

CHAPTER 7 RADICALS, IONS, AND RELATED SPECIES

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P-70 Introduction

P-70.1 General Methodology

The nomenclature for radicals, ions and related species is described in this Chapter. Its rules are based on the same principles as those of organic compounds defined in the Chapters 1 to 6. The nomenclature was revised in 1993 (ref. 3).

P-70.2 Seniority of radicals and ions

As classes, radicals and ions are senior to acids and other classes in the following order:

- (1) radicals;
- (2) anions;
- (3) cations.

P-70.3 Name formation

Substitutive names and functional class names denote radicals and ions and related compounds. Parent hydrides and parent compounds are selected and modified by use of specific suffixes (called cumulative suffixes) and prefixes; traditional endings are used to describe anions derived from acids and related compounds (see Table 7.1). The nomenclature of di- and trivalent radicals does not indicate nor imply an electronic structure or spin multiplicity.

P-70.3.1 The following suffixes, prefixes and endings are also described in Table 3.2. They are as follows:

The suffixes 'elide' and 'elium' are recommended to denote modification of a parent hydride by the addition or the subtraction of one electron to a parent hydride, respectively.

Radicals formed by	Suffix or Ending	Prefix
loss of H•	yl	ylo
loss of 2 H•		
from one atom	ylidene	
from different atoms	diyl	

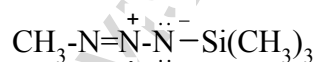
loss of 3 H•	
from one atom	ylidyne
from different atoms	triyyl or ylylidene
addition of H•	hyderyl
Anions formed by	
loss of H ⁺	ide ate, ite (endings)
addition of H ⁻	uide
addition of an electron	elide
Cations formed by	
loss of H ⁻	ylum
addition of H ⁺	ium
loss of an electron	elium

P-70.3.2 Basic multiplying prefixes are used to denote multiplicity of the suffixes ‘yl’, ‘ylidene’, ‘ylidyne’, ‘ide’, ‘uide’, ‘ium’ and of the prefix ‘ylo’. Multiplying prefixes ‘bis’, ‘tris’, etc., are used at the front of the suffix ‘ylum’ and before compound suffixes, such as ‘aminium’, ‘olate’, etc.

P-70.3.3 In names, suffixes and endings are cited in a specific order as described below.

P-70.3.3.1 When two or more cumulative suffixes are present in a name, the order of citation is the reverse of the order of seniority of radicals and ions, i.e., ‘ium’, ‘ylum’, ‘ide’, ‘uide’, ‘yl’, ‘ylidene’, ‘ylidyne’.

Example:

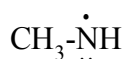


3-methyl-1-(trimethylsilyl)triaz-2-en-2-ium-1-id-2-yl (PIN)_

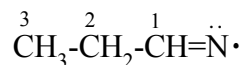
P-70.3.3.2 When functional and cumulative suffixes are present, the order of citation is prescribed by specific rules.

- (a) a cumulative suffix is added to a functional suffix to form a compound suffix (see P-71.3.2):

Examples:



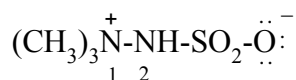
methanaminyll (PIN)
methylazanyl
(traditionally: methylamino)



propan-1-iminyll (PIN)
propylideneazanyl

- (b) in zwitterionic compounds, the cumulative suffixes precede functional suffixes and have seniority for lowest locants:

Example:



1,1,1-trimethylhydrazin-1-ium-2-sulfonate (PIN)

P-70.4 General rules for the selection of preferred names

The concept of preferred IUPAC names as applied to radicals and ions is based on the following principles.

- (1) some names are retained, for example ‘onium cations’, such as ammonium and sulfonium, carbene, $\text{CH}_2\cdot$, and amide, NH_2^- , that are used only in general nomenclature.
- (2) substitutive nomenclature based on carbene and heterane nomenclatures and a set of suffixes and prefixes designed to express the formal operations needed to generate radicals and ions are systematically used to generate preferred IUPAC names.
- (3) when there is a choice, preference is given to names including the largest parent, expressed by means of a functional suffix, for example, methanimide is preferred to methylamide, for $\text{CH}_3\text{-CH}_2\text{-NH}^-$.
- (4) Functional class nomenclature is used to name radicals and ions. These names can be used in general nomenclature, but systematically constructed names are preferred IUPAC names, for example, ‘methylum’ is preferred to ‘methyl cation’, for CH_3^+ .

P-71 Radicals

P-71.1 General methodology

P-71.2 Radicals derived from parent hydrides

P-71.3 Radical centres on characteristic groups

P-71.4 Assemblies of parent radicals

P-71.5 Prefixes denoting radicals

P-71.6 Order of citation and seniority of suffixes ‘yl’, ‘ylidene’, and ‘ylidyne’

P-71.7 Choice of parent structure

P-71.1 General methodology

All radicals are named by modifying a parent hydride name to signal the subtraction or addition of one or more hydrogen atoms, $\text{H}\cdot$. The modification to signal the addition of hydrogen atoms is recommended for the first time. These two operations are expressed by suffixes.

The suffixes 'yl' ($-H\cdot$), 'ylidene' ($-2H\cdot$), 'ylidyne' ($-3H\cdot$) correspond to the subtractive operation, i.e., the removal of hydrogen atoms. The suffix 'hydryl' corresponds to the additive operation, i.e., the addition of hydrogen atoms.

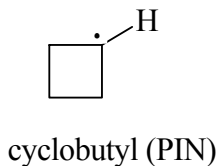
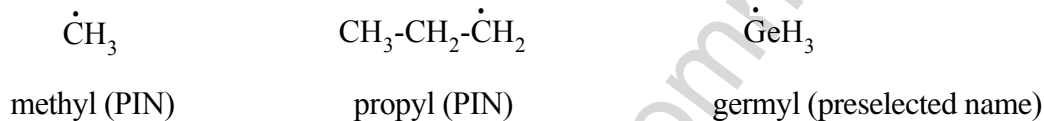
The prefix 'ylo' is used to indicate the removal of $H\cdot$ from a substituent prefix.

P-71.2 Radicals derived from parent hydrides

P-71.2.1 Monovalent radicals.

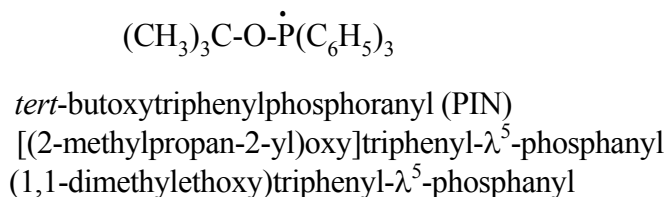
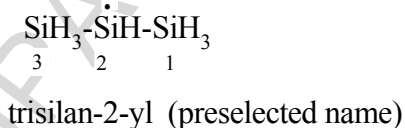
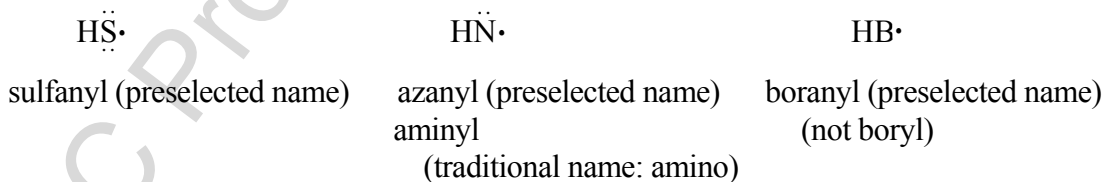
P-71.2.1.1 A radical formally derived by the removal of one hydrogen atom from a mononuclear parent hydride of an element of Group 14, or from a terminal atom of an unbranched acyclic hydrocarbon, or from any position of a monocyclic saturated hydrocarbon ring is named by replacing the 'ane' ending of the systematic name of the parent hydride by 'yl'.

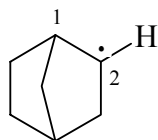
Examples:



P-71.2.1.2 A radical formally derived by the removal of one hydrogen atom from any position of a parent hydride other than those described by P-71.2.1.1, above, is named by adding the suffix 'yl' to the name of the parent hydride, eliding the final letter 'e' of the name of the parent hydride, if any. As exceptions, the names of the radicals $HO\cdot$ and $HOO\cdot$ are 'hydroxyl' and 'hydroperoxyl', respectively. They must not be used when substituted, for example, $CH_3-O\cdot$ is named 'methyloxidanyl', not 'methylhydroxyl'.

Examples:

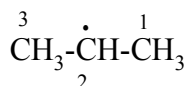




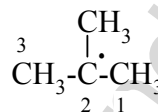
bicyclo[2.2.1]heptan-2-yl (PIN)



spiro[4.5]decan-8-yl (PIN)



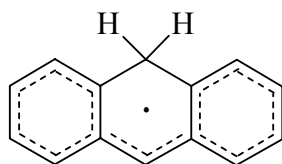
propan-2-yl (PIN)
1-methylethyl
isopropyl



2-methylpropan-2-yl (PIN)
1,1-dimethylethyl
tert-butyl

P-71.2.1.3 The suffix 'hydrl' is used to indicate the addition of H• when the position of the hydrogen atom is to be specified:

Example:



anthracene-9-hydrl (PIN)

P-71.2.2 Divalent and trivalent radicals.

The names of divalent and trivalent radicals are formed substitutively using the suffixes 'ylidene' and 'ylidyne' in two ways:

- (1) replacing the ending 'ane' of a mononuclear parent hydride of an element of Group 14, or from a terminal atom of an unbranched acyclic hydrocarbon, or from any position of a monocyclic saturated hydrocarbon ring by the appropriate suffix (corresponds to P-71.2.1.1)
- (2) adding the appropriate suffix to the name of any position of a parent hydride other than those described by P-71.2.1.1, is named by adding the appropriate suffix 'yl' to the name of the parent hydride, eliding the final letter 'e' of the name of the parent hydride, if any (corresponds to P-71.2.1.2).

These systematic names are preferred to retained names which may be used in general nomenclature.

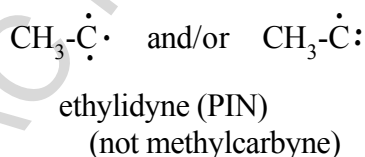
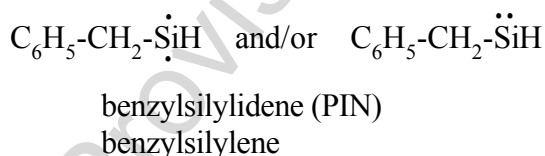
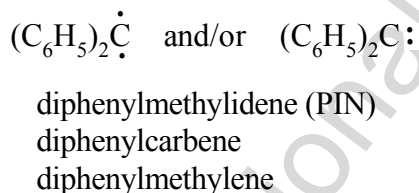
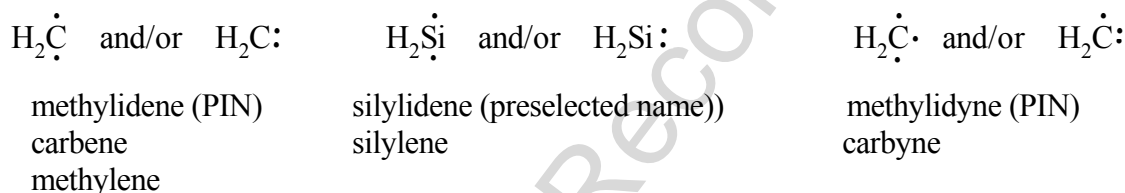
P-71.2.2.1 Specific method and retained names

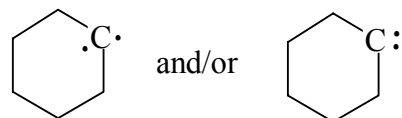
A radical formally derived by the removal of two hydrogen atom from one position of a mononuclear parent hydride of an element of Group 14, or from a terminal atom of an unbranched acyclic hydrocarbon, or from one position of a monocyclic saturated hydrocarbon ring is named by replacing the 'ane' ending of the systematic name of the parent hydride by the suffix 'ylidene'. The suffix 'ylidyne' is used to name radicals formally derived by the removal of three hydrogen atoms from a mononuclear parent hydride of an element of Group 14 or from a terminal atom of an unbranched acyclic hydrocarbon.

Systematic names are the preferred IUPAC names; the retained names carbene or methylene, nitrene or aminylene, silylene, and carbyne, can be used in general nomenclature, with full substitution.

The use of the systematic or retained names does not imply a specific electronic configuration. If needed, such a distinction could be made by using a separate word such as singlet or triplet, or a descriptive phrase.

Examples:



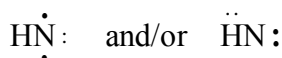


cyclohexylidene (PIN)

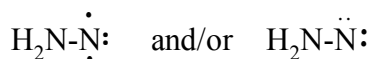
P-71.2.2.2 General method

With the exception of the radicals named in P-71.2.2.1, the names of the divalent and trivalent radicals derived by the removal of two hydrogen atoms from one position of a parent hydride are formed by adding the suffixes 'ylidene' or 'ylydine' to the name of the parent hydride, with elision of the final letter 'e', if present. The name azanylidene is the preferred IUPAC name; nitrene or aminylene are retained names for use in general nomenclature.

Examples:



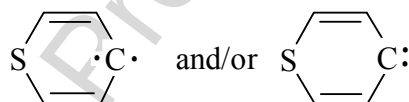
azanylidene (preselected name)
aminylene
nitrene



hydrazinylidene (preselected name)
diazanylidene
(traditional name: hydrazono)
(not aminonitrene)



diphosphanylidene (preselected name)



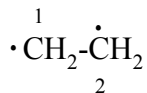
thiopyran-4-ylidene (PIN)

P-71.2.3 Multiple radical centers (Polyradicals)

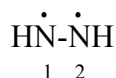
Polyradicals containing two or more radical centers, formally derived by the removal of two or more hydrogen atoms from each of two or more different skeletal atoms of a parent hydride, are named by adding to the name of the parent hydride combinations of the suffix 'yl' for a monovalent radical center, 'ylidene' for a divalent radical center, and 'ylydine' for a trivalent radical center,

together with the appropriate numerical prefixes indicating the number of each kind of radical center. The final letter 'e' of the name of the parent hydride, if present, is elided when followed by 'y'.

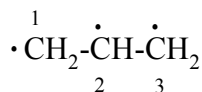
Examples:



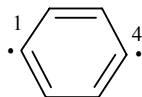
ethane-1,2-diyl (PIN)
(traditional name: ethylene)



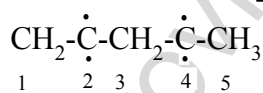
hydrazine-1,2-diyl (preselected name)
diazane-1,2-diyl



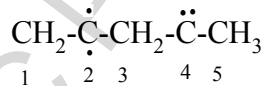
propane-1,2,3-triyl (PIN)



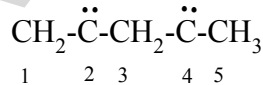
benzene-1,4-diyl (PIN)
(traditional name: *p*-phenylene or 1,4-phenylene)



and/or



and/or



→ pentane-2,4-diylidene (PIN)

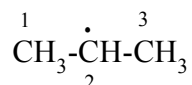
P-71.2.4 Acyclic radicals derived by the removal of one or more hydrogen atoms from nonterminal chain positions are named

(a) by citing the locant of the nonterminal position of the chain, or

(b) by substituting a parent radical that has the free valence(s) at the end of a chain.

Method (a) generates preferred IUPAC names. The principal chain is chosen, if necessary, by the method indicated in Section P-44 for substituent groups.

Examples:

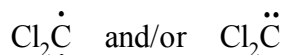


propan-2-yl (PIN)
1-methylethyl

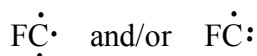
P-71.2.5 The λ -convention

Divalent and trivalent radical centers in a parent hydride formally derived by the removal of two or three hydrogen atoms from the same skeletal atom in its standard valence state may be described by the λ -convention. Locants for the radical centers are followed by the symbol λ^n , where 'n' is the bonding number of the skeletal atom (see P-14.1). This method is only for general nomenclature.

Examples:



dichloro- λ^2 -methane
methylidene (PIN)



fluoro- λ^1 -methane
fluoromethyldyne (PIN)

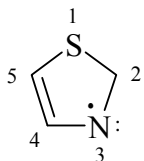


phenyl- λ^1 -azane
phenylazanylidine (PIN)

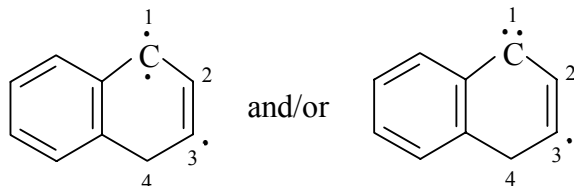
P-71.2.6 Hydro prefixes vs. added hydrogen

A radical center at a position in a mancude parent hydride where there is an insufficient number of hydrogen atoms to apply directly the recommendations for the use of 'yl' or 'ylidene' given in P-71.2.1 and P-71.2.2 is derived formally from a dihydro derivative of the cyclic parent hydride. Such a radical can also be described by applying the principle of 'added hydrogen' (see P-14.6). In this method the 'hydro' derivative is described by specifying the hydrogen atom of a dihydro pair that remains after the radical center is created by citing in italic capital *H* and the locant of the skeletal atom to which the hydrogen atom resides, both enclosed in a set of parentheses and inserted into the name of the corresponding parent hydride immediately after the locant for the radical center. Names formed by the 'added hydrogen' method are preferred.

Examples:



1,3-thiazol-3(2*H*)-yl (PIN)
2,3-dihydro-1,3-thiazol-3-yl



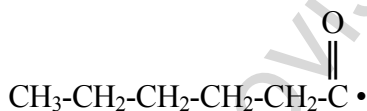
naphthalen-3-yl-1(4*H*)-ylidene (PIN)
1,4-dihydronaphthalen-3-yl-1-ylidene

P-71.3 Radical centers on characteristic groups

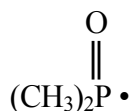
P-71.3.1 Acyl radicals

Acyl radicals, i.e., radicals with at least one chalcogen or nitrogen atom attached to a radical center by a (formal) double bond, which may be considered to be formally derived by the removal of a hydroxy group from acid characteristic groups, are named by replacing the 'ic acid' or 'carboxylic acid' ending of the name of the acid with 'oyl' or 'yl', or 'carbonyl', according to the method for forming names of acyl groups (see P-65.1.8). Substituent groups denoted by prefixes such as 'oxo', 'thioxo', 'sulfanylidene', are not recommended for naming acyl radicals.

