# INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

ORGANIC CHEMISTRY DIVISION COMMISSION ON NOMENCLATURE OF ORGANIC CHEMISTRY\*

# **REVISED NOMENCLATURE FOR RADICALS, IONS, RADICAL IONS AND RELATED SPECIES**

#### (IUPAC Recommendations 1993)

(A Revision of "Subsection C-0.8. Free Radicals, Ions, and Radical Ions" in IUPAC Nomenclature of Organic Chemistry, Section C: Characteristic Groups Containing Carbon, Hydrogen, Oxygen, Nitrogen, Halogen, Sulfur, Selenium, and/or Tellurium)

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# Revised nomenclature for radicals, ions, radical ions and related species (IUPAC Recommendations 1993)

### Summary

These recommendations constitute a comprehensive documentation of nomenclature for organic radicals, ions, and radical ions based primarily on principles given in subsection C-0.8 of the IUPAC *Nomenclature of Organic Chemistry*<sup>1</sup> and illustrated in various subsections of Sections A, B, C, and D of those Rules. They also extend these principles to noncarbon parent hydrides and provide explicit guidance for describing the presence of radical and ionic centers on the principal characteristic groups of organic nomenclature. Recommendations are given for naming polyradicals, and polycationic, polyanionic, and zwitterionic compounds, and are illustrated by complex as well as simple examples.

Two innovations are introduced: (1) the prefix "ylo-" to indicate the presence of a radical center in a substituent group; and (2) the suffix "-uide" to describe an anion formally derived by the addition of a hydride ion to a parent hydride.

Delocalized radicals and ions are not treated in these recommendations except where such delocalization is included in usual structural considerations.

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#### PREAMBLE

The 1979 edition of the IUPAC Nomenclature of Organic Chemistry<sup>1</sup>, hereinafter called the 1979 IUPAC Organic Rules, contains a subsection codifying nomenclature recommendations for radicals\*, ions, and radical ions<sup>2a</sup>, which are illustrated by various recommendations in Sections B<sup>3a</sup>, C<sup>2b</sup>, and D<sup>4a</sup>. Although those recommendations embody all the requirements for a general system of nomenclature for radicals, ions, and radical ions, they have often been interpreted rather narrowly and do not deal thoroughly with some types of compounds, for example, those containing different formal charges in the same parent structure.

This revision retains the essential principles of the 1979 IUPAC Organic Rules<sup>1</sup> for naming organic radicals, ions, and radical ions<sup>2a, 2b, 3a, 4a</sup> and extends them to include parent compounds of the nonmetallic and certain semimetallic elements and to some other characteristic groups. Established recommendations from other IUPAC Nomenclature Commissions have been incorporated and, where appropriate, alternative methods under study by the Comon Nomenclature of Organic Chemistry are noted.

It is not intended for these revised recommendations to deal exhaustively with all aspects of nomenclature for radicals, ions, and radical ions. For example, delocalization is not included even though it was mentioned briefly in the 1979 IUPAC Organic Rules<sup>2C</sup>; this aspect of their nomenclature is currently under study by the Commission. The recommendations presented here are concerned only with classical valence structures and do not deal with concepts such as paired and unpaired electronic configurations.

These recommendations do not legislate for a particular name when more than one is given. Like Section C in the 1979 IUPAC Organic Rules<sup>2</sup>, they provide guidelines for the generation of unambiguous names corresponding to the structural information available. When more than one name appears, the first is the one that reflects the recommendation just preceding, followed by names generated by subsections elsewhere in these recommendations or in previously published IUPAC recommendations, or that reflect established usage elsewhere. Occasionally, a trivial name or a "traditional name", i.e., a name that is, or has been, in common use, is given even though not preferred by these recommendations. Finally, when the difference between a recommended name and a name that would be generated by applying the recommendations in the 1979 IUPAC Organic Rules<sup>1</sup> may be somewhat subtle, the name that would be generated according to the 1979 IUPAC Organic Rules<sup>1</sup> is given, but only for comparison, and identified by a parenthetical note beginning with the phrase "according to" or the word "previously".

<sup>\*</sup> The adjective "free", used in earlier editions of the IUPAC Organic Rules<sup>2a</sup>, is not used in these recommendations. It was used previously to distinguish between radicals as distinct chemical species and the term radical used to describe a substituting group in substitutive nomenclature. In subsequent recommendations on organic nomenclature, the Commission intends to use the term "group" rather than "radical" to designate a substituting group.

These recommendations replace or modify most of Subsection C-0.8 "Free Radicals, Ions, and Radical Ions", in Section C: "Characteristic Groups Containing Carbon, Hydrogen, Oxygen, Nitrogen, Halogen, Sulfur, Selenium, and/or Tellurium"<sup>2a</sup>, and other recommendations in Sections B<sup>3a</sup>, C<sup>2b</sup>, and D<sup>4a</sup> of the 1979 edition of the IUPAC Nomenclature of Organic Chemistry<sup>1</sup>.

These revised recommendations are also published in a brief  $form^5$ .

#### INTRODUCTION

In organic nomenclature, most radicals, ions, and related species are considered formally as derived from parent hydrides or characteristic groups by the loss of hydrogen atoms, or by the addition or loss of hydrogen ions. [Acyl radicals and corresponding cations may be considered as exceptions derived formally from acids by loss of —OH groups as hydroxyl radicals or hydroxide ions, respectively (see RC-81.2.2 and RC-82.2.3.2)]. These operations change the number of substitutable hydrogen atoms at the radical or ionic centers and are described mainly by the operational suffixes\* or prefixes shown in Table 1. The suffixes may be added individually or in combination to the name of a parent hydride, or to some of the traditional suffixes used to express principal characteristic groups in substitutive nomenclature.

These recommendations are concerned only with formal operations for naming radicals, ions, radical ions, and neutral compounds with compensating ionic centers, and related species. They do not include general principles of nomenclature systems, such as the expression of unsaturation or partial saturation in parent hydrides, indicated and "added" hydrogen, locant positions, or numbering priorities, except for those involving the operational suffixes noted in Table 1. However, for convenience, modifications to the 1979 IUPAC Organic Rules<sup>1</sup> to be published in the first part of a complete revision of the 1979 edition<sup>5</sup> that are used in these recommendations are outlined briefly in RC-80.

Even though, traditionally, abbreviated or trivial names for acyclic radicals and ions may be commonly used and even preferred in these recommendations, systematic names for acyclic parent hydrides may be used to generate names of radicals and ions using the operational affixes given in Table 1. These systematic names for acyclic parent hydrides are given in RC-80.9.1 (mononuclear), RC-80.9.2 (polynuclear hydrocarbon), and RC-80.9.3 (polynuclear other than hydrocarbon).

Except for the descriptive method of naming radical ions (RC-85.1), these recommendations provide methods for describing specific structures of radicals, ions, radical ions, and related substances. Methods for naming radicals and ions whose structures are indefinite are not included in these

<sup>\*</sup> Operational suffixes are affixes attached to the end of the name of a parent hydride or functional suffix to indicate that the number of substitutable hydrogen atoms is different from that implied by the parent name or suffix name, for example, "-ium", "-ylium", "-ide", and the traditional subtractive suffixes such as "-yl", "-ene", and "-yne".

	Operation		Suffix		Substituent Prefix Ending*
1.	Addition of H <sup>+</sup>		-onium -ium		-oniumyl -iumyl
	EH <sub>x</sub>	<u>+H</u> +	$[EH_{x+1}]^+$	-H•	[EH <sub>x</sub> ] +
	SH2 sulfane	<u>+</u> H <sup>+</sup> →	[SH3] <sup>+</sup> sulfonium	- <u>H</u> •	-{SH <sub>2</sub> } <sup>+</sup> sulfoniumyl
	CH4 methane	<u>+H</u> +	[CH <sub>5</sub> ] <sup>+</sup> methanium	- <u>H</u> •	[CH4]+ methaniumyl
	C <sub>5</sub> H <sub>5</sub> N pyridine	<u>+</u> H <sup>+</sup> →	[C5H6N] <sup>+</sup> pyridinium	-H•	
2.	Loss of H <sup>+</sup>		-ide		-idvl
	EH <sub>x</sub>	H <sup>+</sup>	[EH <sub>x-1</sub> ] <sup>-</sup>	- <u>H</u> •	[EH <sub>x-2</sub> ]-
	PH3 phosphane	- <u>H</u> +	[PH <sub>2</sub> ] <sup>-</sup> phosphanide	-H•	— [PH] <sup>-</sup> phosphanidyl
	$CH_4$ methane	<u>-</u> H <sup>+</sup> →	[CH3] <sup>-</sup> methanide	<u>-H•</u>	[CH <sub>2</sub> ]- methanidyl
	b.**		-ate		<b>-ato</b> ***
	R-E(X) <sub>x</sub> H <sub>y</sub>	- <u>y</u> H <sup>+</sup>	[R-E(X) <sub>x</sub> ] <sup>y-</sup>	-R•	[E(X) <sub>x</sub> ]Y-
	CH3-SO3H methanesulfonic acid	<u>-</u> H <sup>+</sup> →	[CH3-SO3] <sup>-</sup> méthanesulfonate		[SO <sub>3</sub> ]- sulfonato
	c.**		-ate		-ido
	R-XH	<u>−H</u> +	R-X-	- <u>R</u> •	
	CH3-SH methanethiol	<u>−</u> H <sup>+</sup>	CH3-S <sup>-</sup> methanethiolate	-CH3•	S- sulfido

## TABLE 1: Suffixes and Substituent Prefix Endings for Describing Radical and Ionic Centers

\* Although these prefixes are illustrated here for a mononuclear species, it is understood that the free valency need not reside at the ionic or radical center.

\*\* X = O, S, Se, Te

\*\*\* Used for acid characteristic groups only, attachment being through the characteristic atom, for example,  $-CO_2^-$ , carboxylato.

	Operation		Suffix		Substituent Prefix Ending
з.	Addition of H <sup>-</sup>	_	-uide	_	-uidyl
	EH <sub>X</sub>	+H <sup>-</sup>	[BH <sub>x+1</sub> ] -	-H•	[ EH <sub>x</sub> ] -
	BH3 borane	<u>+H</u> -	[BH4] <sup>-</sup> boranuide*	<u>-H●</u>	[BH3]- boranuidyl
4.	Loss of H <sup>-</sup>		-ylium		-yliumyl
	EH <sub>x</sub>	<u>-H</u> -	$[EH_{x-1}]^+$	-H•	[EH <sub>x-2</sub> ]+
	CH4 methane	<u>H<sup>-</sup></u> →	[CH3] <sup>+</sup> methylium	<u>−H•</u>	[CH2] <sup>+</sup> methyliumyl
5.	Loss of H.		-yl		yloyl
	EHx	<u>-H•</u>	[EH <sub>x-1</sub> ] •	<u>-H•</u>	[EH <sub>x-2</sub> ]•
	CH4 methane	<u>−H•</u>	[CH3] <sup>•</sup> methyl	-H•	[CH <sub>2</sub> ]• ylomethyl

TABLE 1: Suffixes and Substituent Prefix Endings......(cont'd.)

\* In inorganic nomenclature, this anion is named tetrahydroborate (1-)<sup>6a</sup>.

recommendations. In the absence of specific IUPAC recommendations, various methods have been used, such as omission of locants and the use of descriptive phrases, sometimes preceding, but usually following the name of the neutral parent structure, as illustrated by the following examples. Examples\*:

1. Removal of electrons.

[CH2=CH-CH3].+

propene radical cation

2. Addition of electrons.

a.



naphthalene radical anion

<sup>\*</sup> In these recommendations, a radical ion in an empirical formula is denoted by a superscript dot followed by the appropriate charge sign<sup>7</sup>. It is recognized that in mass spectroscopy the opposite sequence is used<sup>8</sup>, following well-established tradition in that field.



3. Removal of hydride ions.

$$\begin{bmatrix} 6 & 7 & 1 \\ 5 & 4 & 3 \end{bmatrix}^{+}$$

$$3H-benzo[d][1,2,3]dithiazole ion(1+)$$

$$3H-1,2,3-benzodithiazole ion(1+)$$

4. Removal of hydrons\*.

$$\begin{bmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}$$
 pentane-2,4-dione ion(1-)  
$$\begin{bmatrix} CH_3 - C & -CH_3 \\ 2 & 3 & 4 & 5 \end{bmatrix}$$
 acetylacetonate ion

5. Addition of hydrons\*



3 2 C2H5 Han 4 1 NHa • HCI bis(N, N-dimethylthiazolidin-2-amine)
sulfate\*\*
bis[2-(dimethylamino)thiazolidine]
sulfate\*\*

2-ethylbenzene-1,4-diamine monohydrochloride\*\*

6. Zwitterions (internally compensating charges).

a.

a.

b.

0  $\frac{1}{4}$   $N^{2}$   $N^{3}$   $H_{F}C_{0}$   $C_{4}H_{1}$ 

3,4-diphenyl-1,2,3-oxadiazolidin-5-one zwitterionic didehydro derivative

\* The name hydron is a generic name for the hydrogen cation, i.e., the naturally occurring mixture of protons, deuterons, and tritons<sup>9</sup>. The name proton is restricted to the hydrogen cation having the mass number 1, i.e.,  $^{1}$ H<sup>+</sup>.

\*\* When the counterion is unknown, terms like "conjugated monoacid" or "hydronated" have been used. When the hydrons have been "substituted", i.e., the unknown cationic center is an "onium" center, terms like "methiodide" and "ethochloride" have been used. However, descriptions like "addition compound of....with methyl iodide" or "....with iodomethane" are preferred.





-O<sub>2</sub>C 4 (4-carboxy-2-hydroxyphenyl)trimethyl-ammonium hydroxide inner salt 4-carboxy-2-hydroxy-N, N, N-trimethylanilinium hydroxide inner salt

#### RECOMMENDATIONS

RC-80. Some general principles of IUPAC organic nomenclature used in these recommendations\*

RC-80.1. Locants for suffixes indicating positions of operation or substitution in a parent hydride are to 'be placed preferably directly before the suffix to which they refer in uncontracted names, for example, but-2-ene, naphthalene-1,4-disulfonic acid, azulen-2-yl, and 9,10-butanoanthracen-2yl. However, in contracted names such locants preferably precede the name, for example, 2-anthryl.

Note: In the 1979 IUPAC Organic Rules, locants are cited before such suffixes only when other locants appear in front of the name of the parent hydride, for example, 3H-indol-2-yl<sup>2d</sup>.

RC-80.2. The subtractive suffixes "-ene", "-yne", etc., and hydro prefixes are used in the manner prescribed by the system in use for designating unsaturated or saturated positions in parent hydrides 3b, 4b, 10a, 11a.

Note 1: Radical or ionic positions are preferred to positions of unsaturation expressed by the subtractive suffixes for assigning low locants, when there is a choice. This is consistent with principles in the 1979 IUPAC Organic Rules<sup>2e</sup>. However, the hierarchy of structural features of organic compounds for numbering preferences is under further study by the Commission and changes may be incorporated in future recommendations.

Note 2: Although the 1979 IUPAC Organic Rules provide that hydro prefixes may be either detachable or nondetachable<sup>2f</sup>, in these recommendations and in the first part of a complete revision of the 1979 edition $^5$ they are treated as nondetachable. Although at this time the Commission favors treatment of hydro prefixes as nondetachable, this principle has important implications for the numbering of organic structures and is therefore under continued study by the Commission.

RC-80.3. Indicated hydrogen is used in the manner given in the 1979 IUPAC Organic Rules for parent hydrides<sup>10b,11b</sup> and for principal characteristic groups and free valence positions ("added hydrogen")<sup>2g</sup>.

Note: The concepts of indicated and "added" hydrogen are under study by the the Commission.

<sup>\*</sup> For convenience, modifications to the 1979 IUPAC Organic Rules $^1$  to be included in the first part of a complete revision of the 1979 edition<sup>5</sup> that are used in these recommendations are outlined here briefly.

**RC-80.4.** All neutral substituents of radical or ionic parent hydrides are expressed by the usual prefixes of organic nomenclature<sup>1,5</sup>. In other words, suffixes expressing neutral characteristic groups are not added to names of radical or ionic parent hydrides. However, suffixes expressing ionic characteristic groups can be added to names of ionic parent hydrides (see RC-82.5.4, RC-83.4.4, and RC-84.1.2), and suffixes expressing neutral or ionic characteristic groups may be added to names of zwitterionic parent hydrides (see RC-84.1.1).

Note: The principle maintained by this recommendation is that the name of a radical should end with a radical suffix and the name of a nonradical ionic compound should end with an ionic suffix.

RC-80.5. The operational suffixes "-ylene" $^{10c}$ , "-ylidene" $^{3c,10d}$ , and "-ylidyne" $^{10e}$  used in Sections A and B of the 1979 IUPAC Organic Rules<sup>1</sup> are retained in these recommendations, but with restricted meanings. The suffix "-ylene" is used to describe the substituent groups  $-CH_2-$  (methylene),  $-CH_2-CH_2-$  (ethylene), and  $-C_6H_4-$  (phenylene) only; methylene is used only when two bonds from the CH<sub>2</sub> group are not attached to a single atom of a parent structure. The suffixes "-ylidene" and "-ylidyne" are used to describe groups in which two and three hydrogen atoms, respectively, have been removed from the same skeletal atom of a parent structure, thereby describing the presence of a double or triple bond, respectively, between the substituting group and a parent structure or a parent substituent.

**RC-80.6.** Substituent acyl groups derived from organic acids are expressed by prefixes derived from the name of the acid, for example, cyclohexanecarbonyl (from cyclohexanecarboxylic acid), and phenylphosphonyl (from phenylphosphonic acid); however, this concept is still under study by the Commission.

Note: In the 1979 IUPAC Organic Rules, acyl groups as substituents are expressed by means of trivial names or by compound prefixes<sup>2h</sup>, for example, acetyl and cyclohexylcarbonyl.

**RC-80.7.** Sulfenic acid<sup>2i</sup>, selenenic acid<sup>2j</sup>, and related names, such as sulfenamide and sulfenyl, are not recommended in the first part of a complete revision of the 1979 edition of the IUPAC Organic Rules<sup>5</sup>, and therefore are not used in these recommendations.

RC-80.8. Substituent prefixes derived from acyclic parent hydrides. In these recommendations, a substituent prefix derived from an acyclic parent hydride named by the full systematic procedure, i.e., by replacement of the final "e" of the parent hydride name by suffixes such as "-yl" and "-ylidene" or by adding suffixes such as "-diylidene" and "-diyl" to the parent hydride name, may designate free valences at any position along an unbranched chain. This procedure is consistent with that given in Section D of the 1979 IUPAC Organic Rules<sup>4C,10f</sup> and supersedes the procedure given in Section A<sup>10</sup>G of the 1979 IUPAC Organic Rules and the ACS recommendations for naming silanes<sup>12a</sup>, in which the principal chain must terminate at the free valence position. It must be noted that this procedure requires the citation of the locant "1" when the free valence position is at a terminal chain position, for example, propan-1-yl. However, use of "contracted" substituent prefix names, for example, propyl, still defines the free valence at a terminal position of the chain and no locant need be cited; thus, the names propyl and propan-1-yl are synonymous for CH<sub>3</sub>-CH<sub>2</sub>-CH<sub>2</sub>--, and the names isopropyl and propan-2-yl are synonymous for (CH<sub>3</sub>)<sub>2</sub>CH--.

The names for the substituent groups HS-, HSe-, and HTe- as prefixes are "sulfanyl-", "selanyl-", and "tellanyl-" in these recommendations, rather than "mercapto-"<sup>2k</sup>, "hydroseleno-"<sup>2</sup>j, (and presumably "hydrotel-luro-"<sup>2m</sup>), as in the 1979 IUPAC Organic Rules<sup>1</sup>.

#### RC-80.9. Systematic names for acyclic parent hydrides

**RC-80.9.1.** Names for mononuclear parent hydrides of twenty-one elements for use in systematic substitutive nomenclature are given in Table 2.

Note: Except for BiH<sub>3</sub>, CH<sub>4</sub>, and the chalcogen hydrides, these names are formed by adding "ne" to the replacement ("a") prefixes<sup>3d,4d</sup>. Because of conflicts with Hantzsch-Widman names for heteromonocycles<sup>3e,11</sup>, stems for mononuclear hydrides of bismuth and the chalcogen elements are "bismuth", "oxid", "sulf", "sel", "tell", and "pol".

TABLE 2. Nan Sys	temati	r mononuclear ic Substituti	ve No	nt Hyaride menclature	s 1n	IUPAC
BH <sub>3</sub> borane CH <sub>4</sub> methane SiH <sub>4</sub> silane GeH <sub>4</sub> germane SnH <sub>4</sub> stannane PbH <sub>4</sub> plumbane	NH3 PH3 AsH3 SbH3 BiH3	azane* phosphane arsane stibane bismuthane	OH <sub>2</sub> SH <sub>2</sub> SeH <sub>2</sub> TeH <sub>2</sub> POH <sub>2</sub>	oxidane sulfane selane tellane polane	FH ClH BrH IH AtH	fluorane chlorane bromane iodane astatane

\* "Amine" is used as a substitutable parent hydride name for  $NH_3$ in one of the traditional methods for naming amines<sup>2n</sup>. However, it is not used as such in these revised recommendations.

**RC-80.9.2.** Polynuclear hydrocarbons<sup>10h</sup>. The names ethane, propane, and butane for the unbranched saturated acyclic hydrocarbons  $C_{2H_6}$ ,  $C_{3H_8}$ , and  $C_{4H_{10}}$  are retained. The names for higher polynuclear unbranched saturated hydrocarbons are formed by combining a numerical prefix equal to the number of carbon atoms in the chain with the ending "ane", for example, pentane, icosane, and tritriacontane.

**RC-80.9.3.** Names for **polynuclear acyclic parent hydrides other than hydrocarbons** are formed by adding a numerical prefix equal to the number of atoms of the element in the chain to the name of the mononuclear hydride in RC-80.9.1<sup>4e</sup>, for example, disilane, triazane, tetrasulfane.

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RC-80.10. Radicofunctional nomenclature<sup>2</sup>P. Since this system of nomenclature is deemphasized in the the first part of a revision of the 1979 edition of the IUPAC Organic Rules<sup>5</sup>, radicofunctional nomenclature, or that which might be considered as such in origin, for example, methylamine, will not be used for naming derived radicals or ions in these recommendations. However, the radicofunctional method for naming ions, i.e., the citation of the class name "cation" or "anion" as a separate word following the name of the radical, is included, but only as a less preferred alternative. Although useful for simple ions, its value for describing complex polyionic structures is severely reduced because prefix names for indicating ionic substituents cannot be generated.

