2N(CH_2)_2N(CH_2–)_2$

(**ethylenedioxy**) = [1,2-ethanediylbis(oxy)] $–O(CH_2)_2O–$

ethylidene $CH_3CH=$

ethylidyne $CH_3C≡$

1-ethylium-1-ylidene $CH_3C^+=$

(**ethyloxy**) = ethoxy EtO–

(**ethylselenyl**) = (ethylseleno) EtSe–

(**ethylthio**) EtS–

eudesman-8-yl = [decahydro-5,8a-dimethyl-2-(1-methylethyl)-2-naphthalenyl] $(C_{15}H_{27})–$

farnesyl (from farnesol) = (3,7,11-trimethyl-2,6,-10-dodecatrienyl) $Me_2C=CH(CH_2)_2CMe=CH-(CH_2)_2CMe=CHCH_2–$

fenchyl = (1,3,3-trimethylbicyclo[2.2.1]hept-2-yl) $(C_{10}H_{17})–$

1,1′-ferrocenediyl $–(C_5H_4)Fe(C_5H_4)–$

fluoranyl = (3-oxospiro[isobenzofuran-1(3*H*),9′-[9*H*]xanthen]yl) $(C_{20}H_{11}O_3)–$

fluoren-9-ylidene = 9*H*-fluoren-9-ylidene $(C_{13}H_8)=$

fluoro F–

formamido = (formylamino) HCONH–

1-formazano = [(hydrazonomethyl)azo] $H_2NN=CHN=N–$

5-formazano = [(diazenylmethylene)hydrazino] HN=NCH=NNH–

formazanyl = (diazenylhydrazonomethyl) $HN=N–C(=NNH_2)–$

formazyl = [(phenylazo)(phenylhydrazono)-methyl] PhN=NC(=NNHPh)–

formimidoyl = (iminomethyl) CH(=NH)–

(**1-formimidoylformimidoyl**) = (1,2-diiminoethyl) HC(=NH)C(=NH)–

(**formimidoylformyl**) = (iminoacetyl) CH(=NH)CO–

(**formimidoylmethyl**) = (2-iminoethyl) $HC(=NH)CH_2–$

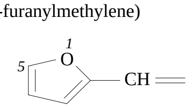
formyl[4] HCO–

fucosyl = (6-deoxygalactosyl) $(C_6H_{11}O_4)–$

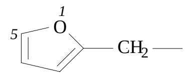
fumaraniloyl = [1,4-dioxo-4-(phenylamino)-2-butenyl] PhNHCOCH=CHCO–

fumaroyl = (1,4-dioxo-2-butene-1,4-diyl) –COCH=CHCO–

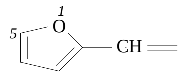
furfural = (2-furanylmethylene)



furfuryl = (2-furanylmethyl)



furfurylidene = (2-furanylmethylene)



furoyl = (furanylcarbonyl) $(C_4H_3O)CO–$

furyl = furanyl $(C_4H_3O)–$

galloyl = (3,4,5-trihydroxybenzoyl) $3,4,5–(HO)_3C_6H_2CO–$

gentisoyl = (2,5-dihydroxybenzoyl) $2,5-(HO)_2C_6H_3CO–$

geranyl (from geraniol) = (3,7-dimethyl-2,6-octadienyl) $Me_2C=CH(CH_2)_2CMe=CHCH_2–$

germacran-6-yl = [5,9=dimethyl-2-(1-methylethyl)cyclodecyl] $(C_{15}H_{25})–$

germanetetrayl =Ge=

germyl $H_3Ge–$

germylene $H_2Ge=$

germylidyne HGe≡

gibbanyl (from gibbane) $(C_{15}H_{23})–$

(**glucosyloxy**) $(C_6H_{11}O_5)O–$

glutaminyl[1] = (2,5-diamino-1,5-dioxopentyl) $H_2NCO(CH_2)_2CH(NH_2)CO–$

α-**glutaminyl**[1] = (4,5-diamino-1,5-dioxopentyl) $H_2NCOCH(NH_2)CH_2CH_2CO–$

glutamoyl[1] = (2-amino-1,5-dioxo-1,5-pentanediyl) $–CO(CH_2)_2CH(NH_2)CO–$

glutamyl = glutamoyl or unspecified glutamyl (see below)

α-**glutamyl**[1] = (2-amino-4-carboxy-1-oxobutyl) $HO_2C(CH_2)_2CH(NH_2)CO–$

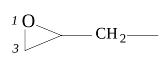
γ-**glutamyl**[1] = (4-amino-4-carboxy-1-oxobutyl) $HO_2CCH(NH_2)(CH_2)_2CO–$

glutaryl = (1,5-dioxo-1,5-pentanediyl) $–CO(CH_2)_3CO–$

glyceroyl = (2,3-dihydroxy-1-oxopropyl) $HOCH_2CH(OH)CO–$

glyceryl = 1,2,3-propanetriyl $–CH(CH_2–)_2$

glycidyl = (oxiranylmethyl)



glycinamido = [(aminoacetyl)amino] $H_2NCH_2CONH–$

glycinimidoyl = (2-amino-1-iminoethyl) $H_2NCH_2C(=NH)–$

glycoloyl = (hydroxyacetyl) $HOCH_2CO–$

glycolyl = (hydroxyacetyl) $HOCH_2CO–$

glycyl[1] = (aminoacetyl) $H_2NCH_2CO–$

glyoxalinyl = imidazolyl $(C_3H_3N_2)–$

glyoxylimidoyl = (1-imino-2-oxoethyl) HCOC(=NH)–

glyoxyloyl = (oxoacetyl) HCOCO–

(**glyoxyloylmethyl**) = (2,3-dioxopropyl) $HCOCOCH_2–$

glyoxylyl = (oxoacetyl) HCOCO–

guaiacyl = (4-hydroxy-3-methoxyphenyl) $4–OH–3–(CH_3O)C_6H_3–$ or (2-methoxyphenyl) $2–(MeO)C_6H_4–$

guaian-8-yl = [decahydro-1,4-dimethyl-7-(1-methylethyl)-6-azulenyl] $(C_{15}H_{27})–$

guanidino = [(aminoiminomethyl)amino] $H_2NC(=NH)NH–$

(**guanidinoazo**) = [3-(aminoiminomethyl)-1-triazenyl] $H_2NC(=NH)NHN=N–$

guanyl = (aminoiminomethyl) $H_2NC(=NH)–$

heptadecanoyl = (1-oxoheptadecyl) $Me(CH_2)_{15}CO–$

heptanamido = [(1-oxoheptyl)amino] $Me(CH_2)_5CONH–$

heptanedioyl = (1,7-dioxo-1,7-heptanediyl) $–CO(CH_2)_5CO–$

heptanoyl = (1-oxoheptyl) $Me(CH_2)_5CO–$

hexadecanoyl = (1-oxohexadecyl) $Me(CH_2)_{14}CO–$

2,4-hexadiynylene = 2,4-hexadiyne-1,6-diyl $–CH_2C≡CC≡CCH_2–$

hexamethylene = 1,6-hexanediyl $–(CH_2)_6–$

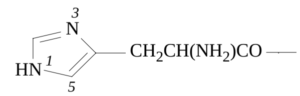
hexanedioyl = (1,6-dioxo-1,6-hexanediyl) $–CO(CH_2)_4CO–$

hexanethioyl = (1-thioxohexyl) $Me(CH_2)_4CS–$

hippuroyl = (*N*-benzoylglycyl)[1] or [(benzoylamino)acetyl] $BzNHCH_2CO–$

hippuryl = (*N*-benzoylglycyl)[1] or [(benzoylamino)acetyl] $BzNHCH_2CO–$

histidyl[1] = [2-amino-3-(1*H*-imidazol-4-yl)-1-oxopropyl]



homocysteinyl[1] = (2-amino-4-mercapto-1-oxobutyl) $HS(CH_2)_2CH(NH_2)CO–$

homomyrtenyl = [2-(6,6-dimethylbicyclo[3.1.1]-hept-2-en-2-yl)ethyl] $(C_9H_{13})CH_2CH_2–$

homopiperonyl = [2-(1,3-benzodioxol-5-yl)ethyl] $(C_7H_5O_2)CH_2CH_2–$

homoseryl[1] = (2-amino-4-hydroxy-1-oxobutyl) $HO(CH_2)_2CH(NH_2)CO–$

homoveratroyl = [(3,4-dimethoxyphenyl)acetyl] $3,4–(MeO)_2C_6H_3CH_2CO–$

homoveratryl [2-(3,4-dimethoxyphenyl)ethyl] $3,4–(MeO)_2C_6H_3CH_2CH_2–$

hydantoyl = [*N*-(aminocarbonyl)glycyl][1] or [[(aminocarbonyl)amino]acetyl] $H_2NCONHCH_2CO–$

hydnocarpoyl (from hydnocarpic acid) = [11-(2-cyclopenten-1-yl)-1-oxoundecyl] $(C_5H_7)(CH_2)_{10}CO–$

hydnocarpyl (from hydnocarpyl alcohol) = [11-(2-cyclopenten-1-yl)undecyl] $(C_5H_7)(CH_2)_{10}CH_2–$

hydracryloyl = (3-hydroxy-1-oxopropyl) $HO(CH_2)_2CO–$

hydratropoyl = (1-oxo-2-phenylpropyl) PhCHMeCO–

hydrazi[5] (see also hydrazo) –NHNH–

1,2-hydrazinediylidene = azino =NN=

hydrazino $H_2NNH–$

1-hydrazinyl-2-ylidene –NHN=

hydrazo[3,6] (see also hydrazi) –NHNH–

hydrazono $H_2NN=$

hydrocinnamoyl = (1-oxo-3-phenylpropyl) $Ph(CH_2)_2CO–$

hydrocinnamyl = (3-phenylpropyl) $Ph(CH_2)_3–$

hydroperoxy[4] HOO–

(**hydroperoxyformyl**) = (hydroperoxycarbonyl) HOOCO–

hydroxamino = (hydroxyamino) HONH–

hydroximino = (hydroxyimino) HON=

hydroxy[4] HO–

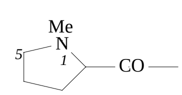
(**hydroxyarsinylidene**) = arsinico[3,4] HOAs(O)=

hydroxyl = hydroxy[4] HO–

(**hydroxyphosphinyl**) HOPH(O)–

(**hydroxyphosphinylidene**) = phosphinico[3,4] HOP(O)=

hygroyl = (1-methylprolyl)[1] or [(1-methyl-2-pyrrolidinyl)carbonyl]



imidazolidyl = imidazolidinyl $(C_3H_7N_2)–$

imidazolinyl = (dihydro-1*H*-imidazolyl) $(C_3H_5N_2)–$

imidocarbonyl = carbonimidoyl[7] –C(=NH)–

(**imidocarbonylamino**) = (carbonimidoylamino) HN=C=N–

imino HN=

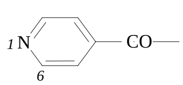
iminio $H_2N^+=$

(**3-iminoacetonyl**) = (3-imino-2-oxopropyl) $HN=CHCOCH_2–$

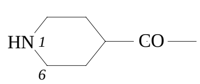
(**iminodisulfonyl**) = [iminobis(sulfonyl)] $–SO_2NHSO_2–$

