

Nomenclature Changes for CA Index Names

Introduction

Effective the week of December 11, 2006, CAS began implementing a number of changes that simplify CA index nomenclature and make CA index names more logical, consistent, and easier to understand. These changes represent the most significant group of modifications to CAS index nomenclature since the introduction of 9th Collective Index (9CI) nomenclature in 1972.

All existing names have been retained on the substance records and the new names are being added during 2007.

The examples show both the new CA index names and the 9CI names for comparison.

Summary of Changes

The key nomenclature changes include:

General Changes

1. New Definition for Ketones
2. Elimination of Unexpressed Amides
3. Elimination of Aldehydo Substituents
4. Binuclear Nitrogen Radicals
5. Names for Sulfur, Selenium, and Tellurium Radicals Double Bonded to Nitrogen
6. New Ranking of Silane for Choice of Parent
7. Acylheteroatom Substances
8. Chalcogen-Substituted Borons
9. Non-traditional Alcohol Esters
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CA Index Names

Effective with 2007, CAS no longer categorizes information by collective index periods. The 15CI period covers 2002-2006. The CA index names in CAS REGISTRYSM no longer have a "CI" label. The "CI" labels (6CI, 7CI, 8CI, 9CI) have been retained for those names that have them.

Updated Registry

The CA index name for all substances in REGISTRY are being updated in 2007 to comply with the new rules. New compounds will receive the new CA index name. The previous CA index name, if different, will appear in the OTHER CA INDEX NAMES portion of the REGISTRY display. No names will be removed.

Questions

If you have questions concerning these changes, please contact CAS Customer Care at help@cas.org or 800-753-4227.

Appendix IV of the CA Index Guide

The full details of the nomenclature changes previously published as Appendix IV of the *CA Index Guide*SM will be published at a later time.

General Changes

1. New Definition for Ketones

Ketones are a class of compounds characterized by the presence of the group



where X is any chalcogen. This group may be attached to carbon or other elements with the exception of hydrogen and those that could form an acid, acid derivative or amide name.

Organometallic and coordination compounds will continue to be named as such.

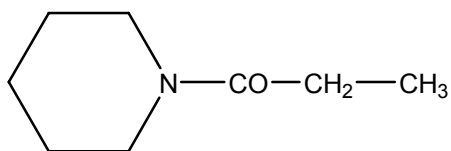


New: 1-Propanone, 1-(trimethylsilyl)-

9CI: Silane, trimethyl(1-oxopropyl)-

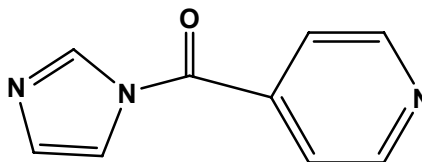
2. Unexpressed Amides

Amides in which the nitrogen atom of the amide group is part of a heterocyclic ring are not treated as unexpressed amides. These substances are named at the highest ranking function present.



New: 1-Propanone, 1-(1-piperidinyl)-

9CI: Piperidine, 1-(1-oxopropyl)-



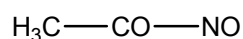
New: Methanone, 1*H*-imidazol-1-yl-4-pyridinyl-

9CI: 1*H*-Imidazole, 1-(4-pyridinylcarbonyl)-

3. Aldehyde Substituents

Replacement of the aldehyde hydrogen is not permitted. Aldehyde names will be restricted to carbonyl groups bonded to hydrogen or an isotope of hydrogen.

Some exceptions to this rule are permitted in carbohydrate nomenclature.



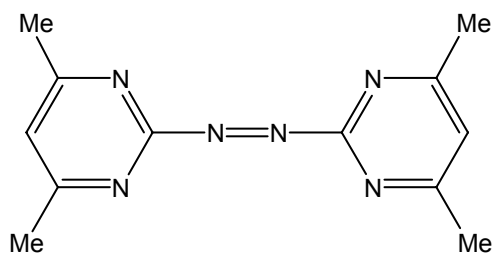
New: Ethanone, 1-nitroso-

9CI: Acetaldehyde, 1-nitroso-

4. Binuclear Nitrogen Radicals

The names for the following binuclear nitrogen radicals are revised as follows:

| <u>9CI</u> | <u>New</u> |
|------------|---|
| azi | 3 <i>H</i> -diaziridine (component ring in a spiro name) |
| azino | 1,2-hydrazinediylidene |
| azo | diazenyl or 1,2-diazenediyl |
| azoxy | (1-oxidodiazenyl) or (2-oxidodiazenyl) or (1-oxido-1,2-diazenediyl) |
| hydrazi | diaziridine (component ring in a spiro name) |
| hydrazino | hydrazinyl |
| hydrazo | 1,2-hydrazinediyl |
| hydrazono | hydrazinylidene |