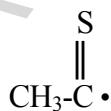
Examples:



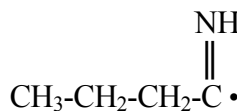
hexanoyl (PIN)
(not 1-oxohexyl)



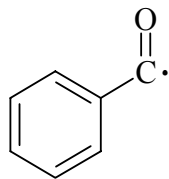
dimethylphosphinoyl (PIN)
P-methylmethanephosphinoyl
dimethyloxo- λ^5 -phosphanyl



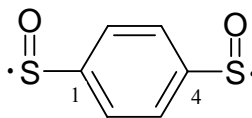
thioacetyl (PIN)
(not sulfanylideneethyl)



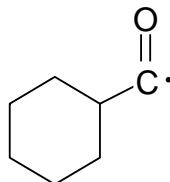
butanimidoyl (PIN)
(not 1-iminobutyl)



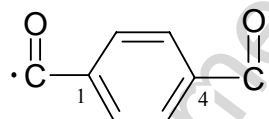
benzoyl (PIN)
phenyl(oxo)methyl



benzene-1,4-disulfinyl (PIN)
1,4-phenylenebis(oxo-λ⁴-sulfanyl)



cyclohexanecarbonyl (PIN)
cyclohexyl(oxo)methyl

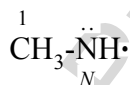


1,4-phenylenebis(carbonyl) (PIN)
terephthaloyl
[not 1,4-phenylenebis(oxomethyl)]

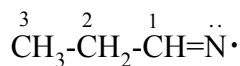
P-71.3.2 A radical derived formally by the removal of one hydrogen atom from an **amine**, **imine**, or **amide** characteristic group is named by adding the corresponding compound suffix formed by adding the suffix 'yl' to the basic suffix:

$-\text{NH}_2$	amine (preselected name)	$-\ddot{\text{N}}\text{H}$	aminyl (preselected name)
$=\text{NH}$	imine (preselected name)	$=\ddot{\text{N}}\cdot$	iminyl(preselected name)
$-(\text{C})\text{O}-\text{NH}_2$	amide (PIN)	$-(\text{C})\text{O}-\ddot{\text{N}}\text{H}$	amidyl (PIN)
$-\text{CO}-\text{NH}_2$	carboxamide (PIN)	$-\text{CO}-\ddot{\text{N}}\text{H}$	carboxamidyl (PIN)

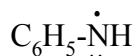
Examples:



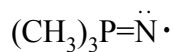
methanaminyl (PIN)
methylazanyl
(traditionally: methylamino)



propan-1- iminyl (PIN)
propylideneazanyl



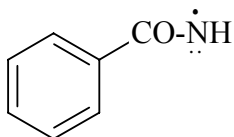
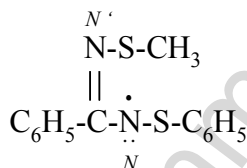
anilinyll (PIN)
benzenaminyl
(not anilino)
(traditionally: phenylamino)
(removal of a hydrogen atom from
the benzene ring generates a radical
named, for example, 4-aminophenyl)



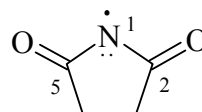
trimethyl- λ^5 -phosphaniminyl (PIN)
(trimethylphosphoranylidene)azanyl
trimethylphosphane imidyl



formamidyl (PIN) N' -(methylsulfanyl)- N -(phenylsulfanyl)benzenecarboximidamidyl (PIN)



pyridine-2-carboxamidyl (PIN)



2,5-dioxopyrrolidin-1-yl (PIN)
succinimidyl

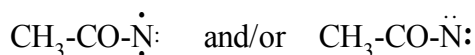
P-71.3.3 Divalent radical centers

A radical derived formally by the removal of two hydrogen atoms from an amine or amide characteristic group is named by substituting the parent radical 'azanylidene' by the appropriate substituent groups. Azanylidene is the preferred IUPAC name; the names nitrene and aminylene are retained for use in general nomenclature.

Examples:



phenylazanylidene (PIN)
phenylnitrene
phenylaminylene



acetylazanylidene (PIN)
acetylnitrene
acetylaminylene

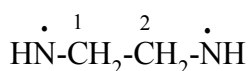
P-71.3.4 Polyamide, polyamine and polyimine radicals

Polyradicals with radical centres identically derived but located on two or more amine, imine, or amide characteristic groups are named in two ways.

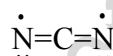
- by using the compound suffixes (see P-71.3.2) denoting the presence of one electron on each characteristic group and the multiplying prefixes 'bis-', 'tris-', etc. or
- by multiplicative nomenclature based on the parent radical 'azanyl'.

In order to avoid any confusion, the name 'aminyl' is reserved for denoting the suffix in substitutive nomenclature; the parent radical 'azanyl' (not 'aminyl') is used in multiplicative nomenclature. Method (a) leads to preferred IUPAC names.

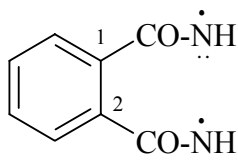
Examples:



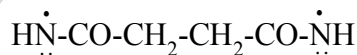
ethane-1,2-bis(aminyl) (PIN)
(ethane-1,2-diyl)bis(azanyl)



methanebis(iminyl) (PIN)
methanediyldienebis(azanyl)



benzene-1,2-bis(carboxamidyl) (PIN)



butanediamidyl (PIN)
butanedioylbis(amidyl)



and/or



and/or



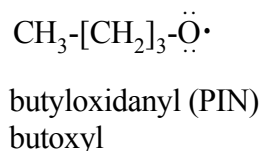
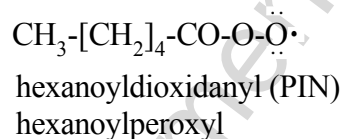
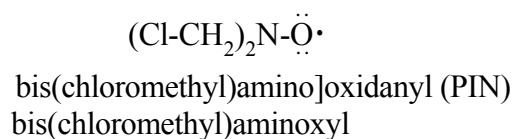
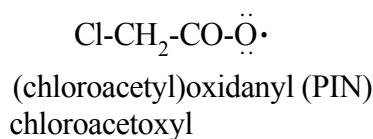
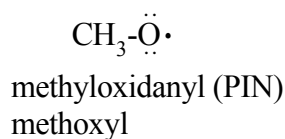
hexanedioylbis(azanvlidene) (PIN)
hexanedioylbis(nitrene)
hexanedioylbis(aminylene)

P-71.3.5 A radical derived formally by the removal of the hydrogen atom of a hydroxy group (or chalcogen analog) of an acid or hydroxy characteristic group is named in two ways.

- by substituting the parent radicals HO•, 'oxidanyl (preselected name)', or HOO•, 'dioxidanyl' (preselected name), by the appropriate substituent groups;
- by using the term 'oxyl' or 'peroxyl' instead of the preselected systematic names 'oxidanyl' and 'dioxidanyl'.

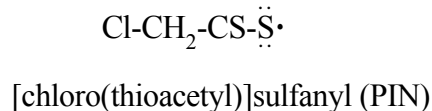
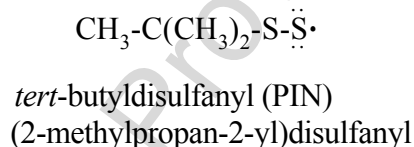
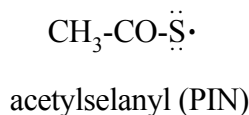
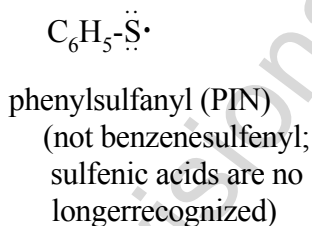
The names methoxyl, ethoxyl, propoxyl, butoxyl and aminoxyl are retained and may be used in general nomenclature; systematic names are preferred. Method (a) generates preferred IUPAC names.

Examples:



Chalcogen analogs are named on the basis of preselected parent radical names, such as ‘sulfanyl’, ‘selanyl’, ‘disulfanyl’, etc.

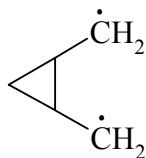
Examples:



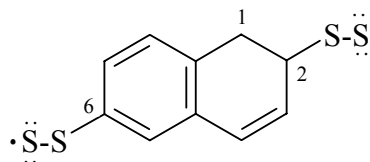
P-71.4 Assemblies of parent radicals

Polyradicals with radical centers identically derived from the same parent hydride or the same characteristic group (except for polyacyl or polyimide radicals) but located in different parts of the structure are named, if possible, according to the principles for nomenclature of assemblies of identical units.

Examples:



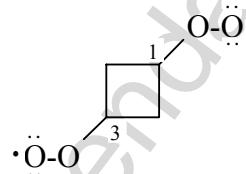
cyclopropane-1,2-diyl dimethyl (PIN)



naphthalene-2,6-diyl bis(disulfanyl) (PIN)



2,4-dimethylpentane-2,4-diyl bis(oxidanyl) (PIN)
1,1,3,3-tetramethylpropane-1-3-diyl bis(oxidanyl)



cyclobutane-1,3-diyl bis(dioxidanyl) (PIN)

P-71.5 Prefixes denoting radicals

The presence of a radical center in a substituent that is to be cited as a prefix is expressed by the prefix 'ylo', indicating the removal of a hydrogen atom. This prefix is a nondetachable prefix, attached to the parent substituent prefix, which is formed by usual methods. The removal of two or more hydrogen atoms from a substituent cited as prefix is indicated by the appropriate multiplying prefix 'di', 'tri', etc. The prefix 'ylo' is also combined with prefixes used additively, such as oxy and carbonyl.

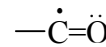
Examples:



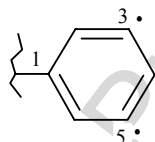
ylomethyl (PIN)



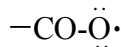
ylooxy (preselected name)
(not ylohydroxy)



ylocarbonyl (PIN)



3,5-diylphenyl (PIN)



(ylooxy)carbonyl (PIN)
(not ylocarboxy)

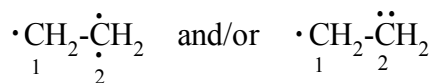


yloamino (preselected name)

P-71.6 Order of citation and seniority of suffixes 'yl', 'ylidene', and 'ylidyne'

The suffixes 'yl', 'ylidene', and 'ylidyne' are cited in that order in a name, if applicable; lowest locants are assigned to radicals as a set, then in the order 'yl', 'ylidene' and 'ylidyne'. The order of citation is identical to that used for naming substituent groups (see P-28.2).

Example:



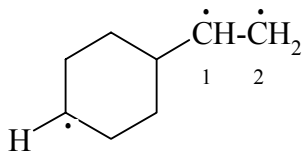
ethan-1-yl-2-ylidene (PIN)

P-71.7 Choice of parent structure

When a choice of a parent radical is necessary, the following criteria are applied, in the order given, until a decision is reached.

- (a) Maximum number of radical centers of any kind in a single parent structure:

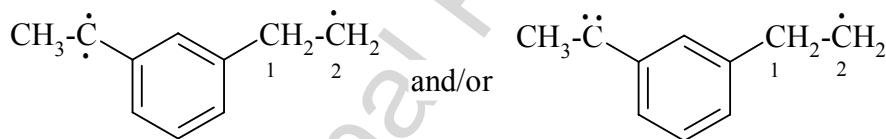
Example:



1-(4-ylcyclohexyl)ethane-1,2-diyl (PIN)

- (b) Maximum number of -yl, then -ylidene radical centers;

Example:



2-[3-(1,1-diyl)phenyl]ethyl (PIN)

- (c) Maximum number of radical centers at the skeletal atom first cited in the seniority order classes: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > C > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl;

Example:



(2-methyl-1-ylpropan-2-yl)oxidanyl (PIN)

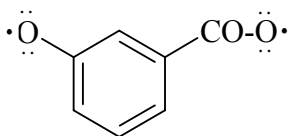
(1,1-dimethyl-2-yl)oxidanyl

- (d) Further choice, if necessary, is made by applying the general criteria for chains and rings given in Chapters 1 to 6 for neutral compounds.

Examples:

- (1) maximum number of radical centers according to the order of suffixes.

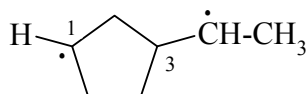
Example:



[3-(ylloxy)benzoyl]oxidanyl (PIN)

(2) rings are senior to chains

Example:



3-(1-ylloethyl)cyclopentyl (PIN)

P-72 Anions

P-72.1 General methodology

P-72.2 Anions formed by subtraction of hydrons

P-72.3 Anions formed by addition of a hydride

P-72.4 Replacement nomenclature

P-72.5 Multiple anionic centers

P-72.6 Anionic centers in both parent compounds and substituent groups

P-72.7 Choice of an anionic parent structure

P-72.1 General methodology

Anions are named in two ways.

- (1) by using suffixes and endings, and
- (2) by functional class nomenclature.

Method (1) leads to preferred IUPAC names. Some names and some contracted names are retained as preferred IUPAC names and for use in general nomenclature.

The following suffixes are used:

‘ide’ (corresponding to removal of a hydron, H^+),

‘uide’ (corresponding to the addition of a hydride, H^-),

‘elide’ (corresponding to the addition of an electron)

The endings ‘ate’ and ‘ite’ are used to indicate removal of a proton from a $-OH$ group of acids and hydroxy compounds.

Functional class nomenclature is based on the class name ‘anion’ in association with the name of the corresponding radical (not necessarily the name of the corresponding substituent group).

P-72.2 Anions formed by removal of hydrons

P-72.2.1 Functional class nomenclature

P-72.2.2 Systematic nomenclature

P-72.2.1 Functional class nomenclature

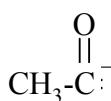
Functional class nomenclature can be used, in general nomenclature, to describe anionic compounds. An anion that can be considered as derived formally by adding an electron to a radical may also be named by adding the class name 'anion' as a separate word to the name of the substituent group. The names are formed by using the names of corresponding radicals (not necessarily the name of substituent groups) and the class name 'anion' as a separate word. The multiplying prefixes 'di', 'tri', etc., are added to the class name to denote multiple anions.

This type of nomenclature is limited to anions having the anionic centers in a same structure. Systematic names (see P-72.2.2) are preferred IUPAC names.

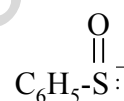
Examples:



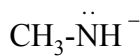
methyl anion
methanide (PIN)



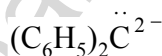
acetyl anion
1-oxoethanide (PIN)



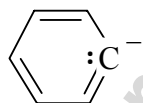
benzenesulfinyl anion
oxophenyl- λ^4 -sulfanide (PIN)



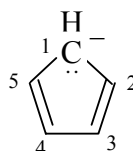
methanaminyl anion
methanaminide (PIN)



diphenylmethylened dianion
diphenylmethanide (PIN)



phenyl anion
benzenide (PIN)



cyclopenta-2,4-dien-1-yl anion
cyclopenta-2,4-dien-1-ide (PIN)

P-72.2.2 Systematic nomenclature

P-72.2.2.1 Anions derived from parent hydrides

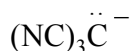
An anion derived formally by the removal of one or more hydrons from any position of a neutral parent hydride is preferably named by using the suffix ‘-ide’, with elision of the final letter ‘e’ of the parent hydride, if any. Numerical prefixes ‘di’, ‘tri’, etc. are used to denote multiplicity; locants identify positions of the negative charges.

The retained names ‘amide’ and ‘imide’ for the anions H_2N^- and HN^{2-} , respectively, can be used in general nomenclature. The systematic names ‘azanide’ and ‘azanedide’, respectively, are preselected names.

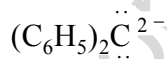
The retained names hydroxide, for HO^- , and hydroperoxide, for HOO^- , are preselected names but cannot be substituted; thus, the preferred IUPAC names for $\text{CH}_3\text{-O}^-$ and $\text{CH}_3\text{-OO}^-$ are methyloxidanyl and methyldioxidanyl, respectively.

The name ‘acetylde’, for $\text{C}\equiv\text{C}^-$, is retained for general use only.

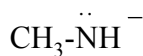
Examples:



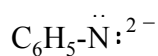
tricyanomethanide (PIN)



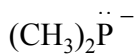
diphenylmethanediide (PIN)



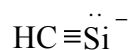
methylazanide
methylamide
methanamide (PIN, see P-72.2.3)



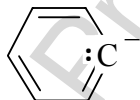
phenylazanedide
phenylimide
benzenaminediide (PIN, see P-72.2.3)



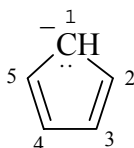
dimethylphosphanide (PIN)
dimethylphosphinide



methylidynesilanide (PIN)



benzenide (PIN)



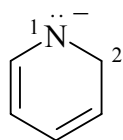
cyclopenta-2,4-dien-1-ide (PIN)

P-72.2.2.1.1 Hydro prefixes vs. added hydrogen

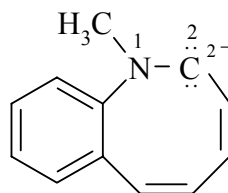
An anionic center at a position in a monocyclic parent hydride where there is an insufficient number of hydrogen atoms to apply directly recommendations for the use of ‘ide’ given in P-72.2.1 is derived formally from a dihydro derivative of the cyclic parent hydride. Such a radical can also be described by applying the principle of ‘added hydrogen’ (see P-14.6). In this method the ‘hydro’ derivative is described by specifying the hydrogen atom of a dihydro pair that remains after the

anionic center is created by citing in italic capital *H* and the locant of the skeletal atom to which the hydrogen atom resides, both enclosed in a set of parentheses and inserted into the name of the corresponding parent hydride immediately after the locant for the radical center. Names formed by the ‘added hydrogen’ method are preferred IUPAC names.

Examples:



pyridin-1(2*H*)-ide (PIN)
1,2-dihydropyridine-1-ide



1-methyl-1-benzazocine-2,2(1*H*)-diide (PIN)
1-methyl-1,2-dihydro-1-benzoazocine-2,2-diide

P-72.2.2.2 Anions derived from characteristic groups

Anions derived from characteristic groups are named in two ways;

- (1) directly for acids, alcohols and amines, by modifying the suffix normally used in substitutive nomenclature:
 - (a) the endings ‘ate’ or ‘ite’ to name anions derived from acids;
 - (b) the ending ‘ate’ to name anions derived from alcohols,
 - (c) the suffix ‘aminide’ (formed by combining the two suffixes ‘amin(e) + ide’) to name anions derived from amines where the negative charge is on the nitrogen atom;
- (2) by using the appropriate preselected anionic parent names in the case of other characteristic groups, such as ‘azanide’ for NH_2^- , ‘azaniide’ for NH^{2-} , ‘oxidanide’ for HO^- . Amides, hydrazides and imides are not named directly by the method (1), as are amines and imines; the reason being that there could be real ambiguity to have the suffix ‘ide’ used at the end of names such as amide, hydrazides, etc; furthermore, the name ‘amide’ may be used in general nomenclature to designate the parent NH_2^- . The use of parents azanide and azaniide eliminates all possible ambiguity.

P-72.2.2.2.1 Anions derived from acids

P-72.2.2.2.2 Anions derived from hydroxyl compounds

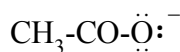
P-72.2.2.2.3 Anions derived from amines and imines

P-72.2.2.2.4 Anions derived from other characteristic groups

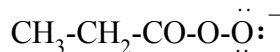
P-72.2.2.2.1 Anions derived from acids

P-72.2.2.2.1.1 An anion formed by the removal of a hydron from the chalcogen atom of an acid characteristic group or functional parent compound is named by replacing the ‘ic acid’ or ‘ous acid’ ending of the acid name by ‘ate’ or ‘ite’, respectively. Names of acids are described in Section P-65.1.

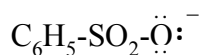
Examples:



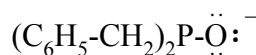
acetate (PIN)



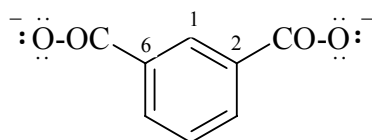
propaneperoxoate (PIN)



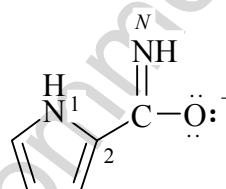
benzenesulfonate (PIN)



dibenzylphosphinite (PIN)



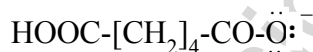
pyridine-2,6-dicarboxylate (PIN)



1*H*-pyrrole-2-carboximidate (PIN)

P-72.2.2.2.1.2 The method of ‘hydrogen salts’ is used to name partially ionized acids and their esters. The name of the anion is preceded, in order, by the name of the cation, the hydrocarbyl group, and finally the word hydrogen. If necessary, lowest locants are assigned in the same order. The resulting names are preferred IUPAC names; they are preferred to those formed substitutively (see P-65.5.1).

