Chemical Abstracts Index Names for Chemical Substances in the Ninth Collective Period (1972–1976)*

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Received November 19, 1973

Index names for chemical substances have been significantly revised by Chemical Abstracts Service (CAS) for Volume 76 [January-June 1972, the first volume of the Ninth Collective Period (1972–1976)] and subsequent volumes of *Chemical Abstracts*. While remaining generally within the framework of IUPAC and other existing nomenclature rules, the most systematic recommended names have been chosen. These names are more easily derived from molecular structural diagrams, and, therefore, are more quickly found by index users. Machine editing of index names and translation of these names into structural representations in the CAS computer-based information system are also aided by the revisions. The index name revisions include (i) conversion of almost all "trivial" or author terminology into more systematic names, (ii) simplification of general name-selection rules, and (iii) elimination of special treatment for certain classes of substances. Specific identifiable alloys, elementary particles, enzymes, and mixtures of substances are now indexed like conventional chemical substances. Difficulties encountered with generation of previous *Chemical Abstracts* index names and indexing rules are described, and comparisons are made of new and former index names for chemical compounds and substituent radicals.

It has been the policy of *Chemical Abstracts* (CA) to make necessary revisions of index terms, including index names for chemical substances, at the beginning of each new collective indexing period so that the Collective Indexes would be self-consistent. Over the years, most improvements in index names have taken one of two forms, (a) conversion of "trivial" or "author" names into more "systematic" names—i.e., names more descriptive of the total molecular structures, and (b) unification and simplification of naming principles for all chemical substances.

For the Ninth Collective Index Period (9CI), covering CA Volumes 76–85 and the years 1972–1976, Chemical Abstracts Service (CAS) has accelerated these improvements. The 9CI revisions are the most extensive changes in index names for chemical substances since systematic index names first began to be used in CA during the Second Decennial Index (1917–1926). Why these changes are important to the user, why they are vital to CA's continued growth and even survival, and how they affect the major classes of organic compounds are explained in this paper. Revised names for substituent prefixes (radicals) are also surveyed.

The paper concludes with a short account of naming procedures for four classes (alloys, elementary particles, enzymes, and mixtures), which are now indexed like conventional chemical substances.[1]

REASONS FOR CA INDEX NAME REVISION

Approximately 250,000 entirely new chemical compounds must be named each year by the staff of Chemical Abstracts Service in order to produce CA indexes. Of all the professional operations performed by CAS staff, this naming function demands the greatest expertise. Anything that simplifies this task means a significant saving in effort and resources. In particular, it is essential that the CA index name for a reported molecular structure be generated quickly, consistently, and with confidence by different indexers working independently. It is equally important that users—i.e., chemists around the world—can employ the same system to gain reliable access to the index and thus retrieve the desired information on these compounds.

CAS has always been reluctant to devise new systems of nomenclature for its own exclusive use. Instead, it has shared its considerable indexing experience with national and international bodies [chiefly the American Chemical Society (ACS) and the International Union of Pure and Applied Chemistry (IUPAC) through the National Academy of Sciences National Research Council (NAS-NRC)] to help devise consistent nomenclature systems for the general use of all chemists. Such systems have then been adapted by CAS for index use. Published rules of these organizations[2] provide methods of supplying one or more unambiguous names to nearly all chemical substances. Often, however, such names are not unique, a state of affairs which, while causing few problems in written and printed communications between chemists, is quite unacceptable in an index. The CA Chemical Substance Index is a formalized, rigidly controlled, alphabetic listing of names that must be quite specific and unique for each substance, totally reproducible by both the indexer and the index user, and preferably designed to bring chemically related substances close together in the alphabetical index listing.

The scientific community is becoming more dependent on the use of mechanization to gain prompt and reliable access to technical information. CAS is committed to the development of a computer-based system for rapid and

* Presented in part before the Division of Organic Chemistry, 164th Meeting, ACS, New York, N. Y., Aug. 27, 1972, and at the Mid-Atlantic Regional Meeting, Washington, D. C., Jan. 15, 1973.

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reliable handling of chemical information. A large part of CAS-processed information is accessible through chemical nomenclature; therefore, automatic handling of such nomenclature and the associated structural diagrams is of great importance to both CAS and the scientific community. Index names must be readily translatable to complete structural representations manually or mechanically and must be amenable to rapid and consistent editing and verification manually or mechanically.

As a corollary, the rules for derivation of CA index names must also be simple, logical, consistent, and dependable. These rules, which are being made widely available throughout the scientific community, are based on those of the ACS and IUPAC,[2] which, however, require substantial extension for CA indexing purposes.

Prior to and during the Eighth Collective Index Period (8CI) (CA Volumes 66–75, 1967–1971), a thorough evaluation was made of CAS nomenclature policies for chemical substances. The result was a 3100-page typewritten compilation of rules. During application of these rules to the indexing of CA Volumes 66–75, several hundred additional pages were required to provide greater detail and clarification. By contrast, the new CA rules for Volumes 76–85 involve a total of only 1850 pages; in addition, they cover a wider range of chemical substances than did the previous rules.

The general rules for naming chemical substances have been improved (and thus the number of such rules reduced) by two interrelated efforts:

(*a*) Elimination of nearly all trivial names (commonly used author, trade, or nonsystematic names that tell little or nothing about the complete molecular structure)

(*b*) Simplification of the rules for selection of the index name from among available systematic recommended names

These are described in the following sections, and illustrated by difficulties encountered with previous rules.

There are usually several acceptable methods by which a compound may be named unambiguously so that its complete structure may be drawn. Even so simple a compound as that shown in Figure 1 may be named Methylamine, 1-benzoyl-; Methanamine, α-benzoyl-; Ethylamine, 2-oxo-2-phenyl-; Acetophenone, 2-amino- (the former CA index name); **Ethanone, 2-amino-1-phenyl-** (the *new* CA name), and so on. [These names are shown in inverted form as in the CA Chemical Substance Indexes with the index heading parent preceding a comma, followed by substituent prefixes (radicals). Ninth CI headings are shown in boldface throughout this paper.] The author may have need of one or more such names when discussing various chemical relationships. CAS does not believe any single name is ideally suited to all contexts. But a single name for each substance is essential in an alphabetical index if scattering is to be avoided, and the particular preferred index name applicable to each presented structure must be readily derivable. The revisions described below are intended to achieve this objective.

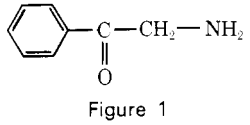


Figure 1

ELIMINATION OF MOST TRIVIAL NAMES

Trivial names for simple compounds of known constitution have long been considered of doubtful value in index construction, and CAS has made index names progressively more systematic at the beginning of collective index periods. Thus, of trivial names that appeared in the first cumulative index (1907–1916), Bivinyl became **1,3-Butadiene** in 1927; γ-Pentenic acid was converted to γ-Pentenoic acid in 1927, and finally to **4-Pentenoic acid** in 1937. Aspirin became Acetylsalicylic acid in 1917, Salicylic acid acetate in 1967, and now **Benzoic acid, 2-(acetyloxy)-.** Chloroform underwent its first and only change (so far) in 1972 to **Methane, trichloro-.**

Beginning with CA Volume 76 (January-June, 1972), trivial names for compounds containing no chiral centers, and for alkaloids and terpenes with simple stereochemistry, have been replaced by more systematic names. Glycosides of known constitution are also indexed at more meaningful names, although monosaccharide names and glycosyl radicals derived from them are retained. Thus, Patulitrin (8CI name) is now indexed at **4*H*-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-7-(β-D-glucopyranosyloxy)-3,5-dihydroxy-6-methoxy-.**

To aid users in searching the proper headings in the Chemical Substance Index, a cross-reference will be found in the CA Index Guide for *every* trivially named heading which has been discontinued in the 1972–1976 indexes.

However, some natural product names are useful. When a simple name defines not only the kinds of atoms and chemical bonds in a compound but also provides stereochemical information, it is not desirable to replace it. This is especially true if the stereochemistry is complex, as in carbohydrates and steroids, and in some alkaloids and terpenes. Amino acids frequently possess only a single center of asymmetry (in the cases of glycine and β-alanine, none at all), but, because common amino acid radical names are so useful in naming peptide chains, the acid names—e.g., alanine and cysteine—have been retained. These natural-product-type names have been dubbed "stereoparents," and they are used as index headings for the substances themselves and their analogs and derivatives. Each stereoparent is accompanied in the Chemical Substance Index by a diagram which indicates the structure, stereochemistry, and locant numbering.

Trivial names are also retained for substances of indefinite or unknown structure—e.g., enzymes and unelucidated natural products—and mixtures of more than nine components.

A classic example of trivial names is the group used prior to this 9CI revision for the isomeric dihydroxybenzoic acids (Figure 2).