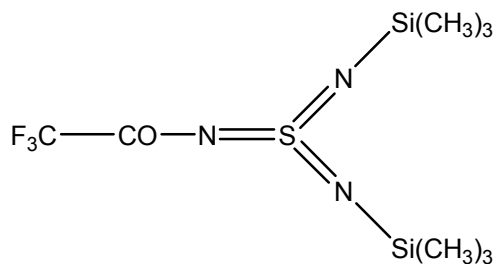
New: Pyrimidine, 2,2'-(1,2-diazenediyl)bis[4,6-dimethyl-

9CI: Pyrimidine, 2,2'-azobis[4,6-dimethyl-

5. Sulfur, Selenium, and Tellurium Radicals

Groups containing a sulfur, selenium, or tellurium atom attached by a double bond to nitrogen are now named as substituents. The following new radical names will be used:

| | S | Se | Te |
|-------------|----------------------------|---------------------------|----------------------------|
| Tetravalent | λ^4 -sulfanylidene | λ^4 -selanylidene | λ^4 -tellanylidene |
| Hexavalent | λ^6 -sulfanylidene | λ^6 -selanylidene | λ^6 -tellanylidene |

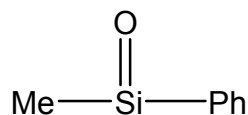


New: Acetamide, *N*-[bis[(trimethylsilyl)imino]- λ^6 -sulfanylidene]-2,2,2-trifluoro-

9CI: Sulfur triamide, (trifluoroacetyl)bis(trimethylsilyl)-

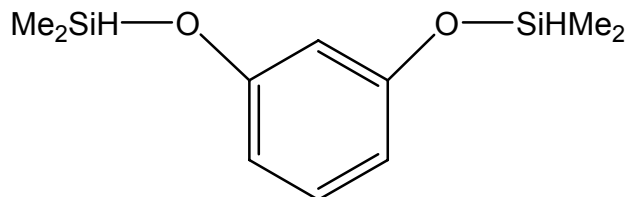
6. New Ranking of Silane

Silanes are now ranked between cyclic carbon parents and acyclic carbon parents. Silyl groups are used primarily as blocking groups and as such are not the primary structural feature of interest.



New: Benzene, (methyloxosilyl)-

9CI: Silane, methyloxophenyl-

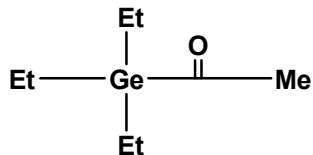


New: Benzene, 1,3-bis[(dimethylsilyl)oxy]-

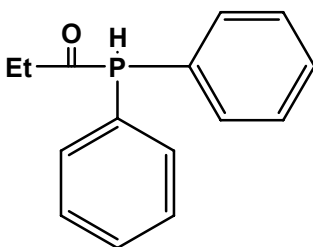
9CI: Silane, [1,3-phenylenebis(oxy)]bis[dimethyl-

7. **Acylheteroatom
Substances**

Acylheteroatom substances are named at the highest function present. The highest functional group is NOT overstepped to preserve the Acylheteroatom grouping.



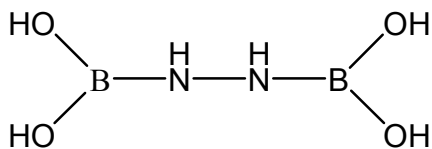
New: Ethanone, 1-(triethylgermyl)-
9CI: Germane, acetyltriethyl-



New: 1-Propanone, 1-(diphenylphosphino)-
9CI: Phosphine, (1-oxopropyl)diphenyl-

8. **Chalcogen
Substituted
Borons**

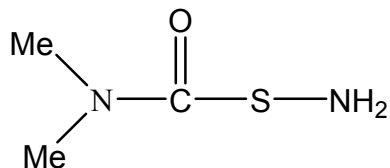
Chalcogen-substituted borons are names as boron acids.



New: Boronic acid, *B,B'*-1,2-hydrazinediylbis-
9CI: Hydrazine, 1,2-diborono-

9. Non-traditional Alcohol Esters

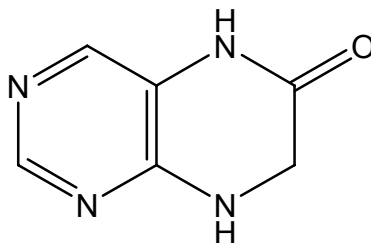
Non-traditional alcohol esters which are esterified with alcohols other than the traditional ones of carbon and silicon are now named as esters. Oximes of aldehydes and ketones are retained.