**RC-80.11.** Multiplicative nomenclature. Two methods extensively used for naming assemblies of identical units that involve divalent or multivalent substituent prefix names will be used in these recommendations.

One method, codified in the 1979 IUPAC Organic Rules<sup>2</sup>9, multiplies only identical parent compounds, i.e., parent hydrides and a principal characteristic group, if any. This method requires that a connecting multipart divalent or polyvalent substituent prefix name be symmetrical. Substituents to the parent hydride, other than the principal characteristic group, are expressed by prefixes cited in front of the divalent or multivalent substituent prefix name.

The other method, used in CAS index nomenclature<sup>13a</sup>, multiplies two or more identical parent hydrides and all attached substituents, including principal characteristic groups, if any. In this method, all substituents attached to the parent hydride must be symmetrically positioned.

Note: Prior to 1972 (Volume 76), unsymmetrical two-part multiplying substituent prefix names were also permitted in CAS index nomenclature.

Example:



*IUPAC name:* 6,6'-dichloro-3,3'-(methylenedioxy)dibenzoic acid *CAS name:* 3,3'-[methylenebis(oxy)]bis[6-chlorobenzoic acid]

#### RC-81. Radicals (replaces C-81<sup>1</sup>)

**RC-81.0.** Introduction. For the purposes of organic nomenclature, a parent radical is a molecular compound formally derived by the removal of one or more hydrogen atoms from one or more atoms of a parent hydride, a parent compound, or a hydro derivative of either. An atom at which the resulting (nonbonding) electron(s) is(are) considered to reside is called a radical center. An atom with one free (nonbonding) electron is a monovalent radical center; an atom with two (or three) free (nonbonding) electrons, which may be paired, i.e., having antiparallel spins (singlet), or unpaired,

i. e., having parallel spins (triplet), but which cannot be nonbonding electron pairs ("lone pairs") of that atom in the parent structure is called a divalent (or trivalent) radical center. A parent radical with two or more monovalent radical centers is called a diradical, triradical, etc.

#### RC-81.1. Radical Centers in Parent Hydrides

RC-81.1.1. Monovalent radical centers in saturated acyclic and monocyclic hydrocarbons, and the mononuclear EH<sub>4</sub> parent hydrides of the carbon family. A monovalent radical center derived formally by removal of one hydrogen atom from a terminal atom of a saturated, unbranched acyclic hydrocarbon; from an atom of a saturated monocyclic hydrocarbon; or from any of the mononuclear parent hydrides methane (CH<sub>4</sub>), silane (SiH<sub>4</sub>), germane (GeH<sub>4</sub>), stannane (SnH<sub>4</sub>), or plumbane (PbH<sub>4</sub>) is named by replacing the "-ane" ending of the name of the parent hydride by "-yl"<sup>4f,10i</sup>. Examples:

H₃C∙	methyl
H₃Ge∙	germyl
$\begin{array}{c} CH_3 - CH_2 - \dot{C}H_2 \\ 3 \qquad 2 \qquad 1 \end{array}$	propyl
<u>с</u> н	cyclobutyl
сн₃—с́н—сн₃	1-methylethyl propan-2-yl (see RC-81.1.2 and RC-80.8) isopropyl (traditional name; see item 1, Appendix, List A)

RC-81.1.2. Monovalent radical centers in parent hydrides other than those described by RC-81.1.1. A radical center formally derived by the removal of one hydrogen atom from any position\* of a parent hydride, except as provided by RC-81.1.1 above, is named by adding the operational suffix "-yl" to the name of the parent hydride, eliding the final "e" of the name of the parent hydride, if present. The trivial name phenyl<sup>10</sup>], and the abbreviated (or contracted) names naphthyl, anthryl, phenanthryl<sup>10k</sup>; furyl, pyridyl, piperidyl, quinolyl, isoquinolyl, thienyl<sup>3f</sup>; and hydrazyl<sup>2r</sup> are retained. Locants describing the position of the radical center for these abbreviated names are placed in front of the names (see RC-80.1).

Note 1: The systematic names phosphane and arsane4g, 6b must be used

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<sup>\*</sup> This recommendation is consistent with the generalized principles for naming and numbering acyclic substituent prefixes as given in Section D of the 1979 IUPAC Organic Rules<sup>4</sup>C,<sup>10</sup>f rather than the principles of Section  $A^{10}$ g and the ACS silicon rules<sup>12</sup>a, where the principal chain must terminate at the free valence position (see also RC-80.8).

for naming the radicals derived from the mononuclear parent hydrides PH<sub>3</sub> and AsH<sub>3</sub> according to this recommendation, because use of the traditional names phosphine and arsine<sup>4</sup>g, <sup>6</sup>b will generate the names phosphinyl<sup>12b</sup> and arsinyl<sup>13b</sup>, which are traditional prefix names for the oxo phosphoric and arsenic acid groups H<sub>2</sub>P(O) — and H<sub>2</sub>As(O) —, respectively, as substituents. Even though the names phosphinoyl and arsinoyl are recommended in the 1979 IUPAC Organic Rules for these groups<sup>4</sup>h, ambiguity would still exist.

Note 2: The traditional names phosphino, arsino, stibino, and bismuthino<sup>41</sup> are less acceptable alternative names for the radicals  $H_2\ddot{P}^{\bullet}$ ,  $H_2\ddot{A}s^{\bullet}$ ,  $H_2\ddot{S}b^{\bullet}$ , and  $H_2\ddot{B}i^{\bullet}$ .

Note 3: The name "aminyl" for the parent radical  $H_2N^{\circ}$  used in the 1979 IUPAC Organic Rules<sup>2</sup>r is continued in these recommendations as an alternative to "azanyl", derived from the parent hydride name azane<sup>6b,14</sup>, even though "amine" is not used as a parent hydride name for NH<sub>3</sub> herein\* (see also footnote to Table 2 in RC-80.9.1).

Note 4: The names of the radicals  $HO^{\circ}$  and  $HO-O^{\circ}$  are hydroxyl<sup>6C</sup> and hydroperoxyl<sup>2S</sup>, respectively, but, in keeping with tradition, are not used as parent radical names in these recommendations. For names of such "substituted" radicals, see RC-81.2.4.

Examples:

HË•	sulfanyl (trivial name: mercapto** <sup>2k</sup> )
H <sub>2</sub> N•	<pre>azanyl*** } (traditional name: amino) aminyl</pre>
H₂B∙	boranyl (previously <sup>4j</sup> and in inorganic nomenclature recommendations <sup>6d</sup> , boryl)
(CH <sub>3</sub> ) <sub>3</sub> C—O—Ρໍ(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub>	[(2-methylpropan-2-yl)oxy]triphenyl-λ <sup>5</sup> - phosphanyl <sup>16</sup> (see RC-80.8) <i>tert</i> -butoxytriphenylphosphoranyl <sup>4k</sup> (see RC-80.8)
SiH <sub>3</sub> —ŠiH — SiH <sub>3</sub> 3 2 1	trisilan-2-yl

\*\* The name mercapto is not used as a parent radical name in these recommendations. For names of such "substituted" radicals, see RC-81.2.5. \*\*\* The trivial name amidogen is used for  $H_2\ddot{N}^{\circ}$  in CAS index nomenclature<sup>13C</sup>.

<sup>\*</sup> Although the name "amine" would be quite consistent with parent hydride names, such as phosphine and arsine, and is used as such by Beilstein, it is not used as a parent hydride name in these recommendations because it has also been added to the name of a radical to form the name of a parent compound<sup>15</sup>, for example butylamine. In these recommendations, the term "amine" is used only as a suffix to denote the attachment of the  $-NH_2$ group to a parent hydride, for example, pyridin-2-amine.

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**RC-81.1.3.** Divalent and trivalent radical centers in a neutral parent hydride are derived formally by the removal of two or three hydrogen atoms from the same skeletal atom of a parent hydride, a parent compound, or a hydro derivative of either.

Nomenclature methods for describing divalent and trivalent radical centers are complicated by current definitions of the term "radical"<sup>7,17</sup>. According to these definitions and many experts in the field, the free (nonbonding) electrons of a radical must be unpaired and therefore a divalent radical center in which the free (nonbonding) electrons are paired (singlet state) is not considered to be a radical. Hence, there is objection to the use of "radical suffixes", such as "-diyl" and "-ylidene", to describe such divalent radical centers. However, in these recommendations, the radical suffixes "-ylidene" and "-ylidyne" are used to describe divalent and trivalent radical centers regardless of the electronic state of the free (nonbonding) electrons. Alternative suffixes, such as "-ylidene" and "-diyl", should not be used to differentiate between a singlet and a triplet state. If necessary, such a distinction should be made by adding the separate word "singlet" or "triplet" to the name of the divalent radical.

**RC-81.1.3.1.** Carbones, carbynes, nitrenes, and silylenes. Divalent radical centers derived formally by the removal of two hydrogen atoms from the mononuclear parent hydrides  $CH_4$ ,  $NH_3$ , and  $SiH_4$ , i.e.,  $H_2^C$  and/or  $H_2^C$ ; HN: and/or HN:, and  $H_2Si$  and/or  $H_2Si$ ;, respectively, may be named carbone (or methylene)<sup>2t</sup>, nitrene\* (or aminylene<sup>2r</sup>), and silylene\*\*, respectively. The mononuclear parent hydride derived formally by removal of three hydrogen atoms from  $CH_4$ , i.e.,  $HC^{\circ}$  and/or HC:, may be named carbyne. Derivatives of these parent hydrides are named according to the usual principles of substitutive nomenclature.

Note: A generally accepted principle of substitutive nomenclature does not allow a structure containing a carbene carbon atom in a carbon chain or ring to be named as a derivative of carbene or methylene; therefore, such structures should be named according to RC-81.1.3.2 or RC-81.1.3.3, below. However, such radicals are included in the general class known as carbenes.

Examples:

(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> ¢ and/or (C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> c:	diphenylcarbene diphenylmethylene
(CH <sub>3</sub> -0-CO) <sub>2</sub> ¢ and/or (CH <sub>3</sub> -0-CO) <sub>2</sub> C:	bis(methoxycarbonyl)- carbene
	bis (methoxycarbonyl) - methylene
ou i and (an ou ii)	methylnitrene
CH <sub>3</sub> —N: and/or CH <sub>3</sub> —N:	methylaminylene
$C_6H_5$ — $CH_2$ — $SiH$ and/or $C_6H_5$ — $CH_2$ — $SiH$	benzylsilylene
c <sub>6</sub> H₅—ċ• and/or c <sub>6</sub> H₅—ċ:	phenylcarbyne

<sup>\*</sup> The name nitrene is widely used in the literature; the name imino also has been used. The trivial name imidogen is used in CAS index nomencla-ture<sup>13c</sup>.

<sup>\*\*</sup> Because the compound  $CH_2=SiH_2$  is quite well known in the literature as silene<sup>18</sup>, this name cannot be used for the mononuclear parent radical  $H_2Si_a^{\dagger}$  and/or  $H_2Si_a^{\bullet}$ . The name "silylene"<sup>12a</sup> is widely used in the literature and in CAS index nomenclature<sup>13c</sup>.

RC-81.1.3.2. Divalent and trivalent radical centers other than those described by RC-81.1.3.1 derived formally by the removal of two or three hydrogen atoms from the same skeletal atom of a parent hydride or a hydro derivative may be described by using an operational suffix "-ylidene" or "-ylidyne" in the same way as prescribed for the suffix "-yl" in RC-81.1.1 and RC-81.1.2.

Note: Although the traditional names methylene<sup>2t</sup>, aminylene<sup>2r</sup>, and silylene<sup>12a</sup>, are used in RC-81.1.3.1 above, the suffix "-ylene" for describing other divalent radical centers is no longer recommended (see RC-80.5).

Examples:

HP: and/or HP: phosphanylidene (the traditional name is phos- phosphinidene <sup>12b</sup> , but phosphinediyl accord- ing to the 1979 IUPAC Organic Rules <sup>4m</sup> )
H <sub>2</sub> N-N: and/or H <sub>2</sub> N-N: 2 i 2 i 2 i b 2 i b diazanylidene hydrazinylidene (traditional parent hydride name <sup>14</sup> ) (trivial name: hydrazono <sup>2u</sup> ) ( <b>not</b> aminonitrene)
H <sub>2</sub> P—P: and/or H <sub>2</sub> P—P: diphosphanylidene 2 1 2 1
$CH_2 = CH = \dot{C}H$ and/or $CH_2 = CH = \dot{C}H$ prop-2-en-1-ylidene 3 2 1 3 2 1
$C_{6}H_{5}-CH_{2}-\dot{C}-CI$ and/or $C_{6}H_{5}-CH_{2}-\ddot{C}-CI$ $2$ 1-chloro-2-phenylethylidene (not benzylchlorocarbene) $C_{6}H_{5}-CH_{2}-\ddot{C}-CI$
CF <sub>3</sub> -CO-Ċ-CF <sub>3</sub> and/or CF <sub>3</sub> -CO-Ċ-CF <sub>3</sub> (see RC-80.8) [3,3,3-trifluoro-2-oxo-1-(trifluoromethyl)- propylidene (see RC-80.8)
C. and/or C: cyclohexylidene
$\int_{6}^{2} \int_{5}^{3} \int_{6}^{4} \cdot \frac{1}{5} d \cdot \frac{1}{5} = \int_{6}^{2} \int_{5}^{3} \cdot \frac{1}{5} d \cdot \frac{1}{5} d \cdot \frac{1}{5} = \int_{6}^{2} \int_{5}^{3} \cdot \frac{1}{5} d \cdot \frac{1}$

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3-phenyl-2-[phenyl(trimethylsilyl)methyl]-4,4-bis(trimethylsilyl)-1-silacyclobut-2-en-1-ylidene\* (replacement name<sup>3g</sup>) 3-phenyl-4-[phenyl(trimethylsilyl)methyl]-2,2-bis(trimethylsilyl)-1,2-dihydrosilet-1-ylidene\* (Hantzsch-Widman name<sup>3e,11</sup>)

 $CH_3 - CH_2 - \dot{C} \cdot and/or CH_3 - CH_2 - \dot{C} \cdot propylidyne$ 3 2 1 3 2 1

**RC-81.1.3.3.** The  $\lambda$ -convention<sup>16</sup> (alternative to RC-81.1.3.1 and RC-81.1.3.2). 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 a standard valence state\*\* may be described by the  $\lambda$ -convention<sup>16</sup>. Locants for the radical centers are followed by the symbol  $\lambda^n$ , where *n* is the bonding number of the skeletal atom, i.e., the sum of the total number of valence bonds to adjacent skeletal atoms, if any, and the number of attached hydrogen atoms.

Examples:

 $c_{l_2}\dot{c}$  and/or  $c_{l_2}c$ :  $c_{gH_5}-\dot{N}$ : and/or  $c_{gH_5}-\ddot{N}$ : phenyl- $\lambda^1$ -azane F $\dot{c}$ . and/or F $\dot{c}$ : fluoro- $\lambda^1$ -methane

<sup>\*</sup> The trivial name "benzyl" is not used as a substituent prefix when  $\alpha$ -substituted (see footnote to item 17 in the Appendix, List A).

<sup>\*\*</sup> Use of the  $\lambda$ -convention<sup>16</sup> to describe a radical center derived by the loss of two hydrogen atoms from a skeletal atom that is in a valence state higher that the standard one is ambiguous because it would not be clear whether the name was describing a standard valence state or a divalent radical center derived from the higher valence state. However, the use of the  $\lambda$ -convention to describe a radical center that is in a lower valence state than the standard one may be useful for naming radical ions (see RC-85.2).

 $CH_2 = CH - \dot{C}H \quad and/or \quad CH_2 = CH - \dot{C}H$ 1λ<sup>2</sup>-prop-2-ene  $5\sqrt[6]{7}$  and/or  $5\sqrt[6]{7}$  c: 2λ<sup>2</sup>-bicyclo[2.2.1]hept-5-ene

RC-81.1.4. Nondetachable hydro prefixes vs. added (indicated) hydrogen. A radical center at a position in a cyclic parent hydride having the maximum number of noncumulative double bonds where there is an insufficient number of hydrogen atoms to apply directly the recommendations for the use of "-yl" or "-ylidene" given above is derived formally from a dihydro derivative of the cyclic parent hydride. Such a radical center may be described by using nondetachable hydro prefixes<sup>2f</sup> (see also RC-80.2) or by applying the principle of indicated (added) hydrogen<sup>2g</sup> (see RC-80.3). In the latter 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 an italic capital H(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 unsaturated parent hydride immediately after the locant for the radical center\*. Example:



 $5 \int_{N}^{S} \frac{2}{3} \frac{2}{N} \frac{2}{3} \frac{2}{3} \frac{1}{3} \frac{2}{3} \frac{1}{3} \frac{2}{3} \frac{1}{3} \frac{1}{3}$ 

RC-81.1.5. A number of trivial and abbreviated names, other than those given in RC-81.1.2, above, have a long and well-established usage for expressing substituent groups as prefixes and for naming radicals; therefore they are recognized throughout the 1979 IUPAC Organic Rules<sup>1</sup>. Although each of these groups can be named easily by the systematic methods given above, their trivial or abbreviated names are acceptable as names for radicals and are given in the Appendix.

RC-81.2. Radical centers on characteristic groups. Although radical centers located on characteristic groups can be described on the basis of parent radicals derived from parent hydrides as given above in RC-81.1, it is often much more convenient and/or desirable to describe a radical center on. the basis of a larger parent structure, such as a parent hydride together

<sup>\*</sup> This procedure is exactly analogous to the use of "indicated hydrogen" to describe saturated ring positions that remain after the introduction of suffixes for principal characteristic groups, such as "-one", into the name of a parent ring or ring system that otherwise expresses the maximum number of noncumulative double bonds $^{2g}$ .

with a principal characteristic group, or to use names that have become established in the literature. The following subsections provide recommendations for describing radical centers on some, but not all, of the characteristic groups of substitutive nomenclature.

**RC-81.2.1. Established or traditional names**. Names for describing radical centers on certain characteristic groups have become established in the literature. Some of these "traditional" names follow the recommendation given in the 1979 IUPAC Organic Rules<sup>2t</sup>, whereby an "1" is added to the name of the substituent prefix for the characteristic group, if a terminal "1" is not already present. Thus,  $HO_2C^{\circ}$  is "carboxyl"<sup>19</sup>; Hö<sup>o</sup> and Höö<sup>o</sup> are "hydroxyl"<sup>6C</sup> and "hydroperoxyl"<sup>2S</sup>, respectively, (see also Note 4 to RC-81.1.2); OC (and/or OCt) is carbonyl<sup>6C</sup>; OS: (and/or OSt) and O<sub>2</sub>S (and/or O<sub>2</sub>St) are "sulfinyl"<sup>2V, 6C</sup> and "sulfonyl"<sup>2V, 6C</sup>, respectively, and their selenium and tellurium analogs are quite analogous, for example, OSe: (and/or OSet) is "seleninyl"<sup>2</sup>J,<sup>6C</sup>; and "ClO<sub>2</sub> and •ClO<sub>3</sub> are chloryl<sup>6C</sup> and perchloryl<sup>6C</sup>, respectively. Contracted names, such as "acetoxyl" and "methoxyl", and even the term "oxyl" (see RC-81.2.4), may also be considered to have been derived in this manner.

A few other established names may be considered to have been derived from a substituent prefix name ending in "o", by replacing the "o" with "yl". Thus, NC• is "cyanyl"<sup>19</sup>; CN• is "isocyanyl"<sup>19</sup>; ON• and O<sub>2</sub>N• are "nitrosyl"<sup>6C</sup> and "nitryl"<sup>6C</sup>, respectively; •N<sub>3</sub> is "azidyl"\*<sup>19</sup>; and •ClO is "chlorosyl"<sup>6C</sup>. The name "aminyl"<sup>2r</sup> and the term "thiyl" (see RC-81.2.5) can also be considered as having been derived in this manner. However, this method cannot be classified as a general one, because it can easily lead to the same name for other groups. For example, replacing the "o" of sulfino", the substituent prefix name for HO<sub>2</sub>S—, by "yl" leads directly to the name for OS: (and/or OS:), given above; and the method cannot be applied to monovalent halo radicals, because the resulting names are the names for O<sub>2</sub>E— groups, for example, chloryl<sup>2w, 6C</sup>.

**RC-81.2.2.** Acyl radicals, i.e., radicals with at least one chalcogen or nitrogen atom attached to the radical center by a (formal) double bond and which may be considered to have been derived formally by the loss of the hydroxy group from all acid characteristic groups expressed by the name of the acid are named by replacing the "-ic acid" or "-carboxylic acid" ending of the name of the acid with -"yl", "-oyl", or "-carboxylic, according to the method for forming the name of the corresponding acid halide<sup>2x</sup>, 4n.

<sup>\*</sup> To avoid any possibility of ambiguity, it is only necessary to keep clearly in mind that this name is derived from "azido", the name for the  $N_3$  group as a substituent prefix, and not from "azide", the name for the  $N_3$ -anion. No confusion should occur if it is remembered that the azide anion lacks hydrogen atoms, which are necessary to generate the "-idyl" suffix for describing systematically an anionic substituent as a prefix (see RC-83.4.7.3).

Note: Compound prefixes for naming acyl substituents<sup>2h</sup> are not used in these recommendations for acyl radicals or ions (see RC-80.6). Examples:



RC-81.2.3. Radical centers on nitrogen atoms of amine, imine, amide, or imide characteristic groups.

**RC-81.2.3.1.** Monovalent radical centers. A monovalent radical center formally derived by the removal of one (or the) hydrogen atom from the nitrogen atom of an amine, imine, amide, or imide characteristic group is named by adding a suffix "-aminyl", "-iminyl", or "-amidyl", "-carboxamidyl", "-sulfonamidyl", "-dicarboximidyl", etc., to the name of the parent hydride attached to the characteristic group with the radical center, eliding the final "e", if any, from the name of the parent hydride; or by replacing the final "e" of a trivial name for an amine, imine, amide, or imide by "-yl". Note 1: Amides of carboximidic and sulfinimidic acids were named as amidines, carboxamidines, or sulfinamidines in the 1979 IUPAC Organic Rules<sup>2</sup>Y; the corresponding suffixes for monovalent radical centers on these suffixes would be "-amidinyl", "-carboxamidinyl", and "-sulfinamidinyl".