(**iminomethyl**) (see also carbonimidoyl) HN=CH–

(**iminonitrilo**) = 1-hydrazinyl-2-ylidene –NHN=
(**iminophosphoranyl**) = phosphinimyl H_2P(=NH)–
indanyl = (2,3-dihydro-1*H*-indenyl) (C_9H_9)–
indenyl = 1*H*-indenyl (C_9H_7)–
1-indolinyl = (2,3-dihydro-1*H*-indol-1-yl) (C_8H_8N)–
2-indolinylidene = (1,3-dihydro-2*H*-indol-2-ylidene) (C_8H_7N)=
indyl = 1*H*-indolyl (C_8H_6N)–
iodo I–
iodoso = iodosyl OI–
iodoxy = iodyl O_2I–
isoallyl = 1-propenyl MeCH=CH–
isoamoxy = (3-methylbutoxy) $Me_2CH(CH_2)_2O$–
isoamyl = (3-methylbutyl) $Me_2CH(CH_2)_2$–
sec-**isoamyl** = (1,2-dimethylpropyl) $Me_2CHCHMe$–
isoamylidene = (3-methylbutylidene) Me_2CHCH_2CH=
isobornyl (from isoborneol) = (1,7,7-trimethylbicyclo[2.2.1]hept-2-yl) ($C_{10}H_{17}$)–
isobutenyl = (2-methyl-1-propenyl) Me_2C=CH–
isobutoxy = (2-methylpropoxy) Me_2CHCH_2O–
isobutyl = (2-methylpropyl) Me_2CHCH_2–
isobutylidene = (2-methylpropylidene) Me_2CHCH=
isobutyryl = (2-methyl-1-oxopropyl) Me_2CHCO–
isocrotyl = (2-methyl-1-propenyl) Me_2C=CH–
isocyanato OCN–
isocyano CN–
isodiazenyl N≡NH– or N=NH–
isodiazenylidene[6] (see also diazo)
isohexyl = (4-methylpentyl) $Me_2CH(CH_2)_3$–
isohexylidene = (4-methylpentylidene) $Me_2CH(CH_2)_2CH$=
2-isoindolinyl = (1,3-dihydro-2*H*-isoindol-2-yl) (C_8H_8N)–
isoleucyl[1] = (2-amino-3-methyl-1-oxopentyl) $EtCHMeCH(NH_2)CO$–
isonicotinoyl = (4-pyridinylcarbonyl)



isonipecotoyl = (4-piperidinylcarbonyl)

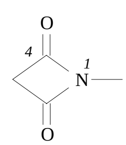


isonitro = *aci*-nitro HON(O)=
isonitroso = (hydroxyimino) HON=
1-isopentenyl = (3-methyl-1-butenyl) Me_2CHCH=CH–
isopentyl = (3-methylbutyl) $Me_2CH(CH_2)_2$–
isopentylidene = (3-methylbutylidene) Me_2CHCH_2CH=
isophthalal = (1,3-phenylenedimethylidyne) 1,3–$C_6H_4(CH=)_2$
isophthalaldehydoyl = (3-formylbenzoyl) 3–$(HCO)C_6H_4CO$–
isophthaloyl = (1,3-phenylenedicarbonyl) 1,3–$C_6H_4(CO–)_2$
isophthalylidene = (1,3-phenylenedimethylidyne) 1,3–$C_6H_4(CH=)_2$
isopropenyl = (1-methylethenyl) H_2C=CMe–
isopropoxy = (1-methylethoxy) Me_2CHO–
isopropyl = (1-methylethyl) Me_2CH–
isopropylidene = (1-methylethylidene) Me_2C=
(**isopropylidenedioxy**) = [(1-methylethylidene)bis(oxy)] –$OCMe_2O$–
isosemicarbazido = [(aminohydroxymethylene)hydrazino] H_2NC(OH)=NNH–
isothiocyanato SCN–
isothiocyano = isothiocyanato SCN–
isovaleryl = (3-methyl-1-oxobutyl) Me_2CHCH_2CO–
isovalyl[1] = (2-amino-2-methyl-1-oxobutyl) $EtCMe(NH_2)CO$–
isoviolanthrenylene = (9,18-dihydrodinaphtho[1,2,3-*cd*:1′,2′,3′-*lm*]perylenediyl) –($C_{34}H_{18}$)–

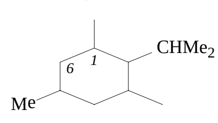
kauranyl (from kaurane) ($C_{20}H_{33}$)–
kauranylene = kauranediyl (from kaurane) –($C_{20}H_{32}$)–
kaurenyl (from kaurene) ($C_{20}H_{31}$)–
keto[11] = oxo O=

labdan-15-yl = [5-(decahydro-2,5,5,8a-tetramethyl-1-naphthalenyl)-3-methylpentyl] ($C_{20}H_{37}$)–
lactosyl = (4-*O*-β-galactapyranosyl-β-D-glucopyranosyl) ($C_6H_{11}O_5$)O($C_6H_{10}O_5$)–
lactoyl = (2-hydroxypropanoyl)[1] or (2-hydroxy-1-oxopropyl) MeCH(OH)CO–
lanostenylene = lanostenediyl (from lanostane) –($C_{30}H_{50}$)–
lauroyl = (1-oxododecyl) $Me(CH_2)_{10}CO$–
leucyl[1] = (2-amino-4-methyl-1-oxopentyl) $Me_2CHCH_2CH(NH_2)CO$–
levulinoyl = (1,4-dioxopentyl) $MeCO(CH_2)_2CO$–
linalyl (from linalool) = (1-ethenyl-1,5-dimethyl-4-hexenyl) $Me_2C=CH(CH_2)_2CMe(CH=CH_2)$–
linolelaidoyl = (1-oxo-9,12-octadecadienyl) $Me(CH_2)_4CH=CHCH_2CH=CH(CH_2)_7CO$–
linolenoyl = (1-oxo-9,12,15-octadecatrienyl) $EtCH=CHCH_2CH=CHCH_2CH=CH(CH_2)_7CO$–
γ-**linolenoyl** = (1-oxo-6,9,12-octadecatrienyl) $Me(CH_2)_4CH=CHCH_2CH=CHCH_2CH=CH(CH_2)_4CO$–
linoleoyl = (1-oxo-9,12-octadecadienyl) $Me(CH_2)_4CH=CHCH_2CH=CH(CH_2)_7CO$–
lupanyl (from lupane) ($C_{30}H_{51}$)–
lysyl[1] = (2,6-diamino-1-oxohexyl) $H_2N(CH_2)_4CH(NH_2)CO$–

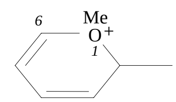
maleoyl = (1,4-dioxo-2-butene-1,4-diyl) –COCH=CHCO–
malonaldehydoyl = (1,3-dioxopropyl) $HCOCH_2CO$–
malonamoyl = (3-amino-1,3-dioxopropyl) H_2NCOCH_2CO–
malonaniloyl = [1,3-dioxo-3-(phenylamino)propyl] $PhNHCOCH_2CO$–
malonimido = (2,4-dioxo-1-azetidinyl)



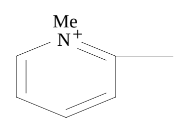
malonyl = (1,3-dioxo-1,3-propanediyl) –$COCH_2CO$–
maloyl = (2-hydroxy-1,4-dioxo-1,4-butanediyl) –$COCH(OH)CH_2CO$–
maltosyl = (4-*O*-α-D-glucopyranosyl-β-D-glucopyranosyl) ($C_6H_{11}O_5$)O($C_6H_{10}O_5$)–
mandeloyl = (hydroxyphenylacetyl) PhCH(OH)CO–
p-**menth-2-yl** = [2-methyl-5-(1-methylethyl)cyclohexyl] 2,5–$Me(Me_2CH)C_6H_9$–
p-**menth-3,5-ylene** = [5-methyl-2-(1-methylethyl)-1,3-cyclohexanediyl]