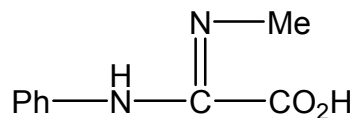
New: Carbamothioic acid, *N,N*-dimethyl-, *S*-azanyl ester
9CI: Thiohydroxylamine, *S*-[(dimethylamino)carbonyl]-

10. Preferred Tautomer

Only structure-based rules are used for selecting the preferred tautomer. In the 9CI system, a combination of nomenclature and structure-based rules were used to select the preferred form of a tautomer to name. Existing names for most tautomers are retained.



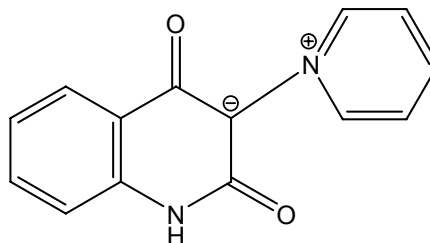
New: 6(*5H*)-Pteridinone, 7,8-dihydro-
9CI: 6(*5H*)-Pteridinone, 1,7-dihydro-



New: Acetic acid, 2-(methylimino)-2-(phenylamino)-
9CI: Acetic acid, (methylamino)(phenylimino)-

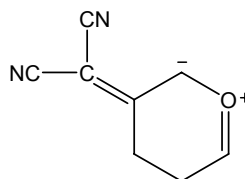
**11. Ylide
Elimination**

Zwitterionic compounds in which the site of the cationic center is known are generally named as inner salts. The term “ylide”, used in 9CI nomenclature, is not used in the new CA index nomenclature.



New: Pyridinium, 1-(1,2,3,4-tetrahydro-2,4-dioxo-3-quinolinyl)-
inner salt

9CI: Pyridinium, 1,4-dihydro-2,4-dioxo-3(2*H*)-quinolinylide

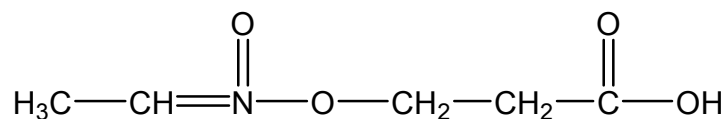


New: Pyrylium, 3-(cyanomethylene)-2,3,4,5-tetrahydro-, inner salt

9CI: Pyrylium, 3-(cyanomethylene)-2,3,4,5-tetrahydro-, ylide

**12. Aci-Nitro
Term**

The term *aci*-nitro will not be retained by overstepping a higher functionality.

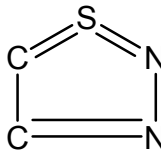


New: Propanoic acid, 3-[(ethylideneoxidoamino)oxy]-

9CI: Ethane, [(2-carboxyethyl)-*aci*-nitro]-

**13. Abnormal
Valent
Heteroatom in
Rings**

The lambda system will be used for naming rings containing an abnormal valent heteroatom.



New: $1\lambda,4\delta$ -1,2,3-Thiadiazole

9CI: 1,2,3-Thia(SIV)diazole

**14. Numerical
Ratios**

Numerical ratios are cited for multicomponent substances. The 9CI system used a combination of numerical ratios and numerical prefixes

New: Glycine, *N*-(aminoiminomethyl)-*N*-methyl-, hydrate (1:1)

9CI: Glycine, *N*-(aminoiminomethyl)-*N*-methyl-, monohydrate

**15.
Multicomponent
Acids**

All multicomponent substances containing an acid are named as "ides" for hydrohalides and "ates" for other acids.

New: Benzenepropanoic acid, hydrochloride (1:1)

9CI: Benzenepropanoic acid, compd. with hydrochloric acid (1:1)

**16. Metal Salt
Terms**

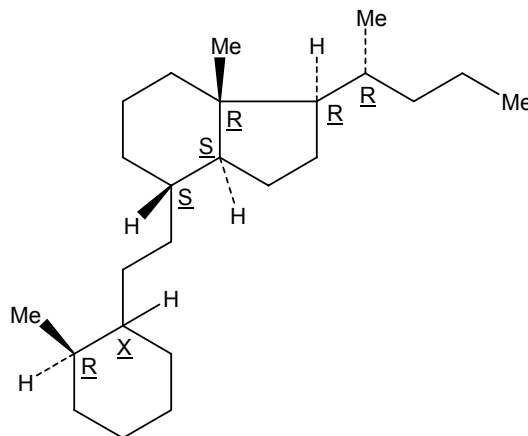
Metal salt terms in uninverted names appear in the expected way.