Note 2: Although not used in these recommendations for radical centers derived from amine, imine, or amide characteristic groups, the names "azanyl" and "aminyl"<sup>2</sup>r can be used as parent radical names in the same way that "amine" has been used as a parent hyride name for derivatives of ammonia (see also footnote to Table 2 in RC-80.9.1 and Note 3 to RC-81.1.2)

Note 3: Trivial and semisystematic names preferred for naming organic compounds according to IUPAC recommendations are used in the first cited names for the examples below.

#### Examples:

Сн₃—-й́н	methanaminyl
C <sub>e</sub> H <sub>s</sub> —ŇH	anilinyl
	benzenaminyl
сн₃—сн₂—сн ≕й•	propan-1-iminyl <sup>2z</sup> propylideneaminyl <sup>2aa</sup> (see Note 2, above)
(CH₃)₃P <b>≕</b> Ñ∙	trimethyl-λ <sup>5</sup> -phosphaniminyl <sup>2z,16</sup> (trimethylphosphoranylidene)aminyl <sup>2aa,4p,12b</sup> (see Note 2, above) trimethylphosphine imidyl <sup>12b</sup>
нсо <sup>й</sup> н	formamidyl
N. CO	

pyridine-2-carboxamidyl

с<sub>6</sub>н<sub>5</sub>—s—<u></u>м́—с<sub>6</sub>н<sub>5</sub>

N- (phenylsulfanyl) anilinyl N- (phenylsulfanyl) benzenaminyl (not N-phenylbenzenesulfenamidyl; see RC-80.7)

 $CH_{3} = S = N$  $H_{3} = C_{6}H_{5} = C_{6}H_{5}$ 



N' - (methylsulfanyl) -N- (phenylsulfanyl) benzenecarboximidamidyl (see Note 1
above)

succinimidyl
2,5-dioxopyrrolidin-1-yl (RC-81.1.2)

pyridine-2,3-dicarboximidyl
5,7-dioxo-5,7-dihydro-6H-pyrrolo[3,4-b]pyridin-6-yl (RC-81.1.2)

**RC-81.2.3.2.** Divalent radical centers. A divalent radical center formally derived by removal of both hydrogen atoms from an amine or amide characteristic group is named as a derivative of nitrene, aminylene (see RC-81.1.3.1), or  $\lambda^{1}$ -azane (see RC-81.1.3.3). Examples:



**RC-81.2.4.** Radical centers on oxygen atoms of acid, peroxy acid, hydroxy, or hydroperoxy characteristic groups. A radical center derived formally by the removal of the hydrogen atom from the oxygen atom of an acid, peroxy acid, hydroxy, or hydroperoxy characteristic group is named on the basis of a compound parent radical name formed by combining the name for the parent hydride or acid residue attached to the oxygen atom with the term "oxyl" or "peroxyl", for example, pentyloxyl, pentan-2-yl-peroxyl. The contracted forms methoxyl, ethoxyl, propoxyl, butoxyl, phenoxyl, acetoxyl, and aminoxyl are retained. Substituents to such compound parent radicals are expressed by prefixes in the usual manner. Except for the contracted forms noted above, the compound parent radical name is enclosed in parentheses or brackets (see third example below).

Note 1: The term peroxyl is more consistent with terms like peroxo, peroxy, and peroxide, even though "dioxyl" is used in the 1979 IUPAC Organic Rules<sup>2t</sup>.

Note 2: The names hydroxyl<sup>6C</sup> and hydroperoxyl<sup>2s</sup> for the radicals  $H\ddot{O}^{\bullet}$  and  $HO-\ddot{O}^{\bullet}$ , respectively (see also Note 4 to RC-81.1.2 and RC-81.2.1), are not used when the hydrogen atom has been substituted by another atom or group.

Examples:

CH3-Ö.methoxylCI-CH2-CO-Ö.chloroacetoxylCH3-O-CH2-CS-Ö.methoxy[(thioacetyl)oxyl]\*CH3-[CH2]4-CO-O-Ö.hexanoylperoxyl

<sup>\*</sup> The contracted form thioacetoxyl is not used because it could be ambiguous. Brackets enclose the compound parent radical name in the presence of the substituent since curves are used to unambiguously describe the structure in the name for the compound parent radical itself.

(CI—CH₂)₂N—Ö∙	bis(chloromethyl)aminoxyl*
сн₃—С(СН₃)₂ сн₃—С(СН₃)₂—С=N—Ö∙	<pre>(2,2,4,4-tetramethylpentan-3-ylidene)- aminoxyl* (see RC-80.8) (1-tert-butyl-2,2-dimethylpropylidene)- aminoxyl* (see RC-80.8)</pre>
H <sub>3</sub> C CH <sub>3</sub> 5 6 4 1N −Ö+ 3 7 H <sub>3</sub> C CH <sub>3</sub>	2,2,6,6-tetramethyl(piperidin-1-yloxyl)

RC-81.2.5. Radical centers on sulfur atoms of thio acid, thiol, or dithiohydroperoxy characteristic groups. Although a radical center formally derived by the removal of the hydrogen atom from the sulfur atom of a thio acid, thiol, or thio hydroperoxy characteristic group can be described in the same manner as a radical center on the corresponding oxygen characteristic group (see RC-81.2.4) using the terms "-thiyl" and "-perthiyl", usage in the literature is not consistent\*\* and therefore it is recommended that these radical centers be named on the basis of the parent radical names sulfanyl and disulfanyl (see RC-81.1.2). Examples:

сн₃—со—ӟ∙	acetylsulfanyl	
	acetylthiyl (by analogy with RC-81.2.4)	
C <sub>6</sub> H₅— S∙	phenylsulfanyl	
	phenylthiyl (by analogy with RC-81.2.4)	
	(not benzenesulfenyl; see RC-80.7)	
СН₃—С(СН₃)₂—Ѕ—Ё∙	(2-methylpropan-2-yl)disulfanyl (see RC-80.8)	
	tert-butyldisulfanyl (see RC-80.8)	
	tert-butylperthiyl (by analogy with RC-81.2.4)	
CI—CH₂—CS—Š∙	[chloro(thioacetyl)]sulfanyl	
	chloro[(thioacetyl)thiyl] (by analogy with	
	RC-81.2.4)	

**RC-81.2.6.** Radical centers on other characteristic groups. A radical center formally derived by the removal of hydrogen atoms from characteristic groups other than those described above in RC-81.2.1 through

<sup>\*</sup> Aminoxyl radicals are named by radicofunctional nomenclature in CAS index nomenclature by using the functional parent compound name "nitroxide" as a class name<sup>13c</sup>, for example, bis(chloromethyl) nitroxide.

<sup>\*\*</sup> For instance both the names benzenethiyl, presumably derived from benzenethiol, and phenylthiyl, by analogy with phenyloxyl, the uncontracted form of phenoxyl (see RC-81.2.4), are used.

RC-81.2.5 is named preferably on the basis of a parent radical named according to RC-81.1 above. Examples:

СН₃—СН₂—О—Ё∙	ethoxysulfanyl
c₅H₅—co—s—o—ö•	(benzoylsulfanyl)dioxidanyl benzoyl(sulfanylperoxyl) (see RC-81.2.4)
c <sub>6</sub> H₅—o—s—s—ö∙	(phenoxydisulfanyl)oxidanyl phenoxy(disulfanyloxyl) (see RC-81.2.4)
c <sub>6</sub> H₅—co—se∙	benzoylselanyl
й∙ Ш сн₃—с—он	(1-hydroxyethylidene)azanyl (1-hydroxyethylidene)aminyl 1-hydroxyethan-1-iminyl (see RC-81.2.3.1)
С <sub>6</sub> Н₅—С—О—СН₃ II N—№Н	2-[methoxy(phenyl)methylidene]hydrazyl*

#### RC-81.3. Multiple radical centers

RC-81.3.1. Polyradicals with radical centers on different skeletal atoms of parent hydrides or hydro derivatives formally derived by removal of one or more hydrogen atoms from each of two or more skeletal atoms are named by using the appropriate operational suffixes, "-yl", "-ylidene", and "-ylidyne", as prescribed by RC-81.1, each preceded by numerical prefixes, as needed, and the locant of the skeletal position for each of the hydrogen atoms removed. Examples:

-	
•CH <sub>2</sub> —ĊH <sub>2</sub> 2 1	ethane-1,2-diyl (traditional name: ethylene <sup>10</sup> P)
•NH — NH 2 1	diazane-1,2-diyl (traditional name: hydrazo <sup>2bb,13b</sup> )
$\cdot \begin{pmatrix} 5 & 6 \\ 4 & 1 \\ 3 & 2 \end{pmatrix}$ .	<pre>benzene-1,4-diyl (traditional names: p-phenylene     or 1,4-phenylene<sup>10</sup>9)</pre>
$ \overset{1}{\overset{2}{\overset{3}{\overset{3}{\overset{3}{\overset{3}{\overset{3}{\overset{3}{3$	7,8,9,10-tetrahydrocyclohepta[ <i>de</i> ]naphthalene- 7,10-diyl

<sup>\*</sup> The trivial name benzyl is not used as a substituent prefix when  $\alpha$ -substituted; see footnote to item 17 in the Appendix, List A.



 $\dot{C}H - - CH_2 - \dot{C}H - - CH_2 - \dot{C} \cdot \dot{C} \cdot \dot{C} + \dot{C}H_2 - \dot{C} \cdot \dot{C} + \dot{C} +$ 

pentan-3-yl-1-ylidene-5-ylidyne

**RC-81.3.2.** 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 of nomenclature for assemblies of identical units<sup>2</sup>q on the basis of a parent radical (see RC-81.1) using the multiplicative prefixes "-bis", "-tris", etc., where necessary to avoid possible confusion that may arise from the use of the numerical prefixes "di-", "tri-", etc.\*.

Polyacyl radicals are included in RC-81.2.2.

**Polyimide radicals** are named as polyradicals derived from heterocyclic ring systems (see RC-81.3.1).

Examples:

cyclopropane-1, 2-diyldimethyl

 $H_2\dot{C} \xrightarrow{6} \dot{C}H_2$  $H_2\dot{C} \xrightarrow{4} \dot{2} \dot{C}H_2$ 

benzene-1,2,4,5-tetrayltetramethyl

<sup>\*</sup> Accordingly, radical centers identically derived from two or more of the same characteristic group are not described in terms of that characteristic group using appropriate multiplicative prefixes.



- (a) IUPAC multiplicative method (see RC-80.11) octakis (pentachlorophenyl) [(1,2-dichloroethene-1,2-diyl) bis(2,4,6-trichlorobenzene-5,1,3-triyl)]tetramethyl\*
- (b) CAS multiplicative method (see RC-80.11)
   [(1,2-dichloroethene-1,2-diyl)bis(2,4,6-trichlorobenzene 5,1,3-triyl)]tetrakis[bis(pentachlorophenyl)methyl]\*



- (a) IUPAC multiplicative method (see RC-80.11) 4,4'-bis(methoxycarbonyl)-1,1'-ethylenebis(1,4-dihydropyridin-4-yl) (see RC-81.1.4)
  - 4,4'-bis(methoxycarbonyl)-1,1'-ethylenedipyridin-4(1*H*)-yl (see RC-81.1.4)
- (b) CAS multiplicative method (see RC-80.11)
  - 1,1'-ethylenebis[4-(methoxycarbonyl)-1,4-dihydropyridin-4-yl]
    (see RC-81.1.4)
    - 1,1'-ethylenebis[4-(methoxycarbonyl)pyridin-4(1H)-yl]
      (see RC-81.1.4)



- (a) IUPAC multiplicative method (see RC-80.11)
  3,3',5,5'-tetra-tert-butyl-N, N'-(1,3-phenylenedisulfonyl)dianilinyl (see RC-80.8)
  3,3',5,5'-tetrakis(2-methylpropan-2-yl)-N, N'-(1,3-phenylenedisulfonyl)bis(benzenaminyl) (see RC-80.8)
- (b) CAS multiplicative method (see RC-80.11)

N, N'-[1, 3-phenylenebis(sulfonyl)]bis[3, 5-di-tert-butylanilinyl] (see RC-80.8)

N, N'-[1, 3-phenylenebis(sulfonyl)]bis[3, 5-bis(2-methylpropan-2-yl)benzenaminyl] (see RC-80.8)

<sup>\*</sup> Since the benzenetriyl component of the multiplying prefix is not the central unit, it is numbered so that the pair of locants describing its attachment to the parent radical, methyl, are the lowest pair and, to reduce the possibility of ambiguity, are cited last, i.e., nearer to the name of the parent radical.



**RC-81.3.3.** Other polyradicals. Polyradicals in which all of the radical centers are in the same structure, but cannot be included in a parent radical derived from a parent hydride according to RC-81.1 (see RC-81.3.1) or by using multiplicative nomenclature (see RC-81.3.2), or when it may not be desirable to do so, are named by selecting as the parent radical that part of the structure containing the largest number of radical centers [see RC-81.3.3.2(a)]; the parts of the structure that contain the other radical centers are then expressed as prefixes.

**RC-81.3.3.1. Radical centers in substituent groups.** 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 attached directly, i.e., nondetachably, to the parent substituent prefix, which is derived by usual methods<sup>1,5</sup>. The removal of two or more hydrogen atoms from a substituent cited as a prefix is indicated by the appropriate numerical prefix, for example, "diylo-". The prefix "ylo-" is also used with prefixes normally used additively, such as oxy and carbonyl.

Examples:

—ċH₂	ylomethyl
— ö•	ylooxy ( <b>not</b> ylohydroxy)
	ylocarbonyl
-co-ö•	(ylooxy) carbonyl
— <u>ю</u> ́н	yloamino
$-1\sqrt[2]{4}_{6}^{3}$ .	4-ylophenyl
CH <sub>2</sub> CH <sub>2</sub> Ċ(CH <sub>3</sub> )[ <sup>1</sup> 1 2 3	CH <sub>2</sub> ] <sub>2</sub> —Ċ(CH <sub>3</sub> )—CH <sub>3</sub> 4–5 6 7

3,6-dimethyl-3,6-diyloheptyl (see RC-80.8)

**RC-81.3.3.2.** Choice of parent structure. Although any portion of a polyradical structure that can be named by the principles of these recommendations can be the parent structure, it is often useful to have some guidelines for making this choice. Thus, when necessary or desirable, a parent radical may be chosen by applying the following criteria in order until a definitive choice is attained:

- (a) the maximum number of radical centers of any kind in a single parent structure (see also RC-81.3.1);
- (b) the maximum number of radical centers that can be expressed by means of a multiplicative name (see also RC-81.3.2);
- (c) the maximum number of "senior" radical centers, according to the nature of the skeletal atom at which the radical center is considered to reside, in the same order as for the corresponding replacement prefixes<sup>3d</sup>,<sup>4d</sup>.

Further choice, if necessary, may be made by applying the general criteria for chains and rings given in the 1979 edition of the organic nomenclature rules<sup>2cc</sup>. Examples:



<sup>\*</sup> The practice of eliding a final "o" or "a" before a following vowel from certain fusion prefix names, as described by the footnote to Rule 21.4 in previous editions of the IUPAC Organic Rules<sup>1</sup>, will no longer be recommended in the forthcoming revision of the 1979 edition<sup>5</sup>.

<sup>\*\*</sup> In order to eliminate possible ambiguity, the locants of the divalent radical phenylene, a component of the multipart multiplying prefix but not the central component, are cited so that the locant "1", the position of attachment to the parent radical, oxidanyl, is nearer to its name.

$$\begin{pmatrix} \dot{\varphi}^{i}_{i} \downarrow_{\varphi}^{i}_{\varphi} & \text{and/or} & \dot{\varphi}^{i}_{i} \downarrow_{\varphi}^{i}_{\varphi} & \text{i:} & \text{and/or} & \overset{(CH}{i} \downarrow_{\varphi}^{i}_{\varphi} & \dot{\varphi}^{i}_{i} \\ [3-(diylomethyl)phenyl]nirphener \} (RC-81.1.3.1) \\ [3-(diylow-h^1-methanyl)phenyl]^{-h^1-azane} (RC-81.1.3.1) \\ (nitrene or mainylene or h^1-azane is preferred to carbene or methylene) \\ C_{eH_{5}} = \dot{\varphi} - (\wp C_{eH_{4}}) - \dot{\varphi} - (\wp C_{eH_{4}}) - \dot{\varphi} - C_{eH_{5}} \\ & \text{and/or} \\ C_{eH_{5}} = \dot{\varphi} - (\wp C_{eH_{4}}) - \dot{\varphi} - (\wp C_{eH_{4}}) - \ddot{\varphi} - C_{eH_{5}} \\ & \text{and/or} \\ C_{eH_{5}} = \dot{\varphi} - (\wp C_{eH_{4}}) - \ddot{\varphi} - (\wp C_{eH_{4}}) - \ddot{\varphi} - C_{eH_{5}} \\ & \text{and/or} \\ C_{eH_{5}} = \dot{\varphi} - (\wp C_{eH_{4}}) - \ddot{\varphi} - (\wp C_{eH_{4}}) - \ddot{\varphi} - C_{eH_{5}} \\ & \text{and/or} \\ C_{eH_{5}} = \dot{\varphi} - (\wp C_{eH_{4}}) - \ddot{\varphi} - (\wp C_{eH_{4}}) - \ddot{\varphi} - C_{eH_{5}} \\ & \text{and/or} \\ C_{eH_{5}} = \ddot{\zeta} - (\wp C_{eH_{4}}) - \ddot{\zeta} - (\wp C_{eH_{4}}) - \ddot{\zeta} - C_{eH_{5}} \\ & \text{and/or} \\ C_{eH_{5}} = \ddot{\zeta} - (\wp C_{eH_{4}}) - \ddot{\zeta} - (\wp C_{eH_{4}}) - \ddot{\zeta} - C_{eH_{5}} \\ & \text{and/or} \\ C_{eH_{5}} = \ddot{\zeta} - (\wp C_{eH_{4}}) - \ddot{\zeta} - (\wp C_{eH_{4}}) - \ddot{\zeta} - C_{eH_{5}} \\ & \text{and/or} \\ C_{eH_{5}} = \ddot{\zeta} - (\wp C_{eH_{4}}) - \ddot{\zeta} - (\wp C_{eH_{4}}) - \ddot{\zeta} - C_{eH_{5}} \\ & \text{and/or} \\ C_{eH_{5}} = \ddot{\zeta} - (\wp C_{eH_{4}}) - \ddot{\zeta} - (\wp C_{eH_{4}}) - \ddot{\zeta} - C_{eH_{5}} \\ & \text{and/or} \\ C_{eH_{5}} = \ddot{\zeta} - (\wp C_{eH_{4}}) - \ddot{\zeta} - (\wp C_{eH_{4}}) - \ddot{\zeta} - C_{eH_{5}} \\ & \text{and/or} \\ (diphenyl (diylomethylenedi-4, 1-phenylene) bis^{-} \\ (RC-81.1.3.1) \\ & \text{diphenyl} (diylomethylenedi-4, 1-phenylene) bis^{-} \\ (methylene)^{*} \\ (diphomyl (\lambda^2 - methanediyldi-4, 1-phenylene) bis [phenylcarbene]^{*} \\ (diylomethylenedi-4, 1-phenylene) bis [phenylcarbene]^{*} \\ (RC-81.1.3.3)^{*} \\ (b) CAS multiplicative method (see RC-80.11) \\ (diylomethylenedi-4, 1-phenylene) bis [phenylcarbene]^{*} \\ (RC-81.1.3.1) \\ & bis [4-(phenyl(diylomethyl)]phenyl] - \lambda^2 - methane] \\ RC-81.1.3.3) \\ \end{cases}$$

<sup>\*</sup> For locant order of phenylene see second footnote, preceding page.

RC-82. Cations [replaces C-82, C-83, C-85, C-551, C-816, C-921.6, C-931.1, C-973.1, C-974 (in part), D-1.63 (in part), D-5.3, and D-6.86<sup>1</sup>]

**RC-82.0.** Introduction. For the purposes of organic nomenclature, a cation is a molecular entity carrying at least one unit of positive charge formally derived from a parent hydride, a parent compound, or a hydro derivative of either, by the gain of one or more hydrons\*, by the loss of one or more hydride ions, or a combination of these operations. An atom at which 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.

RC-82.1. Cationic compounds with cationic centers derived formally by the addition of hydrons\*\*

RC-82.1.1. Cationic centers in parent hydrides

**RC-82.1.1.1.** Monocationic mononuclear parent cations. A parent cation derived formally by the addition of one hydron to a mononuclear parent hydride of the nitrogen, chalcogen, and halogen families (see RC-80.9.1) in its standard bonding number state<sup>16</sup> is named by adding the suffix "-onium" to a root for the element as shown in Table 3\*\*\*.

\* Hydron is a generic name for the hydrogen cation, i.e., the naturally occurring mixture of protons, deuterons, and tritons<sup>9</sup>. The name proton is restricted to the hydrogen cation having the mass number 1, i.e.,  $^{1}\mathrm{H}^{+}$ .

\*\* The procedure of RC-82.2.2.1 or RC-82.2.2.2 could be applied to skeletal atoms of parent hydrides in higher valence states that are described by the  $\lambda$ -convention<sup>16</sup>, but the method given here is preferred.

\*\*\* The term "carbonium" has long been used for a class of hydrocarbon cations derived formally by the loss of a hydride ion from a neutral hydrocarbon. More recently, the terms siliconium and even boronium have been used in an analogous manner. However, in organic nomenclature recommendations, these terms have not been used to name specific cations and they cannot now be used as a name for the cations  $H_5C^+$  or  $H_5Si^+$  by extending RC-82.1.1.1. These cations are to be named methanium and silanium, respectively, according to RC-82.1.1.2. Similarly, names such as carbenium and silenium have been used to describe classes of cations derived formally by addition of a hydron to the appropriate mononuclear divalent species (see RC-81.1.3.1). Except for the names carbenium, carbynium, and nitrenium, which may be used as alternatives to methylium (see RC-82.2.2.1), methyliumyl (see RC-85.2), and azanylium or aminylium (see RC-82.2.2.2), respectively, such names should not be used for naming specific compounds; they should be named according to RC-82.2.2.1 or RC-82.2.2.2, as appropriate. The general class name "carbocation" includes cationic hydrocarbons of both types. Modifying terms, such as tricoordinate and pentacoordinate, are added, if necessary, to differentiate between the two types.
TABLE 3. Names for Mononuclear Parent Cations in IUPAC

Systematic Substitutive Nomenclature					
$H_4N^+$ $H_4P^+$ $H_4As^+$ $H_4Sb^+$ $H_4Bi^+$	ammonium* phosphonium arsonium stibonium bismuthonium	H <sub>3</sub> O <sup>+</sup> H <sub>3</sub> S <sup>+</sup> H <sub>3</sub> Se <sup>+</sup> H <sub>3</sub> Te <sup>+</sup>	oxonium sulfonium selenonium telluronium	H <sub>2</sub> F <sup>+</sup> H <sub>2</sub> Cl <sup>+</sup> H <sub>2</sub> Br <sup>+</sup> H <sub>2</sub> I <sup>+</sup>	fluoronium chloronium bromonium iodonium

\* The name nitronium has been used for  $O_2N^+$  (which could be named nitrylium by applying Rule C-83.1<sup>2dd</sup> to the radicals given in the the IUPAC Inorganic Rules<sup>6C</sup>) and thus cannot be used for  $H_4N^+$ .