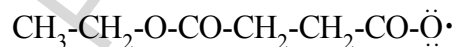
Examples:



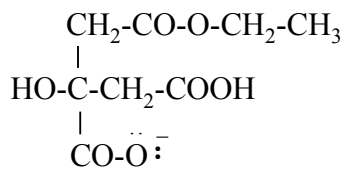
hydrogen hexanedioate (PIN)
5-carboxypentanoate



hydrogen phenylphosphonate (PIN)
hydrogen benzenephosphonate
(not hydroxy(phenyl)phosphinate;
phosphonic acid is senior to
phosphinic acid)



ethyl hydrogen butanedioate (PIN)
ethyl hydrogen succinate



4-ethyl 2-(carboxymethyl)-2-hydroxybutanedioate (PIN)

3-ethyl 1-hydrogen citrate

4-hydrogen 2-(2-methoxy-2-oxoethyl)-2-hydroxybutanedioate

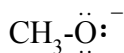
(alphanumerical order makes the first name senior to the third name
and also preferred to the second name)

P-72.2.2.2.2 Anions derived from hydroxy compounds

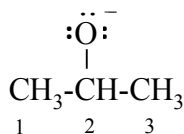
An anion formed by subtracting a hydron from the chalcogen atom of a hydroxy characteristic group, or a chalcogen analog, that can be expressed by a suffix such as 'ol', 'thiol', '-peroxol', etc., is preferably named by using complex suffixes 'olate', 'thiolate', 'peroxolate', etc., formed by addition of the ending 'ate' to the suffixes 'ol', 'thiol', 'peroxol', etc. The multiplying prefixes 'bis', 'tris', etc. are used before compound suffixes, to avoid any ambiguity.

The traditional names methoxide, ethoxide, propoxide, butoxide, isopropoxide, *tert*-butoxide, phenoxide, and aminoxide, for $\text{CH}_3\text{-O}^-$, $\text{C}_2\text{H}_5\text{-O}^-$, $\text{C}_3\text{H}_7\text{-O}^-$, $\text{C}_4\text{H}_9\text{-O}^-$, $(\text{CH}_3)\text{CH-O}^-$, $(\text{CH}_3)_3\text{C-O}^-$, $\text{C}_6\text{H}_5\text{-O}^-$, and $\text{H}_2\text{N-O}^-$ are retained for use in general nomenclature.

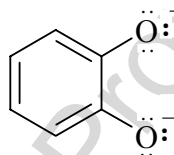
Examples:



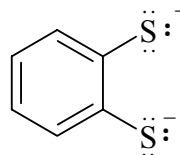
methanolate (PIN)
methoxide



propan-2-olate (PIN)
isopropoxide



benzene-1,2-bis(olate) (PIN)
(not pyrocatecholate)

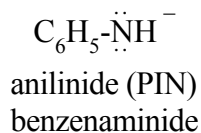
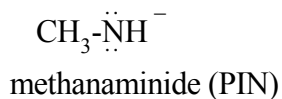


benzene-1,2-bis(thiolate) (PIN)

P-72.2.2.2.3 Anions derived from amines and imines

Amines and imines having one negative charge on the nitrogen atom are named by using the compound suffixes 'aminide' and 'iminide', formed by the addition of the suffix 'ide' to the suffix 'amine' or 'imine', respectively. The resulting names are preferred IUPAC names; for names acceptable in general nomenclature, see P-77.2.2.1. The name 'anilide' is recommended as a retained IUPAC preferred name.

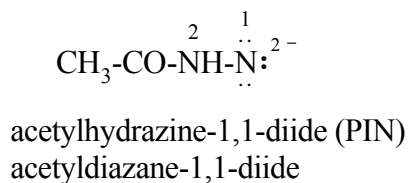
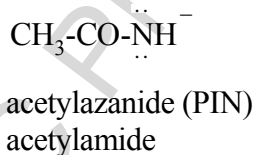
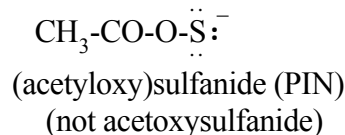
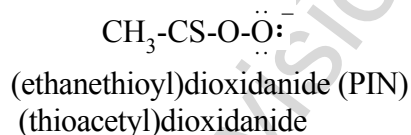
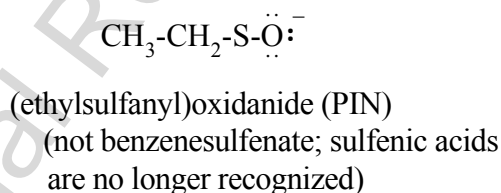
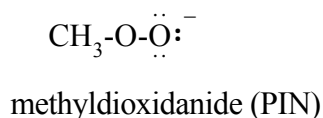
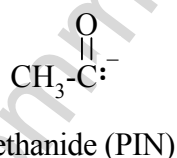
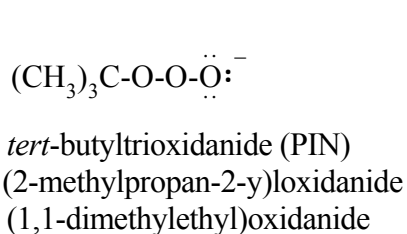
Examples:

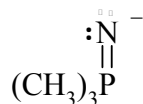


P-72.2.2.2.4 Anionic centers on other characteristic groups

Anionic centers generated formally by the removal of hydrons from atoms of characteristic groups other than those considered in P-72.2.2.1, are named on the basis of the corresponding anionic parent hydrides.

Examples:





(trimethyl- λ^5 -phosphanylidene)azanide (PIN)

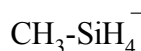
P-72.3 Anions formed by addition of a hydride

Two methods are used to name anions formally formed by adding a hydride ion, H^- .

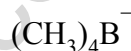
- (1) an anion formally derived by adding a hydride ion, H^- , to a parent hydride is named by the suffix 'uide', preceded by the multiplying prefixes 'di', 'tri' etc. to indicate multiplicity;
- (2) by using the suffix 'ide' with a parent hydride in which the bonding number is expressed by the λ -convention, thus subtracting a hydron, H^+ , as described in Section P-72.2.

Method (1) leads to preferred IUPAC names.

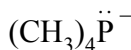
Examples:



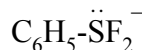
methylsilanuide (PIN)



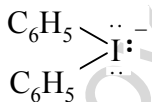
tetramethylboranuide (PIN)



tetramethylphosphanuide (PIN)
tetramethyl- λ^5 -phosphanide
tetramethylphosphoranide



difluoro(phenyl)sulfanuide (PIN)
difluoro(phenyl)- λ^4 -sulfanide



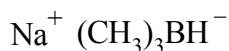
diphenyliodanuide (PIN)
diphenyl- λ^3 -iodanide



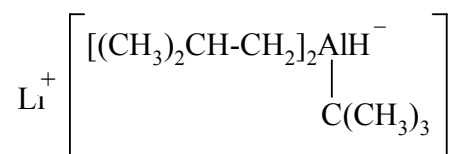
hexafluoro- λ^5 -iodanuide (preselected name)
hexafluoro- λ^7 -iodanide



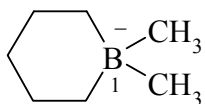
octafluoro- λ^6 -tellanediuide (preselected name)
octafluoro- λ^{10} -tellanediide



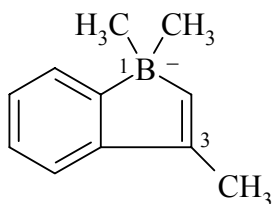
sodium trimethylboranuide (PIN)



lithium *tert*-butylbis(3-methylbutyl)alumanuide (PIN)



1,1-dimethylborinan-1-uide (PIN)



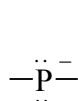
1-methoxy-1,3-dimethyl-1-benzoborol-1-uide

P-72.4 Skeletal replacement nomenclature

Anionic centers in parent hydrides are named by two methods using the principles of skeletal replacement ('a') nomenclature described in Section P-15.4.

- (1) by forming the name of the neutral compound according to skeletal replacement ('a') nomenclature and using the suffixes 'ide' and 'uide' to describe the anionic centers';
- (2) by adding the anionic skeletal replacement ('a') prefixes formed by adding the suffixes 'ida' and 'uida' to the name of the corresponding mononuclear parent hydride, with elision of the final letter 'e'; these replacement prefixes indicate an anionic center having a bonding number one lower or one higher, respectively, than the bonding number of the corresponding neutral mononuclear parent hydride.

Examples:



phosphanida (PIN)
(preselected name)



boranuida (PIN)
(preselected name)

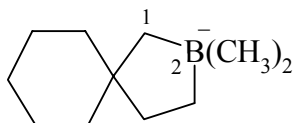


sulfanuida (preselected name)
 λ^4 -sulfanida

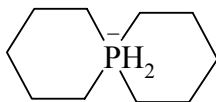
Method (1) results in preferred IUPAC names. Furthermore, names that do not require designation of skeletal heteroatoms in nonstandard valence states using the λ -convention are preferred (see P-72.5).

Skeletal replacement ('a') prefixes ending in 'ata', for example 'borata', are no longer recognized.

Examples:



2,2-dimethyl-2-borasp[iro][4.5]decane-2-uide (PIN)
2,2-dimethyl-2-boranuidasp[iro][4.5]decane
(not 2,2-dimethyl-2-boratasp[iro][4.5]decane)



6 λ^5 -phosphasp[iro][5.5]undecane-6-uide (PIN)
6 λ^5 -phosphanuidasp[iro][5.5]nonane
(not 6-phosphatasp[iro][5.5]nonane)



1-phosphabicyclo[2.2.2]octan-1-uide (PIN)
1-phosphanuidabicyclo[2.2.2]octane
1 λ^5 -phosphabicyclo[2.2.2]octan-1-ide
1 λ^5 -phosphanidabicyclo[2.2.2]octane

P-72.5 Multiple anionic centers

Multiple anionic centers are named by several methods in accordance with the previous rules.

P-72.5.1 Assemblies of parent anions

P-72.5.2 'Ide' and 'uide' centers in the same parent hydride

P-72.5.3 Anionic characteristic groups on anionic parent hydrides

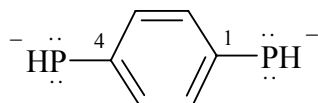
P-72.5.4 Anionic centers in both parent compounds and substituent groups

P-72.5.1 Assemblies of parent anions

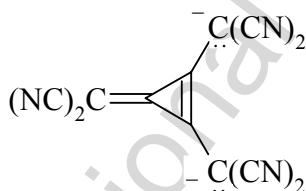
P-72.5.1.1 Assemblies derived from parent anions

Anionic compounds with anionic centers derived from the same parent hydride, but located in different parts of a structure, are named, if possible, according to the principles of multiplicative nomenclature (see P-15.3), using the multiplying prefixes 'bis', 'tris', etc. where necessary.

Examples:



1,4-phenylenebis(phosphanide) (PIN)

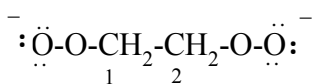


[3-(dicyanomethylidene)cycloprop-1-ene-1,2-diy]bis(dicyanomethanide) (PIN)

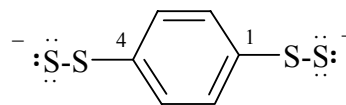
P-72.5.1.2 Polyanions derived from characteristic groups

Anions derived from diacids and polyacids, from diols and polyols, including phenols, and their chalcogen analogues, and also from diamines and polyamines are named substitutively as indicated in P-72.2.2.1. Other characteristic groups are named in accordance with the principles of multiplicative nomenclature, using the multiplying prefixes 'bis', 'tris', etc.

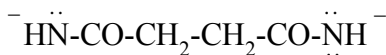
Examples:



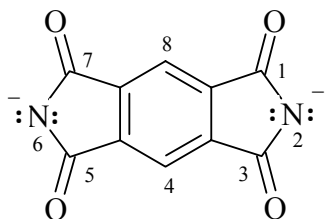
ethane-1,2-diylbis(dioxidanide) (PIN)



1,4-phenylenebis(disulfanide) (PIN)



butanedioylbis(azanide) (PIN)
butanedioylbis(amide)

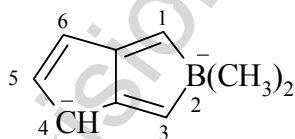


1,3,5,7-tetraoxo-5,7-dihydropyrrolo[3,4-*e*]isoindole-2,6(1*H*,3*H*)-diide (PIN)
(not 1,3,5,7-tetraoxo-5,7-dihydrobenzo[1,2-*c*:4,5-*c'*]dipyrrole-2,6(1*H*,3*H*)-diide)

P-72.5.1.3 'Uide' and 'ide' centers in the same parent hydride

Anionic compounds with two or more anionic centers in the same parent hydride structure, at least one of which is derived formally by removal of a hydron from a skeletal position and one by adding a hydride ion at another position, are named by adding the suffix '-ide', then the suffix '-uide' to the name of the parent hydride, with elision of the final letter 'e' of the parent hydride and of the suffix '-ide'. Each suffix is preceded, where necessary, by the appropriate multiplying prefix. Where there is a choice, low locants of the parent hydride are assigned first to the anionic centers regardless of the kind and then to '-uide' anionic centers.

Example:

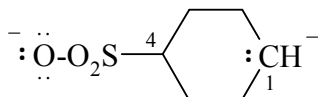


2,2-dimethyl-2,4-dihydrocyclopenta[*c*]borol-4-id-2-uide (PIN)

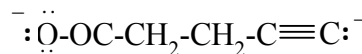
P-72.5.1.4 Anionic characteristic groups on anionic parent hydrides

Polyanions with anionic centers both in the parent hydride part of the structure and on a characteristic group that may be expressed as an anionic suffix are named by adding the anionic suffix to the name of a parent anion formed according to Rules P-72.2.2.1 and P-72.2.3. Where there is a choice, low locants are assigned to the anionic skeletal atoms.

Examples:



cyclohexan-1-ide-4-sulfonate (PIN)



pent-1-yn-1-yl-5-olate (PIN)

P-72.6 Anionic centers in both parent compounds and substituent groups

When anionic centers are not in the same parent structure, one anion is chosen as the parent anion and the other expressed as anionic substituent group(s).

P-72.6.1 Prefixes for anionic centers derived from acid characteristic groups

P-72.6.2 Prefixes for anionic centers derived from hydroxy compounds

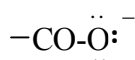
P-72.6.3 Systematically derived prefixes other than those cited in P-72.6.1 and P-72.6.2

P-72.6.4 Choice of parent anionic structure

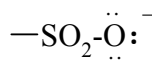
P-72.6.1 Prefixes for anionic centers derived from acid characteristic groups

Substituent anions derived from acid characteristic groups by removal of a hydron from all hydroxy, thiol, etc. groups or a chalcogen analogue, and that are attached to the parent structure by a single bond are named by prefixes formed by changing the ending 'ate' in the name of the anionic suffix to 'ato'.

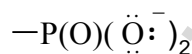
Examples:



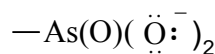
carboxylato (PIN)



sulfonato (preselected name)



phosphonato (preselected name)



arsonato (preselected name)

P-72.6.2 Prefixes for anionic chalcogen atoms

These prefixes are derived from the names oxide, sulfide, selenide, and telluride by changing the final letter 'e', to 'o'.

Examples:



oxido (preselected name)



sulfido (preselected name)

P-72.6.3 Systematically formed prefixes that include anionic center(s)

These prefixes are formed by adding the cumulative suffixes 'yl' or 'ylidene' to the name of the parent anion, with elision of the final letter 'e' in the name of the parent anion. Multiplying prefixes 'di', 'tri', etc, are used to denote multiplicity of free valences. Where there is a choice, low locants are assigned to the free valences.

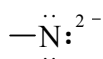
Examples:



methanidyl (PIN)



azanidyl (preselected name)
amidyl



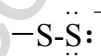
azanediidyl (preselected name)



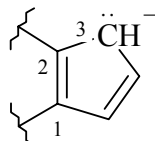
boranuidyl (preselected name)



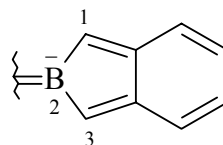
azanidylidene (preselected name)
amidylidene



disulfanidyl (preselected name)



cyclopenta-1,4-dien-3-ide-1,2-diyl (PIN)



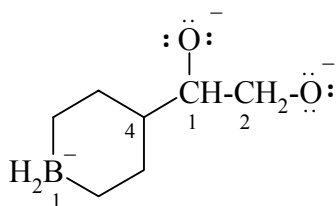
2H-2-benzoborol-2-uid-2-ylidene (PIN)

P-72.7 Choice of an anionic parent structure

When necessary, a parent anionic structure must be chosen by applying the following criteria in order until a definitive choice is achieved.

- (a) maximum number of anionic centers on characteristic groups of any kind, including anionic suffixes;

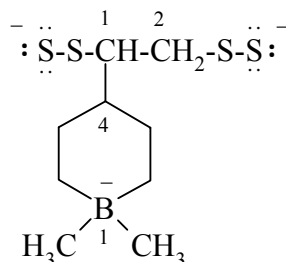
Example:



1-(borinan-1-uid-4-yl)ethane-1,2-bis(olate) (PIN)

- (b) maximum number of anionic centers 'uide' and 'ide';

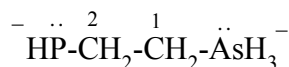
Example:



(1,1-dimethylborinan-1-uide-4-yl)ethane-1,2-diylbis(disulfanide) (PIN)

- (c) Maximum number of 'uide' centers;

Example:



(2-phosphanidylethyl)arsanuide (PIN)

- (d) Maximum number of senior anionic centers, according to the nature of anionic atoms, in the same order as the corresponding replacement prefixes: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > C > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl;

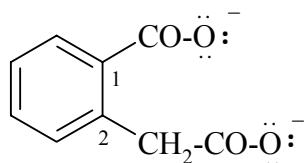
Example:



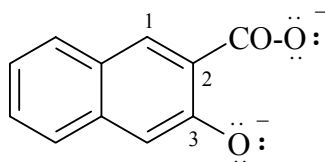
(2-silanidylethyl)phosphanide (PIN)

- (e) Further choice, if necessary, is made by giving priority to corresponding suffixes and by using general priorities.

Examples:



2-(carboxylatomethyl)benzoate (PIN)
(ring senior to a chain)



3-oxidonaphthalene-2-carboxylate (PIN)

P-73 Cations

P-73.0 Introduction

For the purpose of organic nomenclature a cation is a molecular entity carrying at least one unit of positive charge formally derived from a parent hydride or parent compound by adding one or more hydrons, by the removal of one or more hydride ions, or a combination of these operations. An atom where a positive charge is considered to reside is called a cationic center. Cations with two or more cationic centers in the same structure are called dications, trications, etc.

- P-73.1 Cationic compounds with cationic centers derived formally by the addition of hydrons
- P-73.2 Cationic compounds with cationic centers derived formally by the subtraction of hydrides
- P-73.3 Cationic compounds with cationic centers having nonstandard valence states
- P-73.4 Replacement nomenclature for cations
- P-73.5 Cationic compounds with multiple cationic centers
- P-73.6 Cationic prefix names
- P-73.7 Seniority order of cationic centers

73.1 Cationic compounds with cationic centers derived formally by the addition of hydrons

- P-73.1.1 Cationic centers in parent hydrides
- P-73.1.2 Cationic centers on characteristic groups

P-73.1.1 Cations centers in parent hydrides

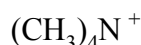
P-73.1.1.1 Retained names of monocationic mononuclear parent cations of Groups 15, 16, and 17

A parent ion derived formally by adding one hydron to a mononuclear parent hydride of the nitrogen, chalcogen and halogen families, in its standard bonding state is named by adding the term 'onium' to a root for the element as indicated in Table 7.1. These cations are parent compounds; they can thus be substituted, but are used only in general nomenclature. For preferred IUPAC names see P-73.1.1.2.