16CI: polymer with sodium hydroxyacetate (1:1)

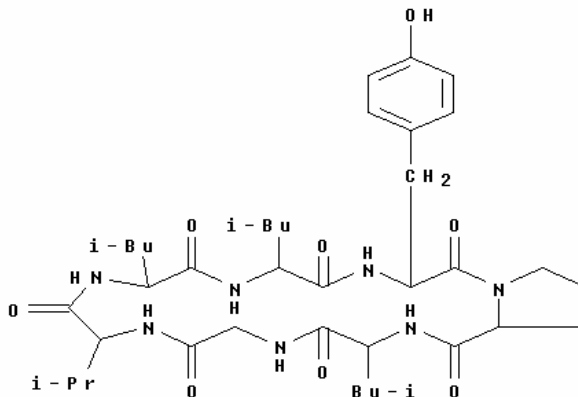
9CI: polymer with hydroxyacetic acid monosodium salt

17.
**Stereoparent
Names**

The number of stereoparent names has been reduced by eliminating nearly 3,000 obscure stereoparents that had to be recognized when naming and searching. Common stereoparents such as insulin, cholane, morphinan, glucose, etc. have been retained.



New: *1H*-Indene, octahydro-7a-methyl-1-[(1*R*)-1-methylbutyl]-4-[2-[(2*R*)-2-methylcyclohexyl]ethyl]-, (1*R*,3a*S*,4*S*,7a*R*)-
9CI : 9,10-Secocholeane



New: Cyclo(glycyl-L-valyl-L-leucyl-L-leucyl-L-tyrosyl-L-prolyl-L-leucyl)
9CI : Pohlianin A

Amino Acid and Peptide Nomenclature

18. Order of Precedence

The order of precedence of standard amino acids now reads as follows:

glutamic acid > aspartic acid > tryptophan > histidine > proline >
tyrosine > phenylalanine > lysine > norleucine > glutamine >
arginine > ornithine > isoleucine > alloisoleucine > leucine >
norvaline > asparagine > threonine > allothreonine > homoserine >
methionine > homocysteine > valine > isovaline > serine >
cystine > cysteine > alanine > β -alanine > glycine

The new rankings attach greater weight to side-chain functional groups. Also, valine outranks the rare isovaline, and cystine is grouped with its reduced form, cysteine, instead of being separated from it by serine.

19. Heterodetic Homomeric Peptides

In most peptides, the amino acid residues are connected solely by amide bonds. However, in a heterodetic homomeric peptide (HHP), at least one of the bonds connecting the residues is an ester bond between the carbonyl group of one amino acid and the oxygen or sulfur of a hydroxy or mercapto amino acid. Prior to the new rules, HHPs were according to the position of the hydroxy or mercapto amino acid in the structure.

The new rule is that regardless of the position of the hydroxy or mercapto amino acid residue in the structure, an amino acid residue attached to the hydroxy or mercapto group will be named as an O or S substituent on that residue.

New: L-Serine, *N,O*-bis[*N*-(1-oxododecyl)-L- α -glutamyl]-
9CI: L-Serine, *N*-(1-oxododecyl)-L- α -glutamyl-, 5-hydrogen *N*-(1-oxododecyl)-L-glutamate (ester)

20.
Unexpressed
Amides of
Peptides

Under the 9CI rule for naming unexpressed amides of peptides, an amino acid amide was the heading parent, and in the process of coming up with that parent one or more residues had to be sacrificed. In some cases, all of them were sacrificed if no acceptable amino acid amide parent were available.

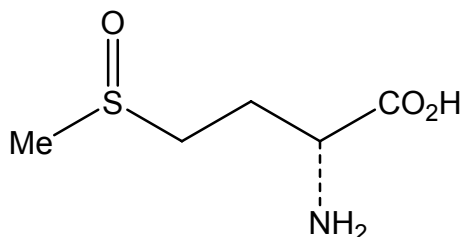
Now all the residue names will be preserved as a peptidyl radical—a substituent on the ring. Users are able to search for many sequences by name that before could be searched only by substructure.

New: Piperidine, 1-(L-methionyl-L-serylglycyl)-

9CI: L-Serinamide, L-methionyl-*N*-[2-oxo-2-(1-piperidinyl)ethyl]-

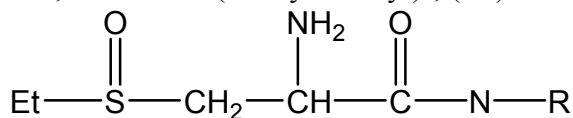
21. S-Oxides

S-Oxides of sulfur-containing amino acids are named at the peptide.