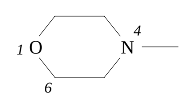
mercapto[4] HS–
mesaconoyl = (2-methyl-1,4-dioxo-2-butene-1,4-diyl) –COCMe=CHCO–
mesidino = [(2,4,6-trimethylphenyl)amino] 2,4,6–$Me_3C_6H_2NH$–
mesityl = (2,4,6-trimethylphenyl) 2,4,6–$Me_3C_6H_2$–
α-**mesityl** = [(3,5-dimethylphenyl)methyl] 3,5–$Me_2C_6H_3CH_2$–
mesoxalyl = (1,2,3-trioxo-1,3-propanediyl) –COCOCO–
mesyl = (methylsulfonyl) $MeSO_2$–
metanilamido = [[(3-aminophenyl)sulfonyl]amino] 3–$H_2NC_6H_4SO_2NH$–
metanilyl = [(3-aminophenyl)sulfonyl] 3–$H_2NC_6H_4SO_2$–
methacryloyl = (2-methyl-1-oxo-2-propenyl) H_2C=CMeCO–
methallyl = (2-methyl-2-propenyl) $H_2C=CMeCH_2$–
methanetetrayl =C=
methene = methylene H_2C=
methenyl = methylidyne HC≡
methionyl (from methionic acid) = [methylenebis(sulfonyl)] –$SO_2CH_2SO_2$–
methionyl[1] (from methionine) = [2-amino-4-(methylthio)-1-oxobutyl] $MeS(CH_2)_2CH(NH_2)CO$–
methoxalyl = (methoxyoxoacetyl) MeO_2CCO–
methoxy MeO–
(**methoxycarbonyl**) MeO_2C–
methyl Me (H_3C)–
[(**methyldithio**)**sulfonyl**] $MeSSSO_2$–
methylene H_2C=
(**methylenedioxy**) = [methylenebis(oxy)] –OCH_2O–
[(**methylenedioxy**)**phenyl**] = 1,3-benzodioxol-*ar*-yl (CH_2O_2)C_6H_3–
(**methylenedisulfonyl**) = [methylenebis(sulfonyl)] –$SO_2CH_2SO_2$–
methylidyne HC≡
methyliumylidene C^+H=
methylol = (hydroxymethyl) $HOCH_2$–
(**methyloxy**) = methoxy MeO–
(**1-methyl-2*H*-pyranium-2-yl**)



(**1-methylpyridinium-2-yl**)

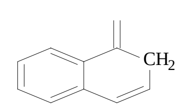


(**methylselenyl**) = (methylseleno) MeSe–
(**methylthio**) MeS–
(**methyltelluro**) MeTe–
(**methyltrioxy**) MeOOO–
morpholino = 4-morpholinyl



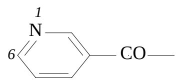
myristoyl = (1-oxotetradecyl) $Me(CH_2)_{12}CO$–

naphthal = (naphthalenylmethylene) ($C_{10}H_7$)CH=
naphthalimido = (1,3-dioxo-1*H*-benz[*de*]isoquinolin-2(3*H*)-yl) ($C_{12}H_6NO_2$)–
naphthenyl = (naphthalenylmethylidyne) ($C_{10}H_7$)C≡
naphthionyl = [(4-amino-1-naphthalenyl)sulfonyl] 4,1–$H_2NC_{10}H_6SO_2$–
naphthobenzyl = (naphthalenylmethyl) ($C_{10}H_7$)CH_2–
naphthothiophene-yl = naphthothienyl ($C_{12}H_7S$)–
naphthoxy = (naphthalenylozy) ($C_{10}H_7$)O–
naphthoyl = (naphthalenylcarbonyl) ($C_{10}H_7$)CO–
naphthyl = naphthalenyl ($C_{10}H_7$)–
naphthylene = naphthalenediyl –($C_{10}H_6$)–
1(2*H*)-naphthylidene = 1(2*H*)-naphthalenylidene

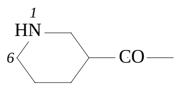


(**naphthylnaphthyl**) = [binaphthalen]yl $C_{10}H_7C_{10}H_6$–
nazyl = (naphthalenylmethyl) ($C_{10}H_7$)CH_2–
neopentyl = (2,2-dimethylpropyl) Me_3CCH_2–
neophyl = (2-methyl-2-phenylpropyl) $PhCMe_2CH_2$–
neryl (from nerol) = (3,7-dimethyl-2,6-octadienyl) –$Me_2C=CH(CH_2)_2CMe=CHCH_2$–
nicotinimidoyl = (imino-3-pyridinylmethyl) (C_5H_4N)C(=NH)–

nicotinoyl = (3-pyridinylcarbonyl)



nipecotoyl = (3-piperidinylcarbonyl)

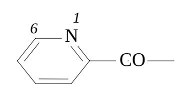


nitramino = (nitroamino) O_2NNH–
aci-**nitramino** = (*aci*-nitroamino) HON(O)=N–
nitrilio HN^+≡
nitrilo N≡
(**nitrilophosphoranyl**) = phosphononitridyl HP(≡N)–
nitro O_2N–
aci-nitro HON(O)=
nitrosamino = (nitrosoamino) ONNH–
nitrosimino = (nitrosoimino) ONN=
nitroso ON–
(**nitrothio**) O_2NS–
nonanedioyl = (1,9-dioxo-1,9-nonanediyl) $–CO(CH_2)_7CO–$
nonanoyl = (1-oxononyl) $Me(CH_2)_7CO$–
norbornyl = bicyclo[2.2.1]heptyl (C_7H_{11})–
norbornylene = bicyclo[2.2.1]heptanediyl –(C_7H_{10})–
norcamphanyl = bicyclo[2.2.1]heptyl (C_7H_{11})–
norcaryl (from norcarane) = bicyclo[4.1.0]heptyl (C_7H_{11})–
norpinyl (from norpinane) = bicyclo[3.1.1]heptyl (C_7H_{11})–
norleucyl[1] = (2-amino-1-oxohexyl) $Me(CH_2)_3CH(NH_2)CO$–
norvalyl[1] = (2-amino-1-oxopentyl) $Me(CH_2)_2CH(NH_2)CO$–
nosyl = [(4-nitrophenyl)sulfonyl] $4–O_2NC_6H_4SO_2$–

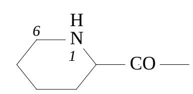
octadecanoyl = (1-oxooctadecyl) $Me(CH_2)_{16}CO$–
octanedioyl = (1,8-dioxo-1,8-octanediyl) $–CO(CH_2)_6CO–$
octanoyl = (1-oxooctyl) $Me(CH_2)_6CO$–
tert-**octyl** = (1,1,3,3-tetramethylbutyl) $Me_3CCH_2CMe_2$–
oenanthyl = (1-oxoheptyl) $Me(CH_2)_5CO$–
oleananyl (from oleanane) ($C_{30}H_{51}$)–
oleoyl = (1-oxo-9-octadecenyl) $Me(CH_2)_7CH{=}CH(CH_2)_7CO$–
ornithyl[1] = (2,5-diamino-1-oxopentyl) $H_2N(CH_2)_3CH(NH_2)CO$–
oxalaldehydoyl = (oxoacetyl) HCOCO–
oxalyl = (1,2-dioxo-1,2-ethanediyl) –COCO–
oxamido = [(aminooxoacetyl)amino] $H_2NCOCONH$–
oxamoyl = (aminooxoacetyl) H_2NCOCO–
oxamyl = (aminooxoacetyl) H_2NCOCO–
oxaniloyl = [oxo(phenylamino)acetyl] PhNHCOCO–
oxazolinyl = (dihydrooxazolyl) (C_3H_4NO)–
oximido = (hydroxyimino) HON=
oxo[5] (See also epoxy and oxy) O=
(**oxoarsino**) = arsenoso OAs–
(**oxobornyl**) = (trimethyloxobicyclo[2.2.1]heptyl) ($C_{10}H_{15}O$)–
(**oxoboryl**) OB–
(**1-oxoethyl**) = acetyl Ac (MeCO–)
(**oxoethylene**) = (1-oxo-1,2-ethanediyl) $–COCH_2–$
(**oxophenylhydrazino**) = (nitrosophenylamino) PhN(NO)–
(**oxophenylmethyl**) = benzoyl Bz (PhCO–)
(**oxophosphino**) = phosphoroso OP–
(**oxopyridinylmethyl**) = (pyridinylcarbonyl) (C_5H_4N)CO–
(**2-oxotrimethylene**) = (2-oxo-1,3-propanediyl) $–CH_2COCH_2–$
(**2-oxovinyl**) = (oxoethenyl) OC=CH–
oxy[9] (see also epoxy and oxo) –O–
[**oxybis**(**methylenecarbonylimino**)] = [oxybis[(1-oxo-2,1-ethanediyl)imino]] $–NHCOCH_2OCH_2CONH–$