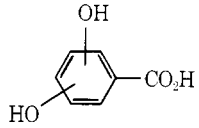


Figure 2

8CI Name	9CI Name
o-Pyrocatechuic acid	**Benzoic acid, 2,3-dihydroxy-**
β-Resorcylic acid	**Benzoic acid, 2,4-dihydroxy-**
Gentisic acid	**Benzoic acid, 2,5-dihydroxy-**
γ-Resorcylic acid	**Benzoic acid, 2,6-dihydroxy-**
Protocatechuic acid	**Benzoic acid, 3,4-dihydroxy-**
α-Resorcylic acid	**Benzoic acid, 3,5-dihydroxy-**

The entries for these compounds were scattered in the 8CI CA Subject Indexes, but they will now all be found at **Benzoic acid** in the 9CI CA Chemical Substance Indexes. In addition, the index user will be aided by a synonym for each compound. Thus,

Benzoic acid, 2,5-dihydroxy- (*gentisic acid*) ([490-79-0] the bracketed term is the CAS Registry Number[1]).

Whereas the name of each isomer is now readily apparent to a searcher, previously a cross-reference in the Index Guide had to be consulted unless the trivial name was recognizable to the user. These cross references are now reversed.

Examples:

8CI cross-reference (in Index Guide)

Benzoic acid, 2,4-dihydroxy-

See *β-Resorcylic acid* [*89-86-1*]

9CI cross-reference (in Index Guide):

β-Resorcylic acid

See *Benzoic acid, 2,4-dihydroxy-* [*89-86-1*]

Another example of widely differing trivial names for closely related compounds is found among hydroxylated and phenylated alkanoic acids—e.g., Hydrocinnamic, Hydratropic, Lactic, Hydracrylic, Glyceric, and Tropic acids. Because the problems associated with derivatives of these acids are exacerbated by the difficulty of choosing the correct index heading parent from among two or more possibilities, they are discussed in the next section.

A related problem has been the use of trivial names for some isomers, and systematic names for others.

Examples:

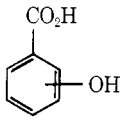


Figure 3

2-OH = Salicylic acid (8CI); **Benzoic acid, 2-hydroxy-** (9CI)

3-OH = Benzoic acid, *m*-hydroxy- (8CI); **Benzoic acid, 3-hydroxy-** (9CI)

4-OH = Benzoic acid, *p*-hydroxy- (8CI); **Benzoic acid, 4-hydroxy-** (9CI)

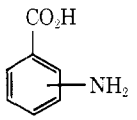


Figure 4

2-NH_2 = Anthranilic acid (8CI); **Benzoic acid, 2-amino-** (9CI)

3-NH_2 = Benzoic acid, *m*-amino- (8CI); **Benzoic acid, 3-amino-** (9CI)

4-NH_2 = Benzoic acid, *p*-amino- (8CI); **Benzoic acid, 4-amino-** (9CI)

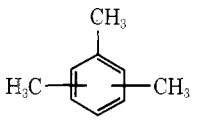


Figure 5

1,3,5-tri-Me = Mesitylene (8CI); **Benzene, 1,3,5-trimethyl-** (9CI)

All other isomers were indexed at Benzene—e.g., Benzene, 1,2,4-trimethyl-—in 8CI, and these names are unchanged in 9CI.

The trivial names previously employed have been cross-referred in the Volume 76 CA Index Guide:

Salicylic acid

See *Benzoic acid, 2-hydroxy-*

Anthranilic acid

See *Benzoic acid, 2-amino-*

Mesitylene

See *Benzene, 1,3,5-trimethyl-*

In this large-scale revision of CA index heading parents, only the following trivial and semisystematic names for simple functional compounds have been retained from earlier indexes. [An index heading parent is that part of the index name which appears in boldface ahead of the "comma of inversion" and substituents (if any). See CA Volume 76 Index Guide, para 104, for a discussion of this and allied terms.]

Acetic acid	**Guanidine**
Benzoic acid	**Hydrazine**
Carbamic acid	**Phenol**
Formic acid	**Urea**

(These are in addition to "stereoparents," which were discussed earlier.)

A selection of discontinued trivial names for benzene derivatives is displayed in Table I. It should be noted that:

(*a*) Aniline and its derivative (items 29–31) are indexed at **Benzenamine**

(*b*) Conjunctive names (items 16–19, 32, 33) such as **Benzeneacetic acid** and **Benzeneethanamine** are now formed in the same manner as those from other ring systems

(*c*) Contracted radicals methoxy and ethoxy (items 4, 34, 35) as well as propoxy, butoxy, and phenoxy, are retained

(*d*) Isopropyl is replaced by (1-methylethyl) (items 24, 25, 40, 41); all other isoalkyl and all *sec-* and *tert-*alkyl radical names are replaced by more systematic compound radical names based on the longest alkyl chains

(*e*) "Multiplication" of hydrocarbon parents including benzene (items 42, 43) is now carried out when appropriate

(*f*) Ethenyl (item 39) replaces vinyl; 1,2-ethanediyl (item 42) replaces ethylene; and 1,2-ethenediyl (item 43) replaces vinylene; many other radical names have been made more systematic (see Table II)

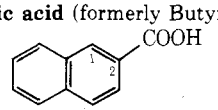
(*g*) Italic letter locants *o-*, *m-*, and *p-* are replaced by numerals, so that Salicylic acid, for example, becomes **Benzoic acid, 2**(not *o-*)**-hydroxy-**, and Resorcinol becomes **1,3** (not *m*)**-Benzenediol**

Examples of various compound classes are shown below. In each case, the former trivial or less systematic 8CI name is given as well as the new 9CI name.

Acids:

$CH_3CH_2CH_2COOH$

Butanoic acid (formerly Butyric acid)

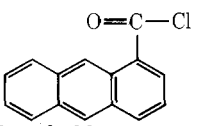


2-Naphthalenecarboxylic acid (formerly 2-Naphthoic acid)

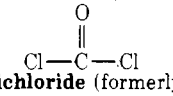
$H_2NNHCOOH$

Hydrazinecarboxylic acid (formerly Carbazic acid)

Acid halides:

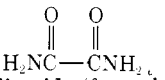


1-Anthracenecarbonyl chloride (formerly 1-Anthroyl chloride)

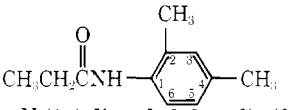


Carbonic dichloride (formerly Phosgene)

Amides:

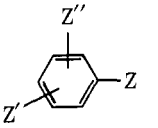


Ethanediamide (formerly Oxamide)

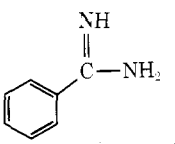


Propanamide, *N*-(2,4-dimethylphenyl)- (formerly 2′,4′-Propionoxylidide)

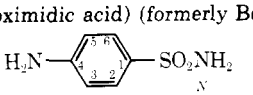
Table I. Revision of CA Index Names for Benzene Derivatives



8CI Name	Z	Z'	Z''	9CI Name
		ACIDS		
1. Benzoic acid	COOH	H	H	**Benzoic acid**
2. Anthranilic acid	COOH	2-NH_2	H	**Benzoic acid, 2-amino-**
3. Salicylic acid	COOH	2-OH	H	**Benzoic acid, 2-hydroxy-**
4. Anisic acid	COOH	OCH_3	H	**Benzoic acid, methoxy-**
5. Toluic acid	COOH	CH_3	H	**Benzoic acid, methyl-**
6. *o*-Pyrocatechuic acid	COOH	OH	OH	**Benzoic acid, 2,3-dihydroxy-**
7. β-Resorcylic acid				**Benzoic acid, 2,4-dihydroxy-**
8. Gentisic acid				**Benzoic acid, 2,5-dihydroxy-**
9. γ-Resorcylic acid				**Benzoic acid, 2,6-dihydroxy-**
10. Protocatechuic acid				**Benzoic acid, 3,4-dihydroxy-**
11. α-Resorcylic acid				**Benzoic acid, 3,5-dihydroxy-**
12. Cresotic acid	COOH	OH	CH_3	**Benzoic acid, hydroxymethyl-**
13. Phthalic acid	COOH	COOH	H	**1,2-Benzenedicarboxylic acid**
14. Isophthalic acid				**1,3-Benzenedicarboxylic acid**
15. Terephthalic acid				**1,4-Benzenedicarboxylic acid**
16. Mandelic acid	CH(OH)COOH	H	H	**Benzeneacetic acid, α-hydroxy-**
17. Hydratropic acid	$CH(CH_3)COOH$	H	H	**Benzeneacetic acid, α-methyl-**
18. Atropic acid	$C(:CH_2)COOH$	H	H	**Benzeneacetic acid, α-methylene-**
19. Hydrocinnamic acid	CH_2CH_2COOH	H	H	**Benzenepropanoic acid**
20. Cinnamic acid	CH:CHCOOH	H	H	**2-Propenoic acid, 3-phenyl-**
		ALCOHOLS AND PHENOLS		
21. Phenol	OH	H	H	**Phenol**
22. Cresol	OH	CH_3	H	**Phenol, methyl-**
23. *ar*-Stilbenol	OH	CH:CHPh	H	**Phenol, (2-phenylethenyl)-**
24. Thymol	OH	2-$CH(CH_3)_2$	5-CH_3	**Phenol, 5-methyl-2-(1-methylethyl)-**
25. *o*-Cymen-5-ol	OH	4-$CH(CH_3)_2$	3-CH_3	**Phenol, 3-methyl-4-(1-methylethyl)-**
26. Pyrocatechol	OH	OH	H	**1,2-Benzenediol**
27. Resorcinol				**1,3-Benzenediol**
28. Hydroquinone				**1,4-Benzenediol**
		AMINES		
29. Aniline	NH_2	H	H	**Benzenamine**
30. Toluidine	NH_2	CH_3	H	**Benzenamine, *ar*-methyl-**
31. Xylidine	NH_2	CH_3	CH_3	**Benzenamine, *ar,ar*-dimethyl-**
32. Benzylamine	CH_2NH_2	H	H	**Benzenemethanamine**
33. Phenethylamine	$CH_2CH_2NH_2$	H	H	**Benzeneethanamine**
		ETHERS		
34. Anisole	OCH_3	H	H	**Benzene, methoxy-**
35. Phenetole	OCH_2CH_3	H	H	**Benzene, ethoxy-**
		HYDROCARBONS		
36. Toluene	CH_3	H	H	**Benzene, methyl-**
37. Xylene	CH_3	CH_3	H	**Benzene, dimethyl-**
38. Mesitylene	CH_3	CH_3	CH_3	**Benzene, 1,3,5-trimethyl-**
39. Styrene	$CH:CH_2$	H	H	**Benzene, ethenyl-**
40. Cumene	$CH(CH_3)_2$	H	H	**Benzene, (1-methylethyl)-**
41. Cymene	$CH(CH_3)_2$	CH_3	H	**Benzene, methyl(1-methylethyl)-**
42. Bibenzyl	CH_2CH_2Ph	H	H	**Benzene, 1,1'-(1,2-ethanediyl)bis-**
43. Stilbene	CH:CHPh	H	H	**Benzene, 1,1'-(1,2-ethenediyl)bis-**