Table 7.1 Retained preselected names of mononuclear parent cations of Groups 15, 16, and 17

H_4N^+	ammonium	H_3O^+	oxonium	H_2F^+	fluoronium
H_4P^+	phosphonium	H_3S^+	sulfonium	H_2Cl^+	chloronium
H_4As^+	arsonium	H_3Se^+	selenonium	H_2Br^+	bromonium
H_4Sb^+	stibonium	H_3Te^+	telluronium	H_2I^+	iodonium
H_4Bi^+	bismuthonium				

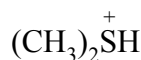
Examples:



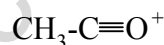
tetramethylammonium
tetramethylazanium
N,N,N-trimethylmethanaminium (PIN)



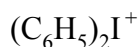
chloro(trimethyl)phosphonium
chloro(trimethyl)phosphanium (PIN)



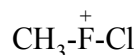
dimethylsulfonium
dimethylsulfanium (PIN)



ethylidyneoxonium
ethylidyneoxidanium (PIN)



diphenyliodonium
diphenyliodanium (PIN)



chloro(methyl)fluoronium
chloro(methyl)fluoranium (PIN)

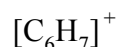
P-73.1.1.2 General rule for systematically naming cationic centers in parent hydrides

A cation derived formally by adding one or more hydrons to any position of a neutral parent hydride (listed in Chapter 2), or whose degree of hydrogenation has been modified (see P-31) is named by replacing the final letter 'e' of the parent hydride name, if any, by the suffix 'ium', preceded by multiplying locants 'di', 'tri', etc., to denote the multiplicity of identical cationic centres. These names for mononuclear cations derived from the mononuclear parent hydrides of Groups 15, 16, and 17, are preferred IUPAC names; these are the preferred IUPAC names and not those given in Table 7.1

Examples:



methanium (PIN)



benzenium (PIN)



azanium (preselected name)
ammonium



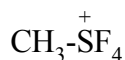
phosphanium (preselected name)
phosphonium



sulfanium (preselected name)
sulfonium



chloranium (preselected name)
chloronium



tetrafluoro(methyl)- λ^4 -sulfanium (PIN)
tetrafluoro(methyl)- λ^4 -sulfonium;



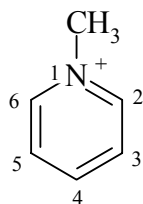
pentamethylhydrazinium (PIN)
pentamethyldiazanium



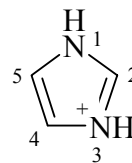
1,2,3-trimethyltrisulfan-2-ium (PIN)



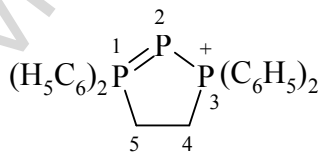
2,2-dichloro-1,1,1-trimethyldiphosphan-1-ium (PIN)



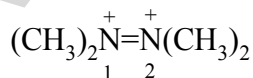
1-methylpyridin-1-ium (PIN)



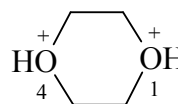
1*H*-imidazol-3-ium (PIN)



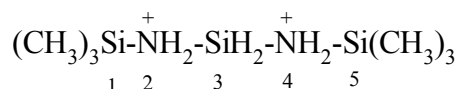
1,1,3,3-tetraphenyl-4,5-dihydro-3*H*-1 λ^5 ,2,3-triphosphol-3-ium (PIN)



tetramethyldiazen-1,2-diium (PIN)



1,4-dioxan-1,4-diium (PIN)



1,1,1,5,5,5-hexamethyltrisilazane-2,4-dium (PIN)

P-73.1.2 Cationic centers on characteristic groups

The principle applied in the naming of cationic centers on characteristic groups is to use the largest neutral parent possible. It is applied particularly in the case of neutral compounds expressed by suffixes containing nitrogen and in the case of oxoacids. Other classes are named on the basis of the largest cationic parent hydride.

P-73.1.2.1 Cationic compounds derived from neutral compounds expressed by suffixes are named in two ways.

- (1) Cationic suffixes expressing oxoacids and functional groups containing nitrogen (amide, imide, nitrile, amine, and imine) are formed by adding the suffix 'ium' to the neutral suffix, as indicated in Table 7.2. These cationic suffixes are used as normal suffixes, with the multiplying prefixes 'bis', 'tris', etc., are used to denote multiplicity. Retained names, used as preferred IUPAC names or in general nomenclature, are modified in the same way.

Table 7.2 Suffixes for cationic characteristic groups

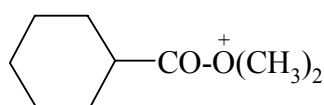
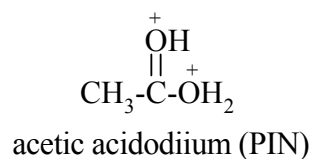
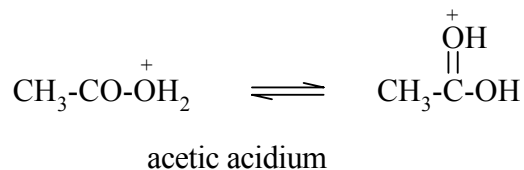
Neutral characteristic group suffix	Cationic characteristic group suffix
ic acid (oxoacids only)	ic acidium
amide, carboxamide	amidium, carboxamidium
imide, carboximide	imidium, carboximidium
nitrile, carbonitrile	nitrilium, carbonitrilium
amine	aminium
imine	iminium

When retained names of amides and nitriles used in general nomenclature imply the presence of two characteristic groups, for example succinonitrile, the corresponding cationic suffix denotes the addition of one hydron to each of the characteristic groups.

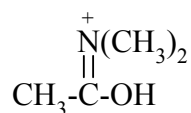
- (2) By substituting cationic parent hydrides described in P-73.1.1.

Method (1) is used to generate preferred IUPAC names

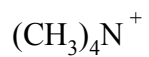
Examples:



O,O-dimethylcyclohexanecarboxylic acidium (PIN)
(cyclohexanecarbonyl)dimethyloxonium



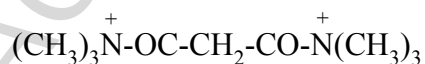
N,N-dimethylacetimidic acidium (PIN)
(1-hydroxyethylidene)dimethylammonium



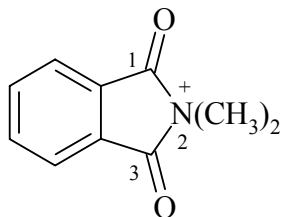
N,N,N-trimethylmethanaminium (PIN)
tetramethylammonium



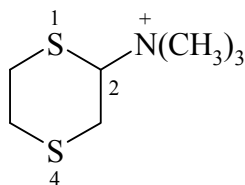
N,N,N-trimethylbenzamidium (PIN)
benzoyltrimethylammonium



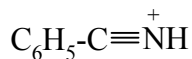
N,N,N,N',N',N'-hexamethylpropanebis(amidium) (PIN)
N,N,N,N',N',N'-hexamethylmalonamidium



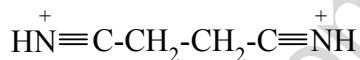
2,2-dimethyl-1,3-dioxo-2,3-dihydro-1*H*-isoindol-2-ium (PIN)
N,N-dimethylphthalimidium



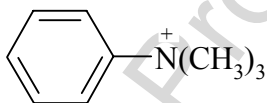
N,N,N-trimethyl-1,4-dithian-2-aminium (PIN)
(1,4-dithian-2-yl)trimethylammonium



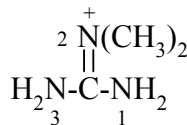
benzonitrilium (PIN)
benzylidyneammonium
benzylidyneazanium



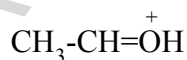
butanebis(nitrilium) (PIN)
butanediylidynebis(ammonium)
butanediylidynebis(azanium)



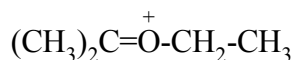
N,N,N-trimethylanilinium (PIN)



2,2-dimethylguanidinium (PIN)



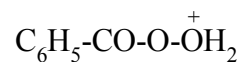
ethylideneoxidanium (PIN)
ethylideneoxonium



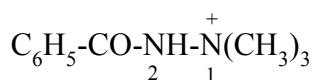
ethyl(propan-2-ylidene)oxidanium (PIN)
ethyl(propan-2-ylidene)oxonium



S,S-dimethylbenzenecarbothioic acidium (PIN)
benzoyldimethylsulfonium
benzoyldimethylsulfanium



benzoyldioxidanium (PIN)
peroxybenzoic *OO*-acidium



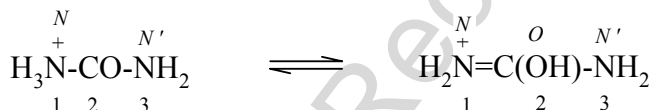
N,N-dimethylbenzenecarbohydrazid-1-ium (PIN)
2-benzoyl-1,1,1-trimethylhydrazinium
2-benzoyl-1,1,1-trimethyldiazanium



acetyl(methyl)chloronium (PIN)

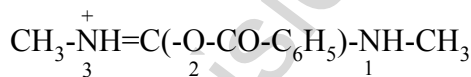
P-73.1.2.2 Uronium ions and chalcogen analogs

Cations derived formally by adding a hydron to urea (or isourea) are named on the basis of the parent cation ‘uronium’, representing the following tautomeric structures:

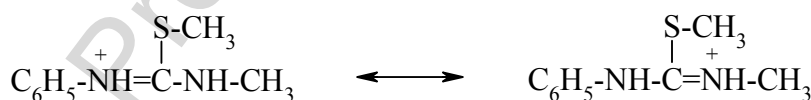


Locants follow those used for urea and isourea. Chalcogen analogues are named on the basis of parent cations, such as ‘thiuronium’, etc. When a choice between two or more tautomeric structures cannot be made, the locants *N*, *N'*, and *O*, *S*, etc. are used.

Examples:



1,3-dimethyl-2-phenyluronium



N-phenyl-*N',S*-dimethylthiuronium

P-73.2 Cations formed by the removal of hydride ions

P-73.2.1 Functional class names

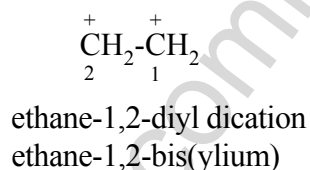
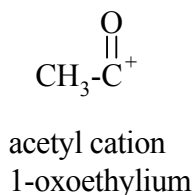
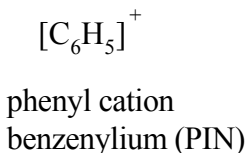
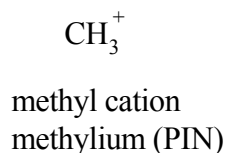
P-73.2.2 Cationic centers in parent hydrides

P-73.2.3 Cationic centers on characteristic groups

P-73.2.1 Functional class names

Cationic compounds that can be considered as being derived formally by removal of electrons from the corresponding radical may be named by adding the class name 'cation' as a separate word after the name of the radical. Polycations are indicated by adding the multiplying prefixes 'di', 'tri', etc., as appropriate, to the class name. Systematic names formed by using the suffix 'ylium' are preferred (see P-73.2.2).

Examples:



P-73.2.2 Cationic centers in parent hydrides

The following recommendations follow closely those for naming radicals, for which see P-71.

P-73.2.2.1 Cationic centers in parent hydrides

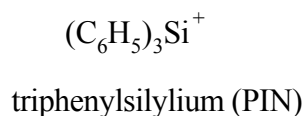
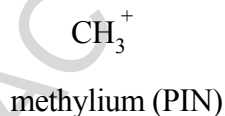
P-73.2.2.2 Cationic centers on characteristic groups

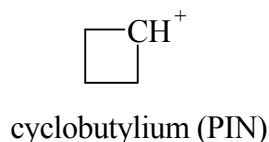
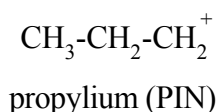
P-73.2.2.1 Cationic centers in parent hydrides

P-73.2.2.1.1 Specific method

Cations formed formally by the removal of a hydride ion, H^- , from a terminal atom of a saturated unbranched acyclic hydrocarbon, a saturated monocyclic hydrocarbon, or a mononuclear parent hydride belonging to Group 14, i.e., methane, CH_4 , silane, SiH_4 , germane, GeH_4 , stannane, SnH_4 , and plumbane, PbH_4 , are named by replacing the 'ane' ending in the name of the parent hydride by the suffix 'ylium'.

Examples:





P-73.2.2.1.2 General method

According to the general method, cations formally derived by the removal of one hydride ion, H^- , from any position of a parent hydride are named by adding the suffix '-ylium' to the name of the parent hydride, with elision of the final 'e' in the name of the parent hydride, if present'. Di- and polycations formally derived by the removal of two or more hydride ions from the parent hydride are named by using the suffix 'ylium' and the multiplying prefixes 'bis', 'tris', etc. Preferred IUPAC names for the parent hydrides are used, as indicated in Chapters 2 and 5. In the examples that follow, preferred IUPAC names are indicated when traditional names are used in general nomenclature.

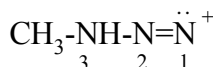
Examples:



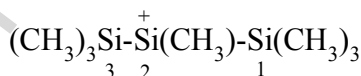
azanylium (preselected name)
aminylium
nitrenium



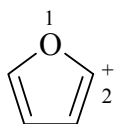
phenylsulfanylium (PIN)



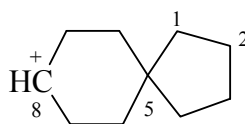
3-methyltriaz-1-en-1-ylum (PIN)



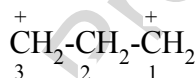
heptamethyltrisilan-2-ylum (PIN)



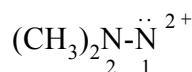
furan-2-ylum (PIN)



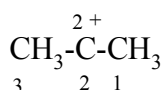
spiro[4.5]decan-8-ylum (PIN)



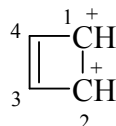
propane-1,3-bis(ylum) (PIN)



2,2-dimethylhydrazine-1,1-bis(ylum) (PIN)
2,2-dimethyldiazane-1,1-bis(ylum)



propane-2,2-bis(ylum) (PIN)
1-methylethane-1,1-bis(ylum)

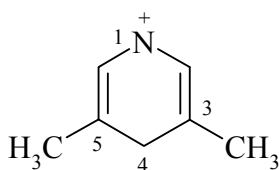


cyclobut-3-ene-1,2-bis(ylum) (PIN)

P-73.2.2.2 Hydro prefixes vs. added hydrogen

A cationic center at a position in a mancude parent hydride where there is an insufficient number of hydrogen atoms to apply directly recommendations for the use of 'ylium' as given in P-73.2.2.1.2 is derived formally from a dihydro derivative of the cyclic parent hydride. Such a radical can also be described by applying the principle of 'added hydrogen' (see P-14.6). In this method the 'hydro' derivative is described by specifying the hydrogen atom of a dihydro pair that remains after the cationic center is created by citing an italic capital *H* and the locant of the skeletal atom at which the hydrogen atom resides, both enclosed in a set of parentheses and inserted into the name of the corresponding parent hydride immediately after the locant for the radical center. Names formed by the 'added hydrogen' method are preferred IUPAC names.

Example:

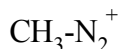


3,5-dimethylpyridin-1(4*H*)-ylium (PIN)
3,5-dimethyl-1,4-dihydropyridin-1-ylium

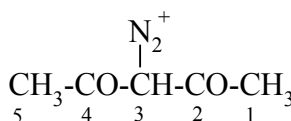
P-73.2.2.3 Diazonium ions

Cations containing a $-N_2^+$ group attached to a parent hydride are traditionally named according to the principles of substitutive nomenclature by using the suffix 'diazonium' and the multiplying prefixes 'bis', 'tris', etc. to denote multiplicity. Diazonium ions may also be named on the basis of the parent cation 'diazenylium', $HN=N^+$. The use of the suffix 'diazonium' yields preferred IUPAC names.

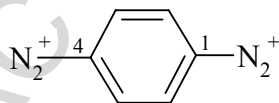
Examples:



methanediazonium (PIN)
methyldiazenylium



2,4-dioxopentane-3-diazonium (PIN)
(2,4-dioxopentan-3-yl)diazenylium



benzene-1,4-bis(diazonium) (PIN)
1,4-phenylenebis(diazenylium)

P-73.2.3 Cationic groups on characteristic groups

P-73.2.3.1 Acylium ions

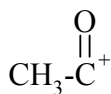
P-73.2.3.2 Cationic groups expressed by suffixes

P-73.2.3.3 Cationic groups expressed as derivatives of parent cations

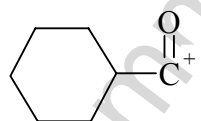
P-73.2.3.1 Acylium cations

Cations formally derived by the removal of all the hydroxy groups as hydroxide ions from acids having systematic or retained names are named by replacing the 'oic acid' or 'ic acid' ending by the suffix 'oylium' or 'ylium', or the 'carboxylic acid' ending by 'carbonylium', in accordance with the rules for naming neutral acyl groups (see P-65.1.8). These names are preferred IUPAC names.

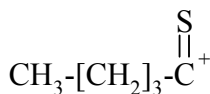
Examples:



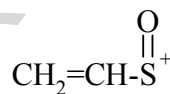
acetylium (PIN)
acetyl cation



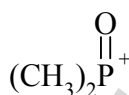
cyclohexanecarbonylium (PIN)
cyclohexanecarbonyl cation



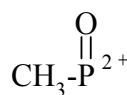
pentanthioylium (PIN)



ethenesulfinylium (PIN)



dimethylphosphinylium (PIN)



methylphosphonylium (PIN)

P-73.2.3.2 Cationic groups expressed by suffixes

Mono- and polycationic centers formally derived by the removal of a hydride ion from the nitrogen atom of an amide, imide, amine, and imine characteristic group are named by using the appropriate suffixes for neutral groups modified by the addition of the suffix 'ylium', with elision of the final 'e' of the neutral suffix. Multiplying prefixes 'bis', 'tris-', etc., are used to denote the multiplicity of these suffixes. These names are the preferred IUPAC names; they are preferred to those formed by substitution of the appropriate parent cation.

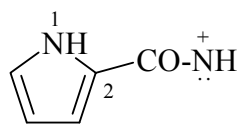
Examples:



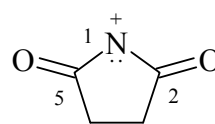
acetamidylium (PIN)



ethanaminylium (PIN)



1*H*-pyrrole-2-carboxamidylum (PIN)



2,5-dioxopyrrolidin-1-ylum (PIN)
succinimidylum

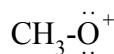
P-73.2.3.3 Cationic groups expressed as substituted parent cations

P-73.2.3.3.1 Cationic centers on oxygen atoms of acids, peroxy acids, hydroxy and hydroperoxy characteristic groups

Cationic centers that are formed by the removal of a hydride ion from an acid, peroxy acid, hydroxy and hydroperoxy characteristic groups are named by substitutive nomenclature on the basis of the corresponding parent cations 'oxidanylium' and 'dioxidanylium'. These are preselected names; a less preferred method uses the terms 'oxylium' and 'peroxylium', respectively.

The names methoxylium, ethoxylium, propoxylium, butoxylium, phenoxylium, and aminoxylium are retained for use in general nomenclature.

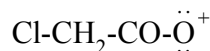
Examples:



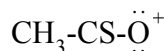
methoxylium (PIN)
methyloxidanylium



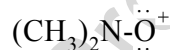
tert-butyldioxidanylium (PIN)
tert-butylperoxylium



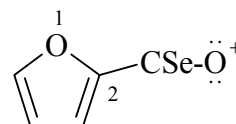
(chloroacetyl)oxidanylium (PIN)
chloracetoxylum



(thioacetyl)oxidanylium (PIN)
(thioacetyl)oxylium



(dimethylamino)oxidanylium (PIN)
dimethylaminoxylium



furan-2-carboselenoyloxidanylium (PIN)
furan-2-carboselenoyloxylium

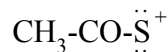
P-73.2.3.3.2 Cationic centers on other characteristic groups

All other cationic centers are named by substituting the appropriate parent cation. The use of the terms 'thiylum' and 'perthiylum' is not recommended in the case of sulfur cationic centers.