palmitoyl = (1-oxohexadecyl) $Me(CH_2)_{14}CO$–
pantothenoyl = *N*-(2,4-dihydroxy-3,3-dimethyl-1-oxobutyl)-β-alanyl[1] or [3-[(2,4-dihydroxy-3,3-dimethyl-1-oxobutyl)amino]-1-oxopropyl] $HOCH_2CMe_2CH(OH)CONH(CH_2)_2CO$–
pelargonoyl = (1-oxononyl) $Me(CH_2)_7CO$–
pelargonyl = (1-oxononyl) $Me(CH_2)_7CO$–
pentadecanoyl = (1-oxopentadecyl) $Me(CH_2)_{13}CO$–
pentamethylene = 1,5-pentanediyl $–(CH_2)_5–$
3-pentanesulfonamido = [[(1-ethylpropyl)sulfonyl]amino] Et_2CHSO_2NH–
1,3-pentazadieno = 1,3-pentazadienyl $H_2NN{=}NN{=}N$–
2-pentenediylidyne = 2-pentene-1,5-diylidyne $≡CCH{=}CHCH_2C≡$
tert-**pentyl** = (1,1-dimethylpropyl) $EtCMe_2$–
pentyl $Me(CH_2)_4$–
pentylidyne BuC≡
perchloryl O_3Cl–
perseleno = seleninoselenoyl Se=Se=
perthio = sulfinothioyl S=S=
phenacyl = (2-oxo-2-phenylethyl) $PhCOCH_2$–
phenacylidene = (2-oxo-2-phenylethylidene) PhCOCH=
phenanthrothiophene-yl = phenanthrothienyl ($C_{16}H_9S$)–
phenanthryl = phenanthrenyl ($C_{14}H_9$)–
phenanthrylene = phenanthrenediyl –($C_{14}H_8$)–
phenenyl = benzenetriyl C_6H_3≡
phenethyl = (2-phenylethyl) $PhCH_2CH_2$–
phenethylidene = (2-phenylethylidene) $PhCH_2CH$=
phenetidino = [(ethoxyphenyl)amino] $(EtO)C_6H_4NH$–
phenetyl = (ethoxyphenyl) $(EtO)C_6H_4$–
phenoxy PhO–
phenyl Ph (C_6H_5)–
phenylalanyl[1] (from phenylalanine) = (2-amino-1-oxo-3-phenylpropyl) $PhCH_2CH(NH_2)CO$–
(**phenylarsinico**) = (hydroxyphenylarsinyl) PhAs(O)(OH)–
[(**phenylazo**)**imino**] = (3-phenyl-2-triazenylidene) PhN=NN=
(**phenylbenzoyl**) = ([1,1′-biphenyl]ylcarbonyl) PhC_6H_4CO
(**phenyldiazenyl**) = (phenylazo) PhN=N–
phenylene –(C_6H_4)–
[**phenylenebis**(**azo**)] $–N{=}NC_6H_4N{=}N–$
[**phenylenebis**[**azo**(**methylimino**)]] = [phenylenebis(1-methyl-2-triazene-3,1-diyl)] $–NMeN{=}NC_6H_4N{=}NNMe–$
[**phenylenebis**(**1-oxo-1-ethanyl-2-ylidene**)] = [phenylenebis(2-oxo-2-ethanyl-1-ylidene)] $=CHCOC_6H_4COCH=$
(**phenylenedimethylene**) = [phenylenebis(methylene)] $–CH_2C_6H_4CH_2–$
(**phenylenedimethylidyne**) $=CHC_6H_4CH=$
(**phenylenedioxy**) = [phenylenebis(oxy)] $–OC_6H_4O–$
(**phenylglyoxyloyl**) = (oxophenylacetyl) PhCOCO–
phenylidene = cyclohexadienylidene (C_6H_6)=
(**phenylimidocarbonyl**) = (phenylcarbonimidoyl)[7] PhN=C=
(**phenyloxalyl**) = (oxophenylacetyl) PhCOCO–
(**phenyloxy**) = phenoxy PhO–
(**phenylphenoxy**) = ([1,1′-biphenyl]yloxy) PhC_6H_4O–
(**phenylsulfenyl**) = (phenylthio) PhS–
(**phenylsulfinyl**) PhS(O)–
(*S*-**phenylsulfonimidoyl**) PhS(O)(=NH)–
phorbinyl (from phorbine) ($C_{22}H_{17}N_4$)–
phosphinico[3,4] HOP(O)=
phosphinidene HP=
phosphinidenio H_2P^+=
phosphinidyne P≡
phosphinimyl H_2P(=NH)–
phosphino H_2P–
phosphinothioyl H_2P(S)–
phosphinothioylidene HP(S)=
phosphinyl H_2P(O)–
phosphinylidene HP(O)=
phosphinylidyne P(O)≡

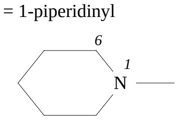
phospho O_2P–
phosphonio H_3P^+–
phosphono[4] $(HO)_2P(O)$–
(**phosphonoformyl**) = (phosphonocarbonyl) $(HO)_2P(O)CO$–
phosphononitridyl HP(≡N)–
phosphoranyl H_4P–
phosphoranylidene H_3P=
phosphoranylidyne H_2P≡
phosphoro = 1,2-diphosphenediyl –P=P–
phosphoroso OP–
phthalal = (1,2-phenylenedimethylidyne) $1,2–C_6H_4(CH{=})_2$
phthalaldehydoyl = (2-formylbenzoyl) $2–(HCO)C_6H_4CO$–
phthalamoyl = [2-(aminocarbonyl)benzoyl] $2–(H_2NCO)C_6H_4CO$–
phthalanyl = (1,3-dihydroisobenzofuranyl) (C_8H_7O)–
phthalidyl = (1,3-dihydro-3-oxo-1-isobenzofuranyl) ($C_8H_5O_2$)–
phthalidylidene = (3-oxo-1(3*H*)-isobenzofuranylidene) ($C_8H_4O_2$)–
phthalimido = (1,3-dihydro-1,3-dioxo-2*H*-isoindol-2-yl) ($C_8H_4NO_2$)–
phthalocyaninyl[1] (from phthalocyanine) ($C_{32}H_{17}N_8$)–
phthaloyl = (1,2-phenylenedicarbonyl) $1,2–C_6H_4(CO–)_2$
phthalylidene = (1,2-phenylenedimethylidyne) $1,2–C_6H_4(CH{=})_2$
phyllocladanyl = kauranyl (from kaurane) ($C_{29}H_{33}$)–
phytyl = (3,7,11,15-tetramethyl-2-hexadecenyl) $Me[CHMe(CH_2)_3]_3CMe{=}CHCH_2$–
picolinoyl = (2-pyridinylcarbonyl)



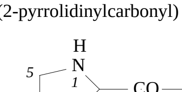
picryl = (2,4,6-trinitrophenyl) $2,4,6–(O_2N)_3C_6H_2$–
pimeloyl = (1,7-dioxo-1,7-heptanediyl) $–CO(CH_2)_5CO–$
4-pinanyl (from pinane) = (4,6,6-trimethylbicyclo-[3.1.1]hept-2-yl) ($C_{10}H_{17}$)–
pinanylene = (trimethylbicyclo[3.1.1]heptanediyl) –($C_{10}H_{16}$)–
pipecoloyl = (2-piperidinylcarbonyl)



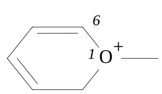
piperidino = 1-piperidinyl



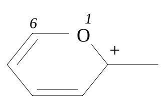
piperidyl = piperidinyl ($C_5H_{10}N$)–
piperidylidene = piperidinylidene (C_5H_9N)=
piperonyl = (1,3-benzodioxol-5-ylmethyl) $3,4–(CH_2O_2)C_6H_3CH_2$–
piperonylidene = (1,3-benzodioxol-5-ylmethylene) $3,4–(CH_2O_2)C_6H_3CH$=
piperonyloyl = (1,3-benzodioxol-5-ylcarbonyl) $3,4–(CH_2O_2)C_6H_3CO$–
pivaloyl = (2,2-dimethyl-1-oxopropyl) Me_3CCO–
pivalyl = (2,2-dimethyl-1-oxopropyl) Me_3CCO–
plumbanetetrayl =Pb=
plumbyl H_3Pb–
plumbylene H_2Pb=
plumbylidyne HPb≡
podocarpan-13-yl = (tetradecahydro-4b,8,8-trimethyl-2-phenanthrenyl) ($C_{17}H_{29}$)–
porphinyl (from porphine) ($C_{20}H_{13}N_4$)–
pregna-5,16-dien-21-yl (from pregnadiene) ($C_{21}H_{31}$)–
prenyl = (3-methyl-2-butenyl) $Me_2C{=}CHCH_2$–
prolyl[1] = (2-pyrrolidinylcarbonyl)



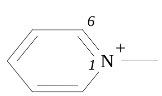
2-propanesulfonamido = [[(1-methylethyl)sulfonyl]amino] Me_2CHSO_2NH–
propargyl = 2-propynyl $HC{\equiv}CCH_2$–
propenyl = 1-propenyl MeCH=CH–
2-propenyl CH_2=CH–CH_2–
propenylene = 1-propene-1,3-diyl –CH=CHCH_2–
propenylidene = 1-propenylidene MeCH=C=
propioloyl = (1-oxo-2-propynyl) $HC{\equiv}CCO$–
propiolyl = (1-oxo-2-propynyl) $HC{\equiv}CCO$–
propionamido = [(1-oxopropyl)amino] EtCONH–
propionyl = (1-oxopropyl) EtCO–
(**propionyldioxy**) = [(1-oxopropyl)dioxy] EtC(O)OO–
propionyloxy = (1-oxopropoxy) $EtCO_2$–
propoxy PrO–
propyl Pr ($CH_3CH_2CH_2$–)
sec-**propyl** = (1-methylethyl) Me_2CH–
propylene = (1-methyl-1,2-ethanediyl) –CHMeCH_2–
propylidene EtCH=
propylidyne $EtC{\equiv}$
(**propyloxy**) = propoxy PrO–
protocatechuoyl = (3,4-dihydroxybenzoyl) 3,4–$(HO)_2C_6H_3CO$–
pseudoallyl = (1-methylethenyl) H_2C=CMe–
pseudocumidino = [(2,4,5-trimethylphenyl)amino] 2,4,5–$Me_3C_6H_2NH$–
as-**pseudocumyl** = (2,3,5-trimethylphenyl) 2,3,5–$Me_3C_6H_2$–
s-**pseudocumyl** = (2,4,5-trimethylphenyl) 2,4,5–$Me_3C_6H_2$–
v-**pseudocumyl** = (2,3,6-trimethylphenyl) 2,3,6–$Me_3C_6H_2$–
pseudoindolyl = 1*H*-indolyl (C_8H_6N)–
pteroyl = [4-[[(2-amino-1,4-dihydro-4-oxo-6-pteridinyl)methyl]amino]benzoyl] ($C_{14}H_{11}N_6O_2$)–
2*H*-pyranio



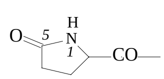
2*H*-pyran-2-ylium-2-yl



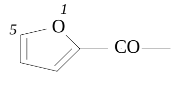
pyrazolidyl = pyrazolidinyl ($C_3H_7N_2$)–
pyrazolinyl = (dihydropyrazolyl) ($C_3H_5N_2$)–
pyridinio



pyridyl = pyridinyl (C_5H_4N)–
pyroglutamoyl = (5-oxoprolyl)[1] or [(5-oxo-2-pyrrolidinyl)carbonyl]