Benzenecarboxamidamide (i.e., the amide from Benzenecarboximidic acid) (formerly Benzamidine)

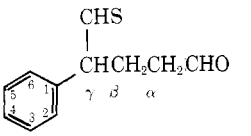


Benzenesulfonamide, 4-amino- (formerly Sulfanilamide)

Aldehydes:

CH_3CH_2CHO

Propanal (formerly Propionaldehyde)



Benzenebutanal, γ-(thioxomethyl)- (formerly Glutaraldehyde, 2-phenyl-1-thio-)

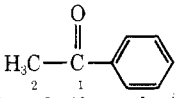
Ketones:

2-Propanone (formerly Acetone)

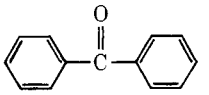
Table II. Revision of Substituent Prefixes (Radicals) for CA Ninth Collective Index Period[a]

8CI Name	9CI Name	8CI Name	9CI Name
acetamido	(acetylamino)	naphthaloyl	(1,8-naphthalenediyldicarbonyl)
acetoacetyl	(1,3-dioxobutyl)	naphthoyl	(naphthalenylcarbonyl)
acetonyl	(2-oxopropyl)	neopentyl	(2,2-dimethylpropyl)
acetoxy	(acetyloxy)	nitramino	(nitroamino)
acryloyl	(1-oxo-2-propenyl)	norbornyl	bicyclo[2.2.1]heptyl
adipoyl	(1,6-dioxo-1,6-hexanediyl)	oxalyl	(1,2-dioxo-1,2-ethanediyl)
allophanoyl	[[(aminocarbonyl)amino]carbonyl]	oxamoyl	(aminooxoacetyl)
allyl	2-propenyl	palmitoyl	(1-oxohexadecyl)
amidino	(aminoiminomethyl)	phenacyl	(2-oxo-2-phenylethyl)
anilino	(phenylamino)	phenanthryl	phenanthrenyl
anthraniloyl	(2-aminobenzoyl)	phenethyl	(2-phenylethyl)
benzamido	(benzoylamino)	phthalamoyl	[2-(aminocarbonyl)benzoyl]
benzenesulfonamido	[(phenylsulfonyl)amino]	phthalimido	(1,3-dihydro-1,3-dioxo-2*H*-isoindol-2-yl)
benzimidoyl	(iminophenylmethyl)		
p-benzoquinonyl	(3,6-dioxo-1,4-cyclohexadien-1-yl)	phthaloyl	(1,2-phenylenedicarbonyl)
4,4′-biphenylylene	[1,1′-biphenyl]-4,4′-diyl	piperidino	1-piperidinyl
2-bornyl	(1,7,7-trimethylbicyclo[2.2.1]-hept-2-yl)	2-piperidyl	2-piperidinyl
		piperonyl	(1,3-dibenzodioxol-5-ylmethyl)
2-butenylene	2-butene-1,4-diyl	propionyl	(1-oxopropyl)
tert-butyl	(1,1-dimethylethyl)	propylene	(1-methyl-1,2-ethanediyl)
butyryl	(1-oxobutyl)	pyruvoyl	(1,2-dioxopropyl)
carbazoyl	(hydrazinocarbonyl)	*m*-quaterphenyl-2′-yl	[1,1′:3′,1″:3″,1‴-quaterphenyl]-2′-yl
carvacryl	[2-methyl-5-(1-methylethyl)phenyl]	quinuclidinyl	1-azabicyclo[2.2.2]octyl
cinnamoyl	(1-oxo-3-phenyl-2-propenyl)	β-resorcyloyl	(2,4-dihydroxybenzoyl)
cinnamyl	(3-phenyl-2-propenyl)	salicyl	[(2-hydroxyphenyl)methyl]
(diazoamino)	1-triazene-1,3-diyl	salicyloyl	(2-hydroxybenzoyl)
disiloxanylene	1,3-disiloxanediyl	semicarbazido	[2-(aminocarbonyl)hydrazino]
(epoxyethyl)	oxiranyl	siloxy	(silyloxy)
ethylene	1,2-ethanediyl	sulfamoyl	(aminosulfonyl)
furyl	furanyl	thenyl	(thienylmethyl)
glyoxyloyl	(oxoacetyl)	toluidino	[(methylphenyl)amino]
guanidino	[(aminoiminomethyl)amino]	toluoyl	(methylbenzoyl)
hexamethylene	1,6-hexanediyl	tolyl	(methylphenyl)
indolyl	1*H*-indolyl	trimethylene	1,3-propanediyl
iodoso	iodosyl	trisiloxanylene	1,5-trisiloxanediyl
iodoxy	iodyl	trityl	(triphenylmethyl)
isobutyl	(2-methylpropyl)	ureido	[(aminocarbonyl)amino]
isobutyryl	(2-methyl-1-oxopropyl)	ureylene	(carbonyldiimino)
isoquinolyl	isoquinolinyl	valeryl	(1-oxopentyl)
isopropyl	(1-methylethyl)	veratroyl	(3,4-dimethoxybenzoyl)
malonyl	(1,3-dioxo-1,3-propanediyl)	vinyl	ethenyl
morpholino	4-morpholinyl	vinylene	1,2-ethenediyl
naphthalimido	(1,3-dioxo-1*H*-benz[*de*]isoquinolin-2(3*H*)-yl)		

[a] A much more complete list of 9CI radical names will be found in the CA Volume 76 Index Guide, para 294 (pp. 126-134I).

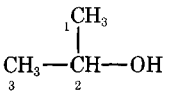


Ethanone, 1-phenyl- (formerly Acetophenone)

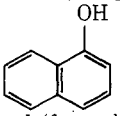


Methanone, diphenyl- (formerly Benzophenone)

Alcohols and phenols:

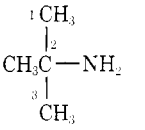


2-Propanol (formerly Isopropyl alcohol)

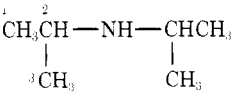


1-Naphthalenol (formerly 1-Naphthol)

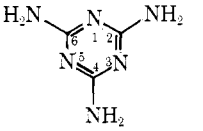
Amines:



2-Propanamine, 2-methyl- (formerly *tert*-Butylamine)

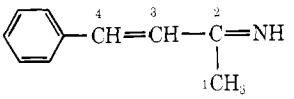


2-Propanamine, *N*-(1-methylethyl)- (formerly Diisopropylamine)



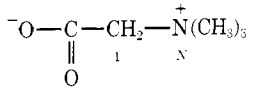
1,3,5-Triazine-2,4,6-triamine (formerly Melamine)

Imines:



3-Buten-2-imine, 4-phenyl- (formerly Cinnamylidenimine, α-methyl-)

Quaternary ammonium compounds:



Methanaminium, 1-carboxy-*N,N,N*-trimethyl- hydroxide, inner salt (formerly Betaine)

(Note that the former index heading Ammonium compounds, substituted, is discontinued; in general, acyclic nitrogen cation names are derived from the preferred primary amine; here, the most substituted Methanamine has been chosen.)