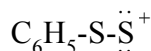
Examples:



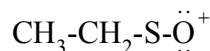
(2,2-dichloroethyl)sulfanylium (PIN)
[not 2,2-dichloro(ethylthiylum)]



acetylsulfanylium (PIN)
(not acetylthiylum)



phenyldisulfanylium (PIN)
(not phenylperthiylum)



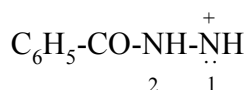
(ethylsulfanyl)oxidanylium (PIN)
ethyl(sulfanyloxylium)



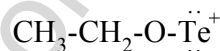
ethylazanebis(ylium) (PIN)



benzoylazanebis(ylium) (PIN)



2-benzoylhydrazin-1-ylium (PIN)
2-benzoyldiazane-1-ylium

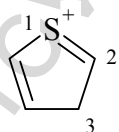


ethoxytellanylium (PIN)

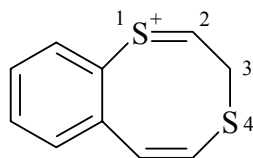
P-73.3 Application of the λ -convention with the suffix ‘ylium’

P-73.3.1 A cationic heterocycle having a cationic center on a heteroatom that has one more skeletal bonds than it has in the corresponding neutral heterocycle is named by adding the suffix ‘ylium’ to the name of the neutral parent hydride for which the λ -convention has been used to describe a nonstandard bonding state of the heteroatom and that heteroatom has at least one hydrogen atom in the neutral heterocycle on which the ‘ylium’ suffix can operate. Indicated hydrogen (see P-14.6) is used as needed.

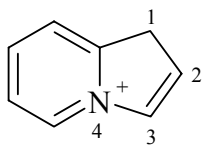
Examples:



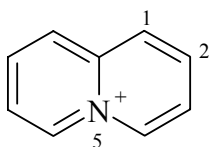
3H-1 λ^4 -thiophen-1-ylium (PIN)



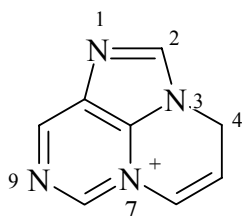
3H-1 λ^4 ,4-benzodithiocin-1-ylium (PIN)
3H-1 λ^4 -benzo[e][1,4]dithiocin-1-ylium



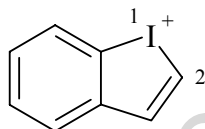
1*H*-4 λ^5 -indolizin-4-ylum (PIN)



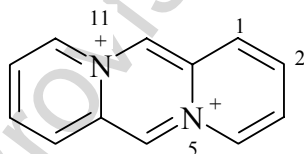
5 λ^5 -quinolizin-5-ylum (PIN)



4*H*-7 λ^5 -pyrimido[1,2,3-*cd*]purin-7-ylum (PIN)



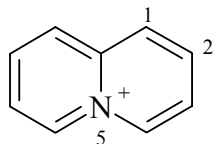
1 λ^3 -benziodol-1-ylum (PIN)



5 λ^5 ,11 λ^5 -dipyrido[1,2-*a*:1',2'-*d*]pyrazine-5,11-bis(ylum) (PIN)

For certain cationic heterocycles of this type, especially those with cationic centers on heteroatoms from the second period elements, it might seem more acceptable to use replacement nomenclature (see P-73.4) or to derive the name by removal of two hydrogen atoms from a cation formed by addition of a hydron using the prefix 'didehydro', for example '4a-azonianaphthalene' or '2,5-didehydro-2*H*-quinolizin-5-ium' for the cation also known as quinolizinium.

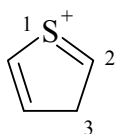
Example:



$5\lambda^5$ -quinolizin-5-ylum (PIN)
4a-azonianaphthalene
2,5-didehydro-2*H*-quinolizin-5-ium

The 'dehydro' method, however, can become quite cumbersome requiring both 'hydro' and 'dehydro' prefixes in some cases.

Example:

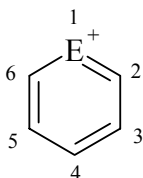


$3H-1\lambda^4$ -thiophen-1-ylum (PIN)
1,2-didehydro-2,3-dihydrothiophen-1-ium

P-73.3.2 Retained names

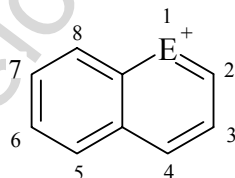
The contracted and traditional names listed in Table 7.3 are retained as preferred IUPAC names and for use in general nomenclature.

Table 7.3 Retained names of 'ylum' cationic parent compounds



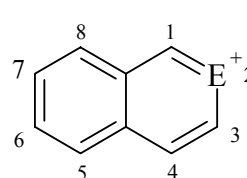
E=O: pyrylium (PIN)

E=S: thiopyrylium (PIN)



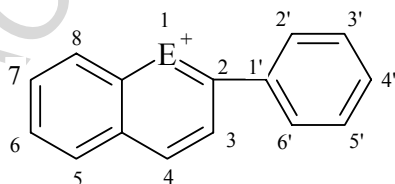
E=O: chromenylium (PIN)

E=S: thiochromenylium (PIN)



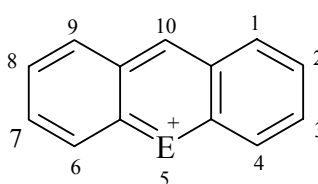
E=O: isochromenylium (PIN)

E=S: isothiochromenylium (PIN)



E=O: flavylum (PIN)

E=S: thioflavylum (PIN)



E=O: xanthylum (PIN)

E=S: thioxanthylum (PIN)

P-73.4 Skeletal replacement ('a') nomenclature for cations

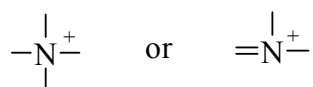
Two methods are used to name cationic centers by skeletal replacement ('a') nomenclature.

- (1) name the compound using neutral skeletal replacement ('a') prefixes and then describe the cationic centers by the appropriate suffix 'ium' and 'ylium'.
- (2) using cationic skeletal replacement ('a') prefixes.

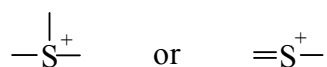
Cationic skeletal replacement ('a') prefixes are formed, except for bismuth, by replacing the 'a' ending of the normal skeletal replacement ('a') prefixes by 'onia'; and, except for carbon, by 'ylia', to indicate a cationic center having a bonding order one higher and one lower, respectively, than the bonding number of the corresponding neutral mononuclear hydride. The cationic skeletal replacement ('a') prefix corresponding to 'bismuthonium' is 'bismuthonia'.

Cationic skeletal replacement ('a') prefixes are used in the same way neutral replacement prefixes

Examples:



azonia (preselected name)



thionia (preselected name)



iodonia (preselected name)



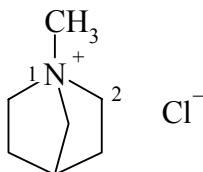
azanylia (preselected name)



boranylia (preselected name)

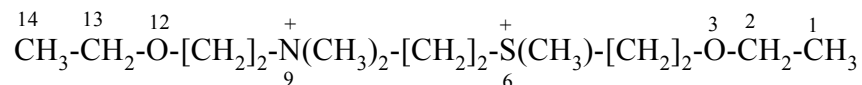
Method (1) gives preferred IUPAC names. Furthermore, names that do not require designation of skeletal in nonstandard valence state by the λ -convention are preferred (see P-73.1 and P-73.2).

Examples:

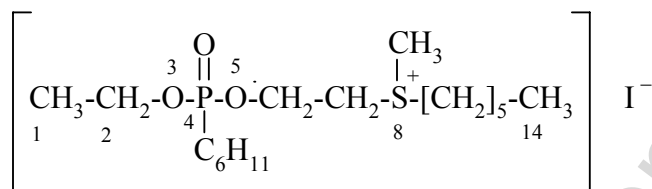


1-methyl-1-azoniabicyclo[2.2.1]heptan-1-ium chloride (PIN)

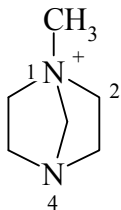
1-methyl-1-azoniabicyclo[2.2.1]heptane chloride



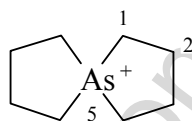
6,9,9-trimethyl-3,12-dioxa-6-thia-9-azatetradecane-6,9-dium (PIN)
6,9,9-trimethyl-3,12-dioxa-6-thionia-9-azoniatetradecane



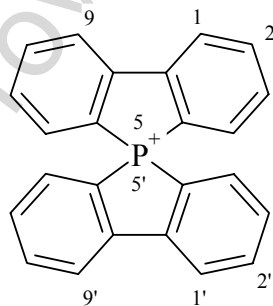
4-cyclohexyl-8-methyl-4-oxo-3,5-dioxa-8-thia-4 λ^5 -phosphatetradecan-8-ium iodide (PIN)
4-cyclohexyl-8-methyl-4-oxo-3,5-dioxa-8-thionia-4 λ^5 -phosphatetradecane iodide



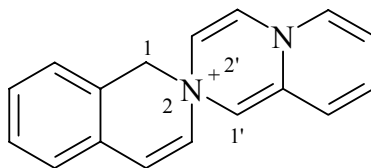
1-methyl-1,4-diazabicyclo[2.2.1]heptan-1-ium (PIN)



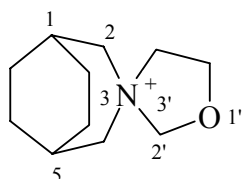
5 λ^5 -arsaspiro[4.4]nonan-5-ylum (PIN)
5-arsoniaspiro[4.4]nonane



5 λ^5 ,5'-spirobi[benzo[*b*]phosphindole]-5-ylum (PIN)
9-phosphonia-9,9'-spirobi[fluorene]
(for construction of the name for the neutral,
noncationic compound, see P-24.8.4)



1*H*-2λ⁵-spiro[isoquinoline-2,2'-pyrido[1,2-*a*]pyrazin]-2-ylum (PIN)



2'*H*-3λ⁵-spiro[3-azabicyclo[3.2.2]nonane-3,3'-[1,3]oxazol]-3-ylum (PIN)

P-73.5 Multiple cationic centers

Cationic compounds with multiple cationic centers are named by several methods in accordance with previous rules.

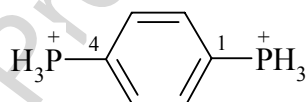
- P-73.5.1 Assemblies of parent cations
- P-73.5.2 'Ium' and 'ylum' centers in the same parent hydride
- P-73.5.3 Cationic characteristic groups on parent cations
- P-73.5.4 Cationic centers in both parent compounds and substituent groups

P-73.5.1 Assemblies of parent cations

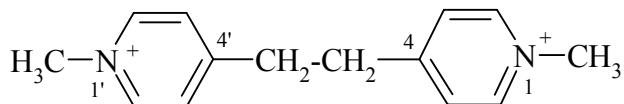
P-73.5.1.1 Assemblies derived from parent cations

Cationic compounds with cationic centers derived from the same parent hydride, but located in different parts of a structure, are named, if possible, according to the principles of multiplicative nomenclature (see P-15.3), using the multiplying prefixes 'bis-', 'tris-', etc. where necessary.

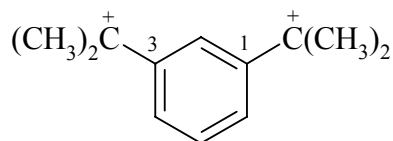
Examples:



- 1,4-phenylenebis(phosphonium) (PIN)
- 1,4-phenylenebis(phosphonium)



4,4'-ethane-1,2-diylbis(1-methylpyridin-1-ium) (PIN)
1,1'-dimethyl-4,4'-ethane-1,2-diylbipyridin-1-ium

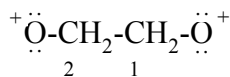


benzene-1,3-diyl(di(propan-2-ylum)) (PIN)
1,3-phenylenedi(propan-2-ylum)

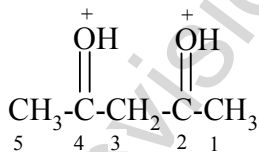
P-73.5.1.2 Polycations with cationic centers on characteristic groups

With the exception of di- and polyamides, di- and polyamines, di- and polyimines, and di- and polyimides, which are named by using direct substitutive nomenclature, polycations with cationic centers on characteristic groups are named by multiplicative nomenclature provided the requirements for the use of multiplicative nomenclature are met.

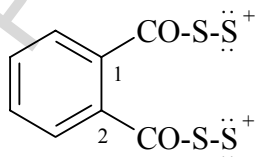
Examples:



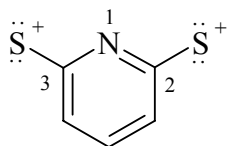
ethane-1,2-diylbis(oxidanylium) (PIN)



pentane-2,4-diylidenebis(oxonium) (PIN)



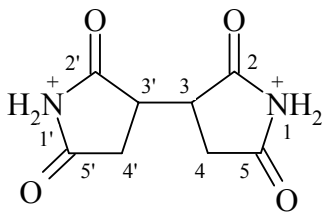
benzene-1,2-diyldicarbonylbis(disulfanylium) (PIN)
benzene-1,2-dicarbonylbis(disulfanylium)



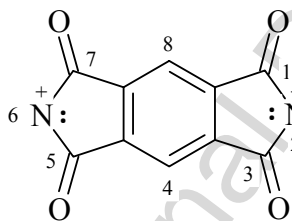
pyridine-2,6-diylbis(sulfanylium) (PIN)

P-73.5.1.3 Polycations derived from cyclic diimides and polyimides are named on the basis of the heterocyclic structure of the imides.

Examples:



2,2',5,5'-tetraoxo[3,3'-bipyrrolidine]-1,1'-dium (PIN)



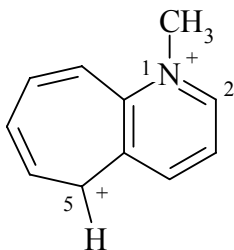
1,3,5,7-tetraoxo-5,7-dihydropyrrolo[3,4-*e*]isoindole-2,6(1*H*,3*H*)-bis(ylium) (PIN)
[not 1,3,5,7-tetraoxo-5,7-dihydrobenzo[1,2-*c*:4,5-*c'*]dipyrrole-2,6(1*H*,3*H*)-bis(ylium)]

P-73.5.2 'ium' and 'ylium' centers in the same parent hydride

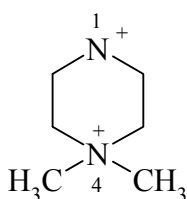
Cyclic compounds with two or more cationic centers in the same parent hydride structure, at least one being denoted by 'ium' and another by 'ylium' suffixes, are named by placing the 'ium' and 'ylium' suffixes, in that order, after the name of the parent hydride, preceded by the appropriate multiplying numerical prefixes and locants, where required.

When there is a choice, low locants are assigned first to the cationic centers irrespective of their kind, then to 'ylium' centers.

Examples:



1-methyl-5*H*-cyclohepta[*b*]pyridin-1-ium-5-ylum (PIN)
(not 1-methyl-5*H*-1-azoniabenz[7]annulen-5-ylum; a skeletal replacement ('a') name is not recommended when fusion names are available)

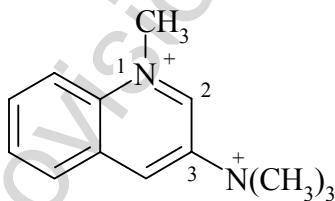


4,4-dimethylpiperazin-4-ium-1-ylum (PIN)

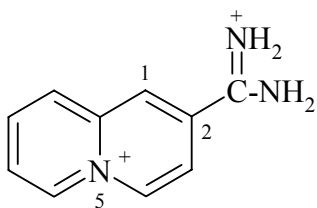
P-73.5.3 Cationic characteristic groups on parent cations

Cationic compounds with cationic centers both in the parent hydride part of the structure and on a characteristic group expressed as a cationic suffix are named by citing both cationic centers, in the order cumulative suffix and cationic suffix.

Examples:



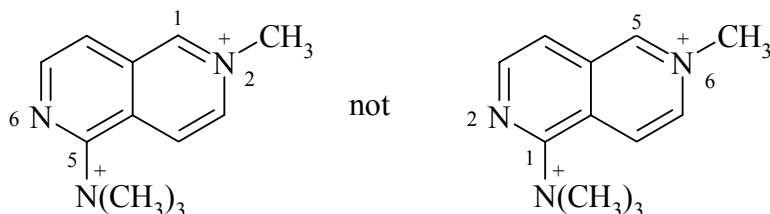
N,N,N,1-tetramethylquinolin-1-ium-3-aminium (PIN)



5λ⁵-quinolizin-5-ylum-2-carboximidamidium (PIN)

Where there is a choice, low locants for skeletal cationic centers are determined before considering locants for cationic suffixes.

Example:



N,N,N,2-tetramethyl-2,6-naphthyridin-5-aminium-2-ium (PIN)
(not *N,N,N,6*-tetramethyl-2,6-naphthyridin-1-aminium-6-ium)

P-73.6 Cationic prefix names

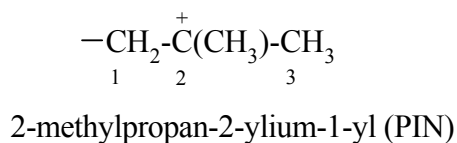
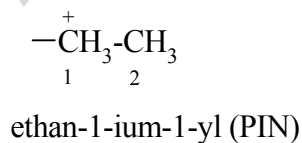
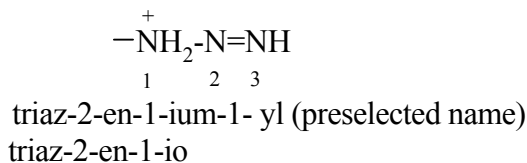
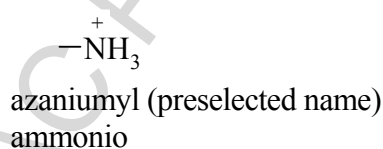
A polycation in which all cationic centers cannot be included in the cationic parent hydride or cationic parent compound is named by selecting one part of the structure as the parent cation and citing the other part(s) as cationic substituent prefixes. The selection of the parent cation is achieved by using the criteria for selecting the cationic parent structure. In zwitterions and in radical cations, the cationic part is always substituted into the anionic portion or into the part including a radical, in accordance with the seniority of anions and radicals over cations.

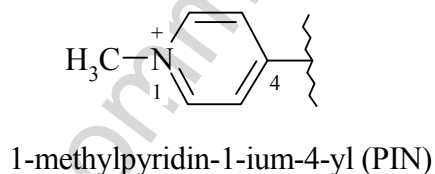
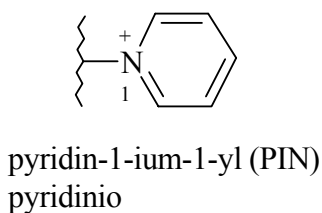
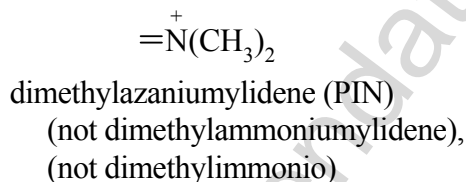
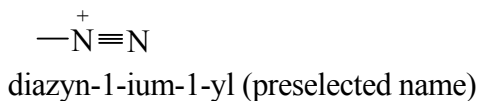
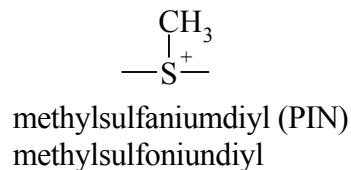
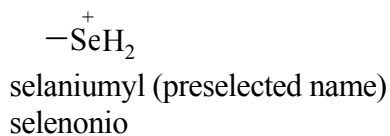
Two methods are used to name substituent structural units containing cationic centers.

- (1) all prefix names are formed by adding to the cation name the suffixes 'yl', 'ylidene', etc. preceded by the multiplying prefixes 'di', 'tri', etc., to indicate multiplicity, where required. Where required, appropriate locants are used. Where there is a choice for numbering, free valences receive lowest possible locants, the suffix 'yl' being senior to 'ylidene'
- (2) prefixes for expressing a monovalent substituent derived from a mononuclear parent cation denoted by 'ium' or by 'onium' described in Table 7.1 are formed by changing the 'onium' ending of the parent cation to 'io' or 'onio'.

Method (1) leads to preferred IUPAC names.

Examples:



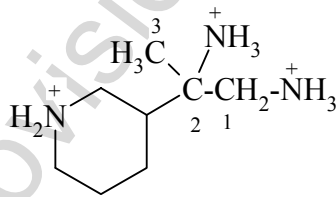


P-73.7 Seniority order of cations and choice of a parent structure

A parent cationic structure is chosen by applying the following criteria in order until a definitive choice is achieved.