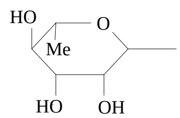
pyromucyl = (2-furanylcarbonyl)



pyrrolidyl = pyrrolidinyl (C_4H_8N)–
pyrrolinyl = (dihydropyrrolyl) (C_4H_6N)–
pyrrol-1-yl = 1*H*-pyrrol-1-yl (C_4H_4N)–
pyrroyl = (pyrrolylcarbonyl) (C_4H_3N)CO–
pyrryl = pyrrolyl (C_4H_4N)–
pyruvoyl = (1,2-dioxopropyl) MeCOCO–

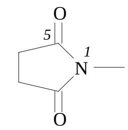
p-**quaterphenylyl** = [1,1′:4′,1″:4″,1‴-quaterphenyl]yl ($C_{24}H_{17}$)–
quinaldoyl = (2-quinolinylcarbonyl) (2–C_9H_6N)CO–
quinolyl = quinolinyl (C_9H_6N)–
quinonyl = (dioxocyclohexadienyl) ($C_6H_3O_2$)–
quinuclidinyl = 1-azabicyclo[2.2.2]octyl ($C_7H_{12}N$)–

α-**resorcyloyl** = (3,5-dihydroxybenzoyl) 3,5–$(HO)_2C_6H_3CO$–
β-**resorcyloyl** = (2,4-dihydroxybenzoyl) 2,4–$(HO)_2C_6H_3CO$–
γ-**resorcyloyl** = (2,6-dihydroxybenzoyl) 2,6–$(HO)_2C_6H_3CO$–
rhamnosyl = (6-deoxymannopyranosyl)



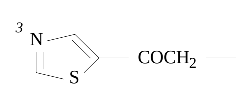
ricinelaidoyl = (12-hydroxy-1-oxo-9-octadecenyl) $Me(CH_2)_5CH(OH)CH_2CH{=}CH(CH_2)_7CO$–
ricinoleoyl = (12-hydroxy-1-oxo-9-octadecenyl) $Me(CH_2)_5CH(OH)CH_2CH{=}CH(CH_2)_7CO$–
rosan-6-yl = (2-ethyltetradecahydro-2,4a,8,8-tetramethyl-9-phenanthrenyl) ($C_{20}H_{35}$)–

salicyl = [(2-hydroxyphenyl)methyl] 2–$HOC_6H_4CH_2$–
salicylidene = [(2-hydroxyphenyl)methylene] 2–HOC_6H_4CH=
salicyloyl = (2-hydroxybenzoyl) 2–HOC_6H_4CO–
sarcosyl = (*N*-methylglycyl)[1] or [(methylamino)acetyl] $MeNHCH_2CO$–
sebacoyl = (1,10-dioxo-1,10-decanediyl) –$CO(CH_2)_8CO$–
seleneno[4] HOSe–
selenino[4] HOSe(O)–
seleninoselenoyl Se=Se=
seleninyl OSe=
seleno[9] (see also episeleno and selenoxo) –Se–
selenocyanato NCSe–
selenono[4] $(HO)SeO_2$–
selenonyl O_2Se=
selenophenyl = selenophene-yl (C_4H_3Se)–
selenoxo[5] (see also episeleno and seleno) Se=
selenyl[4] HSe–
semicarbazido = [2-(aminocarbonyl)hydrazino] $H_2NCONHNH$–
semicarbazono = [(aminocarbonyl)hydrazono] $H_2NCONHN$=
senecioyl = (3-methyl-1-oxo-2-butenyl) Me_2C=CHCO–
seryl[1] = (2-amino-3-hydroxy-1-oxopropyl) $HOCH_2CH(NH_2)CO$–
siamyl = (1,2-dimethylpropyl) $Me_2CHCHMe$–
silanetetrayl =Si=
siloxy = (silyloxy) H_3SiO–
silyl H_3Si–
silylene H_2Si=
silylidyne $HSi{\equiv}$
sorboyl = (1-oxo-2,4-hexadienyl) MeCH=CHCH=CHCO–
spirohex-1-yl (C_6H_9)–
spirostanyl (from spirostane) ($C_{27}H_{43}O_2$)–
stannanetetrayl =Sn=
stannyl H_3Sn–
stannylene H_2Sn=
stannylidyne $HSn{\equiv}$
stearoyl = (1-oxooctadecyl) $Me(CH_2)_{16}CO$–
stibino H_2Sb–
stiboso = (oxostibino) OSb–
stibyl = stibino H_2Sb–
stibylene HSb=
stibylidyne $Sb{\equiv}$
styrene = (1-phenyl-1,2-ethanediyl) –$CHPhCH_2$–
styrolene = (1-phenyl-1,2-ethanediyl) –$CHPhCH_2$–
styryl = (2-phenylethenyl) PhCH=CH–
suberoyl = (1,8-dioxo-1,8-octanediyl) –$CO(CH_2)_6CO$–
succinaldehydoyl = (1,4-dioxobutyl) $HCO(CH_2)_2CO$–
succinamoyl = (4-amino-1,4-dioxobutyl) $H_2NCO(CH_2)_2CO$–
succinamyl = (4-amino-1,4-dioxobutyl) $H_2NCO(CH_2)_2CO$–
succinaniloyl = [1,4-dioxo-4-(phenylamino)butyl] $PhNHCO(CH_2)_2CO$–
succinimido = (2,5-dioxo-1-pyrrolidinyl)

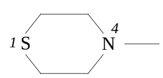


succinyl = (1,4-dioxo-1,4-butanediyl) –$CO(CH_2)_2CO$–
sulfamino = (sulfoamino) $HOSO_2NH$–
sulfamoyl = (aminosulfonyl) H_2NSO_2–
sulfamyl = (aminosulfonyl) H_2NSO_2–
sulfanilamido = [[(4-aminophenyl)sulfonyl]amino] 4–$H_2NC_6H_4SO_2NH$–
sulfanilyl = [(4-aminophenyl)sulfonyl] 4–$H_2NC_6H_4SO_2$–
sulfeno[4] HOS–
sulfhydryl = mercapto[4] HS–
sulfinimidoyl HN=S=
sulfino[4] HOS(O)–
sulfinothioyl S=S=
sulfinyl OS=
sulfinylhydrazono O=S=N–N=
sulfo[4] HO_3S–
sulfonimidoyl HN=S(O)=
sulfonodiimidoyl $(HN{=})_2S$=
sulfonyl –SO_2–
sulfurtetrayl[12] =S=
sulfurtriyl[12] $HS{\equiv}$
sulfuryl = sulfonyl –SO_2–

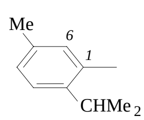
tartaroyl = (2,3-dihydroxy-1,4-dioxo-1,4-butanediyl) –COCH(OH)CH(OH)CO–
tartronoyl = (2-hydroxy-1,3-dioxo-1,3-propanediyl) –COCH(OH)CO–
tauryl = [(2-aminoethyl)sulfonyl] $H_2N(CH_2)_2SO_2$–
telluro[6] (see also telluroxo) –Te–
telluroxo[5] (see also telluro) Te=
telluryl[4] HTe–
terephthalal = (1,4-phenylenedimethylidyne) 1,4–$C_6H_4(CH{=})_2$
terephthalaldehydoyl = (4-formylbenzoyl) 4–$HCOC_6H_4CO$–
terephthalamoyl = [4-(aminocarbonyl)benzoyl] 4–$(H_2NCO)C_6H_4CO$–
terephthalaniloyl = [4-[(phenylamino)carbonyl]benzoyl] 4–$(PhNHCO)C_6H_4CO$–
terephthaloyl = (1,4-phenylenedicarbonyl) 1,4–$C_6H_4(CO–)_2$
terephthalylidene = (1,4-phenylenedimethylidyne) 1,4–$C_6H_4(CH{=})_2$
m-**terphenylyl** = [1,1′:3′,1″-terphenyl]yl ($C_{18}H_{13}$)–
terphenylylene = [terphenyl]diyl –($C_{18}H_{12}$)–
tetradecanoyl = (1-oxotetradecyl) $Me(CH_2)_{12}CO$–
tetramethylene = 1,4-butanediyl –$(CH_2)_4$–
1,4-tetraphosphinediyl –$(PH)_4$–
tetrasiloxanylene = 1,7-tetrasiloxanediyl –$SiH_2(OSiH_2)_2OSiH_2$–
tetrathio[13] –SSSS–
tetrazanediylidene = 1,4-tetrazanediylidene =$N(NH)_2N$=
tetrazanylene = 1,4-tetrazanediyl –$(NH)_4$–
1-tetrazeno = 1-tetrazenyl H_2NNHN=N–
thenoyl = (thienylcarbonyl) (C_4H_3S)CO–
thenyl = (thienylmethyl) (C_4H_3S)CH_2–
thenylidene = (thienylmethylene) (C_4H_3S)CH=
(**thenyloxy**) = (thienylmethoxy) (C_4H_3S)CH_2O–
thexyl = 1,1,2-trimethylpropyl Me_2CHCMe_2–
thianaphthenyl = benzo[*b*]thienyl (C_8H_5S)–
thiazolidyl = thiazolidinyl (C_3H_6NS)–
thiazolinyl = (dihydrothiazolyl) (C_3H_4NS)–
[(**5-thiazolylcarbonyl**)**methyl**] = [2-oxo-2-(5-thiazolyl)ethyl]



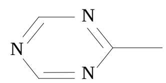
thienyl (C_4H_3S)–
(**thienylthienyl**) = [bithiophen]yl (C_4H_3S)(C_4H_2S)–
thio[9] (see also epithio and thioxo) –S–
(**thioacetonylidene**) = (2-thioxopropylidene) MeCSCH=
thioacetyl = (1-thioxoethyl) MeCS–
(**thioarsenoso**) = (thioxoarsino) S=As–
(**thiobenzoyl**) = (phenylthioxomethyl) PhCS–
(**thiocarbamoyl**) = (aminothioxomethyl) H_2NCS–
thiocarbamyl = (aminothioxomethyl) H_2NCS–
(**thiocarbonyl**) = carbonothioyl[7] –CS–
(**thiocarboxy**)[14] HOSC–
thiocyanato NCS–
thiocyano = thiocysnato NCS–
(**thioformyl**) = (thioxomethyl) HCS–
(**thiohexanoyl**) = (1-thioxohexyl) $Me(CH_2)_4CS$–
thiohydroperoxy = sulfeno[4] HOS– or (mercaptooxy)[4] HSO–
(**thiohydroxy**) = mercapto[4] HS–
thiomorpholino = 4-thiomorpholinyl