Cross references for all discontinued trivially named index parents, including those in Table I, are found in the Volume 76 Index Guide. This Guide also contains cross-references from trivial names found in the literature but never used as CA index headings, as well as synonyms and indexing policy notes. The latter notes have been revised and considerably extended for Volume 76.

SIMPLIFICATION OF SELECTION RULES

Prior to Volume 76, CA indexers and index users faced two problems in selecting an index heading parent for the purpose of generating or finding an entry for a specific substance. The first problem was that of recognizing that the structure was represented in the CA index by a trivially named heading parent—e.g., that 2-chloro-3,4-dihydroxybenzoic acid was entered at Protocatechuic acid, 2-chloro-. This difficulty was alleviated by cross references from more systematic names.

Example (8CI cross-reference):

Benzoic acid, 3,4-dihydroxy-
See *Protocatechuic acid*

In the Volume 76 Index Guide, cross references appear from all discontinued trivially named index heading parents to the more systematic names now employed.

Example (9CI cross-reference):

Protocatechuic acid
See *Benzoic acid, 3,4-dihydroxy-*

The second problem was caused by the difficulty of choosing one particular trivially named index heading parent when the structural elements of two or more were present in the total molecular structure. This was especially true of trivial names representing compounds containing more than one chemical functional group or structural feature, e.g., a ring system and an acyclic chain, such as Salicylic acid, Phenethyl alcohol, or Anisole. The preferred parent prior to Volume 76 might have one or another trivial name or a completely systematic name. In Figure 6, when R = H, the two phenyl groups were treated alike, and the 8CI name was Butyric acid, 2,3-diphenyl-. When R = $CH_2CH_2CH_3$, the two phenyl groups could no longer be treated as like substituents of the largest parent, so the 8CI name was Hydrocinnamic acid, β-methyl-α-phenyl-α-propyl-. When R represented octyl or a larger acyclic substituent, Hydrocinnamic acid was abandoned in favor of the (larger) acyclic parent acid. [The principle of "like treatment of like things," now abandoned, is described in "The Naming and Indexing of Chemical Compounds from *Chemical Abstracts*" (Introduction to the Subject Index of Volume 56) (1962), para 86, p. 13N.]

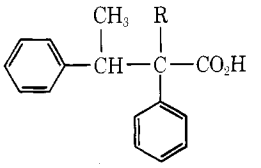


Figure 6

In the 8CI nomenclature manual, over 30 pages of documentation were required to guide one to the preferred names for phenylated acyclic acids. Entries for such acids were scattered in the Index at Hydrocinnamic, Hydratropic, Propionic, Butyric and other acid headings. If hydroxy or oxo groups were present, the choice widened to include Hydracrylic, Hydratropic, Lactic, Mandelic, Acetoacetic, Levulinic, and other acid names.

The carboxylic acid in Figure 7 contains only two phenyl groups, yet the correct 8CI name is not immediately obvious. Hydrocinnamic acid, α-hydroxy-α-phenethyl- is a possible 8CI name, but a cross reference ran from Hydrocinnamic acid, α-hydroxy- to Lactic acid, 3-phenyl-. (This cross reference was an attempt to recognize the "importance" of the subsidiary hydroxyl function and the biological significance of lactic acid.) The correct 8CI name for Figure 7 would thus seem to be Lactic acid, 2-phenethyl-3-phenyl-. But another cross reference led the index user (and indexer) from Lactic acid, 2-phenethyl- to Butyric acid, 2-hydroxy-2-methyl-4-phenyl- in recognition of the longer acyclic chain. Conversion of the "methyl" to "benzyl" in the index name recommended by this cross reference led to the 8CI name Butyric acid, 2-benzyl-2-hydroxy-4-phenyl-, and this merry circular chase came full circle with the cross reference: Butyric acid, 2-benzyl-4-phenyl-. See *Hydrocinnamic acid, α-phenethyl-*. This indeed does indicate the correct 8CI index name for Figure 7: Hydrocinnamic acid, α-hydroxy-α-phenethyl-. (When the presence of conflicting cross references for a particular compound was established, the largest available index heading parent was selected.) The 9CI index name is **Benzenebutanoic acid, α-hydroxy-α-(phenylmethyl)-** (see below).

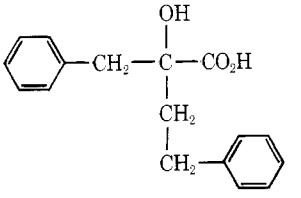


Figure 7

For similar reasons, the choice of an 8CI index heading parent for a phenylated alcohol might lie among Methanol, Ethanol, 1-Propanol, etc., and Benzyl alcohol, Phenethyl alcohol, and Benzhydrol.

Beginning with Volume 76, these problems have been resolved by (a) elimination of all trivial names for phenylated alcohols and acids, and (b) abandonment of the principle of "like treatment of like things." Now, selection of an index heading parent depends on successive consideration of the following principles until (and only until) a decision is reached:

(i) The maximum number of the most preferred chemical functional group. The seniority of such groups and classes of compounds is largely unchanged; the descending order proceeds from free radicals (the highest class) down through cations; neutral coordination compounds (which now include ferrocene); anions; acids (expressed as a suffix) in the order peroxy acids, carbon acids (i.e., carboxylic acids and analogs), sulfur acids, selenium acids, tellurium acids; then other acids in the order carbon acids (i.e., carbonic, formic, etc.), and acids of halogens, chalcogens, ni-

trogen, phosphorus, arsenic, antimony, silicon, and boron; acid halides, azides, isocyanates, etc.; amides; nitriles; aldehydes; ketones, thiones, etc.; alcohols and phenols (which are now of equal rank); thiols, etc.; hydroperoxides; amines; imines. Changes in this order mainly affect peroxy acids and carbonic acids.

(ii) The preferred hetero atom (presence in the molecular skeleton of one or more atoms of nitrogen, phosphorus, arsenic, antimony, bismuth, boron, silicon, germanium, tin, lead, oxygen, sulfur, selenium, tellurium, carbon, in that descending order).

In the absence of a function expressed as a suffix, all these compounds, and those in the following paragraphs, rank below those in (i), above. Thus, **Quinoline** is now less preferred as an index heading parent than **Ethanamine.**

(iii) Preferred ring system (thus, even cyclopropane ranks higher than any acyclic carbon chain)

(iv) Maximum number of acyclic hetero atoms

(v) Largest number of skeletal atoms

(vi) Maximum number of the most preferred acyclic hetero atoms

(vii) Maximum number of multiple bonds

(viii) Lowest locants in the index heading parent

Once chosen by these principles, the index heading parent is not changed by further criteria, such as the discontinued principle of "like treatment of like things." Further selection rules are needed only when the chosen parent occurs in the total molecule more than once. These further rules lead to the choice of that occurrence which:

(ix) is in the most central position (if three or more are present in a linear arrangement)

(x) possesses the most substituent groups

(xi) has these groups attached to positions expressed by lowest locants

(xii) is capable of being "multiplied" so that the index heading parent expresses the maximum number of occurrences

(xiii) when a choice still exists, affords the name which, after inversion in the usual way, appears earliest in the alphabetic sequence of CA Chemical Substance Index names.

Applying these rules to the examples shown above, and taking into account (i) the more systematic name Propanoic acid in place of Propionic acid, as well as (ii) extension of conjunctive names to benzene as previously mentioned, we can see that the preferred index heading parent in Figure 6 (R = H or an acyclic substituent or phenyl) for 9CI is **Benzenepropanoic acid.** If R is a radical derived from a ring system more preferred than benzene—e.g., 4-pyridinyl—then a different conjunctive name parent is chosen—e.g., **4-Pyridineacetic acid**—and the total preferred 9CI index name is **4-Pyridineacetic acid, α-phenyl-α-(1-phenylethyl)-.**

The preferred index name for Figure 7, formerly the object of a perplexing circular chase, can be seen quite clearly to be now **Benzenebutanoic acid, α-hydroxy-α-(phenylmethyl)-.**

As an example of a simple acyclic compound for which selection of a preferred index name was formerly difficult, consider Figure 8:

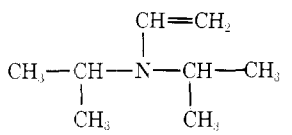


Figure 8

The largest appropriate index heading parent available during the 8CI was Diisopropylamine, of which Figure 8 depicts the *N*-vinyl derivative. But substitution on parents with iso-, *sec-* and *tert-* names has always been avoided by CA. Although derivatives of Isopropyl alcohol were indexed at 2-Propanol, the name 2-Propanamine was not employed prior to the 9CI; instead, radicofunctional names were used for amines. (Radicofunctional names are derived by appending functional class terms, e.g., "amine," "ether," "disulfide" or "peroxide," to substituent radical names. Their use for amines, ethers and chalcogen analogs has been discontinued by CA.) Excluding Diisopropylamine as a parent, the largest one remaining for the 8CI was Diethylamine, of which Figure 8 is the 1,1′-dimethyl-*N*-vinyl derivative. But a further rule preferred an unsaturated skeleton rather than a saturated one, and combination of this rule with the choice of a radical-based name led to the preferred index name Vinylamine, *N,N*-diisopropyl-.