New: D-Methionine, *S*-oxide

9CI: Butanoic acid, 2-amino-4-(methylsulfinyl)-, (*2R*)-



New: *S*-ethyl-*S*-oxidocysteinyl-

9CI: 3-(ethylsulfinyl)alanyl-

22. Peptide Stereoparents

The number of peptide stereoparents has been reduced from about 3,000 to fewer than 100 of the most studied peptides (as judged by the number of derivatives at those index headings). The rest will be assigned sequence names, cyclo names, and occasionally derivative names based on retained stereoparents.

The new peptide stereoparents consist of the following:

Actinomycin D [50-76-0]
Alamethicin I [59588-86-2]
 α -Amanitin [23109-05-9]
Angiotensin I [9041-90-1]
Angiotensin II [11128-99-7]
Angiotensinogen (tetradecapeptide renin substrate) [64315-16-8]
Apamin [24345-16-2]
Apamin (reduced) [28047-76-9]

Bombesin [31362-50-2]
Bradykinin [58-82-2]

Caerulein [17650-98-5]
Calcitonin (human) [21215-62-3]
Calcitonin (human reduced) [27686-18-6]

Calcitonin (salmon) [47931-85-1]
Calcitonin (salmon reduced) [25596-79-6]

α -Calcitonin gene-related peptide (human) [90954-53-3]
 α -Calcitonin gene-related peptide (human reduced) [90877-18-2]
Charybdotoxin [95751-30-7]
Charybdotoxin (reduced) [115422-61-2]
 α^{1-24} -Corticotropin [16960-16-0]
 α^{1-39} -Corticotropin (swine) [9061-27-2]
Corticotropin-releasing factor (human) [86784-80-7]
Corticotropin-releasing factor (sheep) [79804-71-0]
Cyclosporin A [59865-13-3]

Daptomycin [103060-53-3]
Delta sleep-inducing peptide (rabbit) [62568-57-4]
Dermorphin [77614-16-5]
Didemnin A [77327-04-9]
Dynorphin A (swine) [80448-90-4]
Dynorphin B (swine) [83335-41-5]

Echinocandin B [54651-05-7]
Eledoisin [69-25-0]
 α -Endorphin (sheep) [59004-96-5]
 β -Endorphin (sheep) [59887-17-1]
Endothelin 1 (swine) [117399-94-7]
Endothelin 1 (swine reduced) [114640-06-1]

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Fibrinopeptide A (human) [25422-31-5]

Galanin (swine) [88813-36-9]
Gastric inhibitory polypeptide (swine major) [11063-17-5]
Glucagon (swine) [16941-32-5]
Glucagon-like peptide 1 (Rana catesbeiana) [116186-51-7]
Glucagon-like peptide I (human) [87805-34-3]
Gramicidin A [11029-61-1]
Gramicidin S [113-73-5]

Insulin (cattle) [11070-73-8]
Insulin (cattle-A reduced) [17289-65-5]
Insulin (cattle-B reduced) [16941-47-2]
Insulin (human) [11061-68-0]
Insulin (human-A reduced) [24800-07-5]
Insulin (human-B reduced) [27597-36-0]
Insulin (swine) [12584-58-6]

Kallidin [342-10-9]

Luteinizing hormone-releasing factor (swine) [33515-09-2]

Magainin I [108433-99-4]
Mast cell degranulating peptide (*Vespula lewisii*) [72093-21-1]
 α -Melanotropin (swine) [581-05-5]
Melittin (honeybee) [20449-79-0]
Motilin (swine) [9072-41-7]

Neuropeptide Y (human) [90880-35-6]
Neuropeptide Y (swine) [83589-17-7]
Neurotensin (cattle) [55508-42-4]
Nisin A [1414-45-5]

Oxytocin [50-56-6]

Phalloidin [17466-45-4]
Pneumocandin A₀ [120692-19-5]
Pneumocandin B₀ [135575-42-7]
Polymyxin B₁ [4135-11-9]
Polymyxin E₁ [7722-44-3]

Ramoplanin A 1 [81988-87-6]
Ramoplanin A 1 (peptide moiety) [123961-33-1]

Secretin (swine) [17034-35-4]
Somatoliberin (human pancreatic islet) [83930-13-6]
Somatostatin (sheep) [38916-34-6]
Somatostatin (sheep reduced) [40958-31-4]
Somatostatin-28 (sheep) [73032-94-7]
Somatostatin-28 (sheep reduced) [75306-06-8]
Substance P [33507-63-0]

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Thymosin α_1 (cattle) [62304-98-7]
Thymosin β_4 (cattle) [77591-33-4]
Transforming growth factor α (rat) [89899-53-6]
Transforming growth factor α (rat reduced) [89747-89-7]

Valinomycin [2001-95-8]
Vasoactive intestinal octacosapeptide (swine) [40077-57-4]
Vasopressin [11000-17-2]
Virginiamycin S₁ [23152-29-6]

CA Index Name Locant Rules

1.1 Geneva Suffixes

Locants are not cited for Geneva suffixes denoting acid, acid halide or halogenide, amide, nitrile, or aldehyde functional groups that terminate one or both ends of a chain.