- (a) maximum number of cationic centers of any kind, including cationic suffix groups, including those derived from characteristic groups:

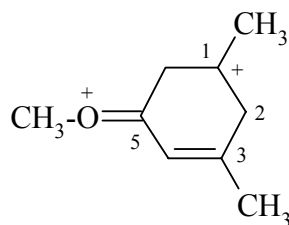
Example:



2-(piperidin-1-ium-3-yl)propane-1,2-bis(aminium) (PIN)

- (b) maximum number of 'ylium' cationic centers:

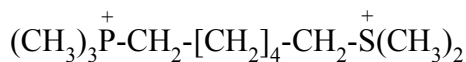
Example:



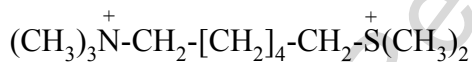
1,3-dimethyl-5-(methyloxidaniumylidene)cyclohex-3-en-1-ylum (PIN)

- (c) maximum number of senior cationic centers, according to the nature of the cationic atom, in the same order as for the corresponding replacement prefixes: F > Cl > Br > I < O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B < Al > Ga > In > Tl.

Examples:



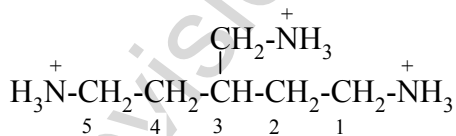
dimethyl[6-(trimethylphosphaniumyl)hexyl]sulfanium (PIN)



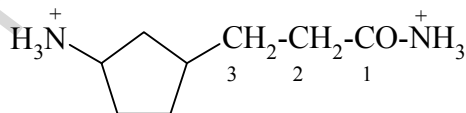
dimethyl[(6-trimethylazaniumyl)hexyl]sulfanium (PIN)

- (d) further choice, if necessary, is made by applying the the general criteria, in accordance with the principles, rules and conventions described in Chapters 1 through 6.

Examples:



3-(azaniumylmethyl)pentane-1,5-bis(aminium) (PIN)



3-(3-azaniumylcyclopentyl)propanamidium (PIN)

P-74 Zwitterionic compounds or zwitterions

Zwitterionic compounds, or zwitterions, are electrically neutral compounds having an equal number of formal unit charges of opposite sign. The structures in this section are all represented as zwitterionic even though some can be drawn as neutral or ionic structures. This section also includes inner salts and dipolar compounds. Section P-74.1 will cover zwitterionic compounds with the ionic centers on the same parent compound and with ionic centers on different parent structures. Section P-74.2 deals with 1,2- and 1,3-dipolar compounds.

According to the seniority of classes, an anionic center has priority over a cationic center in zwitterions. Thus, in zwitterionic compounds anionic centers are preferred for lower locants and are become the parent structure, into which the cationic part is substituted. For the latter CAS uses the reverse order and name.

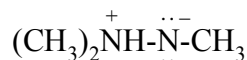
P-74.1 Zwitterionic compounds having equal numbers of anionic and cationic centers on the same parent compound, including ionic centers on characteristic groups expressible as suffixes.

P-74.1.1 Ionic centers in the same parent structure.

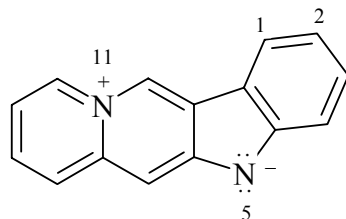
Zwitterionic compounds with the ionic centers in the same parent structure may be named by combining appropriate cumulative suffixes at the end of the name of a parent hydride in the order 'ium', 'ylium', 'ide', 'uide'. This method is preferred to the one using ionic replacement prefixes, as indicated in Sections P-72.4 and P-73.4. In either case anionic suffixes are cited after cationic suffixes in the name, and are given seniority for low locants. The final letter 'e' of the name of a parent hydride, or of an 'ide' or 'uide' suffix, is elided before the letter 'i' or 'y', or before a cumulative suffix beginning with a vowel. Multiplying prefixes 'di', 'tri', etc., appropriate for each type of suffix, are added to specify the number of each kind of ionic center. Where there is a choice, lowest locants are given to the ionic centers in the following order, listed in decreasing order of seniority: 'uide' ('uida'), 'ide' ('ida'), 'ylium' ('ylia'), and 'ium' ('onia').

For nomenclature purposes, zwitterionic compounds having the ionic centers in the same structure are considered as neutral compounds. This concept is important in naming zwitterionic compounds having also a characteristic group denoted by a suffix. These compounds may be named by citing the cumulative suffixes immediately after the name of the parent hydride, in the order given above, and finally the name of the functional suffix denoting the characteristic group, as shown by the last example below.

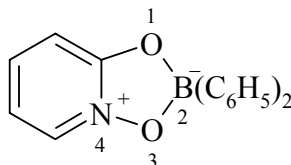
Examples:



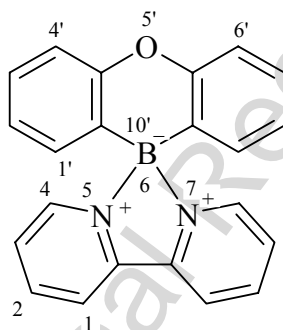
1,2,2-trimethylhydrazin-2-ium-1-ide (PIN)



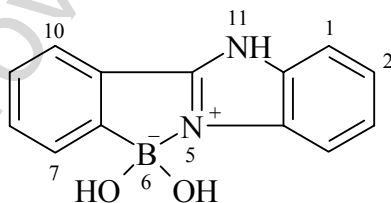
11 λ^5 -5*H*-indolo[2,3-*b*]quinolizin-11-ylum-5-ide (PIN)



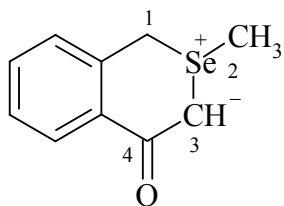
2,2-diphenyl-4 λ^5 -[1,3,4,2]dioxazaborolo[4,5-*a*]pyridin-4-ylum-2-uide (PIN)



5 λ^5 ,7 λ^5 -spiro[1,3,2-diazaborolo[3,4-*a*:5,1-*a*]dipyridine-6,10'-phenoxaborinine]-5,7-bis(ylum)-6-uide (PIN)
(for the name of a structure drawn as an intramolecular adduct, see P-68.1.6.1.1)



6,6-dihydroxy-6,11-dihydro-5 λ^5 -benzimidazolo[3,2-*b*][2,1]benzazaborol-5-ylum-6-uide

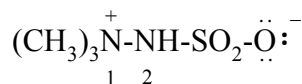


2-methylisosenochroman-2-ium-3-id-4-one

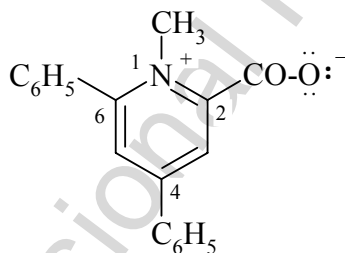
P-74.1.2 Zwitterionic compounds with at least one ionic center on a characteristic group

Zwitterionic compounds with at least one ionic center on a characteristic group may be named by adding the appropriate ionic suffix to the name of the ionic parent hydride. In names, cumulative suffixes are cited before functional suffixes. For assignment of lower locants, ionic centers on skeletal atoms of the parent hydride are preferred to the position of attachment of characteristic groups denoted by ionic suffixes.

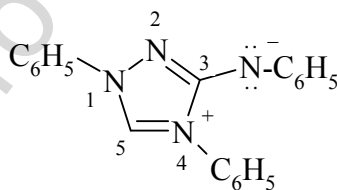
Examples:



1,1,1-trimethylhydrazin-1-ium-2-sulfonate (PIN)



1-methyl-4,6-diphenylpyridin-1-ium-2-carboxylate (PIN)



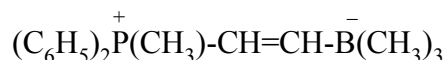
N-(1,4-diphenyl-1*H*-1,2,4-triazole-4-ium-3-yl)anilide (PIN, see P-72.2.2.2.3)

N,1,4-triphenyl-1*H*-1,2,4-triazol-4-ium-3-aminide

P-74.1.3 Anionic and cationic centers on different parent structures

Zwitterionic compounds with anionic and cationic centers on different parent structures may be named by prefixing the name of the cationic center or the parts of the structure containing the cationic centers to the name of the anionic parent compound.

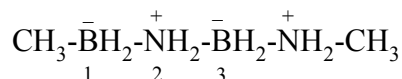
Examples:



[(methylphenylphosphonium)ethenyl]trimethylboranuide (PIN)



(trimethylazaniumyl)acetate (PIN)



1-methyl-3-(methylazaniumyl)diborazan-2-ium-1,3-diide (PIN)

(not 2,4-diaza-3,5-diborahexane-2,4-dium-3,5-diide)

(not 3,5-diazonia-2,4-diboranuidahexane)

(Since diborazane is a nonfunctional parent hydride, there are insufficient heterounits to qualify for a skeletal replacement ('a') name.)

P-74.2 Dipolar compounds

Dipolar compounds are electrically neutral molecules carrying a negative and a positive charge in one of their major canonical descriptions. In most dipolar compounds the charges are delocalized; however the term is also applied to species where this is not the case. 1,2-Dipolar compounds have the opposite charges on adjacent atoms. The term 1,3-dipolar compounds is used for those in which a significant canonical resonance form can be represented by a separation of charge over three atoms.

P-74.2.1 1,2-Dipolar compounds

P-74.2.2 1,3-Dipolar compounds

P-74.2.3 Dipolar substituent groups

P-74.2.1 1,2-Dipolar compounds

P-74.2.1.1 'Ylides'

Compounds in which an anionic site Y^- (originally only on carbon, but now including other atoms) is attached directly to a heteroatom X^+ (usually nitrogen, phosphorus, sulfur, selenium) carrying a formal positive charge are 1,2-dipolar species of the type $\text{R}_m\text{X}^+-\text{Y}^--\text{R}_n$. If X is a saturated atom of an element from the first row of the periodic system, the 'ylide' is commonly represented by a charge separated form; if X is a second, third, etc. row element uncharged canonical forms are available, $\text{R}_m\text{X}=\text{YR}_n$.

These 'ylides' are subdivided into subclasses: nitrogen ylides, phosphorus ylides, oxygen ylides, sulfur ylides, etc. They may be named in different ways depending on the nature of the atoms X and Y.

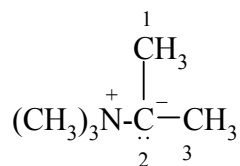
- (1) as zwitterionic compounds, without breaking a homogeneous chain of heteroatoms;
- (2) by applying the λ convention, for X = P, As, S, and Se;
- (3) by functional class using the class names oxide, sulfide, imides.

Method (1) is applicable to all 'ylides' and leads to preferred IUPAC names.

P-74.2.1.1.1 Nitrogen ylides.

Nitrogen ylides have the general structure $R_3N^+-C^-R_2$.

Example:

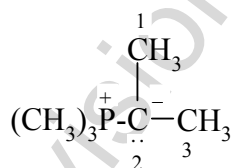


(trimethylazaniumyl)propan-2-ide (PIN)

P-74.2.1.1.2 Phosphorus ylides

Phosphorus ylides have the general structure $R_3P^+-C^-R_2 \leftrightarrow R_3P=CR_2$.

Example:



(trimethylphosphaniumyl)propan-2-ide (PIN)

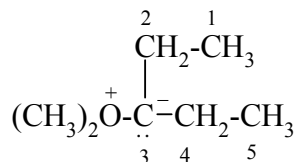
trimethyl(propan-2-ylidene)- λ^5 -phosphane

trimethyl(isopropylidene)phosphorane

P-74.2.1.1.3 Oxygen ylides

Oxygen ylides have the general structure $R_2O^+-C^-R_2$.

Example:

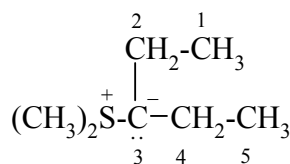


(dimethyloxidaniumyl)pentan-3-ide (PIN)

P-74.2.1.1.4 Sulfur ylides

Sulfur and selenium ylides have the general structure $R_2S^+-C^-R_2 \leftrightarrow R_2S=CR_2$.

Example:



(dimethylsulfaniumyl)pentan-3-ide (PIN)
dimethyl(propan-2-ylidene)- λ^4 -sulfane

This method is also applicable to the analogous selenium compounds.

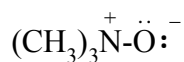
P-74.2.1.2 Amine oxides, imine oxides, and their chalcogen analogues

Amine oxides and imine oxides have the generic formulae $R_3N^+-O^-$ and $R_2=N^+-O^-$, respectively; chalcogen analogues are amine sulfides, imine selenides, etc. (where O is replaced by S, Se, or Te). They may be named:

- (1) as zwitterionic compounds;
- (2) by functional class nomenclature using the functional class name 'oxide'.

Method (2) leads to preferred IUPAC names provided that the resulting name is unambiguous; otherwise, method (1) gives IUPAC preferred names (see also P-62.5).

Example:



N,N-dimethylmethanamine oxide (PIN)
trimethylamine oxide
(trimethylazaniumyl)oxidanide

P-74.2.1.5 Phosphine imides

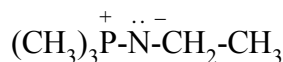
Phosphine imides have the generic structure: $R_3P^+-N^--R \leftrightarrow R_3P=N-R$. They may be named in three ways.

- (1) as zwitterionic compounds;
- (2) by functional class nomenclature using the class name imide;
- (3) as imines of λ^5 -phosphane.

Method (1) leads to preferred IUPAC names.

These methods are extended to arsine and stibine imides.

Example:



ethyl(triphenylphosphaniumyl)azanide (PIN)
triphenylphosphane N-ethylimide
N-ethyl-P,P,P-triphenylphosphane imide
N-ethyl-P,P,P-triphenyl- λ^5 -phosphanimine

P-74.2.2 1,3-Dipolar compounds

The term 1,3-dipolar compounds is used for those compounds in which a significant canonical resonance can be represented by a separation of charge over three atoms. The subclasses of 1,3-dipolar compounds include:

- P-74.2.2.1 the allyl type
- P-74.2.2.2 the propargyl type
- P-74.2.2.3 the carbene type

P-74.2.2.1 Allyl type compounds have the delocalized general structure where Y and/or Z = C, N, or O; and X = N or O.

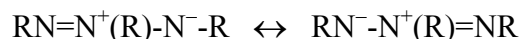


Preferred IUPAC names are based on the first canonical form, although each canonical form can be named, if desired. Names are formed in three different ways.

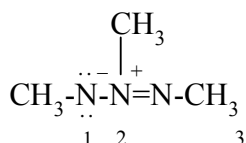
- (1) by substituting a cationic substituent into a parent anion;
- (2) by functional class nomenclature using the class names imide, oxide, etc.;
- (3) by using the λ convention.

Preferred IUPAC names are those expressing the zwitterionic nature of the compounds. Three exceptions are recognized: (1) heteroatom oxides, such as ‘thial’ oxides; (2) azoxy compounds, which are preferably named as diazene oxides; (3) the name nitro, which is retained for $-\text{NO}_2$.

P-74.2.2.1.1 Azo imides, analogous to azoxy compounds, have the delocalized general structure:

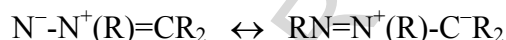


Example:

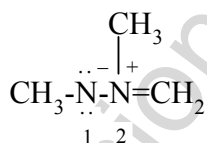


1,2,3-trimethyltriaz-2-en-2-ium-1-ide (PIN; the preferred name is based on the unbroken nitrogen chain)
dimethyldiazene methylimide
trimethyldiazene imide
[methyl(methylimino)ammoniumyl]methanaminide

P-74.2.2.1.2 Azomethine imides have the delocalized general structure:

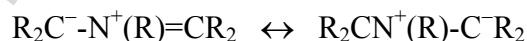


Example:

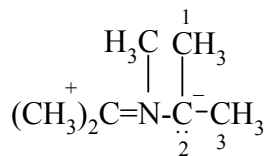


1,2-dimethyl-2-methylidenediazin-2-ium-1-ide (PIN)
N-methylmethanimine methylimide

P-74.2.2.1.3 Azomethine ylides, have the delocalized general structure:



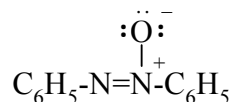
Example:



2-[methyl(propan-2-ylidene)azaniumyl]propan-2-ide (PIN)

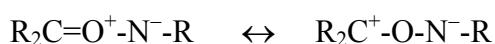
P-74.2.2.1.4 Azoxy compounds, have the general structure $\text{RN}=\text{N}^+(\text{O}^-)\text{-R}$ (see also P-68.3.1.3.2.1)

Example:

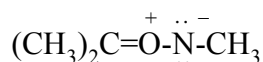


diphenyldiazene oxide (PIN)
(1,2-diphenylhydraziniumyl)oxidanide

P-74.2.2.1.5 Carbonyl imides, have the delocalized general structure:



Example:

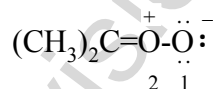


N-[(propan-2-ylidene)oxidaniumyl]methanaminide (PIN)
propan-2-one methylimide
N-methylpropan-2-one imide

P-74.2.2.1.6 Carbonyl oxides, have the delocalized general structure:

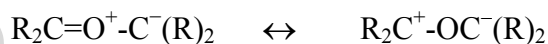


Example:

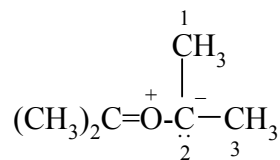


2-(propan-2-ylidene)dioxidan-2-ium-1-ide (PIN)
propan-2-one oxide

P-74.2.2.1.7 Carbonyl ylides, have the delocalized general structure:

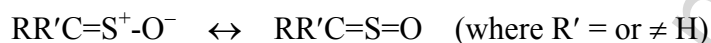


Example:

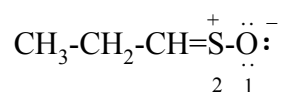


2-[(propan-2-ylidene)oxidaniumyl]propan-2-ide (PIN)

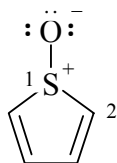
P-74.2.2.1.8 Thioaldehyde *S*-oxides, thioketone *S*-oxides, and heterone *S*-oxides have the generic structure:



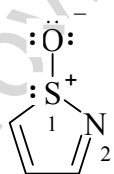
Examples:



propanethial oxide (PIN)
(propylidenesulfaniumyl)oxidanide
propylidene- λ^4 -sulfanone

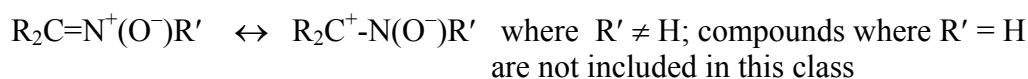


thiophene oxide (PIN)
(thiophen-1-ium-1-yl)oxidanide
 λ^4 -thiophen-1-one

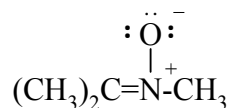


1,2-thiazine 1-oxide (PIN)
1,2-thiazine *S*-oxide

P-74.2.2.1.9 Nitrones have the delocalized general structure:



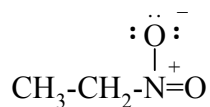
Example:



N-methylpropan-2-imine oxide (PIN)
[propan-2-ylidene(methyl)azaniumyl]oxidanide

P-74.2.2.1.10 Nitro compounds may be named on the basis of the traditional structure R-NO₂, with the permanent prefix 'nitro' (see also P-61.5.1).

Example:



nitroethane (PIN)

P-74.2.2.2 The propargyl type includes compounds having the canonical resonance forms:

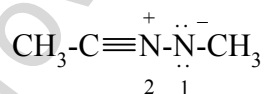


These compounds may be named in different ways:

- (1) as zwitterionic compounds, without breaking the longest chain composed of heteroatoms;
- (2) by functional class nomenclature using the class names imide, oxide, sulfide, etc.