In the 9CI, amines are named by addition of the "-amine" suffix to the preferred molecular skeleton name, and secondary and tertiary amines are indexed as *N*-derivatives of the preferred primary amine. The index name for Figure 8 in Volume 76 can, therefore, be readily derived; it is **2-Propanamine, *N*-ethenyl-*N*-(1-methylethyl)-** (note the more systematic names for the vinyl and isopropyl radicals).

Prior to Volume 76, structures that may be considered as ethers were indexed by a number of methods. The 8CI names were classified as follows:

(a) *Radicofunctional uninverted names* were used for simple symmetrical monoethers.

Example [In this and the following examples, the 8CI name is cited first (in lightface) unless it corresponds to the 9CI name (shown in boldface)]:

$CH_3CH_2OCH_2CH_3$

Ethyl ether **(Ethane, 1,1′-oxybis-)**

(b) *Radicofunctional inverted names* were used for unsymmetrical and substituted monoethers and some more complex ethers.

Examples:

$ClCH_2OCH_2Cl$

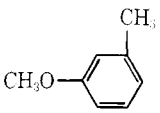
Ether, bis(chloromethyl) **(Methane, oxybis[chloro-)**

$CH_3CH_2OCH_3$

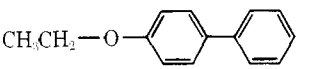
Ether, ethyl methyl **(Ethane, methoxy-)**

(c) *Trivial names* were used for anisole and phenetole and some of their derivatives.

Examples:



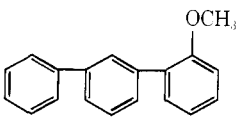
Anisole, *m*-methyl- **(Benzene, 1-methoxy-3-methyl-)**



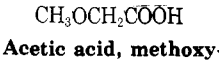
Phenetole, *p*-phenyl- **(1,1′-Biphenyl, 4-ethoxy-)**

(d) *Aryloxy and alkoxy radicals* were used with parents containing functional suffixes and for heterocycles and unsymmetrical ethers containing polycyclic hydrocarbons. (But asymmetry limited to points of attachment on two polycyclic hydrocarbons or ring assemblies led to names based on Ether as parents—e.g., Ether, 1-naphthyl 2-naphthyl.)

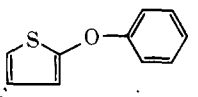
Examples:



m-Terphenyl, 2-methoxy- **(1,1′:3′,1″-Terphenyl, 2-methoxy-)**

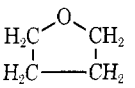


Acetic acid, methoxy-



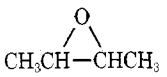
Thiophene, 2-phenoxy-

(e) Cyclic ethers were indexed as heterocyclic compounds if the ring contained five atoms or more.
Example:

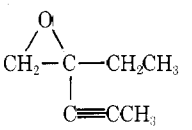


Furan, tetrahydro-

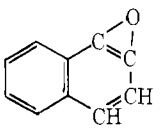
(f) Smaller cyclic monoethers were indexed as epoxy derivatives of acyclic hydrocarbons, etc., not at Oxirane or Oxetane, unless the "correct" hydrocarbon parent could not be employed. The "epoxy" method was also employed for oxireno derivatives of fused hydrocarbons (but not of heterocycles). Unsubstituted oxirane and oxetane were indexed at the radicofunctional names Ethylene oxide and Trimethylene oxide, respectively, and Propylene oxide was used for methyloxirane.
Examples:



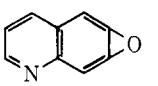
Butane, 2,3-epoxy- (**Oxirane, 2,3-dimethyl-**)



Oxirane, 2-ethyl-2-(1-propynyl)- (the compound could not be named as an epoxy derivative of the preferred hydrocarbon, **2-Hexyne**)

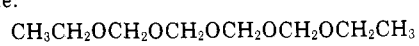


Naphthalene, 1,2-epoxy- (**Naphth[1,2-*b*]oxirene**)



Oxireno[*g*]quinoline

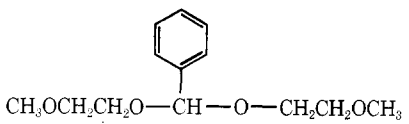
(g) Acyclic polyethers with four or more single oxygen atoms were indexed at replacement ("a") names.
Example:



3,5,7,9,11-Pentaoxatridecane

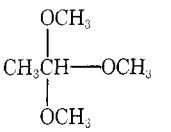
(h) *Acetals,* except acetals of formaldehyde, were indexed at the carbonyl-compound parent.

Example:



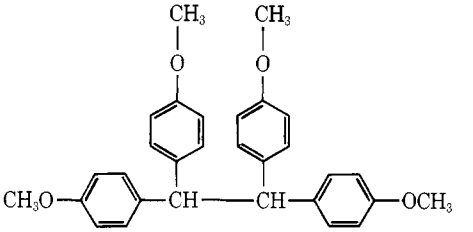
Benzaldehyde bis(2-methoxyethyl) acetal (**2,5,7,10-Tetraoxaundecane, 6-phenyl-**)

(i) *Ortho esters* were indexed at the acid names.
Example:



Orthoacetic acid trimethyl ester (**Ethane, 1,1,1-trimethoxy-**)

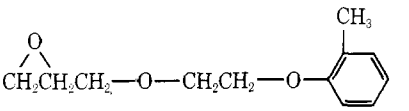
Choice of preferred index names for some ethers, especially polyethers, was therefore a perplexing subject. Consider Figure 9.



Ethane, 1,1,2,2-tetrakis(*p*-methoxyphenyl)- (**Benzene, 1,1′,1″,1‴-(1,2-ethanediylidene)tetrakis[4-methoxy-**)

Figure 9

Benzene might appear to be the preferred 8CI hydrocarbon parent, but anisole is larger. "Like treatment of like things" would require multiplication of the four occurrences of anisole, but this was not permitted (for hydrocarbons or for anisole). Therefore, in the 8CI, the index name was based on the central hydrocarbon parent Ethane. The larger hydrocarbon parent bibenzyl was not used so that the phenyl groups could be all treated alike. Other examples were more difficult, and various rules for polyethers were devised, including choice of a heterocyclic or polycyclic parent if present, use of Ether as a radicofunctional parent (for symmetrical polyethers with a central oxygen atom), and a variety of rules for choice of a hydrocarbon parent. This was often the most central hydrocarbon, rather than the most senior, as in Figure 10:



Ethane, 1-(2,3-epoxypropoxy)-2-(*o*-tolyloxy)- (Oxirane, [[**2-(2-methylphenoxy)ethoxy]methyl**]-)

Figure 10

All the problems of index name selection for ethers were paralleled in the cases of the analogous sulfur, selenium, and tellurium compounds. Examples of these were scattered at Sulfide (or Selenide or Telluride), hydrocarbon and other parents, and "a" names.

Beginning with Volume 76, CA has simplified the rules for ethers, sulfides, etc., as follows:

(a) The index heading parents Ether, Sulfide, etc., are discontinued. Uninverted radicofunctional headings—e.g., Ethyl ether—which included these terms are also abandoned.

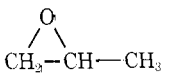
(b) Presence of one or more single oxygen (sulfur, etc.) atoms in an acyclic chain is expressed by "oxy" ("thio," etc.) radicals or, if four or more hetero units are present, by use of a replacement "oxa" ("thia," etc.) name derived from the hydrocarbon [see "Replacement ("a") nomenclature," below].

(c) Cyclic ethers, etc., continue to be named as heterocycles—e.g., at **Furan** or by use of a furanyl radical. Trivial names—e.g., Ethylene oxide—are discontinued.

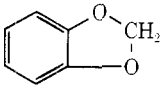
(d) Polyethers, etc., are indexed at hydrocarbon or other parents, and these parents are chosen by the usual rules (highest attached function, hetero-atom chain, etc.). Multiplication of the preferred hydrocarbon is permitted when appropriate. Cyclic hydrocarbons are preferred to acyclic hydrocarbons, regardless of relative size [see selection rule (iii), above].

(e) Acetals are no longer named as such but by the methods employed for other diethers.