Examples:

(CH <sub>3</sub> —CH <sub>2</sub> )₄N <sup>+</sup>	tetraethylammonium
CI(CH <sub>3</sub> ) <sub>3</sub> P⁺	chlorotrimethylphosphonium
(CH₃)₂SH	dimethylsulfonium
(C <sub>6</sub> H <sub>5</sub> )₂I <sup>+</sup>	diphenyliodonium
Cl₂F⁺	dichlorofluoronium
сн₃—с≡о⁺	ethylidyneoxonium

RC-82.1.1.2. Parent cations other than those described by RC-82.1.1.1. A cationic center derived formally by the addition of one or more hydrons to any position of a neutral parent hydride, except for the mononuclear parent hydrides in RC-82.1.1.1, is described by replacing the final "e" of the name of the parent hydride, if present, by the operational suffix "-ium", or by adding the suffixes "-ium", "-diium", "-triium", etc., to the name of the parent hydride. Locants for cationic centers thus created are cited as needed or desired.

Note 1: When a cationic center is fully substituted and locants are cited for the substituents, the locant for the cationic center is often considered unnecessary and omitted.

Note 2: The operational suffix "-ium", when added to the name of a neutral parent hydride, indicates only that the number of substitutable hydrogen atoms at the position given by the appropriate locant has been increased by the addition of a hydron. Accordingly, there is no change in the bonding pattern at that position from that of the neutral parent hydride. Thus, specific structures formally derived by the addition of a hydron to one end of a double bond resulting in the generation of a tricoordinate carbocation at the other end of the double bond are named by RC-82.2. The procedure of Rule C-82.4 in the 1979 IUPAC Organic Rules<sup>2ee</sup> is not included in these revised recommendations.

Examples:

H₅C⁺	methanium
[C₂Hァ] <sup>+</sup>	ethanium
CH₃—ŚF₄	tetrafluoro(methyl)-λ <sup>4</sup> -sulfanium* <sup>16</sup>
(CH <sub>3</sub> ) <sub>2</sub> N—N(CH <sub>3</sub> ) <sub>3</sub>	pentamethyldiazanium pentamethylhydrazinium (traditional parent hydride name <sup>14</sup> )
сн <sub>3</sub> о—о́(сн <sub>3)2</sub>	trimethyldioxidanium
$CI_2P \xrightarrow{P}(CH_3)_3$ 2 1	2,2-dichloro-1,1,1-trimethyldiphos- phan-1-ium
$CH_3 - S - S + (CH_3) - S - CH_3$ 3 2 1	1,2,3-trimethyltrisulfan-2-ium
$H^*$ or $[C_6H_7]^*$	benzenium
	1-methylpyridin-1-ium
5	1 <i>H</i> -imidazol-3-ium
	2-hydroxy-1 <i>H</i> , 3 <i>H</i> -naphtho[1,8- <i>cd</i> ]pyran- 2-ium

<sup>\*</sup> Note that  $\lambda^n$  defines the neutral parent hydride SH4<sup>16</sup>. The suffix "-ium" describes the addition of a hydron, H<sup>+</sup>, just as for a skeletal atom of a parent hydride in its standard valency state.



**RC-82.1.2.** Cationic centers on characteristic groups. Although cationic centers derived formally by the addition of a hydron to a characteristic group can be named on the basis of parent cations derived from parent hydrides as given above in RC-82.1.1, it is often convenient and/or desirable to name a cation on the basis of a larger parent structure. Hence, the following recommendations for describing cationic centers located on some, but not all, of the characteristic groups of substitutive nomenclature are presented.

**RC-82.1.2.1.** Cationic suffixes. A cationic center formally derived by the addition of one hydron to a characteristic group listed in Table 4 is described by adding the appropriate cationic suffix given in Table 4, generated by adding the operational suffix "-ium" to the suffix name for the corresponding neutral suffix, to the name of an appropriate parent hydride.

Characteristic Group Suffix	Cationic Group Suffix
-ic acid (oxo acids only)	-ic acidium
-amide	-amidium*
-imide	-imidium
-nitrile	-nitrilium
-amine	-aminium
-imine	-iminium

TABLE 4: Suffixes for Cationic Characteristic Groups

\* Amides of carboximidic and sulfinimidic acids were named as amidines, carboxamidines, or sulfinamidines in the 1979 IUPAC Organic Rules<sup>2</sup>Y; the corresponding suffixes for monocationic centers on these suffixes would be "-amidinium", "-carboxamidinium", and "-sulfinamidinium".

When one of these characteristic group suffixes (except for "-ic acid") implies two or more of the same characteristic group, as, for example, in the name of a parent compound such as malonamide, the corresponding cationic group suffix denotes the addition of one hydron to each implied characteristic group.

Note: This method does not require knowledge, or assumption, of a specific structure, although the use of italicized element symbols, where unambiguous, can provide specificity. This is a definite advantage where it is not possible, or not desirable, to locate position(s) of the cationic center(s) on specific atoms of a characteristic group; this is particularly useful for unsubstituted cations derived from characteristic groups with two or more heteroatoms. This method also retains a correlation with the functionality of the corresponding neutral compound, and, in most cases, allows the use of a larger parent structure as the basis for the name. Names based on parent hydrides (RC-82.1.1) should be used if it is necessary or desired to indicate a specific structure.

Examples:

сн<sub>3</sub>-со-он<sub>2</sub> = сн<sub>3</sub>-с-он acetic acidium

 $C_{6}H_{5}-CO-O_{2}H_{2}$  peroxybenzoic *OO*-acidium\* perbenzoic 00-acidium\*

<sup>\*</sup> The locant symbol 00, although distinguishing between the carbonyl oxygen atom and the oxygen atoms of the peroxy group, does not distinguish between the oxygen atoms of the peroxy group.



N, N-dimethylphthalimidium 2, 2-dimethyl-1, 3-dioxo-2, 3-dihydro-1Hisoindol-2-ium (RC-82.1.1.2)

N, N, N, N-trimethyl-1,4-dithian-2-aminium  $S \sim S^{N(CH_3)_3}$ 

C<sub>6</sub>H₅—C≡ŃH benzonitrilium

 $Cl_2N-CH=CH-CH=\dot{N}Cl_2$ 

succinonitrilium

## RC-82.1.2.2. Cationic centers on implied characteristic groups

**RC-82.1.2.2.1. Uronium ions and chalcogen analogs.** Cations derived formally by the addition of a hydron to urea (or isourea) are named on the basis of the parent cation "uronium", representing the following tautomeric structures:

 $H_3 \dot{N} - CO - NH_2 \implies H_2 \dot{N} = C(-OH) - NH_2$ 

<sup>\* &</sup>quot;Aminium" is used here in the same way as "aminyl"; see Note 2 and the third and fourth example under RC-81.2.3.1.

Locants follow those used for urea<sup>2ff</sup> or isourea<sup>2gg</sup>. Chalcogen analogs are named on the basis of parent cations, such as "thiouronium", etc. When a choice between two or more tautomeric or mesomeric structures cannot be made the locants N, N', and O, S, etc., are used.

Examples:

$$CH_3 - NH = C(-O - C_8H_5) - NH - CH_3$$
3 2 1

1,3-dimethyl-2-phenyluronium

$$\begin{array}{cccc} S - C_{6}H_{5} & S - C_{6}H_{5} \\ \downarrow & \downarrow \\ C_{6}H_{5} - NH = C - NH - CH_{3} \end{array} \xrightarrow{\phantom{aaa}} C_{6}H_{5} - NH - C = NH - CH_{3}$$

N-methyl-N', S-diphenylthiouronium

$$\begin{array}{cccc} C_{6}H_{5} \longrightarrow S & S \longrightarrow C_{6}H_{5} & S \longrightarrow C_{6}H_{5} \\ (CH_{3})_{2}N \longrightarrow C \longrightarrow NH_{2} & (CH_{3})_{2}N \longrightarrow C \longrightarrow NH_{2} & (CH_{3})_{2}N \longrightarrow C \longrightarrow NH_{2} \end{array}$$

N, N-dimethyl-S-phenylthiouronium

RC-82.1.2.2.2. Cationic centers on implied characteristic groups other than uronium ions or chalcogen analogs. A cation other than a uronium ion, or a chalcogen analog, formally derived by the addition of one or more hydrons to a parent compound, the name of which implies a characteristic group from Table 4 in RC-81.1.2.1, is named by replacing the final "e" of the name of the compound, if present, by "-ium" or by adding "-ium", "-diium", etc., to the name of the parent compound.

Examples:

$$C_{e}H_{5} - N(CH_{2})_{2}$$

$$2, 2-dimethylguanidinium
$$C_{e}H_{5} - N(CH_{2})_{3}$$

$$N, N, N-trimethylanilinium$$

$$V_{H}^{+N} - CO_{2}H$$

$$Prolinium$$$$

RC-82.1.2.3. Cationic centers on characteristic groups other than those given by Table 4 in RC-82.1.2.1 derived formally by the addition of one or more hydrons are named on the basis of cationic parent hydrides, the names of which are formed according to RC-82.1.1. Note: This method also may be used for cations covered by RC-82.1.2.1 and RC-81.1.2.2.

Examples:

СН₃—СН=О́Н	ethylideneoxonium
$CH_3 - CHCI - CH_2 - SH_2$	(2-chloropropyl)sulfonium
(CH₃)₂C=Ó—CH₂—CH₃	ethyl(isopropylidene)oxonium (see RC-80.8) ethyl(propan-2-ylidene)oxonium (see RC-80.8)
C <sub>6</sub> H <sub>5</sub> CO	benzoyldimethylsulfonium
	<pre>2-methyl-1,3-dioxo-1,3-dihydrobenzo[c]- thiophen-2-ium 2-methyl-1,3-dioxo-1,3-dihydro-2-benzo- thiophen-2-ium<sup>3h</sup></pre>
$C_6H_5$ - CO - NH - $\dot{N}(CH_3)_3$ 2 1	2-benzoyl-1,1,1-trimethyldiazan-1-ium 2-benzoyl-1,1,1-trimethylhydrazin-1-ium (traditional parent hydride name <sup>14</sup> )
сн₃—со—сі—сн₃	acetyl (methyl) chloronium
$CH_3 - CH_2$ $CH_3 - C = N - N(CH_3)_3$ 2 - 1	<pre>2-butan-2-ylidene-1,1,1-trimethyldiazan- 1-ium (see RC-80.8) 1,1,1-trimethyl-2-(1-methylpropylidene)- hydrazin-1-ium (traditional parent hydride name<sup>14</sup>) (see RC-80.8)</pre>
Суще N(CH <sub>3</sub> )—ОН	cyclopentylidene (hydroxy)methylammonium

RC-82.2. Cationic compounds with cationic centers derived formally by the loss of hydride ions. These recommendations follow closely those for naming radicals, for which see RC-81.

**RC-82.2.1.** Radicofunctional names. Cationic compounds that can be considered as being derived formally by the 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 (see RC-81). Polycations are indicated by adding the numerical prefixes "di-", "tri-", etc., as appropriate, to the class term.

Note: Although such names are useful for cations where all cationic centers are located in a single parent structure, the method cannot be extended to polycations where one or more of the cationic centers must be expressed in a substituent to a parent structure and is not very useful in naming salts where an anion is specified.

Examples:

H₃C⁺	methyl cation
[C <sub>6</sub> H <sub>5</sub> ] <sup>+</sup>	phenyl cation
0 ॥ CH₃—C⁺	acetyl cation
O C <sub>6</sub> H₅—S <sup>+</sup> U O	benzenesulfonyl cation
сійн	chloroazanyl cation (see RC-81.1.2, Note 3) chloroaminyl cation
нсо—ё⁺	(formyloxyl) cation
<sup>+</sup> CH <sub>2</sub> CH <sub>2</sub> 2 1	ethane-1,2-diyl dication
C2+	cyclohexylidene dication

#### RC-82.2.2. Cationic centers in parent hydrides

RC-82.2.2.1. Monocationic centers in saturated acyclic and monocyclic hydrocarbons and the mononuclear EH4 parent hydrides of the carbon family. A cationic center derived formally by the removal of one hydrogen atom as a hydride ion from a terminal atom of a saturated unbranched acyclic hydrocarbon; from an atom of a saturated monocyclic hydrocarbon; or from any of the mononuclear parent hydrides, methane (CH4), silane (SiH4), germane (GeH4), stannane (SnH4), and plumbane (PbH4) is named by replacing the "-ane" ending of the name of the parent hydride by "-ylium" (see also RC-81.1.1).

Examples:

H₃C⁺	methylium carbenium
(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> Si <sup>+</sup>	triphenylsilylium
(CH₃)₂GeH	dimethylgermylium
$CH_3 - CH_2 - CH_2$ 3 2 1	propylium
сн₃—с́н—сн₃	1-methylethylium propan-2-ylium (see RC-82.2.2.2 and RC-80.8) isopropylium (traditional name, see item 1, Appendix, List A)

cyclobutylium

RC-82.2.2.2. Cationic centers in parent hydrides other than those described by RC-82.2.2.1. A cationic center derived formally by the removal of one or more hydride ions from any position\* of a neutral parent hydride or hydro derivative, except as provided by RC-82.2.2.1, is named by replacing the final "e" of the parent hydride name, if present, by the operational suffix "-ylium", or by adding operational suffixes such as "-bis(ylium)", "-tris(ylium)", etc., to the name of the parent hydride\*\*.

The trivial name phenylium<sup>2dd</sup> for  $[C_{6}H_{5}]^{+}$  and the contracted names naphthylium, anthrylium, and phenanthrylium are retained. Locants describing the position of the cationic center for these abbreviated names, where needed, are placed in front of the names (see RC-80.1).

Note 1: The systematic names phosphane and  $\operatorname{arsane}^{4g,\,6b}$  must be used for naming cations derived from the mononuclear parent hydrides PH<sub>3</sub> and AsH<sub>3</sub> according to this recommendation, because use of the traditional names phosphine and  $\operatorname{arsine}^{4g,\,6b}$  would lead to the names phosphinylium and  $\operatorname{arsinylium}$ , which are the same names that would be generated according to RC-82.2.3.2 from the wellestablished names phosphinyl<sup>12b</sup> and  $\operatorname{arsinyl}^{13b}$ , the names for the acyl groups H<sub>2</sub>P(O) — and H<sub>2</sub>As(O) — derived from phosphinic and arsinic acids, respectively. Even though the names phosphinoyl and  $\operatorname{arsinoyl}$  for these acyl groups are recommended in the 1979 IUPAC Organic Rules<sup>4h</sup>, ambiguity will still exist.

Note 2: The name "aminylium" for the parent cation  $H_2\ddot{N}^+$  used in

\* This recommendation is consistent with the generalized principles for naming and numbering acyclic substituent prefixes as given in Section D of the 1979 IUPAC Organic Rules<sup>4</sup>c,<sup>10</sup>f rather than the principles of Section  $A^{10g}$  and the ACS silicon rules<sup>12a</sup>, where a principal chain must terminate at the free valence position (see also RC-80.8).

\*\* Suffixes based on "-ylene", "-ylidene", and "-ylidyne", such as "-ylenium" or "-ylidenium", are not used for describing cationic centers.

Although suffixes such as "-diylium", "-triylium", etc., should be unambiguous in the context of this rule, a certain amount of ambiguity is clearly possible because of terminology in the 1979 IUPAC Organic Rules<sup>2dd</sup>, where this type of cation is defined as derived formally by "loss of an electron or electrons from a radical at the free valence position(s)". Taken literally, this definition could mean that an ending such as "-diyl-ium" would describe a divalent radical in which only one free valence has lost an electron to form the cation, i.e., the suffix "-diyl" describing the diradical  $\circ$ CH<sub>2</sub>-CH<sub>2</sub>, and the suffix "-diylium" describing the radical cation  $^+$ CH<sub>2</sub>-CH<sub>2</sub>.

the 1979 IUPAC Organic Rules<sup>2dd</sup> is continued in these recommendations as an alternative to "azanylium", derived from the parent hydride name "azane"<sup>6b,14</sup>, even though "amine" is not used as a parent hydride name for NH<sub>3</sub> herein\* (see also footnote to Table 2 in RC-80.9.1, Note 3 to RC-81.1.2, and Note 2 to RC-81.2.3.1). Note 3: The names for the cations  $H\ddot{O}^+$  and  $HO-\ddot{O}^+$  are hydroxylium<sup>6e</sup> and hydroperoxylium<sup>2s,2dd</sup>, respectively, but, in keeping with tradition are not used as parent cations in substitutive nomenclature. For the substituted cations, see RC-82.2.3.4.

Note 4: Although such cations could also be named by adding the suffix "-ium" (see RC-82.1.1.2) to the name of a parent hydride in which the atom at the cationic center is described in the parent hydride name by the  $\lambda$ -convention (see RC-81.1.3.3), the use of "-ylium" with the name for a parent hydride with the atom in the standard valency state is much preferred.

Examples:

Н₂й⁺	azanylium aminylium nitrenium
C₅H₅—Š+	phenylsulfanylium
(CH <sub>3</sub> )₄P <sup>+</sup>	tetramethyl-λ <sup>5</sup> -phosphanylium <sup>16</sup> tetramethylphosphoranylium <sup>2dd,4p</sup> tetramethylphosphonium (see RC- 82.1.1.1)
$CH_3 - NH - N = \ddot{N}^+$ 3 2 1	3-methyltriaz-1-en-1-ylium
$(CH_3)_3SI \stackrel{+}{\longrightarrow} SI(CH_3) \stackrel{-}{\longrightarrow} SI(CH_3)_3$ 3 2 1	heptamethyltrisilan-2-ylium
<b>S</b> −S−S−S−Š <sup>+</sup> 4 3 2 1	4-cyclopropyltetrasulfan-1-ylium
	cyclooct-3-en-1-ylium

<sup>\*</sup> Although the name "amine" would be quite consistent with parent hydride names, such as phosphine and arsine, and is used as such by Beilstein, it is not used as a parent hydride name in these recommendations because it has also been added to the name of a radical to form the name of a parent compound<sup>15</sup>, for example butylamine. In these recommendations, the term "amine" is used only as a suffix to denote the attachment of the ---NH<sub>2</sub> group to a parent hydride, for example, pyridin-2-amine.



furan-2-ylium

$$CH_3 - O - C(C_6H_5) = C_1 - CH_3 - O - CH_3$$

1, 2-bis(4-methoxyphenyl)-2-phenylethen-1-ylium

	bicyclo[2.2.1]heptan-2-ylium
$H_{\mathcal{C}}^{\downarrow} \xrightarrow{9  10}_{7  6  4}^{1} \xrightarrow{2}_{3}$	spiro[4.5]decan-8-ylium
*CH <sub>2</sub> - CH <sub>2</sub> - CH <sub>2</sub> + CH <sub>2</sub> 3 2 2 1	propane-1,3-bis(ylium) (propane-1,3-di- ylium according the 1979 IUPAC Or- ganic Rules <sup>2dd</sup> )
(CH <sub>3</sub> ) <sub>2</sub> N−N <sup>2+</sup> 2 1	2,2-dimethyldiazane-1,1-bis(ylium) 2,2-dimethylhydrazine-1,1-bis(ylium) (traditional parent hydride name <sup>14</sup> )
CH <sub>3</sub> - C - CH <sub>3</sub> 3 2 1	propane-2,2-bis(ylium) 1-methylethane-1,1-bis(ylium) (see RC- 82.2.2.1 and RC-80.8)
⁴́СН зсн	cyclobut-3-ene-1,2-bis(ylium)
$^{+}CH_{2}$ $- CH - CH_{2}$	<pre>propane-1,2,3-tris(ylium)</pre>

RC-82.2.2.3. Diazonium ions, i.e., cations containing a  $-N_2^+$  $(-N=\ddot{N}^+)$  group attached to a parent hydride, are named traditionally by adding the suffix "-diazonium" to the name of the parent hydride<sup>2hh</sup>. The multiplicative prefixes "bis-", "tris-", etc. are used to denote two or more diazonium groups attached to the same parent hydride structure. Diazonium ions may also be named structurally on the basis of the parent cation diazenylium,  $HN=\ddot{N}^+$ .

Examples:

methanediazonium methyldiazenylium

 $CH_3 \rightarrow \dot{N}_2$ 

benzothiazole-2-diazonium benzothiazol-2-yldiazenylium



2,4-dioxopentane-3-diazonium

(1-acety1-2-oxopropy1) diazenylium (see RC-80.8)

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

RC-82.2.2.4. Nondetachable hydro prefixes vs. added (indicated) hydrogen. A cationic center in a cyclic parent hydride having the maximum number of noncumulative double bonds located at a position where there is an insufficient number of hydrogen atoms to apply directly the recommendations for the use of "-ylium" given in RC-82.2.2.2, is derived formally from a dihydro derivative of the cyclic parent hydride. Such a cation may be described by using the principle of indicated hydrogen<sup>2g</sup> or by using nondetachable hydro prefixes<sup>2f</sup>.

In the first method<sup>2</sup>g the "hydro" derivative is described by specifying the hydrogen atom of the dihydro pair that remains after the cationic center is created by citing an italic capital H(H) and the locant for the skeletal atom at which that hydrogen atom resides, both enclosed in a set of parentheses, and inserted into the name of the corresponding unsaturated parent hydride immediately after the locant for the the cationic center\*.

Example:



3,5-dimethyl-1,4-dihydropyridin-1-ylium H<sub>3</sub>C<sup>N</sup><sub>3</sub>C<sub>H<sub>3</sub></sub> 3,5-dimethylpyridin-1(4H)-ylium

RC-82.2.2.5. A number of trivial and abbreviated names, other than those given in RC-82.2.2.2, above, have a long and well-established usage for describing substituent groups as prefixes and for naming radicals, and therefore have been recognized in the 1979 IUPAC Organic Rules<sup>1</sup>. These names are listed in an appendix to these revised recommendations. Although the monocation corresponding to each of these groups can be named easily by the systematic method given in RC-82.2.2, it is quite acceptable to name them by changing the "-yl" ending of the trivial or abbreviated name of the radical to "-ylium", for example: isopropylium, vinylium, acetonylium, tritylium, etc.