(**thionitroso**) SN–
thionyl = sulfinyl –SO–
(**thiophenacyl**) = (2-phenyl-2-thioxoethyl) $PhCSCH_2$–
thiophene-yl = thienyl (C_4H_3S)–
(**thiophosphono**) = (hydroxymercaptophosphinyl (HO)(HS)P(O)–
(**thioseleneno**)[4] HSSe–
(**thiosulfeno**)[4] HSS–
(**thiosulfo**)[14] (HO_2S_2)–
thioxo[5] (see also epithio) S=
(**thioxoarsino**) SAs–
(**thioxomethyl**) (see also carbonothioyl) S=CH–
thiuram = (aminothioxomethyl) H_2NCS–
threonyl[1] (2-amino-3-hydroxy-1-oxobutyl) $MeCH(OH)CH(NH_2)CO$–
4-thujyl = [2-methyl-5-(1-methylethyl)bicyclo-[3.1.0]hex-2-yl] ($C_{10}H_{17}$)–
thymyl (from thymol) = [5-methyl-2-(1-methylethyl)phenyl]



thyronyl = [*O*-(4-hydroxyphenyl)tyrosyl][1] or [2-amino-3-[4-(4-hydroxyphenoxy)phenyl]-1-oxopropyl] $4–(4–HOC_6H_4O)C_6H_4]CH_2CH(NH_2)CO$–
toloxy = (methylphenoxy) MeC_6H_4O–
p-**toluenesulfonamido** = [[(4-methylphenyl)sulfonyl]amino] $4–MeC_6H_4SO_2NH$–
toluidino = [(methylphenyl)amino] MeC_6H_4NH–
toluoyl = (methylbenzoyl) MeC_6H_4CO–
toluyl = (methylbenzoyl) MeC_6H_4CO–
tolyl = (methylphenyl) MeC_6H_4–
α-**tolyl** = (phenylmethyl) $PhCH_2$–
tolylene = (methylphenylene) $–(MeC_6H_3)$–
α-**tolylene** = (phenylmethylene) PhCH=
tosyl = [(4-methylphenyl)sulfonyl] $4–MeC_6H_4SO_2$–
triazano = triazanyl H_2NNHNH–
1-triazeno = 1-triazenyl $H_2NN=N$–
s-**triazin-2-yl** = 1,3,5-triazin-2-yl



trichothecanyl (from trichothecane) ($C_{15}H_{25}O$)–
tridecanoyl = (1-oxotridecyl) $Me(CH_2)_{11}CO$–
(**trimethylammonio**) Me_3N^+–
(**trimethylarsonio**) Me_3As^+–
trimethylene = 1,3-propanediyl $–(CH_2)_3$–
(**1,3,3-trimethyl-2-norbornyl**) = (1,3,3-trimethylbicyclo[2.2.1]hept-2-yl) ($C_{10}H_{17}$)–
(**trimethylphosphonio**) Me_3P^+–
triseleno[13] –SeSeSe–
trisilanylene = 1,3-trisilanediyl $–(SiH_2)_3$–
trisiloxane-1,3,5-triyl = 1,3,5-trisiloxanetriyl $–SiH(OSiH_2–)_2$
trithio[13] –SSS–
trityl = (triphenylmethyl) Ph_3C–
tropanyl = (8-methyl-8-azabicyclo[3.2.1]octyl) ($C_8H_{14}N$)–
tropoyl = (3-hydroxy-1-oxo-2-phenylpropyl) $HOCH_2CHPhCO$–
tryptophyl[1] = [2-amino-3-(1*H*-indol-3-yl)-1-oxopropyl] $(C_8H_6N)CH_2CH(NH_2)CO$–
tyrosyl[1] = [2-amino-3-(4-hydroxyphenyl)-1-oxopropyl] $4–HOC_6H_4CH_2CH(NH_2)CO$–

undecanoyl = (1-oxoundecyl) $Me(CH_2)_9CO$–
uramino = [(aminocarbonyl)amino] H_2NCONH–
ureido = [(aminocarbonyl)amino] H_2NCONH–
ureylene = (carbonyldiimino) –NHCONH–
(**ureylenediureylene**) = [carbonylbis(hydrazocarbonylimino)] –NHCONHNHCONHNHCONH–
ursanyl (from ursane) ($C_{30}H_{51}$)–

valeryl = (1-oxopentyl) BuCO–
valyl[1] = (2-amino-3-methyl-1-oxobutyl) $Me_2CHCH(NH_2)CO$–
vanillal = [(4-hydroxy-3-methoxyphenyl)methylene] $4,3–HO(MeO)C_6H_3CH$=
vanilloyl = (4-hydroxy-3-methoxybenzoyl) $4,3–HO(MeO)C_6H_3CO$–
vanillyl = [(4-hydroxy-3-methoxyphenyl)methyl] $4,3–HO(MeO)C_6H_3CH_2$–
vanillylidene = [(4-hydroxy-3-methoxyphenyl)-methylene] $4,3–HO(MeO)C_6H_3CH$=
vanilmandeloyl = [hydroxy(4-hydroxy-3-methoxyphenyl)acetyl] $4,3–HO(MeO)C_6H_3CH(OH)CO$–
veratral = [(3,4-dimethoxyphenyl)methylene] $3,4–(MeO)_2C_6H_3CH$=
veratroyl = (3,4-dimethoxybenzoyl) $3,4–(MeO)_2C_6H_3CO$–
o-**veratroyl** = (2,3-dimethoxybenzoyl) $2,3–(MeO)_2C_6H_3CO$–
veratryl = [(3,4-dimethoxyphenyl)methyl] $3,4–(MeO)_2C_6H_3CH_2$–
o-**veratryl** = [(2,3-dimethoxyphenyl)methyl] $2,3–(MeO)_2C_6H_3CH_2$–
veratrylidene = [(3,4-dimethoxyphenyl)methylene] $3,4–(MeO)_2C_6H_3CH$=
vinyl = ethenyl $H_2C=CH$–
vinylene = 1,2-ethenediyl –CH=CH–
vinylidene = ethenylidene $H_2C=C$=

xanthen-9-yl = 9*H*-xanthen-9-yl ($C_{13}H_9O$)–
xanth-9-yl = 9*H*-xanthen-9-yl ($C_{13}H_9O$)–
xenyl = [1,1′-biphenyl]-4-yl $4–PhC_6H_4$–
xylidino = [(dimethylphenyl)amino] $Me_2C_6H_3NH$–
xyloyl = (dimethylbenzoyl) $Me_2C_6H_3CO$–
xylyl = (dimethylphenyl) $Me_2C_6H_3$–
xylylene = [phenylenebis(methylene)] $–CH_2C_6H_4CH_2$–

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 phytyl radical is named as 3,7,11,15-tetramethyl-2-hexadecenyl. Because the total stereochemistry of a phytyl compound may be influenced by the presence of other chiral centers, it would be misleading to supply it with the radical name. However, the cross-reference at **Phytol** in the *Index Guide* includes stereochemistry.

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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

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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