Octadecanoic acid
Butanediamide

Under former policy, an exception was sometimes made for a Geneva suffix that terminated one end of a heteroacyclic chain assigned an organic replacement name. Because replacement prefixes were preferred to functional suffixes for lowest locants, the Geneva suffix could end up on the high-numbered end of the chain, necessitating the use of a locant. This exception has been eliminated, because in an organic replacement name for a heteroacyclic chain lowest locants are assigned to functional suffixes, not replacement prefixes. When that functional suffix is a single Geneva suffix, it will always have an implied locant of “1”.

New: 3,7,9-Trioxa-8-siladecanal
9CI: 2,4,8-Trioxa-3-siladecan-10-al

1.2 Conjunctive Suffixes

A locant is not cited for a single conjunctive suffix on benzene or a saturated homogeneous monocyclic ring.

Benzeneethanol
Cyclohexanepropanoic acid

For all other conjunctive suffixes, a locant is cited to denote the position of attachment to the ring.

New: 1,1,2,2,3,3-Cyclopropanehexamethanol
9CI: Cyclopropanehexamethanol

New: 2-Cyclohexene-1-acetaldehyde
9CI: 2-Cyclohexeneacetaldehyde

1.3 Other Functional Suffixes

For functional suffixes that are not Geneva (oic acid, amide, etc.) suffixes and not part of conjunctive suffixes, locants are cited.

New: 1-Disiloxanol
9CI: Disiloxanol

New: 1,2-Ethanediiimine
9CI: Ethanediiimine

New: 1,2-Diazenedicarboxylic acid
9CI: Diazenedicarboxylic acid

New: 1,2,3,4,5-Benzenepentacarbonitrile
9CI: Benzenepentacarbonitrile

New: 2-Oxiranecarboxylic acid
9CI: Oxiranecarboxylic acid

New: Bicyclo[2.2.2]octan-2-one
9CI: Bicyclo[2.2.2]octanone

2. Subtractive Suffixes

A locant is not cited for a subtractive suffix denoting unsaturation if the suffix is for a single site of unsaturation on one of the following:

- A homogeneous molecular skeleton parent with two skeletal atoms (with or without a functional suffix) or a parent radical derived therefrom.

Ethynamine

Diazene

1,2-diphosphenediyl

- A homogeneous monocyclic ring parent with no functional or conjunctive suffix.

Cyclooctene

Cyclotetrasilene

For all other double and triple bonds, locants are cited.

New: 2-Propynoic acid

9CI: Propynoic acid

New: 1-Triazene

9CI: Triazene

New: 1,3-cyclobutadien-1-yl

9CI: cyclobutadien-1-yl

3. Free Valences

A locant is not cited for a free valence if the radical is one of the following:

- An acyclic radical with only one possible site of attachment, or whose site of attachment is implicit in the radical name itself. Among the many examples that could be cited are the following:

acetyl

chloro

methylene

amino

ethoxy

nitro

arsinothioyl

imino

phosphono

benzoyl

methyl

sulfonimidoyl

- A radical derived from a saturated homogeneous molecular skeleton parent with two or more skeletal atoms by the loss of one or more hydrogen atoms from one terminal atom.

hexyl

pentasilanyl

ethylidyne

diphosphinylidene

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- A radical derived from an unsaturated homogeneous molecular skeleton parent with two skeletal atoms by the loss of one or more hydrogen atoms from one terminal atom.
diazenyl
ethenylidene
- A radical derived from a homogeneous chalcogen molecular skeleton parent or parent oxide, with either one or two free valences.
dioxy
disulfonyl
- A radical derived from a saturated homogeneous monocyclic ring parent by the loss of one or more hydrogen atoms from one skeletal atom.
cyclopentyl
cyclotrisilanylidene
- A radical derived from a heterocyclic ring parent not assigned an organic replacement name and with a single heteroatom that is cationic and the site of the free valence.
oxiranio
3H-indolio
- A phenyl radical, either substituted or unsubstituted.

For all other radicals, locants are cited for the free valences.