<sup>\*</sup> This procedure is exactly analogous to the use of "indicated hydrogen" to describe saturated ring positions that remain after the introduction of suffixes for principal characteristic groups, such as "-one", into the name of a parent ring or ring system that otherwise expresses the maximum number of noncumulative double bonds<sup>2g</sup>.

RC-82.2.3. Cationic centers on characteristic groups. Although cationic centers derived formally by the loss of a hydrogen atom as a hydride ion from a characteristic group can be named on the basis of parent cations derived from parent hydrides as given in RC-82.2.2, it is often convenient and/or desirable to name a cation on the basis of a larger parent structure. Hence, the following recommendations for describing cationic centers located on some, but not all, of the characteristic groups of substitutive nomenclature are presented.

RC-82.2.3.1. Established or traditional names. Names describing certain cationic species related to characteristic groups are established in the literature. The names hydroxylium and hydroperoxylium for HÖ<sup>+</sup> and HOÖ<sup>+</sup>, respectively, were mentioned in Note 3 to RC-82.2.2.2. Such cations may be considered to have been derived by the loss of an electron from the corresponding radical<sup>2s, 6c</sup> and named according to method (b) of Rule C-83.1 in the 1979 IUPAC Organic Rules<sup>2dd</sup> by replacing the "-yl" ending of the univalent radical name by "-ylium". The name nitrylium for  $O_2N^+$  was mentioned in the footnote to Table 3 in RC-82.1.1.1, and the name nitrosylium for  $ON^+$  follows directly. The name carboxylium for  $HO_2C^+$  has been proposed<sup>19</sup>. The method could be extended to the oxy halogen radicals, such as chloryl, but not to multivalent radicals, such as carbonyl or sulfonyl because of potential ambiguity (see also RC~81.2.1). Nevertheless, names such as hydroxysulfonylium and chlorosulfonylium for  $HO_3S^+$  and  $ClO_2S^+$ , respectively, have been proposed<sup>19</sup>.

RC-82.2.3.2. Acylium ions, i.e., cations having at least one chalcogen atom or nitrogen atom bonded to the cationic center(s) by a formal double bond that can be considered as derived formally from an acid characteristic group (except peroxy acid groups) by the loss of all hydroxy groups as hydroxide ions are named by replacing the "-ic acid" ending of the name, except for acids named by the carboxylic acid suffix, with "-ylium" or, occasionally, "-oylium", according to the rules for naming the corresponding acid halides $^{2x}$ , <sup>4n</sup>. The carboxylic acid suffix is changed to "carbonylium".

Note: The use of compound prefixes for expressing acyl substituents is not applied in these rules<sup>2h</sup> (see RC-80.6).

Examples:

о СH<sub>3</sub>—С\* СH<sub>3</sub>—[СH<sub>2</sub>]<sub>4</sub>—С\* acetylium hexanethicylium

cyclohexanecarbonylium



RC-82.2.3.3. Monocationic centers on nitrogen atoms of amine, imine, amide, or imide characteristic groups. A cationic compound in which a cationic center is formally derived by the removal of one hydrogen atom as a hydride ion from the nitrogen atom of an amine, imine, amide, or imide characteristic group is named by replacing the final "e" of the appropriate suffix (see Table 4 in RC-82.1.2.1) by the operational suffix "-ylium".

Note: Trivial and semisystematic names preferred for naming organic compounds according to IUPAC recommendations are used in the first cited names for the examples below.

Examples:

CH3-CH2-NH

ethanaminylium

С<sub>6</sub>Н<sub>5</sub>—<u>Ň</u>Н

anilinylium benzenaminyliun

acetamidylium

cyclohexaniminylium<sup>2z</sup> cyclohexylideneaminylium<sup>2aa</sup> (see Note 2 under RC-82.2.2.2)

CH3-CO-NH

1H-pyrrole-2-carboxamidylium



succinimidylium 2,5-dioxopyrrolidin-1-ylium (RC-82.2.2.2)



RC-82.2.3.4. Cationic centers on oxygen atoms of acid, peroxy acid, hydroxy, or hydroperoxy characteristic groups. A cationic center formally derived by removal of the hydrogen atom as a hydride ion from the oxygen atom of an acid, peroxy acid, hydroxy, or hydroperoxy characteristic group is named on the basis of a compound parent cation name formed by combining the appropriate prefix for the parent hydride or acid residue attached to the oxygen atom with the term "oxylium" or "peroxylium"; for example, pentyloxylium, pentan-2-ylperoxylium.

The contracted forms methoxylium, ethoxylium, propoxylium, butoxylium, phenoxylium, acetoxylium, and aminoxylium are retained.

Substituents to such compound parent cations are expressed by prefixes in the usual manner. Except for the contracted forms noted above, the compound parent cation is enclosed in parentheses.

Note 1: The term "peroxylium" is more consistent with terms like peroxo, peroxide, and peroxy, even though "dioxyl", and presumably therefore "dioxylium", is used in the 1979 IUPAC Organic Rules<sup>2t</sup>.

Note 2: The names hydroxylium and hydroperoxylium for the cations  $H\ddot{O}^+$  and  $HO-\ddot{O}^+$ , respectively (see Note 3 to RC-82.2.2.2), are not used when the hydrogen atom has been substituted by another atom or group.

Examples:

сн₃—ё⁺	methoxylium
(CH₃)₃C—O—Ö+	<pre>tert-butylperoxylium (see RC-80.8) 2-methyl(propan-2-ylperoxylium) (see RC-80.8)</pre>
сюн₂ —со—ё⁺	chloroacetoxylium
Сн₃—сѕ —ö⁺	(thioacetyl)oxylium*

\* The contracted form thioacetoxylium is not used because it could be ambiguous. Compare with the second example under RC-82.2.3.5 (CH₃)₂N —Ö⁺

dimethylaminoxylium

furan-2-carboselenoyloxylium

RC-82.2.3.5. Cationic centers on sulfur atoms of thio acid, thiol, or dithiohydroperoxy characteristic groups. Although a cationic center derived formally by the removal of the hydrogen atom as a hydride ion from the sulfur atom of a thio acid, thiol, or dithiohydroperoxy characteristic group can be described in the same manner as a cationic center on the corresponding oxygen characteristic group (RC-82.2.3.4) using the terms "-thiylium" and "-perthiylium", in these recommendations such cationic centers are described on the basis of the parent cation names sulfanylium and disulfanylium (RC-82.2.2.2) (see also RC-81.2.5).

Examples:

Cl₂CH — CH₂ — Š⁺ 2 1	<pre>(2,2-dichloroethyl)sulfanylium 2,2-dichloro(ethylthiylium) (by analogy with RC-82.2.3.4)</pre>
сн₃со—ӟ⁺	acetylsulfanylium acetylthiylium (by analogy with RC-82.2.3.4)
c <sub>6</sub> H₅—s—ä⁺	phenyldisulfanylium phenylperthiylium (by analogy with RC- 82.2.3.4)

RC-82.2.3.6. Cationic centers on other characteristic groups. A cationic center formally derived by the removal of hydrogen atoms as hydride ions from characteristic groups other than those covered by RC-82.2.3.1 through RC-82.2.3.5 are named on the basis of a cationic parent hydride named according to RC-82.2.2.

Examples:

C <sub>6</sub> H₅—Se—Äe⁺	phenyldiselanylium
CH₃—CH₂—S—Ö⁺	(ethylsulfanyl)oxidanylium ethyl(sulfanyloxylium) (see RC-82.2.3.4)
1 CH <sub>2</sub> -O-Š <sup>+</sup>	(2-naphthylmethoxy) sulfanylium
CH₃—CH₂—N <sup>²+</sup>	ethylazanebis (ylium)
C <sub>e</sub> H₅—CO—Ñ <sup>2+</sup>	benzoylazanebis(ylium)

# RC-82.3. Cationic heterocycles in which the cationic center results from skeletal bonding of a heteroatom\*.

RC-82.3.1. The  $\lambda$ -convention with "-ylium". A cationic heterocycle having a cationic center on a heteroatom that has one more skeletal bond than it has in the corresponding neutral heterocycle is named by adding the operational suffix "-ylium" to the name of a neutral parent heterocycle for which the  $\lambda$ -convention<sup>16</sup> 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.

Note: 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 RC-82.4) or to derive the name by the removal of two hydrogen atoms (didehydro) from a cation formed by addition of a hydron, for example, 4a-azonianaphthalene or 2,5-didehydro-2*H*-quinolizin-5ium, respectively, for the cation known also as quinolizinium<sup>2</sup>jj. The latter method, however can become quite cumbersome in some cases, requiring both hydro and dehydro prefixes; for example, the structure in the first example below would have to be named 1,2-didehydro-2,3dihydrothiophen-1-ium.

Examples:

5 5<sup>3+</sup> 1 2

 $3H-1\lambda^4$ -thiophen-1-ylium

<sup>\*</sup> Cationic heteroatoms of this type result usually from the involvement of a "free" electron pair of the heteroatom in the skeletal bonding of the heterocycle, either in the formation of a ring or in the double bond system of the ring. These cations cannot be treated systematically by either or both of the methods described in Rules RC-82.1.1 or RC-82.2.2 as such. They have been described by trivial names<sup>211</sup>, named by replacement methods (see RC-82.4), or simply indicated as being cationic by adding the suffix "-ium" to the name of the neutral heterocycle<sup>2</sup>jj, regardless of the formal derivation of the cation. None of these methods is satisfactory for a broad range of structural types.



\* This cation is commonly called 1,3-dithiolium, but it must be noted that this name also could refer to the structure shown to the right:



\*\* For recommendations to be published<sup>5</sup> on elision in names of fused ring systems, see the footnote to example 4 under RC-81.3.3.2.

RC-82.3.2. The following well-established contracted and trivial names<sup>2</sup>ii are retained; other chalcogen analogs can be named similarly.





E=O: pyrylium

E=O: chromenylium



E=O: isochromenylium E-S: thiopyrylium E-S: thiochromenylium E-S: isothiochromenylium



E=O: flavylium E=S: thioflavylium



E=O: xanthylium E=S: thioxanthylium

RC-82.4. Replacement nomenclature for cations. Cationic centers in parent hydrides may be described by the principles of replacement ("a") nomenclature<sup>2kk</sup>, 3g, 3i, 4q. Cationic replacement prefixes are derived, except for bismuth\*, by replacing the final "a" of the corresponding replacement prefix<sup>3d,4d,11</sup> by "-onia", or, except for carbon\*\*, by replacing the final "e" of the corresponding mononuclear parent hydride name (see RC-80.9.1) by "-ylia"\*\*\*, and indicate a cationic center having a bonding number one higher (see RC-82.1) or one lower (see RC-82.2), respectively, than the bonding number of the corresponding neutral mononuclear parent hydride. Examples:

> azonia \_s<sup>⊥</sup>\_ or =s<sup>⊥</sup>\_ thionia

\* This cationic replacement prefix for bismuth is formed by adding "-onia" to the element name<sup>4r</sup>.

\*\* Although the name "carbenia" has been proposed as a replacement prefix for the tricoordinate carbon cation (an "-ylia" cationic center)<sup>20</sup>, the name "carbanylia" would be consistent with the principles of these recommendations. The term "carbonia" cannot be used as a replacement prefix for a pentacoordinate carbon cationic center, because of previous usage of the term "carbonium" for a tricoordinate carbon cationic center (see also footnote to RC-82.1.1.1).

\*\*\* The only replacement prefix of this type noted in the previous rules was borvlia4s.

I <del>*</del>	iodonia
—в⁺	boranylia
—N <u>+</u>	azanylia

Cationic replacement prefixes are nondetachable, i.e., they are cited directly in front of the parent hydride name<sup>2f</sup>.

Cationic replacement prefixes are cited and the skeletal positions they represent are numbered, where there is a choice, in the same order as the the corresponding neutral replacement ("a") prefixes given in Table I of Rule B-1.1<sup>3d</sup> or in Table I in the Appendix to Section D of the 1979 IUPAC Organic Rules<sup>4d</sup>. Cationic replacement prefixes are cited immediately after the corresponding neutral replacement prefix<sup>3i</sup> occurring in the same name in the order "-onia" followed by "-ylia"; and, where there is a choice, are preferred to the corresponding neutral skeletal atom for assignment of low locants<sup>2mm</sup> in the order "-ylia" followed by "-onia" (see also RC-82.5.2).

Note: In general, the Commission favors the use of the suffixes "-ium" and "-ylium" with nonreplacement names of parent hydrides or with neutral replacement names, to the use of cationic replacement prefixes. In addition, names that do not require designation of skeletal atoms in nonstandard valency states by the  $\lambda$ -convention<sup>16</sup> are preferred (see also Note 4 to RC-82.2.2.2).

Examples:



1-methyl-1-oxoniacyclopentane 1-methyltetrahydrofuran-1-ium (RC-82.1.1.2)



1-methyl-4-aza-1-azoniabicyclo[2.2.1]heptane
1-methyl-1,4-diazabicyclo[2.2.1]heptan-1-ium
(RC-82.1.1.2)



2-bromo-9-hydroxy-9-oxoniabicyclo[4.2.1]nonane 2-bromo-9-hydroxy-9-oxabicyclo[4.2.1]nonan-9-ium (RC-81.1.1.2)



1-methyl-1-phosphonianaphthalene	
1-methylphosphinolin-1-ium	
1-methylbenzo[b]phosphinin-1-ium <sup>11</sup>	
1-methyl-1-benzophosphinin-1-ium <sup>3h,11</sup>	)



6,6,9,9-tetramethyl-3,12-dioxa-6-thia-9-azatetradecane-6,9-diium (RC-82.1.1.2)

## RC-82.5. Cationic compounds with multiple cationic centers.

**RC-82.5.1.** Polycations with cationic centers identically derived at two or more positions on the same parent hydride are named using appropriate numerical prefixes and operational suffixes as given in RC-82.1.1.2 and RC-82.2.2.2 or replacement prefixes as given in RC-82.4.

**RC-82.5.2.** "Ium" and "ylium" centers in the same parent hydride. Cationic compounds with two or more cationic centers in the same parent hydride structure, at least one being derived formally by the addition of a hydron to a skeletal position and at least one by the loss of a hydrogen atom as a hydride ion from another skeletal position, are named by replacing the final "e" of the parent hydride name by the operational suffix "-ium", followed by the operational suffix "-ylium", each preceded, where necessary, by appropriate numerical or multiplicative prefixes and locants (see RC-82.1.1.2 and RC-82.2.2.2).

<sup>\*</sup> For recommendations to be published<sup>5</sup> on elision in names of fused ring systems, see the footnote to example 4 under RC-81.3.3.2.

Where there is a choice, low locants of the parent hydride are given first to the cationic centers regardless of their type, and then to "-ylium" cationic centers.

Examples:



RC-82.5.3. Polycations with cationic centers identically derived by the addition of one hydron to each of two or more of the characteristic groups given by Table 4 in RC-82.1.2.1, except for imides (for which see RC-82.5.7) and acids, are named by using multiplicative prefixes, such as "bis-", and "tris-" with the appropriate cationic suffix.

Dications and polycations so derived from diacids and polyacids are named by adding numerical prefixes, such as "di-" and "tri-", to the term "acidium".

Examples:

(CH<sub>3</sub>)<sub>2</sub>NH-CH<sub>2</sub>-CH<sub>2</sub>-NH(CH<sub>3</sub>)<sub>2</sub>

N, N, N', N' -tetramethylethane-1, 2-bis(aminium)
N, N, N', N' -tetramethylethylenebis(aminium)

H20-CO-[CH2]4-CO-0H2

hexanedioic diacidium

**RC-82.5.4.** 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 expressible as a cationic suffix (see RC-82.1.2.1, RC-82.2.3.2, and RC-82.2.3.3) may be named by adding the cationic suffix to the name of a parent cation formed according to RC-82.1.1, RC-82.2.2, RC-82.3, RC-82.4, or RC-82.5.2. Examples:



N, N, N, 1-tetramethylquinolin-1-ium-3-aminium



5λ<sup>5</sup>-quinolizin-5-ylium-2-carboximidamidium (see footnote to Table 4 in RC-82.1.2.1) Where there is a choice, low locants for skeletal cationic centers are determined before considering low locants for positions at which cationic suffixes are attached.

Example:



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

**RC-82.5.5.** Assemblies of parent cations. Cationic compounds with cationic centers identically derived from the same parent hydride but located in different parts of the structure are named, if possible, by the principles for naming assemblies of identical units<sup>2</sup>q using the multiplicative prefixes "bis-", "tris-", etc., where necessary\*.

Examples:

1,4-phenylenebis(phosphonium) 1,1'-dimethyl-4,4'-ethylenedipyridin-1-ium (IUPAC multiplicative л́м—сн₃ method; see RC-80.11) 4,4'-ethylenebis[1-methylpyridin-1-ium] (CAS multiplicative method; see RC-80.11) 1,1'-oxydicyclohepta-2,4,6-trien-1-ylium 1,1',3,3'-tetramethyl-2,2'-oxybis(2,5-dihydro-1H-imidazol-3-ium) (IUPAC multiplicative method; see RC-80.11) 2,2'-oxybis[1,3-dimethyl-2,5-dihydro-1H-imidazole-3-ium] (CAS multiplicative method; see RC-80.11) 2,2'-(1,3-phenylene)dipropan-2-ylium (see RC-82.2.2.2 and RC-80.8) 1,1'-dimethyl-1,1'-(1,3-phenylene)diethylium (see RC-82.2.2.1 and RC-80.8 ) (IUPAC multiplicative method; see RC-80.11) 1,1'-(1,3-phenylene)bis[1-methylethylium] (see (RC-82.2.2.1 and RC-80.8 ) (CAS multiplicative method; see RC-80.11)

<sup>\*</sup> The multiplicative prefixes "bis-", "tris-", etc. are used to avoid the possibility of confusion that could arise from the use of the numerical prefixes "di-", "tri-", etc.

RC-82.5.6. Other polycations with cationic centers on characteristic groups. Cationic compounds with two or more cationic centers identically derived from the same characteristic group, except for diimides and polyimides (for which see RC-82.5.7), diacids and polyacids (for which see RC-82.2.3.2 and RC-82.5.3), and the other characteristic groups given by Table 4 in RC-82.1.2.1, as described in RC-82.5.3, are named if possible on the basis of a cationic parent hydride according to the principles for naming assemblies of identical units<sup>2q</sup> using the multiplicative prefixes "bis-", "tris-", etc., where necessary to avoid possible confusion that may arise from the use of the numerical prefixes "di-", "tri-", etc.\*.

Examples:

$$\begin{array}{cccc} H\ddot{O}^+ & H\ddot{O}^+ & pentane-2,4-diylidenebis(oxonium) & (see RC-80.8) \\ \parallel & \parallel & \\ CH_3-C-CH_2-C-CH_3 & (1,3-dimethylpropan-1,3-diyl)bis(oxonium) \\ 5 & 4 & 3 & 2 & 1 & (see RC-80.8) \end{array}$$

 $C_6H_5 \rightarrow O(CH_3) \rightarrow CH_2 \rightarrow CH_2 \rightarrow O(CH_3) \rightarrow C_8H_8$ 

0,0'-dimethyl-0,0'-diphenyl[ethylenebis(oxonium)] (IUPAC multiplicative method; see RC-80.11)

ethylenebis[methylphenyloxonium] (CAS multiplicative method; see RC-80.11)

phthaloylbis (disulfanylium)

ethylenebis (azanylium) ethylenebis (aminylium)

ethylenebis (oxidanylium)

 $^{\dagger}N = CH - CH_2 - CH_2 - CH = N^{\dagger}$ 

HN-CH2-CH2-NH

⁺ö—сн,—сн,—ö⁺



pyridine-2, 6-diylbis(sulfanylium)

butane-1,4-diylidenebis(azanylium)

butane-1,4-diylidenebis(aminylium)

\*ġ−0−S0₂-√ S0₂−0−ġ\* benzene-1,4-disulfonylbis (dioxidanylium)

<sup>\*</sup> Accordingly, cationic centers derived from two or more of the same characteristic group are not described in terms of that characteristic group using appropriate multiplicative prefixes.

[ethane-1, 2-disulfonylbis(sulfanediyl)]bis(oxidanylium)

**RC-82.5.7.** Polycations derived from diimides and polyimides by either addition of hydrons to, or removal of hydrogen atoms as hydride ions from, two or more nitrogen atoms of a diimide or polyimide are described on the basis of a heterocyclic parent cation name derived according to RC-82.1.1.2, RC-82.2.2.2, or RC-82.5.2.

Examples:

H2N1' 3' 3 1NH2 H5' 4' 4 51

NH2 2,2',5,5'-tetraoxo[3,3'-bipyrrolidine]-1,1'-diium



1,3,5,7-tetraoxo-1,2,3,5,6,7-hexahydrobenzo[1,2-c;-4,5-c']dipyrrole-2,6-bis(ylium) (RC-82.2.2.4) 1,3,5,7-tetraoxo-5,7-dihydrobenzo[1,2-c:4,5-c']dipyrrole-2,6(1H,3H)-bis(ylium) (RC-82.2.2.4)



1,3,6,8-tetraoxo-1,2,3,6,7,8-hexahydrobenzo[1mn][3,8]phenanthrolin-7-ium-2-ylium (RC-82.2.2.4)
1,3,6,8-tetraoxo-3,6,7,8-tetrahydrobenzo[1mn][3,8]phenanthrolin-7-ium-2(1H)-ylium (RC-82.2.2.4)

**RC-82.5.8.** Cationic centers in both parent compounds and substituent groups. A polycation in which all catonic centers cannot be included in a cationic parent hydride or parent compound (or when it may not be desirable to do so) is named by selecting part of the structure that contains most of the cationic centers as the cationic parent hydride or parent compound [see RC-82.5.8.4(a)] to be named by the principles of these recommendations. Parts of the structure containing other cationic centers are then expressed by prefixes formed as described in the following subsections.