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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, *ace*naphthene.
aci- the *acid* form: as *aci*-acetoacetic ester, $CH_3C(OH){:}CHCOOC_2H_5$; *aci*-nitro group HON(O):.
aldo-, ald- from *aldehyde;* as, *aldo*hexose, *ald*oxime.
allo- (Greek *allos*, other) indicating *close relation*; as, *allo*-telluric acid, *allo*ocimene (a structural isomer of ocimene). Specifically, designating the more stable of two geometrical isomers; as, *allo*maleic acid (fumaric acid).
amphi- (Greek, both, around) relating to both sides or both kinds; as, *amphi*-naphthoquinone (2,6-naphthalenedione), *amphi*phile.
andro-, andr- (Greek) relating to *man*, *male*; as *andro*gen, *andro*sterone.
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, *anhydro*glucose. Cf. *dehydro*-.
antho-, anth- (Greek) of *flowers*; as, *antho*cyanin, *antho*xanthin.
anthra-, anthr- (Greek, *anthrax*, coal) of *coal* or *anthracene*; as, *anthra*cite, *anthra*quinone, *anthra*pyrrole.
anti- (Greek, against) *opposite*, *opposed to*; as, *anti*oxidant; specifically, equivalent to *trans*- (which see) as, *anti*-benzaldoxime.
apo- (Greek, from) denoting formation from, or relationship to, another compound; as, *apo*morphine, $C_{17}H_{17}NO_2$ (morphine is $C_{17}H_{19}NO_3$).
ar- abbreviation of *aromatic*; as, *ar*-derivatives of Tetralin.
as- abbreviation of *asymmetric*; as, *as*-trichlorobenzene (1,2,4-$Cl_3C_6H_3$).
benzo-, benz- of *benzene*; as, *benzoic*; specifically, denoting fusion of a benzene ring; as, *benzo*quinoline.
bi- (Latin) *twice*, *two*, *double*; specifically: (a) in double proportion; as, *bi*carbonate (no longer considered good usage); (b) denoting the doubling of an organic radical or molecule; as, *bi*phenyl, $C_6H_5C_6H_5$; *bi*pyridine, $C_5H_4N.C_5H_4N$.
bicyclo- of *two rings*; specifically, designating certain *bicyclic* bridged compounds, as; *bicyclo*[2.2.1]heptane.
bili- (Latin) of *bili*rubin, as, *bili*verdin.
bisnor-, dinor- indicating removal of two CH_2 groups; as, *bisnor*cholanic acid or *dinor*cholanic acid $C_{22}H_{36}O_2$ (cholanic acid is $C_{24}H_{40}O_2$).
bufo-, buf- (Latin *bufo*, toad) derived from the *toad*; as, *bufo*talin.
chole-, cholo, chol- (Greek) of *bile*; as, *chole*sterol, *chol*ine.
chromo- (Greek *chroma*, color) *color*, *colored*; as, *chromo*phore, *chromo*protein, *chromo*isomer (a colored isomer of a colorless compound).
chryso-, chrys- (Greek) *gold*, *golden yellow*, *yellow*; as *chryso*phanic acid, *chrys*azin.
cincho-, cinch- of *cinchoma* or *cinchonine*; as *cincho*meronic acid, *cinch*onan.
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, *copro*sterol.
cyclo- (Greek *kyklos*, circle) of ring structure, *cyclic*; as, *cyclo*hexane.
D- denoting configurational relationship to D-glyceraldehyde; as, D-fructose.
d- (a) abbreviation of *dextro* or *dextrotatory*; as, *d*-strychnine; (b) less properly = D.
de-, des- (Latin) indicating *removal* of something from the molecule; as, deoxybenzoin, $C_6H_5CH_2COC_6H_5$ (benzoin with one oxygen atom removed).
dehydro- denoting (a) *removal of hydrogen*; as, *dehydro*cholic acid; (b) sometimes, *removal of water*; as, *dehydro*mucic 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*-methylenecyclohexane (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*rhamnose (epimer of rhamnose); (c) a bridge connection; as, 9,10-*epi*dioxyanthracene (anthracene 9,10-peroxide).
ergo-, ergot- relating to *ergot*; as, *ergo*sterol, *ergot*amine.
erythro-, erythr- (Greek) *red*; as *erythro*mycin, *erythro*sine.
eso- (Greek, within) denoting immediate attachment to a ring atom. Cf. *exo*-.
etio-, aetio- (Greek *aitia*, cause) denoting a *degradation product*; as, *etio*-cholanic acid, *etio*cobalamin.
exo- (Greek) *outside*, *out of*; as, *ex*otoxin (an excreted toxin); specifically, denoting attachment in a side chain. Cf. *endo*, *eso*-.
flavo-, flav- (Latin *flavus*, yellow) *yellow*; as, *flavo*protein, *flav*one; specifically, designating certain series of coordination compounds.
fuco-, fuc- of *fucus* (a seaweed); as, *fuco*xanthin, *fuc*ose.
gala-, galacto-, galact- (Greek, milk, milky) relating to: (a) *milk*; as, *galac*tase, *galact*ose; (b) *galactose*; as, *galacto*cerebroside, *galacto*lipin.
gallo-, gall- relating to *gallnuts* or *gallic acid*; as, *gallo*tannic 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, *gluco*pyranose, *gluc*uronic acid; (b) less properly = *glyco*-, *glyc*-.
glyco-, glyc- (Greek) *sweet*, or relating to *sugars* or *glycine*; as, *glyco*gen, *glyco*side, *glyco*cholic acid.
hemato-, hemat-, hemo-, hem- (also haemato-, etc.) (Greek) of *blood* or its color; as, *hemato*porphyrin, *hemat*ein, *hemo*globin, *hem*in.
hetero-, heter- (Greek *heteros*, other) *other*, *different*; as, *hetero*poly acids, *hetero*cyclic.
holo- (Greek) *whole*, *complete*; as, *holo*cellulose; *holo*phosphoric acid, H_5PO_5.
homo- (Greek) *same*, *similar*; as, *homo*cyclic, *homo*logous (differing by an increase of CH_2; as, *homo*phthalic acid).
hydro-, hydr- (Greek) (a) denoting presence or addition of *hydrogen*; as, *hydro*chloric, *hydr*acrylic; (b) sometimes, relating to *water*; as *hydr*ate.
hyo- (Greek) of *swine*; as, *hyo*deoxycholic acid (from hog bile), *hyo*scyamine (from *Hyoscyamus* (hog bean)).
hypo- (Greek, under, beneath) indicating a lower (or the *lowest*) state of oxidation; as, *hypo*chlorous acid, *hypo*xanthine.
i- abbreviation of (a) *inactive*; as, *i*-tartaric acid; (b) *iso*-; as, *i*-pentane.
iso- (Greek) *equal*, *alike*; as, *iso*mer; usually, denoting an *isomer* of a compound; as, *iso*cyanic acid; specifically, denoting an isomer having a single, simple branching at the end of a straight chain; as, *iso*pentane, $(CH_3)_2CHCH_2CH_3$.
keto-, ket- from *ketone*; as, *keto*hexose, *ket*oxime.
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, *lano*sterol (from wool fat).
leuco-, leuc- (Greek) *colorless*, *white*; as, *leuc*ine; specifically, a colorless reduced derivative of a triphenylmethane dye; as, *leuco*methylene 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, *lith*arge, *litho*cholic acid (from gallstones).
luteo- (Latin *luteus*) *orange-yellow*, *brownish yellow*; as *luteo*lin; specifically, the coordination compounds $[M(NH_3)_6]Cl_3$.
m- abbreviation of *meta* (sense c).
meso-, mes- (Greek) *middle*, *intermediate*; specifically; (a) an intermediate hydrated form of an inorganic acid; as, *meso*periodic acid, H_3IO_6; (b) optically inactive owing to internal compensation; as, *meso*tartaric acid; (c) (abbreviated μ-) centrally substituted; as, *meso*-chloroanthracene (9-chloroanthracene), *meso*-phenylimidazole (2-phenylimidazole); (d) (abbreviated *ms*-) centrally fused; as, *meso*naphthodianthrene (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, *meta*phosphoric acid, HPO_3; (b) a closely related compound (sometimes, a polymer); as, *met*aldehyde (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, *neo*arsphenamine; (of a hydrocarbon) having one carbon atom connected directly to four others; as, *neo*pentane, $(CH_3)_4C$.
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, *oligo*saccharide.
ortho- (Greek, straight, right, true) (a) the fully hydrated form of an acid; as, *ortho*nitric acid, H_5NO_5; (b) the highest-hydrated stable form; as, *ortho*-phosphoric acid, H_3PO_4; (c) the common or symmetrical molecular form of an element; as, *ortho*hydrogen; (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 *para*xanthine (1,7-dimethylxanthine). Specifically, (a) a higher hydrated form of an acid; as, *para*periodic acid, H_3IO_5 (preferably called orthoperiodic); (b) a polymer; as, *par*aldehyde; (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, *per*chloric acid, manganese *per*oxide (better, dioxide); (b) pres-

ence of the peroxide group (O_2); as, barium *per*oxide, *per*benzoic acid, *per* acid (better, peroxy acid); (c) exhaustive substitution or addition; as, *per*chloroethylene, C_2Cl_4; *per*hydronaphthalene, $C_{10}H_{18}$.
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, *peri*naphthindene (phenalene).
peroxy- containing the *peroxide* group (O_2); as, *peroxy*monosulfuric acid, $HOSO_2OOH$.
pheno-, phen- (from *phene*, benzene) related to *phenyl* or *benzene*; as, *phena*cyl; specifically, an anthracene analogue having two hetero atoms in the central positions; as, *phen*azine, *pheno*thiazine.
phloro-, phlor- relating to *phlorizin*; as, *phloro*glucinol, *phlor*etin.
phthalo-, phthal- relating to *phthalic acid*; as, *phthalo*cyanine, *phthal*ide.
phyllo-, phyll- (Greek *phyllos*) of *leaves*; as, *phyllo*porphyrin.
phyto-, phyt- (Greek) relating to *plants*; as, *phyto*sterol, *phyto*hormon*es.*
picro-, picr- (Greek) *bitter*; as, *picro*toxin, *picr*ic acid.
pino-, pin- (Latin *pinus*, pine) relating to *pine* or *pinene*; as, *pin*ic acid, *pino*carvone.
poly- (Greek) many; as, *poly*mer, *poly*sulfide, *poly*saccharide.
pro- (Greek, before) a precursor; as *pro*enzyme, *pro*vitamin.
proto-, prot- (Greek) *first*; specifically, designating: (a) first in an inorganic series; as, *prot*oxide (lowest in oxygen content); (b) parent or immediate antecedent; as, *prot*actinium, *proto*chlorophyll.
pseudo-, pseud- abbreviated ψ or *ps* (Greek, false) indicating *resemblance* to, or *relation* (especially isomerism) with; as, ψ-cumene, *pseud*aconitine, *pseudo*base. Abbreviation: as, ψ-cumene.
purpuro- (Latin *purpura*, purple) indicating *purple* or *red* color; as, *purpuro*gallin.
pyo- py- (Greek) relating to *pus*; as, *pyo*cyanine.
pyro-, pyr- (Greek *pyr*, fire) indicating *formation by heat*; as, *pyro*cinchonic acid, *pyr*ene; specifically, designating an acid derived from two molecules of an “ortho” acid by loss of $1H_2O$; as, *pyro*phosphoric acid, $H_4P_2O_7$ ($2H_3PO_4$-H_2O).
pyrrolo-, pyrro-, pyrr- containing the *pyrrole* ring; as, *pyrrolo*pyridine, *pyrro*coline.
reso-, res- relating to *resorcinol*; as, *res*orufin, *res*azurin.
rhodo-, rhod- (Greek *rhodon*, rose) *rose-red;* as, *rhodo*porphyrin, *rhod*amine.
s- abbreviation of (a) *symmetric*(*al*); (b) *secondary*.
sapo- (Latin, soap) relating to *soap* or *soap bark*; as *sapo*nin, *sapo*genin.
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, *sub*iodide, *sub*oxide, aluminum *sub*acetate.
super- (Latin, above, over) denoting a *high proportion* (or superfluity, as in an acid salt); as, *super*oxide (peroxide), *super*phosphate.
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, *tauro*cholic acid, *tauro*cyamine.
tere- (Latin *terebinthus*, terebinth) relating to *terebene* or *terpenes*; as, *tere*phthalic, *tere*santalic.
tert- abbreviation of *tertiary*; as, *tert*-butyl.
thymo-, thym- relating to (a) *thyme*; as, *thymo*quinone, *thym*ol; (b) the *thymus*; as, *thymo*nucleic.
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, CH_3CHCl_2.
uro-, ur- (Greek *ouro*-, *our*-) relating to *urine* or *urea*; as, *uro*bilin, *ur*ethane, *ur*ic acid.
urso-, urs- (Latin *ursus*, bear) relating to *bears* or the *bearberry*; as, *ur*solic acid.
v- abbreviation of *vicinal*; as, *v*-triazine.
verdo- (French, *verd*, *vert*, green) indicating *green* color; as, *verdo*hemin.
vic- abbreviation of *vicinal*; as, *vic*-triazole.
xantho-, xanth- (Greek) *yellow*; as, *xantho*toxin, *xanth*ic acids, *xanth*ine.
xylo-, xyl- (Greek *xylon*, wood) relating to *wood*, *xylene*, or *xylose*; as, *xyl*an, *xyl*idine, *xylo*quinone, *xylo*caine.
zymo-, zym- (Greek *zyme*, leaven) relating to a *ferment* or *fermentation*; as, *zymo*sterol, *zym*ase.