New: 1-disilazanyl
9CI: disilazanyl

New: 1,2-ethanediylidene
9CI: ethanediylidene

New: 2-propen-1-yl
9CI: 2-propenyl

New: 2-oxiranylidene
9CI: oxiranylidene

New: 2-pyrazinyl
9CI: pyrazinyl

New: cyclotrisiloxan-2-yl
9CI: cyclotrisiloxanyl

**4.1 Substituent
Prefixes:
Multiplying
Radicals**

Locants are cited for every multiplying radical to denote the points of attachment to each occurrence of the parent.

Methane, 1,1'-oxybis-
Acetic acid, 2,2'-thiobis-
Hydrazine, 1,1'-methylenebis-

If the multiplied parent has other substituent prefixes besides the multiplying radical, locants are cited for those as well.

New: Methane, 1,1'-oxybis[1-chloro-
9CI: Methane, 1,1'-oxybis[chloro-

The same rules apply without exception to radicofunctional parents.

New: Hydroperoxide, 1,1'-[oxybis(methylene)]bis-
9CI: Hydroperoxide, [oxybis(methylene)]bis-

New: Nitroxide, N,N'-1,4-phenylenebis[N-ethenyl
9CI: Nitroxide, 1,4-phenylenebis[ethenyl-

New: Disulfide, 1,1'-(1,2-ethanediyl)bis[2-(1-naphthalenyl)-
9CI: Disulfide, 1,2-ethanediylbis[1-naphthalenyl-

4.2 Other Substituent Prefixes

For a substituent prefix other than a multiplying radical, a locant is not cited if the substituent prefix is one of the following:

- One or more substituent prefixes on a single occurrence of a mononuclear molecular skeleton parent or parent oxide, sulfide, selenide, or telluride.
Methane, dichloro-
Phosphine oxide, triphenyl-
Silane, tetramethyl-
- One or more substituent prefixes on a single occurrence of a mononuclear molecular skeleton parent with an attached functional suffix, provided that suffix has no substitutable hydrogens and no alcohol or acid hydrogens.
Methanone, diphenyl-
Silanecarbonitrile, trimethyl-
- One or more substituent prefixes on a single occurrence of a mononuclear nitrogen parent.
Nitroxide, methylene
Amidogen, difluoro-
- One or more substituent prefixes on a mononuclear radical all of whose substitutable hydrogens are on a single atom.
trifluoromethyl
dimethylphosphino
diphenylphosphinothioyl
methylcarbonimidoyl
diphenylamino
cyclohexylimino
- A single substituent prefix on a single occurrence of a saturated or unsaturated homogeneous molecular skeleton parent with two skeletal atoms and no functional suffix.
Hydrazine, bromo-
Ethyne, chloro-
- One or two substituent prefixes on a single occurrence of a homogeneous chalcogen molecular skeleton parent or two substituent prefixes on a single occurrence of the parent oxide.
Hydroperoxide, phenyl
Disulfone, dimethyl

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- A single substituent prefix on a single occurrence of a homogeneous monocyclic ring parent with no functional suffix.

Benzene, methyl-

Triaziridine, nitro-

Cycloheptatrienylium, methyl-

For all other substituent prefixes, locants are cited.

New: Methanol, 1-chloro-

9CI: Methanol, chloro-

New: Disiloxane, 1-ethyl-

9CI: Disiloxane, ethyl-

New: Methanesulfonic acid, 1,1,1-trifluoro-

9CI: Methanesulfonic acid, trifluoro-

New: Benzene, 1,2,3,4,5,6-hexamethyl-

9CI: Benzene, hexamethyl-

New: Pyrazine, 2-butyl-

9CI: Pyrazine, butyl-

New: 2,3,4,5,6-pentafluorophenyl

9CI: pentafluorophenyl

New: 2-iodoacetyl

9CI: iodoacetyl

New: Butanedioic acid, 2-sulfo-

9CI: Butanedioic acid, sulfo-

New: Propanedinitrile, 2-oxo-

9CI: Propanedinitrile, oxo-

New: 2-oxoethylidene

9CI: oxoethylidene

New: Ethynol, 2-bromo-

9CI: Ethynol, bromo-

New: 2-(2-quinolinyl)ethynyl

9CI: 2-quinolinylethynyl

New: Diazene, 1,2-diiodo-

9CI: Diazene, diiodo-

New: Cyclotrisiloxane, 2-methylene-

9CI: Cyclotrisiloxane, methylene-

All substituent prefixes on functional parent compounds—with the exception of formaldehyde—require heteroatom locants.

New: Carbamic acid, N,N-dimethyl-

9CI: Carbamic acid, dimethyl-

New: Diphosphonic dichloride, P,P'-diphenyl-

9CI: Diphosphonic dichloride, diphenyl-

New: Imidodisulfamide, N,N',N'',N'''-pentaethyl-

9CI: Imidodisulfamide, pentaethyl-

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BUT

New: Formaldehyde, nitro-
9CI: Formaldehyde, C-nitro-

All substituent prefixes on hydrazides, hydrazones, and oximes will require locants.