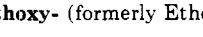
Examples:



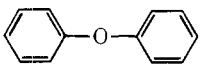
Oxirane, methyl- (formerly Propylene oxide)



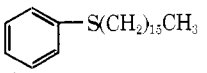
1,3-Benzodioxole (formerly Benzene, 1,2-(methylenedioxy)-)



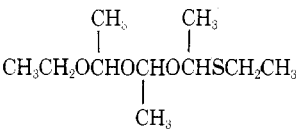
Ethane, methoxy- (formerly Ether, ethyl methyl)



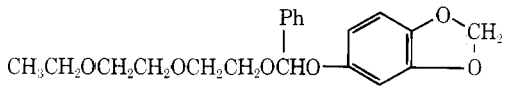
Benzene, 1,1'-oxybis- (formerly Phenyl ether)



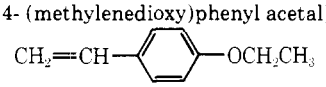
Benzene, (hexadecylthio)- (formerly Sulfide, hexadecyl phenyl) (principle: cyclic parent preferred)



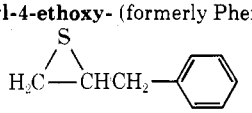
3,5,7-Trioxa-9-thiaundecane, 4,6,8-trimethyl- (formerly Acetaldehyde, 1-ethoxyethyl 1-(ethylthio)ethyl acetal).



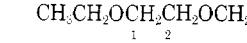
1,3-Benzodioxole, 5-[(2-(2-ethoxyethoxy)ethoxy]phenylmethoxy]- (formerly Benzaldehyde, 2-(2-ethoxyethoxy)ethyl 3,4- (methylenedioxy)phenyl acetal)



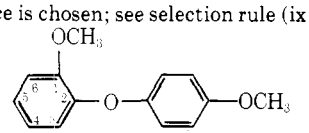
Benzene, 1-ethenyl-4-ethoxy- (formerly Phenetole, *p*-vinyl-



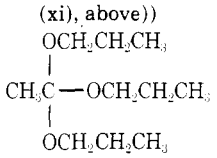
Thiirane, (phenoxymethyl)- (formerly Ether, 2,3-epithiopropyl phenyl) (principle: the heterocyclic parent is preferred; see selection rule (ii), above)



Ethane, 1-ethoxy-2-(2-methoxyethoxy)- (principle: **Ethane** is preferred to **Methane** as parent; the central occurrence is chosen; see selection rule (ix), above)



Benzene, 1-methoxy-2-(4-methoxyphenoxy)- (principle: lowest locants for substituent prefixes (see selection rule (xi), above))

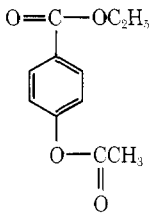


Propane, 1,1',1''-[ethylidynetris(oxy)]tris- (formerly Orthoacetic acid, tripropyl ester)

SUMMARY OF OTHER CHANGES

Functional Derivatives. Nonionic derivatives of the principal chemical function (that chemical function that is expressed by the index heading parent) are cited in the index modification as previously, but derivatives of subsidiary chemical functions are named as prefixes in the bold-faced index heading. (The index modification is that part of the total index entry which appears in lightface and modifies or adds to the information supplied by the bold-faced main heading.) This brings some information formerly expressed in the light-faced modification up into the heading and results in more consistent names. Esters and other subsidiary derivatives of parts of the molecule structurally removed from the principal index heading parent are also named as prefixes.

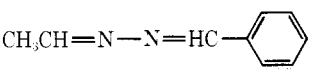
Example:



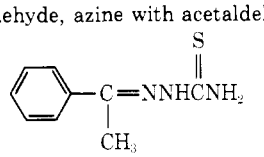
Benzoic acid, 4-(acetyloxy)- ethyl ester (formerly Benzoic acid, ethyl ester, acetate)

Derivatives of principal chemical functions still named in index modifications are esters, hydrazides, hydrazones, and oximes. (Azines and phosphazines of principal chemical functions are named in modifications as substituted hydrazones.) Semicarbazones, carbohydrazones, semioxamazones, and acetals of index heading parents, other than stereoparents, are named by the general rules outlined above by which the preferred index heading parent is first chosen and the remaining substituents (except for derivatives of the principal chemical function) are expressed by prefixes cited in alphabetical order.

Examples:



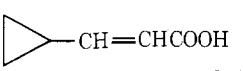
Benzaldehyde, ethylidenehydrazone (formerly Benzaldehyde, azine with acetaldehyde)



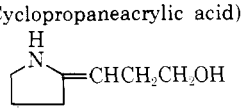
Hydrazinecarbothioamide, 2-(1-phenylethylidene)- (formerly Acetophenone, thiosemicarbazone)

Conjunctive Nomenclature. Conjunctive nomenclature has been extended to benzene (which had been the sole exception) when attached to one or more saturated acyclic chains, each of which contains a chemical function (see Benzeneacetic acid, Benzeneethanamine, etc., in Table I). Conjunctive names are no longer formed for unsaturated or polyfunctional acyclic parents (this had been done only for trivially-named parents such as Acrylic acid), or for compounds in which the ring attachment is by a double bond. Conjunctive (or "additive") names have been used by CA since the First Decennial Index (1916). They are formed by conjunction of a ring-system name with an acyclic chain bearing a chemical function. It is always understood that the ring is located at one end of the chain and the function at the other. Thus, **2-Naphthalenebutanamine** is formed by conjunction of naphthalene at the 4-position of 1-butanamine, the locant "2" indicating the position on the naphthalene ring system.

Examples:



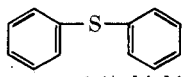
2-Propenoic acid, 3-cyclopropyl- (formerly Cyclopropaneacrylic acid)



1-Propanol, 3-(2-pyrrolidinylidene)- (formerly $\Delta^{2,\gamma}$-Pyrrolidinepropanol)

Multiplicative Nomenclature. Multiplicative nomenclature has been extended to hydrocarbons, as explained in the discussion of ethers, above. If the index heading parent contains more than one position with replaceable hydrogen, locants are used. "Bis," "tris," etc. (not "di," "tri," etc.) are now always used in multiplying a substitutive index parent.

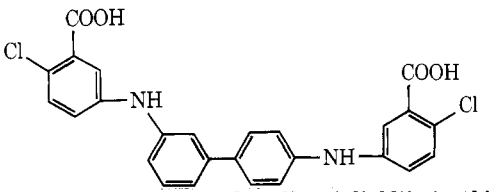
Example:



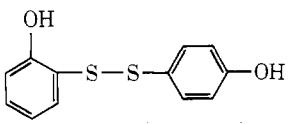
Benzene, 1,1′-thiobis-

The use of multiplicative nomenclature is now restricted to cases in which each occurrence of the index heading parent is substituted in equivalent positions by equivalent atoms or groups, and in which any asymmetry is restricted to a central (substituted or unsubstituted) one-part multivalent radical.

Examples:



Benzoic acid, 3,3′-([1,1′-biphenyl]-3,4′-diyldiimino)bis[6-chloro- (formerly Benzoic acid, 3,3′-(3,4′-biphenylylenediimino)bis[6-chloro-)



Phenol, 2-[(4-hydroxyphenyl)dithio]-formerly Phenol, 2,4′-dithiodi-) (principle: the lowest locant for attachment to the index heading parent is preferred)

Replacement ("a") Nomenclature. The use of replacement ("a") nomenclature for ring systems in CA indexes is essentially unchanged. For acyclic compounds, replacement nomenclature is continued but has been made more consistent. (Replacement nomenclature employs aza, oxa, thia, etc., terms to indicate replacement of carbon atoms by nitrogen, oxygen, sulfur, etc. See CA Volume 76 Index Guide, Section IV, paras 127–9.) Prior to Volume 76, various criteria were applied to determine whether the preferred index name was formed by replacement nomenclature. Usually, four hetero atoms were needed, but exceptions were made for acetals and for compounds containing two or three silicon atoms. Consideration also was given to whether like groups were treated alike. Sometimes more than one index entry was made for a specific compound if three hetero atoms were present.

Now, the concept of "hetero units" has been introduced, and the rules have been simplified and are applied without exception. A hetero unit is (a) a single hetero atom, (b) a chain of contiguous, like hetero atoms, e.g., —O—O—O—, or (c) a chain of unlike hetero atoms named by CA as a simple multivalent radical, e.g., -SiH_2-O-SiH_2- (1-3-disiloxanediyl).

A replacement ("a") name is chosen if carbon is present and:

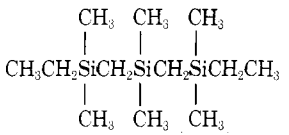
(1) Four or more hetero units are present in the index heading parent

(2) The chain is terminated by C, P, As, Sb, Bi, Si, Ge, Sn, Pb, or B

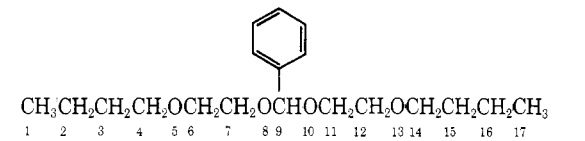
(3) The replacement name does not rank lower than the conventional name; i.e., it must express, as a suffix, at least the same number of equivalent functions

(4) All atoms in the chain must be in the standard substitutive valency state, or any abnormal valency must be clearly expressible—e.g., by use of an additive term such as "oxide" on a phosphorus atom.