RC-82.5.8.1. Prefixes for expressing the mononuclear parent cations described by RC-82.1.1.1 as monovalent substituents are formed by changing the "-onium" ending of the parent cation to "-onio"<sup>2nn</sup>. Examples:

ŇH₃	ammonio
SeH₂	selenonio
— <sup>†</sup> Cl₃	trichlorophosphonio

-1-C<sub>6</sub>H<sub>5</sub>

phenyliodonio

RC-82.5.8.2. Prefixes for expressing monocationic polynuclear parent hydrides with the free valence at a heteroatomic cationic center may be derived by changing the "-ium" ending of the parent cation to "-io"<sup>2</sup>PP. Locants may be omitted provided that there is no resulting ambiguity.

Examples:

-N NH<sub>2</sub>-N=NH 1 2 3 pyridinio triaz-2-en-1-io

RC-82.5.8.3. Systematically derived prefixes for expressing cationic structural units as substituents are formed by adding the operational suffixes "-yl", "-ylidene"\*, "-diyl", etc., with appropriate locants, to the name of the parent cation derived according to RC-82.1.1, RC-RC-82.2.2, RC-82.3, or RC-82.5.2, or by replacing the final "e", if present, of a cationic replacement name (see RC-82.4) by these operational suffixes.

Note: This method is also applicable to the cationic prefix groups considered in RC-82.5.8.1 and RC-82.5.8.2.

Examples:

—ŅH₃

ammoniumyl ammonio (RC-82.5.8.1)

 $-\dot{C}H_3-CH_3$  ethan-1-ium-1-yl

 $-CH_2 - \dot{C}(CH_3) - CH_3$  2-methylpropan-2-ylium-1-yl

1-methylpyridin-1-ium-3-yl

1-methyl-1-azoniabicyclo[2.2.1]heptan-3-yl
(RC-82.4)
1-methyl-1-azabicyclo[2.2.1]heptan-1-ium-3-yl
(RC-82.1.1.2)

<sup>\*</sup> The operational suffix "-ylidene" is to be used only to describe the presence of a double bond between the substituting group and a parent hydride or parent substituent (see RC-80.5).



**RC-82.5.8.4.** Choice of parent cationic structure. Although, in theory, any portion of a polycationic structure that can be named by the principles in these recommendations can be the parent structure, it is often useful to have some guidelines for making this choice. Thus, when necessary or desirable, a parent cationic structure may be chosen by applying the following criteria in order until a definitive choice is achieved.

- (a) the maximum number of cationic centers of any kind\*\*, including cationic suffix groups;
- (b) the maximum number of "ylium" cationic centers;
- (c) the maximum number of senior cationic centers, according to the nature of the cationic atom, in the same order as for the corresponding replacement prefixes<sup>3d</sup>, 4d, 11.

Further choice, if necessary, is made by applying the general criteria for chains and rings given in the 1979 IUPAC Organic Rules<sup>2cc</sup>. Examples:

$(CH_3)_3 \overset{1}{N} - CH_2 - [CH_2]_4 - CH_2 - \overset{1}{S}(CH_3)_2$	<pre>dimethyl[6-(trimethylammonio)hexyl]- sulfonium (RC-82.1.1.1, RC-</pre>
	82.5.8.1, and RC-80.8)
	6-(dimethylsulfonio)-N, N, N-trimethyl-
	hexan-1-aminium (RC-82.1.2.1 and
	RC-82.5.8.1)
	2,9,9-trimethyl-2-thionia-9-azonia-
	decane (RC-82.4)

\* Note that the traditional name "diazonio" describes both structures,  $-\dot{N} \equiv N$  and  $-N = \dot{N}^+$ , whereas the systematic name given here describes only the first of these structures; the name diazen-2-ylium-1-yl describes the second structure.

\*\* This is in agreement with the principles for choosing a preferred component for naming fused heterocyclic ring systems<sup>3j</sup>.



Rule RC-83. Anions [replaces C-84 (in part), C-86, C-206 (in part), C-461.1 (in part), C-462.1 (in part), C-511.3 (in part), C-511.4, C-542.1 (in part), D-1.63 (in part), D-5.8, D-6.87, D-7.63 (in part)]

**RC-83.0.** Introduction. For the purposes of organic nomenclature, an anion is a molecular entity carrying at least one unit of negative charge formally derived from a parent hydride, a parent compound, or a hydro derivative of either, by the removal of one or more hydrogen atoms as hydrons\*, by the addition of one or more hydride ions, or by a combination of these operations. An atom at which the negative charge is considered to reside is called an anionic center. Anions with two or more anionic centers are called dianions, trianions, etc..

<sup>\*</sup> Hydron is a generic name for the hydrogen cation, i.e., the naturally occurring mixture of protons, deuterons, and tritons<sup>9</sup>. The name proton is restricted to the hydrogen cation having the mass number 1, i.e., <sup>1</sup>H<sup>+</sup>.

RC-83.1. Anionic compounds with anionic centers derived formally by removal of hydrons.

**RC-83.1.1.** Radicofunctional names. Anionic compounds that can be considered as being derived formally by addition of electrons to the corresponding radical (see RC-81) may be named by adding the class name "anion" as a separate word after the name of the radical. Polyanions are indicated by adding the numerical prefixes "di-", "tri-", etc., as appropriate, to the class name.

Note: Although such names are useful for anions where all anionic centers are located in a single parent structure, the system cannot be extended to polyanions where one or more of the anionic centers must be expressed in a substituent to a parent structure.

Examples:

H₃Ċ⁻

<u>\_\_\_\_</u>

methyl anion

O II CH<sub>3</sub>--C<sup>-</sup> acetyl anion

phenyl anion

benzenesulfinyl anion

H<sub>3</sub>---NH<sup>-</sup> methanaminyl anion methylazanyl anion

jCH<sup>-</sup> cyclopenta-2,4-dien-1-yl anion

(C<sub>6</sub>H<sub>5</sub>)<sub>2</sub><sup>2</sup>

diphenylmethylene dianion

1,4-dihydronaphthalene-1,4-diyl dianion

### RC-83.1.2. Anionic centers in parent hydrides.

**RC-83.1.2.1.** The operational suffix "-ide". An anionic center derived formally by the removal of one or more hydrons from any position of a neutral parent hydride is named by replacing the final "e" of the name of the parent hydride, if present, by the operational suffix "-ide", or by adding the suffixes "-ide", "-diide", etc., to the name of the parent hydride.

The trivial names "amide" and "imide" for the anions  $H_2\ddot{N}$ : and  $H\ddot{N}$ :<sup>2-</sup>, respectively<sup>6f,14</sup>, are retained, and may be used as parent anions in substitutive nomenclature, but see also RC-83.1.5. The trivial name "acetylide" for the anion  $[C_2]^{2-}$  is also retained<sup>6g</sup>.

Note 1: Contracted names for hydrocarbon anions, such as methide, are not recommended, since other contracted names, such as boride, sulfide, and phosphide, cannot be used because they are names for the monoatomic anions  $:\ddot{B}^{3-}$ ,  $:\ddot{S}:^{2-}$ , and  $:\ddot{P}:^{3-}$ , respectively<sup>6h</sup>.

Note 2: The names for the anions HÖ:-, HO-Ö:-, and HS:-, HS-S:-, etc., are hydroxide<sup>6f</sup>, hydroperoxide<sup>21a</sup>, and hydrosulfide<sup>21b</sup>, hydrodisulfide, etc., respectively, but, in keeping with tradition, are are not used as parent anion names in substitutive nomenclature. For the substituted anions, see RC-83.1.4 and RC-83.1.6.

Examples:

сн₃—ён⁻	methylamide methylazanide (see also RC-83-1.5)
(CH <sub>3)2</sub> ₽ <sup></sup>	dimethylphosphanide <sup>4</sup> g,6b dimethylphosphinide*
$(CH_3 - CH_2 - CH_2 - CH_2)_3 \ddot{Sn}^-$	tributylstannanide
HC≡≡ä⁻	methylidynesilanide
(C <sub>6</sub> H <sub>5</sub> )₂B—ĊH₂ <sup>−</sup>	(diphenylboryl)methanide
(NC)₃C <sup>−</sup>	tricyanomethanide
CH₃—ČH—CH₃ 3 2 1	propan-2-ide
CH <sub>3</sub> —CH₂—C <del>=</del> C <sup>−</sup> 4 3 2 1	but-1-yn-1-ide
C <sub>6</sub> H₅—CH=CH—C̄H —C <sub>6</sub> H₅ 3 2 1	1,3-diphenylprop-2-en-1-ide
$HN = \frac{1}{2} C(CN) - \overline{C}(CN)_2$ $H = \frac{1}{2} C(CN) - \overline{C}(CN)_2$	1,1,2-tricyano-2-(3,4-dicyano-5-imino- 1,5-dihydro-2H-pyrrol-2-ylidene)- ethan-1-ide

\* Although the traditional names phosphine, arsine, etc.<sup>4g,6b</sup>, can be used for deriving parent anion names, the systematic names are preferred. 4-chlorobenzen-1-ide





cyclopenta-2,4-dien-1-ide



 $H_{3}C \xrightarrow{N=N} \underbrace{N=N-N=N}_{5 \ 4 \ 3 \ 2 \ 1} \underbrace{-CH_{3}}_{1}$ 

1,5-di-p-tolylpentaaza-1,4-dien-3-ide



1H-benzotriazol-1-ide

C6H5-N:2-

phenylimide

(C<sub>6</sub>H<sub>5</sub>)₂Ë<sup>2 −</sup>

diphenylmethanediide



9H-fluorene-9,9-diide



1,4-dihydronaphthalene-1,4-diide

(CH<sub>3</sub>)<sub>3</sub>Si-N<sup>-</sup>SiH<sub>2</sub>-N<sup>-</sup>Si(CH<sub>3</sub>)<sub>3</sub> 1,1,1,5,5,5-hexamethyltrisilazane-5 4 3 2 1 2,4-diide

 $C_{\theta}H_{5}$  -  $\overline{C}H$  -  $\overline{C}H$  -  $\overline{C}H$  -  $C_{\theta}H_{5}$ 3 2 1



1,4,6,9-tetrahydropyrene-1,4,6,9-tetraide

1,3-diphenylpropane-1,2,3-triide

**RC-83.1.2.2.** Nondetachable hydro prefixes vs. added (indicated) hydrogen. An anionic center at a position in a ring or ring system having the maximum number of noncumulative double bonds where there is an insufficient number of hydrogen atoms to apply the recommendations for the use of "-ide" given in RC-83.1.2.1 is formally derived from a dihydro derivative of the cyclic parent hydride. Such an anion may be named by adapting the principle of "indicated hydrogen"<sup>2g</sup> or by using nondetachable hydro prefixes<sup>2f</sup>.

In the first method<sup>2g</sup>, the "hydro" derivative is described by specifying the hydrogen atom of the dihydro pair that remains after the anionic center has been created by citing an italic capital H(H) and the locant for the skeletal atom at which that hydrogen atom resides, both enclosed in a set of parentheses and inserted into the name immediately after the locant for the anionic center\*.

Examples:



1,2-dihydropyridin-1-ide pyridin-1(2*H*)-ide



1,10b-dihydrocyclopenta[*ef*]heptalen-10b-ide cyclopenta[*ef*]heptalen-10b(1*H*)-ide



1-methyl-1, 2-dihydrobenzo[b] azocine-2, 2-diide\*\*
1-methyl-1-benzoazocine-2, 2 (1H) -diide\*\*<sup>3h</sup>

RC-83.1.3. Anionic centers on chalcogen atoms of acid characteristic groups.

**RC-83.1.3.1.** Acid groups expressed as suffixes. An anion formed by the loss of the hydrogen atom as a hydron from the chalcogen atom of each acid characteristic group expressed by an "ic acid" suffix (except for mixed chalcogen peroxy acids, such as R-CS-O-OH or R-CO-S-SH\*\*\*), or implied by a semisystematic or trivial "-ic acid"

\*\* For recommendations to be published<sup>5</sup> on elision in names of fused ring systems, see the footnote to example 4 under RC-81.3.3.2.

\*\*\* Application of this method to mixed chalcogen peroxy acids does not necessarily produce an unambiguous name.

<sup>\*</sup> This procedure is exactly analogous to the use of "indicated hydrogen" to describe saturated ring positions that remain after the introduction of suffixes for principal characteristic groups, such as "-one", into the name of a ring or ring system that otherwise expresses the maximum number of noncumulative double bonds<sup>2</sup>9.

acid" name is named by replacing the "-ic acid" ending of the acid name by the suffix "-ate". Examples\*:



**RC-83.1.3.2.** Mononuclear parent "oxo" acids. An anion formed by loss of the hydrogen atom as a hydron from each hydroxy group, or a chalcogen analog, of a mononuclear parent "oxo" acid, except for mixed chalcogen analogs of peroxy acids, is named by replacing the "-ic acid" or "-ous "acid" ending of the acid name by "-ate" or "-ite", respectively.

Examples:

<sup>\*</sup> Even though it is common practice to represent the structure of such acid anions in a condensed form, such as  $-CO_2^-$  and  $-SO_3^-$ , anionic acid groups are shown here in an extended form, as  $-CO_2^-$  and  $-S(0)_2^-$ . in order to explicitly show nonbonding electron pairs at anionic centers, as is done throughout these recommendations for radical and ionic centers.

CH3-AsO(---Ö: --)2

methylarsonate

**RC-83.1.3.3. Partly ionized acids and their esters.** An anion formed by the loss of the hydrogen atom as a hydron from one or more, but not all, of the hydroxy groups of a polybasic acid expressed by a suffix, or implied by a parent acid name, a semisystematic name, a trivial name, or an acid ester, may be named by indicating the hydrogen atoms remaining by the term "hydrogen" prefixed by an appropriate numerical prefix (except for mono) and cited as a separate word\* in front of the name of the anion derived according to Rule RC-83.1.3.1 and RC-83.1.3.2.

Note: Although locants prefixed to the hydrogen term can provide specificity in some cases, this is not always possible. The lack of specificity in this method can be an advantage when positions of remaining hydrogen atoms or charge cannot be determined, or when such specificity is neither necessary nor desirable. This method retains a correlation with the functionality of the corresponding neutral compound.

If specificity is required, the anionic center should be named on the basis of a fully ionized structure according to RC-83.1.3.1 or RC-83.1.3.2, and the free acid or ester groups expressed as substituents. Names of this type are included for the examples below.

Examples:

hydrogen heptanedioate HO<sub>2</sub>C-[CH<sub>2</sub>]<sub>5</sub>-CO-Ö:-6-carboxyhexanoate ethyl phenylmalonate  $CH_3 - CH_2 - O - OC - CH(C_6H_5) - CO - \ddot{O}$ (ethoxycarbonyl)phenylacetate hydrogen phenylphosphonate C<sub>6</sub>H<sub>5</sub>--- P(O)(OH)--- Ö:-hydroxy (phenyl) phosphinate 0<sup>3</sup>-ethyl 0<sup>1</sup>-hydrogen citrate  $CH_3 - CH_2 - O - CO - CH_2$ HO<sub>2</sub>C - CH<sub>2</sub> - C - OH O<sup>4</sup>-ethyl 2-(carboxymethyl)-2-hydroxybutanedioate O<sup>4</sup>-hydrogen 2-[(ethoxycarbonyl)methyl]-2-hydroxybutanedioate 2-(carboxymethyl)-3-(ethoxycarbonyl)-2hydroxypropanoate

<sup>\*</sup> According to IUPAC inorganic nomenclature recommendations, the word hydrogen should be attached directly to the name of the anion<sup>61</sup>; in this guide to IUPAC organic nomenclature practices, the word hydrogen is separated from the name of the anion, a continuation of the practice used in previous organic rules and recommendations<sup>2rr</sup>.

 $O^4$ -hydrogen 2-chloro-1,4-dithioterephthalate  $O^4$ -hydrogen 2-chlorobenzene-1,4-dicarbothioate 2-chloro-4-[hydroxy(thiocarbonyl)]thiobenzoate

RC-83.1.4. Anionic centers on hydroxy characteristic groups and their chalcogen analogs.

**RC-83.1.4.1.** Anions from  $C_1 - C_4$  acyclic alcohols, phenol, or hydroxylamine. The traditional contracted radicofunctional names<sup>2ss</sup>, such as methoxide (from methyl oxide) and aminoxide (presumably from aminyl oxide) are the names for anions formally derived by the loss of the hydrogen atom as a hydron from the oxygen atom of these hydroxy compounds. The unbranched acyclic structures are parent anions for substitutive nomenclature; the branched structures, such as isopropoxide (from isopropyl oxide), are not.

Examples:

CI—CH₂—CH₂—Ö:	2-chloroethoxide
(CH <sub>3</sub> )₂C(CI)—Ö: <sup>-</sup>	1-chloro-1-methylethoxide 2-chloropropan-2-olate (see RC-83.1.4.2)
(CH₃)N — Ö;-	dimethylaminoxide

RC-83.1.4.2. Anions from hydroxy groups other than those described by RC-83.1.4.1 and chalcogen analogs of all hydroxy groups. An anion formed by the loss of the hydrogen atom as a hydron from the chalcogen atom of a hydroxy characteristic group or a chalcogen analog that is expressed as a suffix such as "-ol", "-thiol", etc., except as provided by RC-83.1.4.1, is named by adding the operational suffix "-ate" to the appropriate suffix\*, for example, "-olate" and "-thiolate". When the suffix in the name of a parent compound implies two or more hydroxy characteristic groups, or a chalcogen analog, the suffix "-ate" implies the loss of a hydron from each each such characteristic group implied by that suffix.

Note 1: The trivial names picric  $acid^{2uu}$  (2,4,6-trinitrophenol) and styphnic  $acid^{2uu}$  (2,4,6-trinitrobenzene-1,3-diol) are used to

<sup>\*</sup> The limited practice of naming anions derived in this way from alcohols in radicofunctional nomenclature by adding the suffix "ate" to the class name "alcohol", or by changing the ending "yl alcohol" to "ylate" (in some languages other than English), permitted by the previous edition of the IUPAC Organic Rules<sup>2tt</sup>, is not included in these revised recommendations.

derive the names picrate and styphnate for the corresponding anions with anionic centers on the (both) oxygen atom(s), according to RC-83.1.3.1, just as if an actual acid characteristic group were present.

Note 2: The names hydroxide, hydroperoxide, and hydrosulfide, hydrodisulfide, etc., for the anions HÖ:-, HOÖ:-, and HS:-, HS-S:-, etc., respectively, are not used when the hydrogen atom has been substituted by another atom or group (see Note 2 to RC-83.1.2.1).

Examples:

CH₃[CH₂]₄Ö;-	pentan-1-olate
C <sub>6</sub> H <sub>11</sub> —Se:-	cyclohexaneselenolate
<u>ة:</u> - ق:-	resorcinolate benzene-1,2-bis(olate)*

RC-83.1.5. Monoanionic centers on the nitrogen atom of an amine characteristic group formally derived by the removal of one hydrogen atom from the nitrogen atom as a hydron may be named by replacing the final "e" of the amine suffix or parent compound name by the operational suffix "-ide", or by substitutive nomenclature based on the parent anion names amide or azanide (see RC-83.1.2.1).

Examples:

СН₃—СН₂—ЁН⁻	ethanaminide ethylamide ethylazanide
С <sub>6</sub> н₅—ён-	anilinide benzenaminide phenylamide phenylazanide

**RC-83.1.6.** Anionic centers on other characteristic groups\*\*. Anions with anionic centers generated formally by the removal of hydrogen atoms as hydrons from atoms of characteristic groups other than those covered

<sup>\*</sup> The multiplicative prefixes "bis-", "tris-", etc. are used to avoid the possibility of ambiguity by interpreting a suffix such as "-diolate to mean a monoanion derived from a diol.

<sup>\*\*</sup> Suffixes such as "-imidide" and "-amidide" are not recommended and "ylideneaminide" names are not included herein.
by RC-83.1.3 through RC-83.1.5, are named on the basis of an anionic parent hydride name formed according to RC-83.1.2. Examples:

сн₃–с̈-	1-oxoethanide	
сн₃—о—ё:-	methyldioxidanide*	
C <sub>6</sub> H₅—S— ö: <sup>-</sup>	<pre>(phenylsulfanyl)oxidanide (not benzene- sulfenate; see RC-80.7)</pre>	
CH₃— CS— O— Ö:¯	(thioacetyl)dioxidanide	
(CH₃)₃C— O— O— Ö:¯	<i>tert-</i> butyltrioxidanide (see RC-80.8) (2-methylpropan-2-yl)trioxidanide (see RC-80.8)	
CH <sub>3</sub>	acetoxysulfanide	
5 5 Se - S	(2-furyl)diselanide	
сн₃— о— <u>ё</u> ∶-	methoxysulfanide	
Сн₃—С(Он)—й∶-	(1-hydroxyethylidene)amide (1-hydroxyethylidene)azanide	
O Ⅱ (CH <sub>3</sub> )₂P <sup>-</sup>	dimethyloxo-λ <sup>5</sup> -phosphanide <sup>16</sup> dimethyloxophosphoranide <sup>4</sup> P	
(CH₃)₃P== <u>N</u> <sup>–</sup>	(trimethyl- $\lambda^5$ -phosphanylidene) amide <sup>16</sup> (trimethylphosphoranylidene) amide <sup>4</sup> p, 12b (trimethyl- $\lambda^5$ -phosphanylidene) azanide <sup>16</sup> (trimethylphosphoranylidene) azanide <sup>4</sup> p, 12b	
C <sub>6</sub> H₅—CO—NH— <u>N</u> ∷ <sup>2−</sup>	<pre>2-benzoyldiazane-1,1-diide 2-benzoylhydrazine-1,1-diide (traditional     parent hydride name<sup>14</sup>)</pre>	
сн₃—со—ён⁻	acetylamide acetylazanide	

<sup>\*</sup> Although the radicofunctional name methyl peroxide is in fact an accurate description for this anion, such names are not recommended herein because of the widespread use of such names to describe symmetrical peroxides, such as dimethyl peroxide.



RC-83.2. Anionic compounds with anionic centers derived formally by the addition of a hydride ion. The nomenclature systems in the 1979 IUPAC Organic Rules<sup>1</sup> do not provide an operational suffix for indicating addition of a hydride ion to a parent compound comparable to the "-ium" suffix for naming cations (see Rule RC-82.1.1.2). Although many such compounds can be named by the principles of coordination nomenclature<sup>6</sup>, for example, tetrahydroborate<sup>6a</sup>, for [BH<sub>4</sub>]<sup>-</sup>, and hexachlorophosphate<sup>6k</sup>, for [PCl<sub>6</sub>]<sup>-</sup>, anions of this type occurring in more complicated organic systems cannot be named easily in this way. Therefore, two methods, other than replacement techniques (see RC-83.3), are included in these revised recommendations for use in naming such anions.