New: 2-(phenylmethylene)hydrazide
9CI: (phenylmethylene)hydrazide

New: 2-phenylhydrazone
9CI: phenylhydrazone

New: O-benzoyloxime
9CI: benzoyloxime

4.3 Prefixes with Greek and Capitalic Locants

When a Greek or capitalic letter locant occurs only once in a structure, it requires no superscript or prime when it is cited in the name.

Benzenemethanamine, N,N-dimethyl- α,α -diphenyl-

But multiple occurrences of the same Greek or capitalic letter locant in a structure must be distinguished because they refer to different positions on the parent. In the new system, Greek and capitalic letter locants with superscript Arabic numerals are now preferred to primed and unprimed locants.

New: 1,2-Benzenediacetic acid, α^1,α^2 -diamino-
9CI: 1,2-Benzenediacetic acid, α,α' -diamino-

New: 1,2-Ethanediamine, N^1,N^2 -dimethyl-
9CI: 1,2-Ethanediamine, N,N' -dimethyl-

New: Butanediamide, N^1 -phenyl-
9CI: Butanediamide, N -phenyl-

But primes must be used if Arabic numerals are not available. For example, if the parent is a functional parent compound.

Imidodicarbonimidic diamide, $N,N,N',N',2$ -pentamethyl-

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And primes alone are used if Arabic numerals are available but are the same for each Greek or capital letter locant.

1,1-Cyclopropanedimethanol, α, α' -dimethyl-
Ethanimidamide, N, N' -diphenyl-

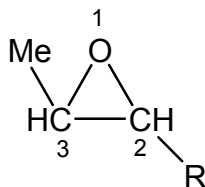
Primes are combined with superscript Arabic numerals if (1) the parent includes a ring assembly or other ring with primed locants, (2) a multiplying radical is attached at positions whose locants include superscript Arabic numerals, or (3) the same primed locant occurs at different positions on the parent.

New: [1,1'-Biphenyl]-4,4'-diacetic acid, α^4, α^4 -dihydroxy-
9CI: [1,1'-Biphenyl]-4,4'-diacetic acid, α, α' -dihydroxy-

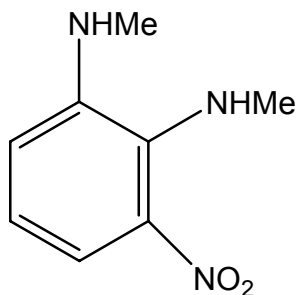
New: 1,4-Benzenediamine, $N^1, N^{1'}$ -1,6-hexanediylbis[N^4 -methyl-
9CI: 1,4-Benzenediamine, N, N'' -1,6-hexanediylbis[N' -methyl-

New: 1,3-Benzenedicarboximidamide, N^1, N^3 -diphenyl-, [$C^1(Z), C^3(Z)$]-
9CI: 1,3-Benzenedicarboximidamide, N', N''' -diphenyl-, [$C(Z), C'(Z)$]-

Examples of the Changes

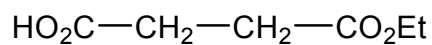


New: 3-methyl-2-oxiranyl-
9CI: 3-methyloxiranyl-



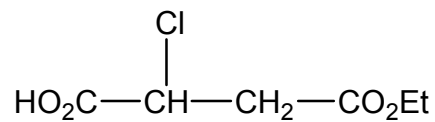
New: 1,2-Benzenediamine, N^1, N^2 -dimethyl-3-nitro-
9CI: 1,2-Benzenediamine, N, N' -dimethyl-3-nitro-

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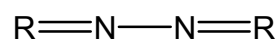
New: Butanedioic acid, 1-ethyl ester

9CI: Butanedioic acid, monoethyl ester



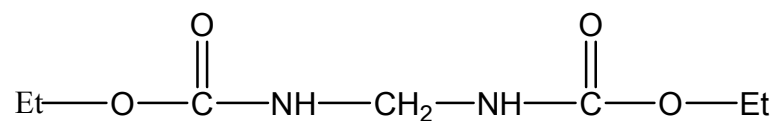
New: Butanedioic acid, 2-chloro-, 3-ethyl ester

9CI: Butanedioic acid, chloro-, 1-ethyl ester



New: 1,2-hydrazinediylidene

9CI: azino-



New: Carbamic acid, *N,N'*-methylenebis-, *O,O'*-diethyl ester

9CI: Carbamic acid, methylenebis-, diethyl ester