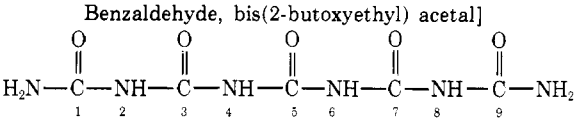
Examples:



Silane, bis[(ethyldimethylsilyl)methyl]dimethyl- (formerly 3,5,7-Trisilanonane, 3,3,5,5,7,7-hexamethyl-)



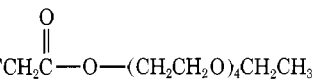
5,8,10,13-Tetraoxaheptadecane, 9-phenyl- [formerly Benzaldehyde, bis(2-butoxyethyl) acetal]



2,4,6,8-Tetraazanonanediamide, 3,5,7-trioxo- (formerly Pentauret)

Radicals are named by "a" nomenclature on a routine basis for the first time. The criteria are similar to those for index heading parents, the free valencies (not the hetero atoms) are numbered low, and locants for free valencies are always cited.

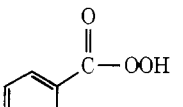
Example:



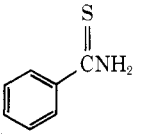
Acetic acid, fluoro- 3,6,9,12-tetraoxatetradec-1-yl ester (formerly Acetic acid, fluoro-, 2-[2-[2-(ethoxyethoxy)ethoxy]ethoxy]ethyl ester

Another type of replacement nomenclature[3] has long been used to express replacement of oxygen in phosphorus acids by other atoms or groups. Thus, analogs of **Phosphoric acid,** $(HO)_3P(O)$, include **Phosphorodithioic acid,** $(HO)(HS)_2P(O)$, and Phosphoramidic acid, $(HO)_2(H_2N)P(O)$. These names are retained in the 9CI, and the nomenclature system, which may be called *functional replacement nomenclature,* has been extended to peroxy acids and hydrazonic acids, and made fully consistent for chalcogen analogs of acids, acid halides, amides, and aldehydes.

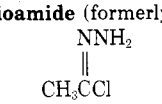
Examples:



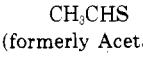
Benzenecarboperoxoic acid (note that this name and the next one are derived from Benzenecarboxylic acid, not Benzoic acid) (formerly Peroxybenzoic acid)



Benzenecarbothioamide (formerly Benzamide, thio-)



Ethanehydrazonoyl chloride (formerly Acetyl chloride, hydrazone)

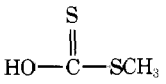


Ethanethial (formerly Acetaldehyde, thio-)

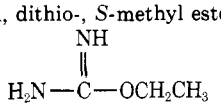
Such functional replacement names are also extended

to mononuclear carbon acids, arsenic acids, and related compounds.

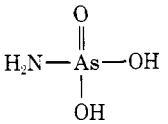
Examples:



Carbonodithioic acid, *S*-methyl ester (formerly Carbonic acid, dithio-, *S*-methyl ester)



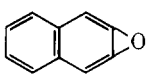
Carbamimidic acid, ethyl ester (the contracted form is used for Carbamic acid (not Carbonamidic acid) and its analogs) (formerly Pseudourea, 2-ethyl-)



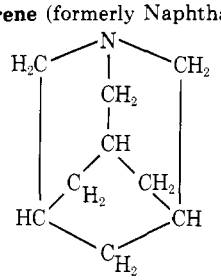
Arsenamidic acid (formerly Arsine oxide, aminodihydroxy-)

Ring Systems. Former ring names[4] are generally unchanged. In those that contained *o*, *m*, or *p* locants, these have been replaced by numerals. The locant *v* has also been replaced and in most cases *as* and *s* (except for *as*- and *s*-indacenes and their fused derivatives). Fused oxirene and thiirene derivatives of hydrocarbon systems are now named systematically; adamantane is renamed Tricyclo[3.3.1.1^{3,7}]decane. The position of indicated hydrogen is left unexpressed only for saturated ring atoms located between two bivalent ring atoms. Special names for *partially* hydrogenated systems, e.g., Indan, Acenaphthene, etc., are replaced by "hydro" names—e.g., 1*H*-Indene, 2,3-dihydro-; Acenaphthylene, 1,2-dihydro-. (A complete set of ring-system diagrams in name order up to date through 1971 appears in the CA Volume 75 and Eighth Collective Index Guides, accompanied by an Index of Ring Systems arranged according to the number, size and content of component rings in the systems. CAS will soon publish a Parent Compound Handbook devoted to ring systems and cyclic stereoparents, with emphasis on the relations between members of the two classes. See CA Volume 76 Index Guide, para 8.)

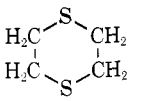
Examples:



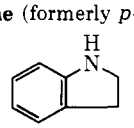
Naphth[2,3-*b*]oxirene (formerly Naphthalene, 2,3-epoxy-)



1-Azatricyclo[3.3.1.1^{3,7}]decane (formerly 1-Azaadamantane)



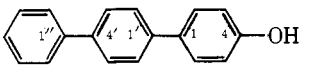
1,4-Dithiane (formerly *p*-Dithiane)



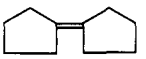
1*H*-Indole, 2,3-dihydro- (not Indole, 2,3-dihydro-) (formerly Indoline)

Ring-assembly names are now preceded by locants for points of attachment—e.g., **1,1′-Biphenyl**—except for two-component assemblies of cycloalkenes—e.g., **Bi-2-cyclohexen-1-yl.** Ring assembly names are no longer used when the component rings are connected by double bonds. Binaphthyl and Bianthryl are renamed Binaphthalene and Bianthracene, respectively. (Ring assemblies are formed by junction of two or more rings (or ring systems) by valence bonds, the number of bonds being one fewer than the number of cyclic components.)

Examples:



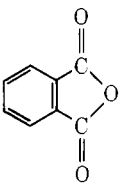
[1,1′:4′,1″-Terphenyl]-4-ol (formerly [*p*-Terphenyl]-4-ol)



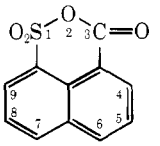
Cyclopentane, cyclopentylidene- (formerly Bicyclopentylidene)

Cyclic anhydrides, esters, etc., are now indexed at ring-system names unless a stereoparent is involved. Such compounds were often, but not always, named in the "open" form in the 8CI, with cross-references at ring names.

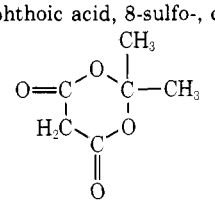
Examples:



1,3-Isobenzofurandione (formerly Phthalic anhydride)



3*H*-Naphth[1,8-*cd*][1,2]oxathiin-3-one, 1,1-dioxide (formerly 1-Naphthoic acid, 8-sulfo-, cyclic anhydride)



1,3-Dioxane-4,6-dione, 2,2-dimethyl- (formerly Malonic acid, cyclic isopropylidene ester)

Substituent Prefixes (Radicals). The changes adopted for index heading parents have been applied in a similar way to radicals. Trivially named radicals have been replaced by more systematic names, and the selection of a name for a branched-chain radical follows rules parallel to those for choice of an index heading parent. Major changes in substitutive prefix names include:

(a) Branched-chain alkyl radicals are named as derivatives of the longest alkyl chain; all iso-, *sec*-, and *tert*-alkyl names are discontinued. Trivial names like allyl and vinyl are replaced by more systematic equivalents. The contracted forms methoxy, ethoxy, propoxy, butoxy, and phenoxy are retained. Acyclic "-ylene" radicals (except methylene) from carbon chains have been converted to "diyl" radicals and locants for the free valencies (which must be at terminal positions) are always cited; thus, butylene becomes 1,4-butanediyl, trimethylene becomes 1,3-propanediyl, and vinylene is replaced by 1,2-ethenediyl.

(b) Trivalent benzene radicals are named 1,2,3-benzenetriyl, etc., in place of *v*-phenenyl, etc. Phenylene radicals are retained, but numerical locants replace *o*-, *m*-, and *p*-.

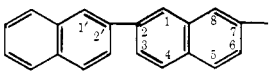
(c) Most other ring-system radicals are unchanged; the contracted radicals naphthyl and anthryl are spelled out as

naphthalenyl and anthracenyl; bivalent "-ylene" radicals for cyclic hydrocarbons are replaced by "-diyl" radicals (e.g., 1,4-cyclohexylene becomes 1,4-cyclohexanediyl).

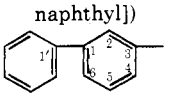
(d) Trivially named (alkylphenyl), (phenylalkyl), etc., radicals are named systematically as compound (i.e., two-part) radicals. Thus, benzyl becomes (phenylmethyl); styryl becomes (2-phenylethenyl); 2,4-xylyl becomes (2,4-dimethylphenyl); and so on.

(e) Ring-assembly radicals are now based on the assembly names, not on the components. Biphenyl radicals are retained, but with added brackets and ring-junction locants.