- (a) The operational suffix "-uide". An anionic center at any position of a neutral parent hydride may be described by replacing the final "e" of the name of the parent hydride, if present, by the operational suffix "-uide", or by adding the operational suffixes "-uide", "-diuide", etc., to the name of the parent hydride; locants for the anionic centers thus created are cited as needed or desired.
- (b) The operational suffix "-ide" with the  $\lambda$ -convention<sup>16</sup>. An anionic center derived from any position of a neutral parent hydride where the  $\lambda$ -convention defines at least two more hydrogen atoms than are present in the standard neutral parent hydride may be described by replacing the final "e" of the parent hydride name, if present, by the operational suffix "-ide", or by adding the operational suffixes "ide", "-diide", etc., to the name of the parent hydride. Locants for the anionic centers thus defined are cited, if necessary, even though locants are given with the " $\lambda$ " symbolism.

Since method (b) often requires use of bonding states that may be too artificial for some to accept readily, method (a) is to be preferred in such cases; for example, this method would require  $[AsF_6]^-$  and  $[GeF_5]^-$  to be named hexafluoro- $\lambda^7$ -arsanide and pentafluoro- $\lambda^6$ -germanide, respectively.

<sup>\*</sup> For recommendations to be published<sup>5</sup> on elision in names of fused ring systems, see the footnote to example 4 under RC-81.3.3.2.

### Examples:

CH <sub>3</sub> —SiH <sub>4</sub> <sup>-</sup>	(a)	methylsilanuide	
(CH₃)₄Ë-	(a) (b) (b)	tetramethylphosphanuide <sup>4</sup> g, 6b tetramethyl- $\lambda^5$ -phosphanide <sup>16</sup> tetramethylphosphoranide <sup>4</sup> P	
(C <sub>6</sub> H <sub>5</sub> )F₂S <sup>−</sup>	(a) (b)	difluoro (phenyl) sulfanuide difluoro (phenyl) −λ <sup>4</sup> -sulfanide <sup>16</sup>	
(C <sub>8</sub> H <sub>5)2</sub> Ï: <sup></sup>	(a) (b)	diphenyliodanuide diphenyl-λ <sup>3</sup> -iodanide <sup>16</sup>	
F <sub>6</sub> Ï <sup>→</sup>	(a) (b)	hexafluoro-λ <sup>5</sup> -iodanuide <sup>16</sup> hexafluoro-λ <sup>7</sup> -iodanide <sup>16</sup>	
F <sub>8</sub> Te <sup>2−</sup>	(a) (b)	octafluoro- $\lambda^6$ -tellanediuide <sup>16</sup> octafluoro- $\lambda^{10}$ -tellanediide <sup>16</sup>	
H <sub>3</sub> C CH <sub>3</sub>	(a)	<pre>1,3-dihydro-1-methyl-1,1,1-tri-p-tolyl-3,3- bis(trifluoromethyl)-1λ<sup>5</sup>-benzo[c][1,2]- oxastibol-1-uide*<sup>16</sup></pre>	
5 4 F <sub>3</sub> C CF <sub>3</sub>	(a)	<pre>1,3-dihydro-1-methyl-1,1,1-tri-p-tolyl-3,3- bis(trifluoromethyl)-2,1λ<sup>5</sup>-benzooxa- stibol-1-uide*<sup>3h</sup>,16</pre>	

**RC-83.3.** Replacement nomenclature for anions. Anionic centers in parent hydrides may be described by the principles of replacement ("a") nomenclature<sup>2kk</sup>, 3g, 3i, 4q. Anionic replacement prefixes are derived by replacing the final "e" of the name of the mononuclear parent hydride (see RC-80.9.1) by the operational suffixes "-ida" or "-uida", and indicate an anionic center having a bonding number one lower (see RC-83.1) or one higher (see RC-83.2), respectively, than the bonding number of the corresponding neutral mononuclear parent hydride.

Note 1: In the 1979 IUPAC Organic Rules, replacement prefixes for describing anionic skeletal atoms with a bonding number one higher than that of the corresponding neutral heteroatom had the ending "-ata"<sup>4s,4t</sup>. Note 2: The 1979 IUPAC Organic Rules<sup>1</sup> make no provision for replacement prefixes to describe anionic skeletal atoms with bonding numbers one lower than that of the corresponding neutral heteroatom.

Examples:

-<u>p</u>phosphanida<sup>4</sup>g, 6b -<u>B</u>boranuida

<sup>\*</sup> For recommendations to be published<sup>5</sup> on elision in names of fused ring systems, see the footnote to example 4 under RC-81.3.3.2.

<u>)</u>š.—

## sulfanuida λ<sup>4</sup>-sulfanida<sup>16</sup>

Anionic replacement prefixes are nondetachable, i.e., they are cited directly in front of the name of the parent hydride<sup>2f</sup>.

Anionic replacement prefixes are cited and the skeletal atoms they represent and are numbered, where there is a choice, in the same order as the corresponding neutral replacement ("a") prefixes given by Table I in Rule  $B-1.1^{3d}$  or in Table I in the Appendix to Section D of the 1979 IUPAC Organic Rules<sup>4d</sup>. An anionic replacement prefix is cited immediately after the corresponding neutral replacement prefix<sup>3i</sup> occurring in the same name; where there is a choice, an anionic skeletal atom is preferred to the corresponding neutral skeletal atom for assignment of low locants. An "-uida" anionic prefix is cited after the corresponding "-ida" prefix; where there is a choice, an "-uida" anionic center is preferred to an "-ida" anionic center for assignment of low locants.

Note: In general, the Commission favors the use of the suffixes "-ide" and "-uide" with nonreplacement names of parent hydrides or with neutral replacement names according to RC-83.2 over the use of "ida" or "uida" replacement prefixes. In addition, names that do not require designation of skeletal atoms in nonstandard valency states by the  $\lambda$ -convention<sup>16</sup> are preferred (see also Note 4 to RC-82.2.2.2 and the Note to RC-82.4).

Examples:



2,2-dimethyl-2H-2-boranuidaindene 2,2-dimethyl-2H-2-borainden-2-uide [RC-83.2(a)]



decahydro-4a-phosphanuida-1,3,6,8-tetrasilanaphthalene decahydro-4a<sup>5</sup>-phosphanida-1,3,6,8-tetrasilanaphthalene 1-phosphanuida-3,5,7,9-tetrasilabicyclo[4.4.0]decane 1<sup>5</sup>-phosphanida-3,5,7,9-tetrasilabicyclo[4.4.0]decane

octahydro-2*H*-4a-phospha-1,3,6,8-tetrasilanaphthalen-4a-uide [RC-83.2(a)] 1-phospha-3,5,7,9-tetrasilabicyclo[4.4.0]decan-1-uide [RC-83.2(a)] decahydro-4a $\lambda^5$ -phospha-1,3,6,8-tetrasilanaphthalen-4a-ide [RC-83.2(b)] 1 $\lambda^5$ -phospha-3,5,7,9-tetrasilabicyclo[4.4.0]decan-1-ide [RC-83.2(b)]



5λ<sup>5</sup>-phosphanuidaspiro[4.4]nonane 5λ<sup>5</sup>-phosphaspiro[4.4]nonan-5-uide [RC-83.2(a)]

## RC-83.4. Multiple anionic centers.

RC-83.4.1. Polyanions identically derived at different positions on the same parent hydride are named using appropriate numerical prefixes and operational suffixes as given in RC-83.1.2 and RC-83.2.

RC-83.4.2. "Ide" and "uide" 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 the removal of a hydron from a skeletal position, and one by the addition of a hydride ion at another skeletal position, are named by replacing the final "e" of the name of the parent hydride, if present, by the operational suffix "-ide", followed by the operational suffix "-uide", each preceded, where necessary, by the appropriate numerical or multiplicative prefix (see RC-83.1.2.1 and RC-83.2). The "e" of the "-ide" suffix is elided before "-uide" unless a multiplicative prefix precedes the latter. Where there is a choice, low locants of the parent hydride are assigned first to the anionic centers regardless of type and then to "-uide" anionic centers. Example:



RC-83.4.3. Polyanions identically derived from hydroxy characteristic groups or chalcogen analogs by the loss of the hydrogen atom as a hydron from each of two or more hydroxy groups or chalcogen analogs attached to a parent hydride are named by adding a suffix such as "-bis(olate)", or "-tris(thiolate)" to the name of the parent hydride\*.

Examples:



cyclohexane-1, 4-bis(olate)

naphthalene-2,6-bis(thiolate)

RC-83.4.4. 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 (see RC-83.1.3 through RC-83.1.5) may be named by adding the anionic suffix to the name of a parent anion formed according to Rules RC-83.1.2 and RC-83.2. Where there is a choice, preference for low locants goes to the anionic skeletal atom.

Examples:

cyclohexan-1-ide-4-sulfonate

<sup>\*</sup> The multiplicative prefixes "bis-", "tris-", etc. are used to avoid the possibility of ambiguity which would result if a suffix such as "-diolate" were to be interpreted as describing a monoanion derived from a diol.

 $\begin{array}{c} \vdots \ddot{O} - OC - CH_2 - CH_2 - C \equiv \ddot{C} \vdots \\ 5 & 4 & 3 & 2 & 1 \end{array} \qquad \text{pent-1-yn-1-id-5-oate}$ 

RC-83.4.5. Assemblies of 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 for naming assemblies of identical units<sup>2</sup>q using the multiplicative prefixes "bis-", "tris-", etc., where necessary\*.

Examples:

1, 4-phenylenebis (phosphanide)

tetracyano[3-dicyanomethylidene)cycloprop-1- $(NC)_2C \xrightarrow{3}_2C(CN)_2$ ene-1,2-divl]dimethanide (IUPAC multiplicative method; see RC-80.11) [3-(dicyanomethylidene)cycloprop-1-ene-1,2diyl]bis[dicyanomethanide] (CAS multiplicative method; see RC-80.11)

RC-83.4.6. Other polyanions with anionic centers on characteristic groups. Anionic compounds with two or more anionic centers identically derived from the same characteristic group, except for diacids and polyacids, dialcohols and polyalcohols or phenols and their chalcogen analogs (for which see RC-83.1.3, RC-83.1.4.2, and RC-83.4.3), and diimides and polyimides, are named, if possible, on the basis of an anionic parent hydride according to the principles for naming assemblies of identical units<sup>2</sup> using the multiplicative prefixes "bis-", "tris-", etc., instead of the numerical prefixes "di-", "tri-", etc., where necessary\*\*. Examples:

-:<u><u>s</u>-s-<u>s</u>-<u>s</u>-<u>s</u>:-</u>

<sup>-</sup>:Ö—O—CH₂—CH₂—O— Ö:<sup>-</sup>

1,4-phenylenebis(disulfanide)

ethylenebis (dioxidanide)

-HN-CH2CH2CH2CH2Airde)321propane-1, 3-diylbis (amide)321propane-1, 3-diylbis (azanide)

\* The multiplicative prefixes "bis-" and "tris-", etc., are used to avoid the possibility for confusion that could arise from the use of the numerical prefixes "di-", "tri-", etc..

\*\* Accordingly, anionic centers derived from two or more of such same characteristic groups are not described in terms of such characteristic groups using appropriate multiplicative prefixes.

**Polyanions** derived from **diimides** and **polyimides** are named on the basis of heterocyclic parent anions in accordance with RC-83.1.2. Example:

**RC-83.4.7.** Anionic centers in both parent compounds and substituent groups. A polyanion in which not all anionic centers can be included in an anionic parent hydride or parent compound (or where it may not be desirable to do so) is named by selecting the part of the structure that includes most of the anionic centers [see RC-83.4.7.4(a)] as the anionic parent hydride or parent compound to be named by the principles of these recommendations. Parts of the structure containing the other anionic centers are then expressed by prefixes as described in the following subsections.

RC-83.4.7.1. Prefixes for anionic centers derived from acid characteristic groups by removal of the hydrogen atoms from all hydroxy, thiol, etc., groups of an acid characteristic group or a chalcogen analog, and that are attached to the parent structure by a single bond\* are named by changing the "ic acid" ending of the name of the acid suffix or parent mononuclear oxo acid to "- ato"<sup>2vv</sup>, <sup>4</sup>u.

Examples:

—co—ö:-	carboxylato
— so₂ — ö:-	sulfonato
PO(Ö:)5	phosphonato
— AsH(O)(Ö: <sup>-</sup> )	arsinato**

**RC-83.4.7.2. Prefixes for anionic chalcogen atom**s may be derived by replacing the final "e" of the name of the corresponding monoatomic anion<sup>6h</sup> with an "o"<sup>2</sup>WW.

Example:

---Ö:-- oxido

\* In the 1979 IUPAC Organic Rules, these prefixes<sup>4</sup> were not limited to attachment by a single bond.

\*\* In the 1979 IUPAC Organic Rules, this prefix<sup>4</sup><sup>u</sup> was used for the anionic substituent group —As(0)- $\ddot{o}$ :<sup>-</sup>.

RC-83.4.7.3. Systematically derived prefixes for expressing anionic structural units as substituents are formed by replacing the final "e" of the name of the parent anion derived according to RC-83.1.2 with an operational suffix, "-y1" or "-ylidene" or by adding an operational suffix such as "-diy1" to the parent anion name. Where there is a choice, low locant numbers are assigned to the point of attachment to the parent structure.

Examples:

---¨CH₂- methanidyl

----BH3

boranuidyl

- amidylidene\* azanidylidene (see RC-80.5) azanidediyl

-s--s<sup>--</sup> disulfanidyl



cyclohexa-2,5-dien-4-id-1-ylidene (see RC-80.5)



cyclopenta-1,4-dien-3-ide-1,2-diyl (see RC-80.5)



2H-benzo[c]borol-2-uid-2-ylidene 2H-2-benzoborol-2-uid-2-ylidene3h (see RC-80.5)

**RC-83.4.7.4.** Choice of parent anionic structure. Although, in theory, any portion of a polyanionic structure that can be named by the principles of these recommendations can be the parent structure, it is often useful to have a few guidelines for making this choice. Thus, when necessary, or desirable, a parent anionic structure may be chosen by applying the following criteria in order until a definitive choice is achieved.

\* The use of "-diyl" with the anion name "amide" is not recommended.

- (a) the maximum number of anionic centers of any kind\*, including anionic suffix groups;
- (b) the maximum number of senior anionic centers, according to the nature of the anionic atoms, in the same order as the corresponding replacement prefixes<sup>3</sup>d,<sup>4</sup>d,<sup>11</sup>.

Further choice, if necessary, is made by applying the general criteria for chains and rings given in the 1979 IUPAC Organic Rules<sup>2</sup>cc. Examples:



Rule RC-84. Cationic and anionic centers in a single structure (replaces C-87<sup>1</sup>)

**RC-84.1.** Zwitterionic compounds having equal numbers of cationic and anionic centers in the same parent compound (including ionic centers on characteristic groups expressible as suffixes).

RC-84.1.1. Zwitterionic parent hydrides are named by combining appropriate operational suffixes (see RC-82.1.1.2, RC-82.2.2.1, RC-82.2.2.2, RC-83.1.2.1, and RC-83.2) at the end of the name of a neutral parent hydride, in the order "-ium", "-ylium", "-ide", and "-uide" or by citing ionic replacement prefixes (see C-82.4 and RC-83.3) in front of the name of the neutral parent hydride. In either case, anionic affixes are cited after cationic affixes in the name, and are given preference for low locants. An ionic or neutral characteristic group suffix, if present, may be added, if desired. The final "e" of the name of the parent hydride, or of an "-ide" or "-uide" suffix, is elided before "i" or "y", or before a functional suffix beginning with a vowel. Numerical prefixes, appropriate for each type of affix, 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 priority: "-uide" ("uida-"), "-ide" ("ida-"), "-ylium" ("ylia-"), and "-ium" ("onia-").

<sup>\*</sup> This is in agreement with the principles for choosing a preferred component in naming fused heterocyclic ring systems<sup>3j</sup>.



<sup>\*</sup> Several trivial names for this compound have appeared in the literature, of which dimethylisodiazene and dimethylazamine are the least objectionable. The name 1,1-dimethyldiazene does not correspond to the structure and the name (dimethylamino)nitrene is considered to break a traditional principle of systematic substitutive nomenclature long established for naming acyclic hydrocarbons, i.e., that a homogeneous chain of atoms should not be broken. However, the effect of this principle in noncarbon systems is under study by the Commission.





- 2, 2-diphenyl- $4\lambda^5$ ,  $2\lambda^5$ -[1, 3, 4, 2] dioxazaborolo-[4,5-a]pyridin-4-ylium-2-ide [RC-82.3.1 and RC-83.2(b)]
- 2, 2-diphenyl-1, 3-dioxa-3a-azonia-2-boranuidaindene (RC-82.4 and RC-83.3) (formerly 2,2-diphenyl-1, 3-dioxa-3a-azonia-2-borataindene<sup>48</sup>)

2-methylisoselenochroman-2-ium-3-id-4-one (RC-82.1.1.2 and RC-83.1.2.1)

CH<sub>3</sub>---BH<sub>2</sub>--NH<sub>2</sub>--BH<sub>2</sub>---NH<sub>2</sub>--CH<sub>3</sub>

2,4-diaza-3,5-diborahexane-2,4-diium-3,5-diuide [RC-82.1.1.2 and RC-83.2(a)] 2, 4-diaza- $3\lambda^5$ ,  $5\lambda^5$ -diborahexane-2, 4-diium-3, 5-diide (RC-82.1.1.2 and RC-83.1.2.1) 3,5-diazonia-2,4-diboranuidahexane (RC-82.4 and RC-83.3) (formerly 3, 5-diazonia-2, 4-diboratahexane<sup>4s</sup>)

(Note: In the third name, the ionic replacement name, the anionic centers are given preference for lowest locants, but in the first two names, in which neutral replacement prefixes and ionic suffixes are used, the neutral heteroatoms have priority for lowest locants.)

RC-84.1.2. Zwitterionic parent compounds with at least one ionic center on a characteristic group expressible as a suffix (see RC-82.1.2.1, RC-82.2.3.2, RC-82.2.3.3, RC-83.1.3.1, RC-83.1.3.3, RC-83.1.4, and RC-83.1.5) may be named by adding the appropriate ionic suffix to the name of an ionic parent hydride. Ionic centers on skeletal atoms of the ionic parent hydride are preferred to the position of attachment of ionic suffixes for assignment of lowest locants. Examples:

> 1,1,1-trimethyldiazan-1-ium-2-sulfonate (CH<sub>3</sub>)<sub>3</sub>N-NH-SO<sub>2</sub>-Ö:-(RC-82.1.1.2 and RC-83.1.3.1) 1,1,1-trimethylhydrazin-1-ium-2-sulfonate (traditional parent hydride name<sup>14</sup>) (RC-82.1.1.2 and RC-83.1.3.1)



\* This is one of the canonical forms of a sydnone. Other canonical forms can also be treated by these methods as shown by the following example:

HO<sub>2</sub>C 5 4 11 0 H<sub>3</sub>C 3 <u>N</u>: 3-methyl-5-oxo-2,5-dihydro-1,2,3-oxadiazol-3-ium-2-ide-4-carcarboxylic acid (RC-82.1.1.2, RC-83.1.2.1, and RC-83.1.2.2) 3-methyl-5-oxo-1,2,3-oxadiazol-3-ium-2(5H)-ide-4-carboxylic acid (RC-82.1.1.2, RC-83.1.2.1, and RC-83.1.2.2) RC-84.2. Prefixes for zwitterionic parent hydrides as substituents are formed by replacing the final "e" of the name of the zwitterionic parent hydride (see RC-84.1.1), if present, by an operational suffix "-yl" or "-ylidene", or by adding a suffix such as "-diyl" to the name of the zwitterion. Where there is a choice, the free valence of the zwitterionic substituent prefix has preference for assignment of lowest locants. Example:

3-methyl-1*H*-imidazol-3-ium-1-id-4-yl (RC-82.1.1.2 and RC-83.1.2.1)

RC-84.3. Ionic centers not in the same parent structure. A zwitterionic compound or an ionic compound in which all ionic centers are not in a single parent structure, or when it is not desired to include all ionic centers in one parent structure, is named by expressing the cationic centers or the parts of the structure containing the cationic centers as substituent prefixes to the name of an anionic parent compound (see RC-83). Examples:

H <sub>2</sub> C= <sup>+</sup> CH <sub>2</sub> <sup>-</sup>	(methylideneoxonio)methanide (RC-82.5.8.1 and RC-83.1.2.1) (methylideneoxoniumyl)methanide (RC-82.5.8.3 and RC- 83.1.2.1)		
[(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> 中] <sub>2</sub> c <sup>²−</sup>	<pre>bis(triphenylphosphonio)methanediide (RC-82.5.8.1 and RC-83.1.2.1) bis(triphenylphosphoniumyl)methanediide (RC-82.5.8.3 and</pre>		
	RC-83.1.2.1)		
(C <sub>6</sub> H <sub>5</sub> )₂ <sup>+</sup> (CH <sub>3</sub> )—C <del>=</del>	<pre>CB(C<sub>e</sub>H<sub>5</sub>)<sub>3</sub> [[diphenyl(methyl)phosphonio]ethynyl]triphenyl- boranuide [RC-82.5.8.1 and RC-83.2(a)] [[diphenyl(methyl)phosphoniumyl]ethynyl]tri- phenylboranuide [RC-82.5.8.3 and RC-83.2(a)]</pre>		
³∕⊂H <sup>−</sup>	2-(dimethylsulfonio)cyclopropan-1-ide (RC-82.5.8.1 and RC-83.1.2.1)		
H <sup>™</sup> S(CH <sub>3</sub> )2	2-(dimethylsulfoniumyl)cyclopropan-1-ide (RC-82.5.8.3 and RC-83.1.2.1)		
(NC) <sub>2</sub> C	dicyano[2-(dicyanomethylidene)-3-(triethyl- ammonio)cyclopropyl]methanide (RC-82.5.8.1 and RC-83.1.2.1)		
H * N(CF	<pre>dicyano[2-(dicyanomethylidene)-3-(triethyl- ammoniumyl)cyclopropyl]methanide (RC-82.5.8.3 and RC-83.1.2.1)</pre>		
<b>1</b>	3-(trichlorophosphonio)cyclopenta-2,4-dien-1-ide		
CLA CH	(RC-82.5.8.1 and RC-83.1.2.1)		
UI3F 9 2	3-(trichlorophosphoniumyl)cyclopenta-2,4-dien-1-ide (RC-82.5.8.3 and RC-83.1.2.1)		

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$$(CH_{ij})_{i}\dot{N}-CH_{2}-CO-\dot{O}^{-}$$

$$(trimethylammonio)acetate (RC-82.5.8.1 and RC-83.1.3.1)$$

$$(trimethylammoniumyl)acetate (RC-82.5.8.3 and RC-83.1.3.1)$$

$$(trivial name: betaine*)$$

$$CH_{3}-\dot{N}_{3}^{-}\dot{+}_{3}(-H_{2}-CO-\dot{O}^{-}$$

$$(1-methylpyridin-1-ium-4-yl)acetate (RC-82.5.8.3 and RC-83.1.3.1)$$

$$\dot{T}^{-}(1\lambda^{4}, 2-dithiol-1-ylium-4-yl)-2-naphtholate (RC-82.5.8.3 and RC-83.1.4.2)$$

$$\dot{T}^{-}_{O}-\dot{+}_{3}\dot{-}_{4}\dot{-}_{5}\dot{-}_{7}\dot{-}$$

$$(-(1\lambda^{4}, 2-dithiol-1-ylium-4-yl)-2-naphtholate (RC-82.5.8.3 and RC-83.1.4.2)$$

$$\dot{T}^{-}_{O}-\dot{+}_{3}\dot{-}_{4}\dot{-}_{7}\dot{-}_{7}\dot{-}_{7}\dot{-}(1\lambda^{4}, 2-dithiol-1-ylium-4-yl)-2-naphtholate (RC-82.5.8.3 and RC-83.1.4.2)$$

$$\dot{T}^{-}_{O}-\dot{+}_{3}\dot{-}_{4}\dot{-}_{7}\dot{-}_{7}\dot{-}_{7}\dot{-}(1\lambda^{4}, 2-dithiol-1-ylium-4-yl)-2-naphtholate (RC-82.5.8.3 and RC-83.1.4.1)$$

$$\dot{T}^{-}_{O}-\dot{+}_{3}\dot{-}_{4}\dot{-}_{7}\dot{-}_{7}\dot{-}_{7}\dot{-}_{7}\dot{-}_{7}\dot{-}(1\lambda^{4}, 2-dithiol-1-ylium-4-yl)phenoxide (RC-82.5.8.1, RC-83.1.4.1)$$

$$(CH_{0})_{k}C=CH-CH_{2}-\dot{S}(CH_{0})-\dot{-}_{4}\dot{-}_{7}\dot{+}_{7}\dot{-}_{9}\dot{-}_{7}\dot{-}_{9}\dot{-}_$$

\* The name "betaine" is also used as a class name for such zwitterionic compounds.