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 lowercase 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	ο	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	tricosa-, 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

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Deriving a chemical structural diagram	314
Index heading parents	315
Substituent prefixes	¶ 316
Modifications	317
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312. Introduction. The foregoing sections of Appendix IV 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]

Sources of structural data include the *Ring Systems Handbook*, the *Index Guide*, and (when information concerning a substance has been published) the Volume and Collective issues of the *Chemical Substance Index*. The reader is also referred to other paragraphs of Appendix IV, when appropriate, for more detailed discussion of complex subjects. It is not the purpose of this section to cover every subject. Discussion of subjects not covered in this section can be found by reference to the Index at the end of Appendix IV.

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:

Basic skeleton name Principal functional suffix

Methan | amine

$MeNH_2$

[1]A. L. Goodson, "Graphical Representation of Chemical Structures in Chemical Abstracts Service Publications", *J. Chem. Inf. Comput. Sci.* **1980**, 20, 212-217.

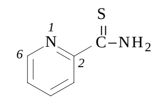
The basic skeleton is the one-carbon unit "Methane" (¶ 141), the final "e" being elided before a vowel. The principal (here, the only) functional group is the amine (¶ 176).

Example:

Basic skeleton name

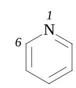
Locant Principal functional suffix

2- | Pyridine | carbothioamide



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).

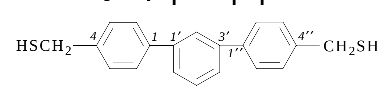
Another type of two-part name, known as a "conjunctive name" (see ¶ 124), is a combination of the name of a cyclic molecular skeleton and the name(s) of one or more identical, saturated acyclic hydrocarbon chains, each terminated by the same functional group.

Example:

Locant Greek multiplicative prefix

Cyclic molecular skeleton Acyclic hydrocarbon chain terminated by a functional group

[1,1′:3′,1′′-Terphenyl] | -4,4′′- | di | methanethiol

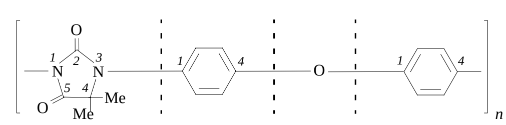


The structure of the phenyl group is found in the Illustrative List of Substituent Prefixes (¶ 294). That "ter" is a Latin prefix meaning "three" is found in ¶ 311. The first set of locants (1,1′:3′,1″) indicates that the three benzene rings are connected as shown. The second set of locants (4,4″) shows 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.

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 (Al_2CaTiO_6)

Aluminum calcium titanium oxide ($Al_2Ca_4Ti_2O_{11}$)

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:

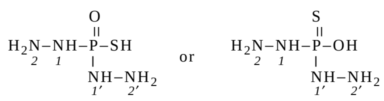
Aluminum calcium titanium oxide

III. Index heading parents with chemical structural diagrams.

A *chemical structural diagram* is provided in the *Index Guide* and *Chemical Substance Index* where the structure of an inorganic substance (¶ 219) may not be readily apparent from the name.

Example:

Phosphorodihydrazidothioic acid

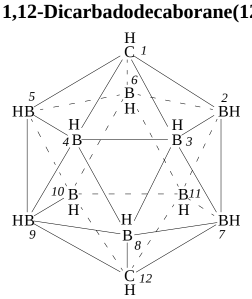


A similar procedure is followed for other types of index heading parents such as *cage parents, ring parents,* and *stereoparents*. Here, however, the structural diagrams are published in the *Ring Systems Handbook* as well as the *Chemical Substance Index*.

Examples:

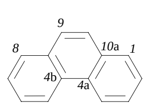
Cage Parent:

1,12-Dicarbadodecaborane(12)



Ring Parent:

Phenanthrene

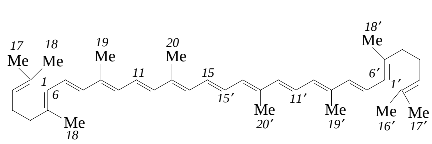


As stated in ¶ 313, the complexity of chemical substances generally dictates the complexity of *CA* index names. This is particularly true for natural products whose names must imply standard orientation and stereochemical representation as well as structure and numbering (compare ¶ 318). Such complexity 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:

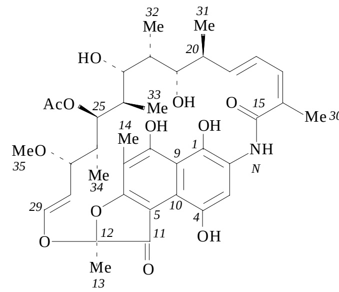
Acyclic stereoparent:

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-dotria-contatridecaene*)



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-heptamethyl-2,7-(ep-oxypentadeca[1,11,13]trienimino)naphtho[2,1-b]furan-1,11(2H)-dione)*



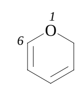
316. Substituent prefixes (see ¶ 10A) follow the "comma of inversion" (see ¶ 104) in *CA* index names and their structures can be determined from ¶ 294, the Illustrative List of Substituent Prefixes.

Example:

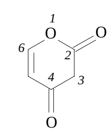
2*H*-Pyran-2,4(3*H*)-dione
——, **3-[[(4-aminophenyl)amino]phenylmethylene]-6-phenyl-**

The structure of the chemical substance represented by this name is derived by first obtaining the structure of **2*H*-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 **2*H*-Pyran** is RF 2133. Entry RF 2133 in the *Ring* Systems *Handbook* is as follows:

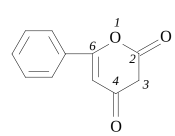
RF 2133 **289-66-7**
2*H*-Pyran
C_5H_6O



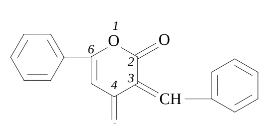
The *index heading parent* contains two functional groups which ¶ 174 identifies as ketone groups. However, putting an oxygen on position 4 requires "adding" a hydrogen at position 3. The indicated and added hydrogen terms (see ¶¶ 135 and 136) in the index heading parent thus define the bonding in the 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 **(2*H*-Pyran-2,4(3*H*)-dione)** is therefore:



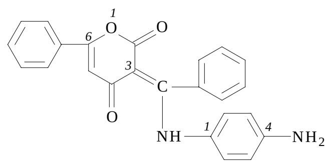
The *substituent* fragment of the name indicates that a simple substituent (i.e., "phenyl", see ¶ 294) is attached to the ring at position 6:



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:

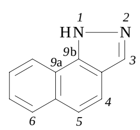


317. Modifications of the principal functions or other groups follow the substituent(s) (¶ 104). Where derivatives of more than one functional group must be named, the derivative terms are cited in the order described in ¶ 113.
Example:

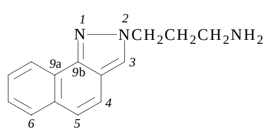
2*H*-Benzo[*g*]indazole-2-propanamine
——, 3,3a,4,5-tetrahydro-*N*,*N*-dimethyl-3-phenyl-
trihydrochloride

Only the form **1*H*-Benzo[**g**]indazole** is illustrated in the *Chemical Substance Index* and the *Ring Systems Handbook:*

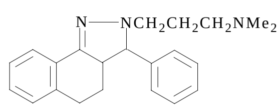
1*H*-Benz[*g*]indazole



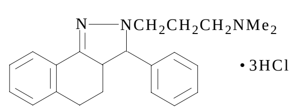
The structure is converted into the 2*H*-isomer and the propanamine group (¶¶ 141 and 176) is attached at the 2-position. (It should be noted that, in conjunctive nomenclature, the function is located at the end of the saturated, acyclic chain furthest from the ring system of the index heading parent (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 "trihydrochloride" 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:

$$\underset{4}{\text{Me}}-\underset{3}{\overset{\text{Me}}{\text{CH}}}-\underset{2}{\overset{\text{Me}}{\text{C}}}=\underset{1}{\text{CH}_2}$$

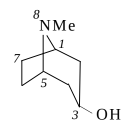
The homopolymer is represented as follows:

$$(\text{Me}_2\text{CHCMe}{=}\text{CH}_2)_x$$

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:

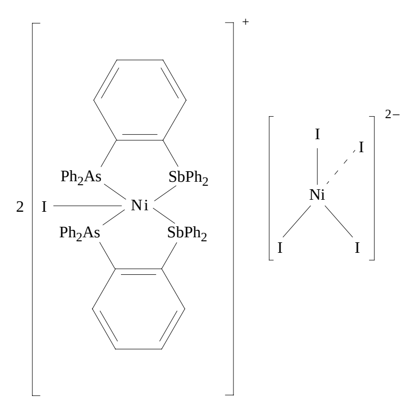


As stated in ¶ 315, *stereoparent names* (see ¶ 203 II) in the *Chemical Substance Index* imply (in the absence of cited stereochemical descriptors) a standard structure, including specific stereochemistry, as illustrated by an accompanying structural diagram complete with the numbering system from which 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)phenyl]diphenylarsine-
***As*,*Sb*]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) 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.

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