Examples:



[2,2'-binaphthalen]-7-yl (formerly [7-(2-naphthyl)-2-naphthyl])



[1,1'-biphenyl]-3-yl (formerly 3-biphenylyl)

(f) Among special radical names retained are azo (—N=N—) (but the unsubstituted radical HN=N— is diazenyl instead of diazeno), hydrazino (H_2NNH—), hydrazo (—NHNH—), hydrazono (NH_2N=), thienyl (not thiophenyl), and all formazan radicals.

(g) Except for carbonyl, formyl (when unsubstituted), acetyl, and benzoyl, acyl radicals in systematic index names are replaced by substituted alkyl radicals; thus, acetimidoyl $CH_3C(:NH)$— becomes (1-iminoethyl); propionyl becomes (1-oxopropyl), succinoyl becomes (1,4-dioxo-1,4-butanediyl), etc. Carboxy and cyano groups are always treated as units. In multiplicative names, carbonothioyl is used for —C(:S)—, carbonimidoyl for —C(:NH)—, and carbonohydrazonoyl for $—C(:NNH_2)$—; these names are also used when both valencies are attached to a single atom of a parent, otherwise the names (thioxomethyl), (iminomethyl), and (hydrazonomethyl) are employed. Carbamoyl is replaced by (aminocarbonyl), and sulfamoyl is replaced by (aminosulfonyl).

The names of former and revised names for radicals of various types are shown in Table II.

EXTENSION OF CHEMICAL SUBSTANCE REGISTRATION

Beginning in CA Volume 76, the CAS Registry System includes specific members of the following classes (for further details of these special classes, see the CA Volume 76 Index Guide, paras 214, 217, 218, 221): (a) Alloys, (b) Elementary particles, (c) Enzymes, and (d) Mixtures.

This has been done to obtain all the advantages of registration, including storage and retrieval of chemical composition and preferred index names by CA indexers, and improved search capabilities for users of CAS products. These classes of substances are entered in the Chemical Substance Index, each with its CAS Registry Number, in the same way as are conventional chemical compounds as follows:

(a) *Alloys* are indexed at each component (down to 1% concentration), and the composition is described in the modification by use of element symbols and rounded-off percentage figures (down to 0.1%). The component present in greatest concentration is indexed at a "base" heading, the other indexed components at "nonbase" headings. A concentration range is shown where appropriate.

Example (9CI):

Copper alloy, base Cu 68-73, Ni 15-20, Al 9, Co 1.7, Fe 0.8

Nickel alloy, nonbase Cu 68-73, Ni 15-20, Al 9, Co 1.7, Fe 0.8

(Similar "nonbase" entries are made for aluminum and cobalt; an entry is made at **Iron** (not **Iron alloy, nonbase**) if its presence is considered significant in the reported study.)

The index heading **Steel** is used when appropriate and (when no further information is available) also the headings **Brass** and **Bronze.**

(b) *Elementary particles* are indexed at headings such as **Alpha particle; Meson,** π**; Meson,** K**; Proton;** and **Positronium chloride** (e^+Cl).

(c) *Enzymes* are entered at names approved by IUPAC-IUB. Cross references at E.C. numbers in the Volume 76 Index Guide lead to these index names, which are inverted when this is feasible. Parenthetical qualifying phrases are sometimes included in the headings.

Examples:

Phosphatase, adenosine tri-
Dehydrogenase, lactate
Papain
Dehydrogenase, malate (decarboxylating)

(d) *Mixtures* are indexed and registered as such if they have significance as mixtures, e.g., as pharmaceuticals or pesticides with trade names, or are specially prepared mixtures with properties reported in original documents. Solvents, fillers, etc., are not indexed. Mixtures appear in the Chemical Substance Index at each significant ingredient; one or more of such ingredients may be indexed (because of their indefinite nature) in the General Subject Index.

Example:

Glycine
mixt. with egg white and sodium chloride (preferred Chemical Substance and Formula Index entry) (cross reference to this name from the trade name, Yumol)
Sodium chloride
mixt. with egg white and glycine (additional Chemical Substance and Formula Index entry)
Egg white
mixt. with glycine and sodium chloride (General Subject Index entry, not retrievable from the CAS Registry System)

Mixtures containing more than nine registrable components are indexed only at the accepted trivial or trade name, but each component is registered as usual and "see also" cross references to the index name appear in the Index Guide at the names of the components.

SUMMARY

Chemical Abstracts index names for chemical substances have been significantly revised for the Ninth Collective Period (Volumes 76-85, 1972-1976), particularly in the following respects:

(a) Except for natural product names that include stereochemical information, nearly all trivial or author names have been abandoned in favor of more systematic names. Radical names have also been made more systematic.

(b) Special treatment of various compound classes has been eliminated so far as possible. Rules are applied consistently to all the areas of general index nomenclature.

(c) Name selection rules have been simplified appreciably. The principle of "like treatment of like things" has been abandoned, and the principle of centrality (applied to a linear arrangement of three or more occurrences of an index heading parent) has been clarified.

(d) Alloys, elementary particles, enzymes, and mixtures are now indexed and registered like chemical substances

when sufficient information about their composition is available.

This paper was designed to call attention to some of the major revisions in the CAS handling of chemical substance index nomenclature. A more detailed (120-page) account is included in the Volume 76 CA Index Guide, Section IV (Selection of Index Names for Chemical Substances).

The complete new documentation used by CAS staff in naming all classes of chemical substances is also available in typewritten form from the CAS Marketing Department. It comprises nearly 2000 pages, including a comprehensive index and alphabetical list of substituent radical names, and is titled "Chemical Substance Name Selection Manual for the Ninth Collective Index Period (1972–1976)."

LITERATURE CITED

(1) Rowlett, R. J., Jr., and Tate, F. A., *J. Chem. Doc.* **12,** 125 (1972); CA Vol. 76 Index Guide (1972), para 13, p. 101.
(2) CA Volume 76 (1972) Index Guide, Section IV, paras 296–300.
(3) *Chem. Eng. News* **30,** 4515 (1952).
(4) Patterson, A. M., Capell, T., and Walker, D. F., "The Ring Index," 2nd ed., Washington, D. C., 1960; Suppl. I-III (1963, 1964, 1965).
(5) *Enzyme nomenclature:* Recommendations of the International Union of Pure and Applied Chemistry and the International Union of Biochemistry. Elsevier, Amsterdam, 1973. This is a revision of the recommendations (1964) of IUB.

The CA Integrated Subject File. II. Evaluation of Alternative Data Base Organizations*

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Received October 9, 1973

The relative retrieval performances of the *CA Integrated Subject File* (CAISF), *CA Condensates,* and a Merged File created from these two data bases have been measured. Retrieval performance is reported in terms of recall and precision values as well as costs. The precision and recall retrieval failures—i.e., irrelevant documents and missed documents—have been analyzed for each data base and characterized according to the five major types of failures: index language, indexing, searching, clerical, and miscellaneous. Over-all analysis of the performance suggests that an effective data base can be created by augmenting the *CA Condensates* data base with Registry Numbers and some representation of the CAISF General Subject concept headings, which results in a file approximately half the size of the corresponding CAISF data base and is suitable for search using existing retrieval system software.

A research study was designed to investigate alternative methods of using the *CA Integrated Subject File* (CAISF) (the acronym ISF was used in the previous paper in this series[4]) for computer-based bibliographic retrieval and to compare these approaches to retrieval from *CA Condensates.* Both of these data bases are produced and distributed by Chemical Abstracts Service (CAS). The CAISF contains the index entries in the printed *CA Subject Index,* plus molecular formulas, the CA section numbers, and the CA abstract numbers. It is distributed in two parts for each six-month volume, the Chemical Substance (CS) segment containing the index entries for specific chemical substances and the General Subject (GS) segment containing the conceptual index entries. *CA Condensates* corresponds to *Chemical Abstracts* and includes the bibliographic citation data, keywords, and the CA abstract number.

The purpose of this study was to determine quantitatively the relative retrieval performances of these three data bases and of others constructed from them in terms of both cost and retrieval capacity. The CAISF contains largely controlled indexing information while *CA Condensates* contains bibliographic information and some uncontrolled descriptive information, such as titles and keywords. Both files represent the same set of documents. The comparison, then, includes these data bases organized as distributed by CAS as well as other combinations which can be created through computer processing. The major tasks included the measurement of recall and precision values for several file organizations, comparison of natural language and controlled vocabularies, evaluation of alternative search strategies, and projection of implementation and operational costs for the alternative approaches.

RESEARCH DESIGN

The approach which was taken to evaluate alternative data content and file organizations for the CA-related files was the construction and use of files as near opposite ends of the retrieval continuum as could reasonably be derived from the resources available—that is, a file containing natural language vocabulary and a file with controlled vocabulary; a file designed for postcoordinate index term retrieval *vs.* one with a highly structured, hierarchical, precoordinate retrieval structure; and a single file which collects both chemical compound and general subject entries at a single point suitable for Boolean logic operations *vs.* split files which require postcorrelation of document refer-

* Presented in part before the Division of Chemical Literature, 166th Meeting, ACS, Chicago, Ill., Aug. 28, 1973.
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