P-74.2.2.2.1 Nitrile imides. Zwitterionic names generate preferred IUPAC names.

Example:



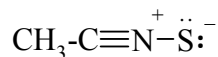
2-ethylidyne-1-methylhydrazin-2-ylum-1-ide (PIN)
acetonitrile methylimide
N-methylacetonitrile imide

P-74.2.2.2.2 Nitrile oxides and sulfides. Functional class names are preferred IUPAC names (see also P-66.5.3.1).

Examples:



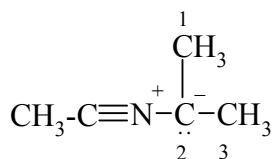
acetonitrile oxide (PIN)
(ethyldiyneazaniumyl)oxidanide



acetonitrile sulfide (PIN)
(ethyldiyneazaniumyl)sulfanide

P-74.2.2.2.3 Nitrile ylides. Zwitterionic names are preferred IUPAC names.

Example:



(ethyldiyneazaniumyl)propan-2-ide

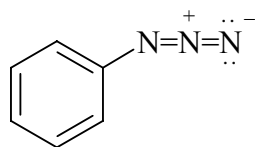
P-74.2.2.2.4 Azides

Azides may be named by two methods.

- (1) substitutively by using the prefix azido (P-61.6, azido = compulsory prefix)
- (2) by functional class nomenclature using the class name azide.
- (3) as derivatives of the zwitterionic parent hydride name: triazadien-2-ium-1-ide.

Method (1) yields preferred IUPAC names (see also P-61.6)

Example:



azidobenzene (PIN)
phenyl azide
phenyltriazadien-2-ium-1-ide.

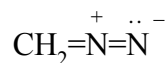
P-74.2.2.2.5 Diazo compounds

Diazo compounds may be named in two ways:

- (1) substitutively by using the prefix diazo.
- (2) As derivatives of the zwitterionic parent hydride name diazen-2-ium-1-ide

Method (1) leads to preferred IUPAC names (see also P-61.4).

Example:



diazomethane (PIN)
methylidene diazen-2-ium-1-ide

P-74.2.2.3 The carbene type includes compounds having the canonical resonance forms:

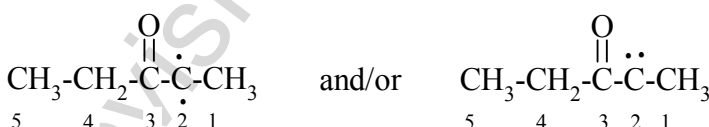


P-74.2.2.3.1 Acyl carbenes have the generic structure acyl- $\text{C}^{2\bullet}$ -R. In organic chemistry, an unspecified acyl carbene is generally a carbonyl carbene. They may be named in two ways:

- (1) by using the longest carbon chain, according to the principles of substitutive nomenclature for radicals (see P-29.3.2), priority being given to the radical to be cited as the suffix; or
- (2) substitutively on the basis of the corresponding carbene.

Method (1) generates preferred IUPAC names.

Example:



3-oxopentan-2-ylidene (PIN)
1-propanoylethylidene

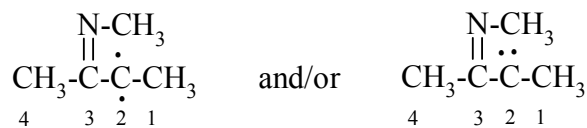
P-74.2.2.3.2 Imidoyl carbenes

Compounds having the structure $\text{RC}(=\text{NH})\text{C}^{2\bullet}$ -R are imidoyl carbenes. Imidoyl is a shortened but imprecise term for carboximidoyl, $\text{RC}(=\text{NH})-$. These carbenes may be named:

- (1) by using the longest carbon chain, according to the principles of substitutive nomenclature for radicals, low locants being assigned to the radical to be cited as suffix;
- (2) substitutively on the basis of carbene used as parent structure.

Method (1) leads to preferred IUPAC names.

Example:



3-(methylimino)butan-2-ylidene (PIN)
1-(dimethylcarbonimidoyl)ethylidene

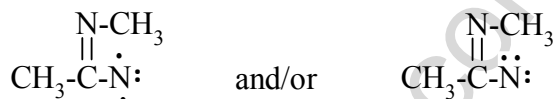
P-74.2.2.3.3 Imido-yl nitrenes

Imido-yl nitrenes have the general structure:



They may be named substitutively using the parent names azanylidene, nitrene, or aminylene.

Example:

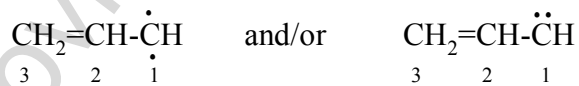


(*N*-methylacetimidoyl)azanylidene (PIN)
(*N*-methylacetimidoyl)nitrene
(*N*-methylacetimidoyl)aminylene

P-74.2.2.3.4 Vinyl carbenes

Vinyl carbenes have the structure $\text{RR}'=\text{CR}''-\text{C}^{2\bullet}-\text{R}'''$. They may be named using the longest carbon chain according to the principles of substitutive nomenclature for radicals, low locants being assigned to the suffix ylidene.

Example:

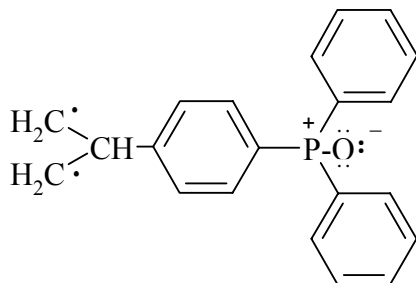


prop-2-en-1-ylidene (PIN)

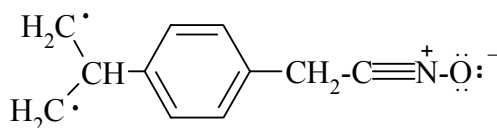
P-74.2.3 Dipolar substituent groups

Names of dipolar substituent groups are formed by using prefixes for naming ions in the substituent group and using the suffixes 'yl', 'ylidene' and 'ylidyne' to designate the free valences.

Examples:



2-[4-(oxidophosphaniumyl)phenyl]propane-1,3-diyl (PIN)



2-[4-[2-(oxidoazaniumyl)ethyl]benzyl]propane-1,3-diyl (PIN)

P-75 Radical Ions

For the purpose of nomenclature of organic chemistry, a radical ion is a molecular entity having at least one radical center and one ionic center, which may be on the same or on different atoms. They are formally classified as:

- P-75.1 Radical ions formed by the addition or subtraction of electrons
- P-75.2 Radical ions derived from parent hydrides
- P-75.3 Radical ions on characteristic groups
- P-75.4 Ionic and radical centers in different parent structures

P-75.1 Radical ions formed by the addition or removal of electrons

Radical ions formed by the addition or removal of electrons may be named in two ways.

- (1) by using the suffixes 'elide' and 'elium' in substitutive nomenclature

Radical ions derived formally from a neutral parent hydride, parent compound, or hydro derivative of either, by the addition or removal of electrons may be named by adding the suffixes 'elide' or 'elium' to the name of the neutral parent. The number of radical centers is denoted by numerical prefixes.

This new method may be used to indicate a global structure, when the positions of the radical and/or ionic centers are not known, or when it is not necessary, nor desirable, to name a specific structure.

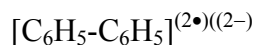
- (2) by functional class nomenclature

Radical ions derived formally from a neutral parent hydride, parent compound,

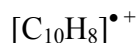
or hydro derivative of either by the addition or removal of electrons may be named by adding the terms 'radical cation' or 'radical anion' as separate words to the name of the neutral parent hydride or parent compound having the same molecular formula. The multiplying prefixes 'di', 'tri' etc. are used to denote multiple radical or ionic centers. The terms 'radical ion' can also be used, followed by a Ewens-Basset number indicating the appropriate charge sign.

The substitutive method, (1), leads to preferred IUPAC names.

Examples:



biphenyldielide (PIN)
biphenyl diradical dianion
biphenyl diradical ion(2-)



azulenelium (PIN)
azulene radical cation
azulene radical ion(1+)

P-75.2 Radical ions derived from parent hydrides

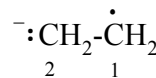
The order of seniority, radicals > anions > cations, is reflected in a preferred IUPAC name. Suffixes assigned to anionic and/or cationic centers are placed first after the name of the parent structure (parent hydride, functional parent hydride, or functionalized parent hydride), followed by suffixes attributed to radical centers.

A radical ion derived formally by the removal of one or more hydrogen atoms from a single skeleton atom or from different skeletal atoms of an ionic or zwitterionic parent hydride is named by adding to its name the suffixes 'yl' or 'ylidene' with appropriate multiplying prefixes before 'yl' or 'ylidene', with elision of the final letter 'e' of the name of the ionic parent hydride. Skeletal positions with radical centers have preference over those with ionic centers for assignment of low locants.

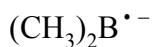
P-75.2.1 Examples of radical anions:



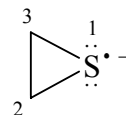
azanidyl (preselected name)



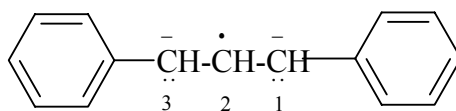
ethan-2-id-1-yl (PIN)



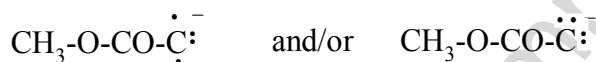
trimethylboranidyl (PIN)
trimethyl-1 λ^5 -boranidyl



1 λ^4 -thiiran-1-id-1-yl (PIN)



1,3-diphenylpropan-1,3-diyl-2-yl (PIN)



(methoxycarbonyl)methanidylidene (PIN)

P-75.2.2 Examples of radical cations:



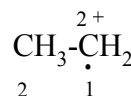
methyliumyl (PIN)



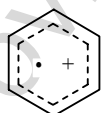
silaniumyl (preselected name)



ethaniumyl (PIN)

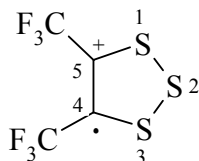


ethan-1-ium-1-ylum-1-yl (PIN)



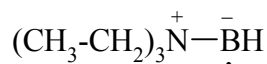
or $[\text{C}_6\text{H}_6]^{\bullet+}$

benzenelium

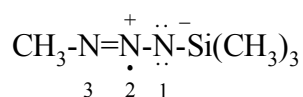


4,5-bis(trifluoromethyl)-1,2,3-trithiolan-5-ylum-4-yl

P-75.2.3 Examples of zwitterionic radical ions:



(triethylazaniumyl)boranuidyl (PIN)
(triethylazaniumyl)-λ⁵-boranidyl

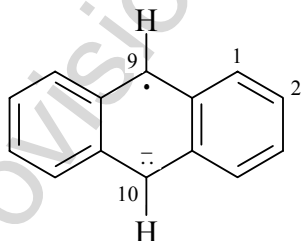


3-methyl-1-(trimethylsilyl)triaz-2-en-2-ium-1-id-2-yl

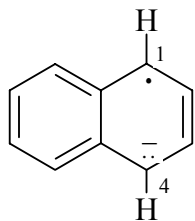
P-75.2.4 Hydro prefixes vs. added hydrogen

Radical and ionic centers at positions in a mancude parent hydride where there is an insufficient number of hydrogen atoms to directly apply recommendations for the use of ‘yl’, ‘ylidene’, ‘ide’ or ‘ylium’ as given in P-72.1, P-72.2 and P-72.3, respectively are derived formally from a dihydro derivative of the cyclic parent hydride. Radical ions can also be described by applying the principle of ‘added hydrogen’ (see P-14.6). In this method, the ‘hydro’ derivative is described by specifying the hydrogen atom of a dihydro pair that remains after the radical center is created by citing in *italic capital H* and the locant of the skeletal atom to which the hydrogen atom resides, both enclosed in a set of parentheses and inserted into the name of the corresponding parent hydride immediately after the locant for the radical center. The ionic center is created next, by subtraction of a hydron. For clarity of names, the ‘added hydrogen’ is cited in names. Preferred IUPAC names are formed by the ‘added hydrogen’ method.

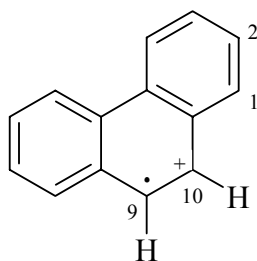
Examples:



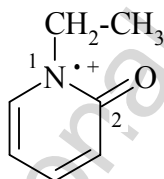
anthracen-10-id-9(10H)-yl (PIN)
9,10-dihydroanthracen-10-id-9-yl
anthracenelide (unspecified)



naphthalen-4-yl-1(4H)-yl (PIN)
1,4-dihydronaphthalen-4-yl-1-yl



phenanthren-10-ylum-9(10H)-yl (PIN)
9,10-dihydrophenanthren-10-ylum-9-yl
phenanthrenium (unspecified)



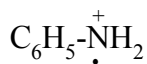
1-ethyl-2-oxopyridin-1-ium-1(2H)-yl (PIN)
1-ethyl-2-oxo-1,2-dihydropyridin-1-ium-1-yl

P-75.3 Radical ions on characteristic groups

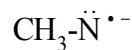
P-75.3.1 Radical ions on ionic suffix groups

When ions may be named by using modified suffixes (see P-73.121 and P-73.2.3.2), the suffixes denoting radical centers are added to the name of the anionic parent hydride.

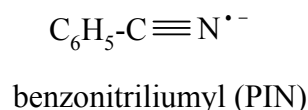
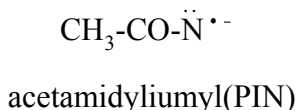
Examples:



aniliniumyl (PIN)
benzenaminiumyl

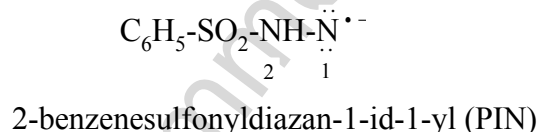
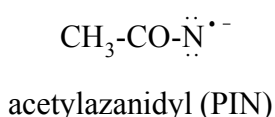
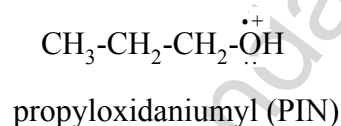
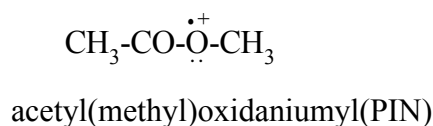


methanaminidyl (PIN)



P-75.3.2 Radical ions other than those named by using ionic suffix groups

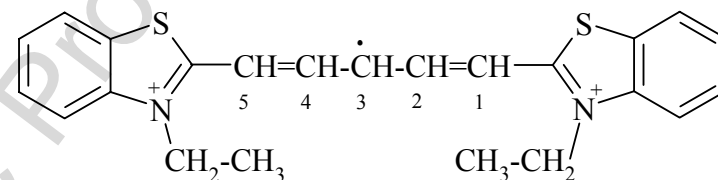
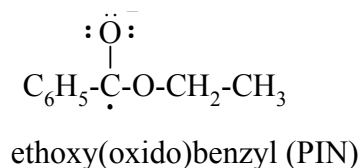
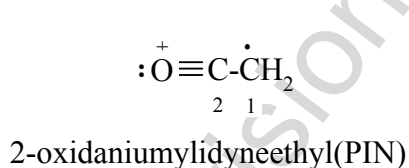
Examples:



P-75.4 Ionic and radical centers in different parent structures

Radical centers have priority over ionic centers. A radical ion derived formally by the subtraction of one or more hydrogen atom(s) from an ionic or zwitterionic compound in which the ionic and radical centers cannot be included in the same parent structure is named by expressing the ionic center(s), or the part of the structure containing the ionic center(s), by means of substituent prefixes attached to the name of the parent radical.

Examples:



1,5-bis(3-ethyl-1,3-benzothiazol-3-ium-2-yl)penta-1,4-dien-3-yl (PIN)

P-76 Delocalized and non-classical radicals and ions

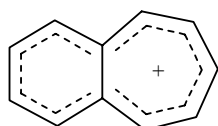
P-76.1 Delocalized radicals and ions

P-76.1.1 Delocalization in names involving one radical or anionic center in an otherwise conjugated double bonds structure is denoted by the appropriate suffix, without locants.

Examples:



- x = • : cyclopentadienyl (PIN)
x = + : cyclopentadienylum (PIN)
x = - : cyclopentadienide (PIN)



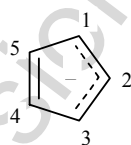
benzo[7]annulenylium (PIN)



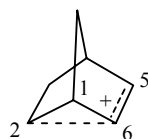
pentadienyl (PIN)

P-76.1.2 Partial delocalization is denoted by the descriptor *deloc* preceded by the locants indicating the extent of delocalization. This descriptor and its locants are cited immediately before the appropriate suffix and enclosed in parentheses.

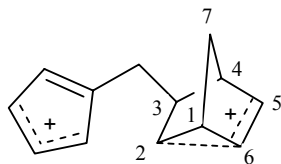
Examples:



cyclopenta-2,4-dien(1,2,3-*deloc*)ide (PIN)



bicyclo[2.2.1]hept-5-en(2,5,6-*deloc*)ylum (PIN)



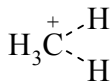
3-[[cyclopenta-2,4-dien(2,3,4-*deloc*)ylum-1-yl]methyl]bicyclo[2.2.1]hept-5-en(2,5,6-*deloc*)ylum

P-76.2 Nonclassical carbocations

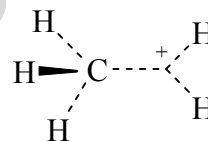
A nonclassical carbocation is a structure having cationic center(s) that cannot be represented by the normal valence system. Hypercoordinated and bridged carbocations belong to this class.

P-76.2.1 Hypercoordinated carbocations (ref. 25)

The prototype of a hypercoordinated carbocation is methanium, CH_5^+ , which results from the addition of a proton to methane. It is best represented by a two-electron three-center system involving the carbon atom and two hydrogen atoms, and three normal valences for the remaining three carbon-hydrogen bonds.



methanium (PIN)



P-76.2.2 Bridged carbocations (see ref. 25)

A carbocation (real or hypothetical) in which there are two (or more) carbon atoms that could be designated as carbenium centers in alternative Lewis formulas but which instead is represented by a structure in which a group (a hydrogen atom or a hydrocarbon residue, possibly with substituent in non involved positions) bridges these potential carbenium centers. One may distinguish ‘electron-sufficient bridged carbocations’ and ‘electron-deficient bridged carbocations’.

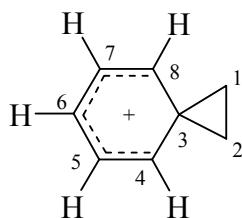
Examples of ‘electron-sufficient bridged carbocations’ are phenyl-bridged ions (for which the trivial name ‘phenonium’ has been used), described in P-76.2.2.1. These ions are straightforwardly classified as carbenium ions.

The three types of ‘electron-deficient bridged carbocations’ described in P-76.2.2.2 necessarily involve three-center bonding. The ‘hydrogen-bridge-carbocation’ shown in P-76.2.2.2.1 contains a two-coordinate hydrogen atom. The ‘bridged carbocations’ in P-76.2.2.2.2 contain five-coordinate carbon atoms. Hypercoordination (see P-76.2.1), which includes two-coordination for hydrogen and five- but also higher coordination for carbon, is generally observed in bridged carbocations.

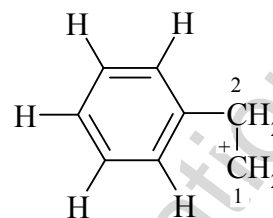
P-76.2.2.1 Phenonium ions (electron-sufficient bridged carbocations)

The class name ‘phenonium ion’ designates cyclohexadienyl cations (cyclohexadienylum cations) that are spiro-fused with a cyclopropane unit. Individual compounds may be named as carbenium ions of the corresponding spiro compounds, by using the suffix ‘ylum’.

Examples:



spiro[2.5]octa-5,7-dien(4,5,6,7,8-*deloc*)ylum (PIN)



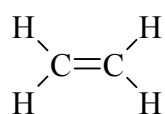
2-phenylethylum (PIN)

P-76.2.2.2 Electron-deficient bridged carbocations

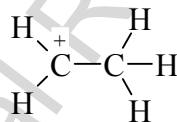
P-76.2.2.2.1 Hydrogen-bridged-carbocations

It is specifically stated in the document Radicals and Ions (RC-82.1.1.2) that specific structures obtained by the addition of a hydron to one end of a double bond resulting in the formation of a tricoordinate carbocation at the other end of the double bond may be named by using the 'ylum' suffix. However, according to the recommendations given herein for naming delocalized cations the name for a delocalized ethylum would be ethen(1,2-*deloc*)ium. The name ethenium would then be used only to describe the formula $[C_2H_5]^+$.

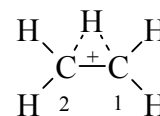
Example:



ethene (PIN)



ethylum(PIN)

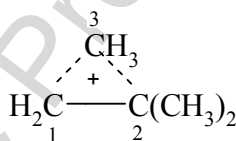


ethen(1,2-*deloc*)ium (PIN)
ethyl(1,2-*deloc*)ylum

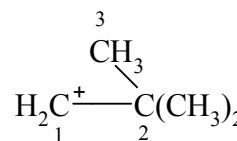
P-76.2.2.2.2 Carbon-bridged carbocations

Locants describing delocalized carbocation systems are cited in names in ascending order following the path of the two delocalized bonds.

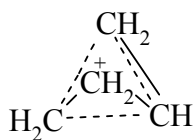
Examples:



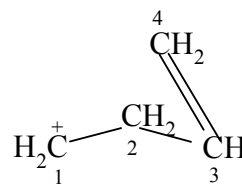
2,2-dimethylpropan(1,3,2-*deloc*)ylum (PIN)



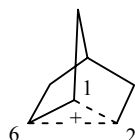
2,2-dimethylpropylum (PIN)



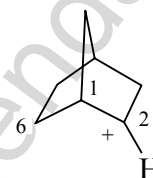
but-3-ene(3,1,4-deloc)ylum (PIN)



but-3-en-1-ylum (PIN)



bicyclo[2.2.1]heptane-(1,2,6-deloc)-2-ylum (PIN)



bicyclo[2.2.1]heptan-2-ylum (PIN)

P-77 Preferred names for radicals, ions, radical ions

Preferred names for radicals, ions, and radical ions are selected either between systematically formed and retained names, or between systematic names.

P-77.1 Selection of preferred names between systematically formed and retained names

Traditional names are retained for naming radicals and ions (see Table 7.3). Most of them are recommended only for use in general nomenclature. Preferred IUPAC names, with a few exceptions, are systematically formed.

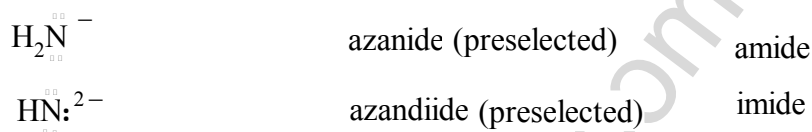
Table 7.3 Retained names used as preselected or preferred IUPAC names and in general nomenclature

Structure	Preselected or Preferred IUPAC name	Retained name for general nomenclature
Radicals		
$\text{H}_2\text{N}\cdot$	azanyl (preselected)	aminyl
$\text{H}_2\text{C}\cdot$	methylidene (PIN)	carbene, methylene
$\text{HC}\cdot$	methylidyne (PIN)	carbyne
$\text{H}_2\text{Si}\cdot$	silylidene (preselected)	silylene
$\text{HN}\cdot$	azanylidene (preselected)	nitrene, aminylene
$\text{R-O}\cdot$	(see P-71.3.3)	

R = CH ₃ -	methyloxidanyl (PIN)	methoxyl
R = CH ₃ -CH ₂ -	ethyloxidanyl (PIN)	ethoxyl
R = CH ₃ -CH ₂ -CH ₂ -	propyloxidanyl (PIN)	propoxyl
R = CH ₃ -[CH ₂] ₂ -CH ₂ -	butyloxidanyl (PIN)	butoxyl
R = CH ₃ -CO-	acetyloxidanyl (PIN)	acetoxyl
R = H ₂ N-	aminooxidanyl (PIN)	aminoxyl



Anions



R = CH ₃ -	methanolate (PIN)	methoxide
R = CH ₃ -CH ₂ -	ethanolate (PIN)	ethoxide
R = CH ₃ -CH ₂ -CH ₂ -	propan-1-olate (PIN)	propoxide
R = CH ₃ -[CH ₂] ₂ -CH ₂ -	butan-1-olate (PIN)	butoxide
R = H ₂ N-	aminooxidamide (preselected)	aminoxide

Cations



R = CH ₃ -	methyloxidanylium (PIN)	methoxylium
R = CH ₃ -CH ₂ -	ethyloxidanylium (PIN)	ethoxylium
R = CH ₃ -CH ₂ -CH ₂ -	propyloxidanylium (PIN)	propoxylium
R = CH ₃ -[CH ₂] ₂ -CH ₂ -	butyloxidanylium (PIN)	butoxylium
R = CH ₃ -CO-	acetyloxidanylium (PIN)	acetoxylum
R = H ₂ N-	aminooxidanylium (preselected)	aminoxylium



dioxidanylium (preselected)	peroxylium, dioxylium
pyrylium (PIN)	(see P-73.3.2)

chromenylium (PIN)	(see P-73.3.2)
isochromenylium (PIN)	(see P-73.3.2)
flavylium (PIN)	(see P-73.3.2)
xanthylium (PIN)	(see P-73.3.2)

P-77.2 Preferred systematic names

P-77.2.1 Preferred names derived from mancude parent hydrides and fullerene

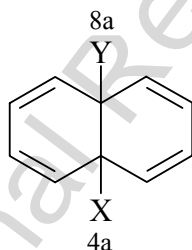
P-77.2.2 Preferred names for anions

P-77.2.3 Preferred names for cations

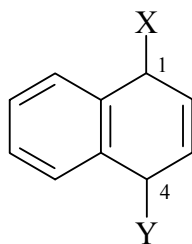
P-77.2.1 Preferred names derived from mancude parent hydrides and fullerenes

Preferred names for radicals, ions and radicals-ions derived from mancude parent hydrides and fullerenes are formed by using the 'added hydrogen' method. In general nomenclature, the addition of hydrogen atoms and the creation of radicals and ions by the subtraction of hydrogen atom, hydrons or hydrides as appropriate, is an acceptable method.

Examples:

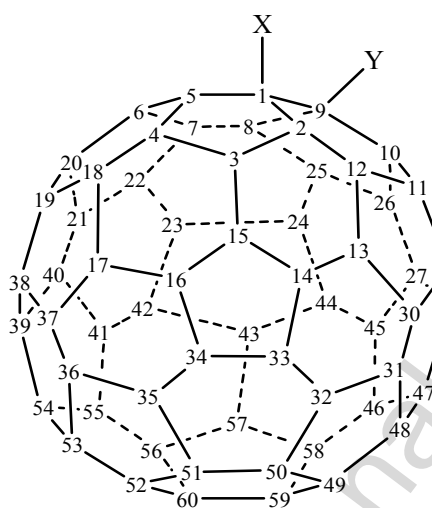


X = •	Y = H	naphthalen-4a(8aH)-yl (PIN) 1,4-dihydronaphthalen-1-yl
X = •	Y = •	naphthalene-4a,8a-diyl (PIN) 4a,8a-dihydronaphthalene-4a,8a-diyl
X = ⊕	Y = H	naphthalen-4a(8aH)-ylium (PIN) 4a,8a-dihydronaphthalen-4a-ylium
X = •	Y = ⊕	naphthalen-8a-ylium-4a(8aH)-yl (PIN) 4a,8a-dihydro-naphthalen-8a-ylium-4a-yl



X = • Y = - naphthalen-4-id-4(8a*H*)-yl (PIN)
1,4-dihydronaphthalen-4-id-1-yl

X = Y = - naphthalene-1,4-diide (PIN)
1,4-dihydronaphthalen-1,4-diide



- I X = • ; Y = H
- II X = + ; Y = H
- III X = • ; Y = +
- IV X = - ; Y = H
- V X = • ; Y = -
- VI X = • ; Y = •

I (C₆₀-I_h)[5,6]fulleren-1(9*H*)-yl (PIN)
1,9-dihydro(C₆₀-I_h)[5,6]fulleren-1-yl

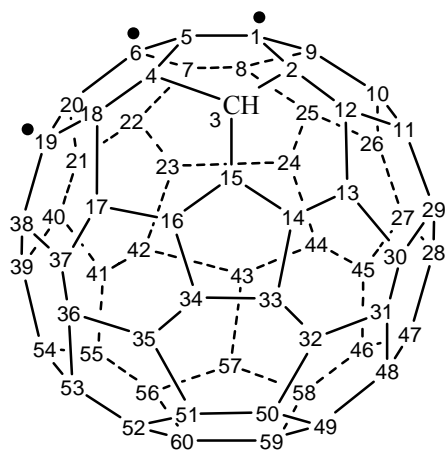
II (C₆₀-I_h)[5,6]fulleren-1(9*H*)-ylium (PIN)
1,9-dihydro(C₆₀-I_h)[5,6]fulleren-1-ylium

III (C₆₀-I_h)[5,6]fulleren-9-ylium-1(9*H*)-yl (PIN)
1,9-dihydro(C₆₀-I_h)[5,6]fulleren-1,9-diyl

IV (C₆₀-I_h)[5,6]fulleren-1(9*H*)-ide ((PIN)
1,9-dihydro(C₆₀-I_h)[5,6]fulleren-1-ide

V (C₆₀-I_h)[5,6]fulleren-9-id-1(9*H*)-yl (PIN)
1,9-dihydro(C₆₀-I_h)[5,6]fulleren-9-id-1-yl

VI (C₆₀-I_h)[5,6]fullerene-1,9-diyl (PIN)
1,9-dihydro(C₆₀-I_h)[5,6]fulleren-9-ylium-1-yl

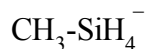


(C60-Ih)[5,6]fullerene-1,6,19(3H)-triyl (PIN)
1,3,6,19-tetrahydro(C60-Ih)[5,6]fullerene-1,6,19-triyl

P-77.2.2 Anions

P-77.2.2.1 Substitutive names that involve the suffix ‘uide’ are preferred to those that are denoted by the suffix ‘ide’ with the λ -convention.

Examples:



methylsilanuide (PIN)
methyl- λ^6 -silanide



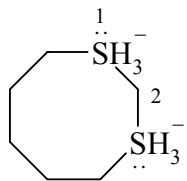
hexafluoro- λ^5 -iodanuide (preselected name)
hexafluoro- λ^7 -iodanide

P-77.2.2.2 The use of the suffix ‘ide’ is preferred to that of the suffix ‘uide’ added to a parent hydride modified by the λ -convention; the suffix ‘ide’ is also preferred over ‘uide’ when the λ -convention must be used to denote both anionic centers.

Examples:



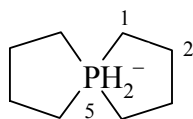
methanide (PIN)
 λ^2 -methanuide



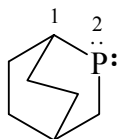
$1\lambda^4, 3\lambda^4$ -dithiocane-1,3-diide (PIN)
 $1\lambda^6, 3\lambda^6$ -dithiocane-1,3-diide
 $1\lambda^4, 3\lambda^6$ -dithiocane-3-ide-1-uide

P-77.2.2.3 Names denoted by the suffixes ‘uide’ or ‘ide’ added to neutral replacement names of parent hydrides are preferred to those formed by anionic replacement prefixes ‘uida’ or ‘ida’ (see P-72.4).

Examples:



$5\lambda^5$ -phospha-5-uide (PIN)
 $5\lambda^5$ -phosphanuida-5-uide



2-phospha-2-uide (PIN)
 2-phosphanida-2-uide

P-77.2.3 Cations

P-77.2.3.1 ‘Onium cations’

Names of mononuclear cations of Groups 15, 16, and 17, formed by adding the suffix ‘ium’ to the name of the mononuclear parent hydride are preferred to those formed by using the ending ‘onium’.

Examples:



azanium (preselected name)
ammonium



sulfanium (preselected name)
sulfonium

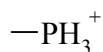


bromanium (preselected name)
bromonium

P-77.2.3.2 Prefixes for denoting cations

Prefixes formed by adding the suffix 'yl' to the systematic name of the cation are preferred to those derived from 'onium cations', ending with the letter 'o'.

Examples:



phosphaniumyl (preselected name)
phosponio



seleniumyl (preselected name)
selenonio



iodaniumyl (preselected name)
iodonio

P-77.2.3.3 Preference between 'ylium' and 'ium' suffixes

P-77.2.3.3.1 The use of the suffix '-ylium' is preferred to that of the suffix '-ium' added to a parent hydride modified by the λ -convention.

Example:



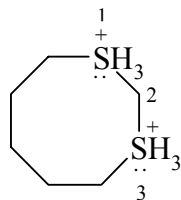
azanylium (preselected name)
 λ^1 -azanium
aminylium
nitrenium

P-77.2.3.3.2 The use of the suffix 'ium' is preferred to that of the suffix 'ylium' added to a parent hydride modified by the λ -convention; the suffix 'ium' is also preferred over 'ylium' when the λ -convention must be used to denote both cationic centers.

Examples:



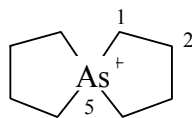
phosphanium (preselected name)
phosponium
 λ^5 -phosphanylium



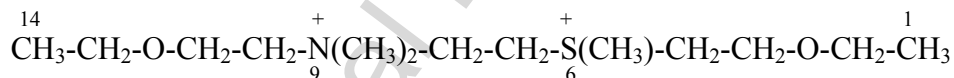
$1\lambda^4, 3\lambda^4$ -dithiocane-1,3-dium (PIN)
 $\lambda^6, 3\lambda^6$ -dithiocane-1,3-bis(ylium)
 $1\lambda^6, 3\lambda^4$ -dithiocane-3-ium-1-ylium

P-77.2.3.3.3 Names denoted by the suffixes ‘ium’ or ‘ylium’ added to neutral replacement names of parent hydrides are preferred to those formed by cationic replacement prefixes (see P-73.4).

Examples:



$5\lambda^5$ -arsaspiro[4.4]nonan-5-ylum (PIN)
 5-arsoniaspiro[4.4]nonane



6,9,9-trimethyl-3,12-dioxa-6-thia-9-azatetradecane-6,9-dium (PIN)
 6,9,9-trimethyl-3,12-dioxa-6-thionia-9-azoniatetradecane

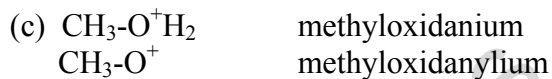
P-77.3 Preferred parent structures

Names of radicals and ions are constructed on the basis of functional parents (e.g. acetic acid) or functionalized parents (e.g. methanamine), and on radical and ionic parents derived from parent hydrides (e.g. acetylazaniide, methyloxidanyl). Preferred names are based on these two principal types.

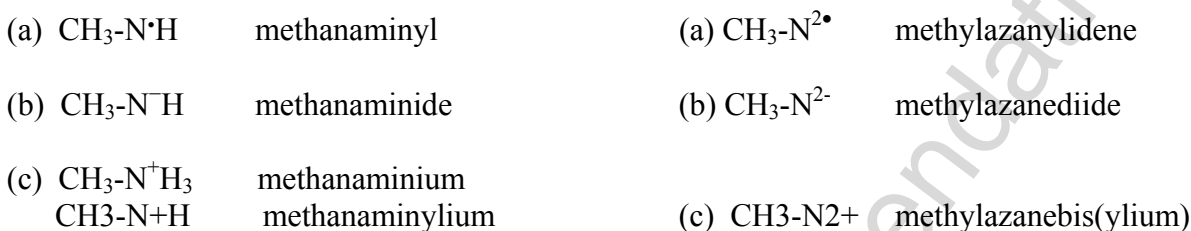
Table 7.4 illustrates this dichotomy.

Table 7.4 Preferred IUPAC names for radicals and ions derived from functionalized and functional parents

Type I: Functional and functionalized parents		Type II: Derivatives of radical and ionic parents	
Acids			
		(a) $\text{CH}_3\text{-CO-O}\cdot$	acetyloxidanyl
(b) $\text{CH}_3\text{-COO}^-$	acetate		
(c) $[\text{CH}_3\text{-COOH}]\text{H}^+$	acetic acidium	(c) $\text{CH}_3\text{-CO-(O}^+\text{H}_2)$ $\text{CH}_3\text{-CO-O}^+$	acetyloxidanium acetyloxidanylium
Amides			
(a) $\text{CH}_3\text{-CO-N}\cdot\text{H}$	acetamidyl	(a) $\text{CH}_3\text{-CO-N}^2\cdot$	acetylazanylidene
(b)		(b) $\text{CH}_3\text{-CO-N}^-\text{H}$	acetylazanide
(c) $[\text{CH}_3\text{-CO-NH}_2]\text{H}^+$	acetamidium	(c) $\text{CH}_3\text{-CO-N}^+\text{H}_3$	acetylazanium
$\text{CH}_3\text{-CO-N}^+(\text{CH}_3)_3$	<i>N,N,N</i> -trimethyl-acetamidium	$\text{CH}_3\text{-CO-N}^+(\text{CH}_3)_3$	acetyltrimethyl azanium
$\text{CH}_3\text{-CO-N}^+\text{H}$	acetamidylum	$\text{CH}_3\text{-CO-N}^{2+}$	acetylazanebis(ylum)
Nitriles			
(c) $\text{CH}_3\text{-C}\equiv\text{N}^+\text{H}$	acetonitrilium		
Aldehydes/Ketones		(c) $\text{CH}_3\text{-CH=O}^+\text{H}$	ethylideneoxidanium
Hydroxy compounds			
		(a) $\text{CH}_3\text{-O}\cdot$	methyloxidanyl
(b) $\text{CH}_3\text{-O}^-$	methanolate		



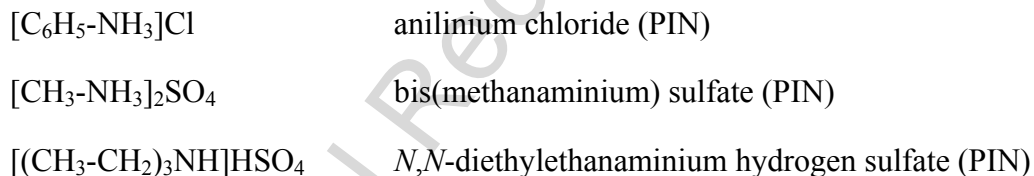
Amines - imines



P-77.4 Preferred names for salts of organic bases

P-77.4.1 Preferred names are binary names formed by citing the name of the cation followed by that of the anion.

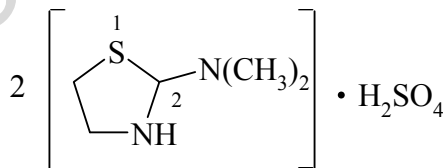
Examples:



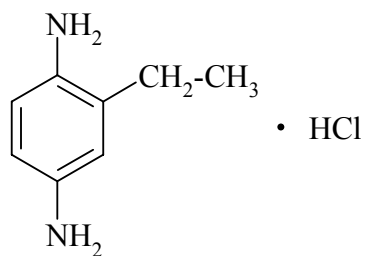
P-77.4.2 When the above rule cannot be applied, recourse is found in two traditional methods of naming salts of organic bases, namely:

- the unaltered name of the base is followed by the name of the anion;
- for salts of hydrohalogen acids only, the unaltered name of the base is followed by hydrofluoride, hydrobromide, hydrochloride, or hydroiodide, as the case may be.

Examples:



bis(*N,N*-dimethyl-1,3-thiazolidin-2-amine) sulfate (PIN)



2-ethylbenzene-1,4-diamine monohydrochloride (PIN)

IUPAC Provisional Recommendations