#### Rule RC-85. Radical ions (replaces C-83.3 and C-84.4<sup>1</sup>)

**RC-85.0.** Introduction. For the purposes of organic nomenclature, a radical ion is a molecular entity having at least one radical center (see RC-81.0) and one cationic center (see RC-82.0) or anionic center (see RC-83.0) or both (see RC-84.0), which may be on the same or on different atoms.

**RC-85.1.** Descriptive names. 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 phrase "radical cation" or "radical anion" as separate words following the name of the neutral parent hydride or parent compound with the same molecular formula. The numerical prefixes "di-", "tri-", etc., are added to each term to indicate indicate multiple radical or ionic sites.

Alternatively, the phrase "radical ion" may be used with the type and amount of charge given by an appended parenthetical arabic number and appropriate charge sign (often called a Ewens-Bassett number<sup>21c</sup> or a charge number<sup>6m</sup>, for example, radical ion(2-). Numerical prefixes are used to denote the number of radical centers, when more than one are present.

Note 1: These names are most useful when the positions of the radical and/or ionic sites are unknown, or when it is not necessary or desirable to indicate specific positions for such sites.

Note 2: It should be noted that, since the suffix denoting a radical center is cited last in systematic structural names, the phrase following the name of the neutral parent hydride or parent compound perhaps should be "cation radical", "anion radical", or "ion radical". This format is being used in the literature and, although not used in these recommendations, may be considered as an acceptable alternative.

#### Examples\*:

[C <sub>2</sub> H <sub>6</sub> ] **	ethane radical cation ethane radical ion(1+)		
[C <sub>4</sub> H <sub>6</sub> ] **	butadiene radical cation butadiene radical ion(1+)		
[(CH <sub>3</sub> ) <sub>2</sub> Se — Se(CH <sub>3</sub> ) <sub>2</sub> ]**	tetramethyl-1 $\lambda^4$ , 2 $\lambda^4$ -diselene radical cation <sup>16</sup> tetramethyl-1 $\lambda^4$ , 2 $\lambda^4$ -diselene radical ion(1+) <sup>16</sup>		
[CH <sub>3</sub> SF <sub>5</sub> ]**	pentafluoro (methyl) $-\lambda^6$ -sulfane radical anion <sup>16</sup> pentafluoro (methyl) $-\lambda^6$ -sulfane radical ion (1-) <sup>16</sup>		

<sup>\*</sup> In this document, a radical ion in an empirical formula is denoted by a superscript dot followed by the appropriate charge sign<sup>7</sup>. It is recognized that in mass spectroscopy the opposite sequence is used<sup>8</sup>, following well-established tradition in that field.

(CH <sub>3</sub> ) <sub>3</sub> SI	(trimethylsilyl)benzene radical anion (trimethylsilyl)benzene radical ion(1-)	
H <sub>2</sub> C>	<pre>bicyclo[5.3.1]undeca-1,3,5,7,9-pentaene radical anion bicyclo[5.3.1]undeca-1,3,5,7,9-pentaene radical ion(1-)</pre>	
[C <sub>6</sub> H <sub>5</sub> C <sub>6</sub> H <sub>5</sub> ] <sup>(2 •)(2−)</sup>	biphenyl diradical dianion biphenyl diradical ion(2-)	
[C <sub>14</sub> H <sub>10</sub> ] <sup>(•)(3–)</sup>	phenanthrene radical trianion phenanthrene radical ion(3-)	

RC-85.2. Radical ions derived from parent hydrides. A radical ion derived formally by the removal of one or more hydrogen atoms from a single skeletal atom or from different skeletal atoms of an ionic or zwitterionic parent hydride is named by replacing the final "e" of its name, if present, or by adding to its name, operational suffixes, such as "-yl", "-ylidene", "-diyl", etc. The  $\lambda$ -convention<sup>16</sup> may offer a considerable advantage for naming such radical ions. However, the use of names in which the skeletal atoms are in standard valency states is preferred (see also Note 4 to RC-82.2.2.2 and the Notes to RC-82.4 and RC-83.3). Skeletal positions with radical centers have preference over skeletal positions with ionic centers for assignment of lowest locants.

Note: Added hydrogen (see RC-81.1.4, RC-82.2.2.4, and RC-83.1.2.2) is not considered necessary where the radical center is derived from a position at which a hydron or hydride ion has been added, i.e., at an "-ium" or "-uide" center.

Examples of radical cations:

H₂C**	methyliumyl λ <sup>2</sup> -methaniumyl <sup>16</sup> (see also RC-81.1.3.3) carbynium (see also RC-81.1.3.1)	
H₄Si*+	silaniumyl	
[CH <sub>3</sub> CH <sub>2</sub> ] <sup>(•)(2+)</sup>	ethaniumyliumyl	
CH₃ <sup>2</sup> + 2 1	ethan-1-ium-1-ylium-1-yl	
$H_{c}^{\dagger} = \stackrel{\circ}{\underset{2}{\overset{\circ}{\underset{1}{\overset{1}{\overset{1}{\overset{1}{\overset{1}{\overset{1}{\overset{1}{1$	ethen-2-ylium-1-ylidene 1λ <sup>2</sup> -ethen-2-ylium <sup>16</sup> (see also RC-81.1.3.3)	
() or [C <sub>6</sub> H <sub>6</sub> ]**	benzeniumyl	
	cyclohexa-2,5-dien-4-ylium-1-yl	

# Examples of radical anions:





 $CH_3 \longrightarrow N \underset{3}{\longrightarrow} N \underset{2}{\longrightarrow} N \underset{1}{\longrightarrow} N \underset{3}{\longrightarrow} SI(CH_3)_3 \qquad \qquad 3-methyl-1-(trimethylsilyl)triaz-2-en-2-ium-1-id-2-yl$ 

RC-85.3. Radical ions on characteristic groups.

**RC-85.3.1. Radical ions on ionic suffix groups.** A radical ion derived formally by the removal of one or more hydrogen atoms from a cationic characteristic group given by Table 4 in RC-82.1.2.1 (except for acid suffixes), or the anionic characteristic group "-aminide" (RC-83.1.5), is named by adding an operational suffix, such as "-yl, "-ylidene" and "-diyl" to the ionic suffix, or by replacing the final "e" of the ionic suffix, if present, by an operational suffix.

Examples:

C <sub>6</sub> H <sub>5</sub> №H <sub>2</sub>	aniliniumyl benzenaminiumyl
Сн₃—й•-	methanaminidyl methylamidyl methylazanidyl
Сн₃—со—й**	acetamidyliumyl
C <sub>6</sub> H₅—C <b>≡</b> N <sup>•+</sup>	benzonitriliumyl
N <sup>+</sup> and/or	v: succinimidiumylidene
	cyclohexylmethanaminidyl (cyclohexylmethyl)amidyl (cyclohexylmethyl)azanidyl

RC-85.3.2. Radical ions on characteristic groups other than those described by RC-85.3.1. A radical ion derived formally by the removal of a hydrogen atom from an ionic characteristic group other than those in RC-85.3.1 above is named on the basis of a parent radical ion, named according to RC-85.2.

Examples:

C <sub>6</sub> H₅—SO₂—NH — №́* <sup>-</sup>	2-benzenesulfonyldiazan-1-id-1-yl	
сн₃—со—й∙-	acetylamidyl acetylazanidyl	
CH₂ === C === Ö**	vinylideneoxoniumyl	
СН₃—СН₂—СН₂ —О́́н	propyloxoniumyl	
сн₃—со—о́—сн₃	acetyl (methyl) oxoniumyl	

**RC-85.4.** Ionic and radical centers in different parent structures. A radical ion derived formally by the removal of one or more hydrogen atom(s) from an ionic or zwitterionic compound in which the ionic centers and the radical positions 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 a parent radical the name of which is derived according to RC-81.1 or RC-81.2.

Examples:





#### REFERENCES

 International Union of Pure and Applied Chemistry. Organic Chemistry Division. Commission on Nomenclature of Organic Chemistry, Nomenclature of Organic Chemistry, Sections A, B, C, D, E, F, and H, 1979 ed., Pergamon Press, Oxford, 1979, 559 p.

<sup>\*</sup> The trivial name "benzyl" is not used as a substituent prefix when  $\alpha$ -substituted (see footnote to item 17 in the Appendix, List A).

- 2. Reference 1, Section C, pp. 79-322: [a] Subsection C-0.8, pp. 133-43; [b] Rules C-107, pp. 146-7; C-206(in part), pp. 155-6; C-511.3, p. 212; C-511.4 (in part), p. 213; C-551, pp. 227-8; C-816, pp. 259-61; C-861, pp. 275-6; C-921.6, p. 287; C-931.1, pp. 289-90; C-931.2(in part); p. 290; C-931.3(in part), p. 290; C-973, p. 299; and C-974(in part), pp. 299-300; [c] Rule C-83.1, Note 1, p. 138; [d] Preamble, Conventions (1), p. 80; [e] Subsection C-0.15, pp. 105-7; [f] Rule C-16.1, p. 108; [g] Rule C-315.1, p. 172; [h] Rule C-403.2, pp. 185,188, Note, p. 188; and Rule C-631.1, pp. 230-1; [i] Rule C-521, p. 217; and Rule C-641.1, p. 233-4, Table XII, p. 234; [j] Rule C-701.1, p. 247-8, Table XIII; p. 248; [k] Rule C-502, pp. 210-1; [m] Rule C-701.2, p. 248; [n] Rule C-11.41, p. 91; [p] Subsection C-0.2, pp. 112-3; [q] Rules C-72, p. 130-1; and C-73, p. 132; [r] Rule C-81.2, p. 134; [s] Rules C-218.1, p. 161; and C-81.1, pp. 133-4; [t] Rule C-81.1, pp. 133-4; [u] Rule C-922.1, p. 288; [v] Rule C-631.2, p. 231; [w] Rule C-106.2, p. 146; [x] Rules C-403, pp. 185,188; C-481, pp. 206-7; C-641.7, pp. 236-7; and C-642.4, pp. 240-1; [y] Rules C-641.9, pp. 238-9; C-951.1, p. 292; C-951.2, p. 292; and C-951.3, p. 293; [z] Rule C-815.3(a), pp. 258-9; [aa] Rule C-815.3(b), pp. 258-9; [bb] Rule C-921.2, pp. 285-6; [cc] Subsections C-0.13, pp. 97-101; and C-0.14, pp. 101-5; [dd] Rule C-83.1, pp. 137-9; [ee] Rule C-82.4, p. 136-7; [ff] Rules C-971.1, p. 297; and C-971.2, pp. 297-8; [gg] Rule C-972.1, p. 298; [hh] Rule C-931.1, pp. 289-90; [ii] Rule C-83.2, p. 139; [jj] Rule C-83.1, pp. 137-9, Note 2, p. 138; [kk] Subsection C-0.6, pp. 123-7; [mm] Rule C-62.1, pp. 124-5; [nn] Rules C-82.1, p. 134-5, Table V, p. 135; and C-816.3, p. 260; [pp] Rule C-82.1, p. 134-5, Table V, p. 135, footnote; [qq] Rule C-441, pp. 196-7, Exceptions, p. 197; [rr] Rule C-462.1, p. 200; [ss] Rule C-206.2, p. 156, Exceptions; [tt] Rule C-206.2, p. 156, Note (1); [uu] Rule C-202.2, pp. 151-2; [vv] Rules C-461, pp. 199-200; C-462, p. 200; and C-86.1, p. 142; [ww] Rule C-86.2, p. 142.
- 3. Reference 1, Section B, pp. 53-76: [a] Rules B-6, pp. 71-2; B-10.1(in part), p. 72; and B-11(in part), p. 73; [b] Rule B-1.2(in part), p. 54;
  [c] Rule B-5.12, pp. 70-1; [d] Rule B-1.1, pp. 53-5, Table I, p. 53;
  [e] Rule B-1.1, pp. 53-5; [f] Rule B-5.11, p. 70; [g] Rule B-4, p. 68-70; [h] Rule B-3.5, pp. 67-8; [i] Rules B-6, pp. 71-2; B-10.1(in part), p. 72; and B-11(in part); [j] Rule B-3.1, pp. 64-5.
- 4. Reference 1, Section D, pp. 323-471; [a] Rules D-1.63, p. 336; D-3.73, p. 371; D-4.53, p. 379; D-5.3, pp. 392-3; D-5.42, p. 394; D-5.52(in part), p. 396; D-5.8, p. 408; D-6.85, pp. 425-6; D-6.86, p. 426; D-6.87, p. 426; and D-7.6(in part), pp. 447-54; [b] Rules D-4.12, p. 374; D-4.13, p. 374; D-4.14, pp. 374-5; D-4.22, pp. 375-6; and D-4.23, p. 376; [c] Rule D-4.14, p. 374-5, esp. † footnote, p. 374; and Rule D-6.12, pp. 409-10, Note, p. 410; [d] Appendix, Table I, pp. 459-60; [e] Rules D-4.11, p. 373; and D-6.11, p. 409; [f] Rules D-4.14, pp. 374-5; and D-6.12, pp. 409-10; [g] Rule D-5.11, p. 384, footnote; [h] Rule D-5.66, pp. 403-4; [i] Rule D-5.12, pp. 385-6; [j] Rule D-7.3, pp. 433-4; [k] Rule D-5.74, p. 407; [m] Rule D-5.14, p. 387; [n] Rules

D-5.66, pp. 403-4; and D-5.67, p. 404; [p] Rule D-5.71, p. 406; [q] Rule D-1.6, pp. 334-6; [r] Rule D-5.34, p. 393; [s] Rule D-7.63, pp. 449-50; [t] Rule D-1.63, p. 336; [u] Rule D-5.52, p. 396.

- 5. International Union of Pure and Applied Chemistry. Organic Chemistry Division. Commission on Nomenclature of Organic Chemistry, A Guide to IUPAC Nomenclature of Organic Compounds, Recommendations 1993, (in press). [Publication as a book by Blackwell Scientific Publications, Oxford, 1993]
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# APPENDIX: TRIVIAL AND ABBREVIATED NAMES FOR COMPOUNDS WITH RADICAL CENTERS ON CARBON ATOMS

List A. Names retained in "A Guide to the Use of IUPAC Nomenclature of Organic Compounds", Recommendations, 1993 (in press)<sup>5</sup>

	Structure	Trivial Name*	Systematic Name(s) According to the Recommendations Herein*
1.	(CH₃)₂ĊH	isopropyl**	1-methylethyl (RC-81.1.1) propan-2-yl (RC-81.1.2)
2.	(CH₃)₂CH—ĊH₂	isobutyl**	2-methylpropyl (RC-81.1.1) 2-methylpropan-1-yl (RC-81.1.2)
3.	сн₃—сн₂—сн —сн₃	sec-butyl**	1-methylpropyl (RC-81.1.1) butan-2-yl (RC-81.1.2)
4.	(CH3)3C.	tert-butyl**	1,1-dimethylethyl (RC-81.1.1) 2-methylpropan-2-yl (RC-81.1.2)
5.	(CH₃)₂CH−CH₂−ĊH₂	isopentyl**	3-methylbutyl (RC-81.1.1) 3-methylbutan-1-yl (RC-81.1.2)
6.	(CH₃)₃C—ĊH₂	neopentyl**	2,2-dimethylpropyl (RC-81.1.1) 2,2-dimethylpropan-1-yl (RC-81.1.2)
7.	СН <sub>3</sub> —СН <sub>2</sub> —с(СН <sub>3)2</sub>	tert-pentyl**	1,1-dimethylpropyl (RC-81.1.1) 2-methylbutan-2-yl (RC-81.1.2)
8.	сн₂шс́н	vinyl (Rule A-3.5 <sup>1</sup> )	ethenyl (RC-81.1.2)
9.	СН <sub>2</sub> === СН — СН	allyl (Rule A-3.5 <sup>1</sup> )	prop-2-en-1-yl (RC-81.1.2)
10.	сн₂ — с – сн₃	isopropenyl** (Rule A-3.5 <sup>1</sup> )	prop-1-en-2-yl (RC-81.1.2)

<sup>\*</sup> Where appropriate, the suffixes "-ylidene" and "-ylidyne" are used with the trivial and abbreviated names given here (see RC-81.1.3.2).

<sup>\*\*</sup> This name is used for unsubstituted structures only; see Rule A-2.25<sup>1</sup>.

	Structure	Trivial Name*	Systematic Name(s) According to the Recommendations Herein*
11.	C <sub>6</sub> H₅—CO—ĊH₂	phenacyl** (Rule C-318.1 <sup>1</sup> )	2-oxo-2-phenylethyl
12.	ĊH <sub>2</sub>	furfuryl (Rule B-5.11 <sup>1</sup> )	2-furylmethyl (see RC- 81.1.1 and RC-81.1.2)
13.	ČH <sub>2</sub>	thenyl (Rule B-5.11 <sup>1</sup> )	2-thienylmethyl (RC-81.1.1 and RC-81.1.2)
14.	сн₃—со—сн₂	acetonyl (Rule C-318.1 <sup>1</sup> )	2-oxopropyl (RC-81.1.1)
15.	н₃с-∕СУ∙	tolyl** (Rule A-13.1 <sup>1</sup> ) (4-isomer shown)	methylphenyl (RC-81.1.2) (4-isomer shown)
16.	H <sub>3</sub> C, CH <sub>3</sub> CH <sub>3</sub>	mesityl** (Rule A-13.1 <sup>1</sup> )	2,4,6-trimethylphenyl (RC-81.1.2)
17.	с <sub>6</sub> н₅—с́н₂	benzyl*** (Rule A-13.3 <sup>1</sup> )	phenylmethyl (RC-81.1.1 and RC-81.1.2)
18.	(C <sub>6</sub> H₅)₂ĊH	benzhydryl*** (Rule A-13.3 <sup>1</sup> )	diphenylmethyl (RC-81.1.1 and Rule RC-81.1.2)
19.	(C <sub>6</sub> H <sub>5</sub> )₃C •	trityl*** (Rule A-13.3 <sup>1</sup> )	triphenylmethyl (RC-81.1.) and RC-81.1.2)
20.	C <sub>6</sub> H₅—CH₂ —ĊH₂	phenethyl*** (Rule A-13.3 <sup>1</sup> )	2-phenylethyl (RC-81.1.1 and RC-81.1.2)

Trivial and Abbreviated Names for Compounds With Radical Centers on Carbon Atoms. List A (cont'd.)

\* Where appropriate, the suffixes "-ylidene" and "-ylidyne" are used with the trivial and abbreviated names given here (see RC-81.1.3.2).

\*\* This name is included in "A Guide to the Use of IUPAC Nomenclature of Organic Compounds", Recommendations, 1993 (in press)<sup>5</sup>, but substitution is not allowed.

\*\*\* This name is included in "A Guide to the Use of IUPAC Nomenclature of Organic Compounds", Recommendations, 1993 (in press)<sup>5</sup>, but substitution is allowed only on the ring.

	Structure	Trivial Name*	Systematic Name(s) According to the Recommendations Herein*
21.	с₀н₅—сн <u>—</u> с́н	styryl** (Rule A-13.3 <sup>1</sup> )	2-phenylvinyl (RC-81.1.2 and entry 8, above) 2-phenylethenyl (RC-81.1.2)
22.	с <sub>е</sub> н₅—сн <i>—</i> сн,	cinnamyl** (Rule A-13.3 <sup>1</sup> )	<pre>3-phenylallyl (RC-81.1.2 and entry 9, above) 3-phenylprop-2-en-1-yl (RC-81.1.2)</pre>

Trivial and Abbreviated Names for Compounds With Radical Centers on Carbon Atoms. List A (cont'd.)

# List B. Names not retained in "A Guide to the Use of IUPAC Nomenclature", Recommendations, 1993 (in press), but included in the 1979 IUPAC Organic Rules<sup>1</sup>

	Structure	Trivial Name*	Systematic Name(s) According to the Recommendations Herein*
1.	(CH <sub>3</sub> ) <sub>2</sub> CH[CH <sub>2</sub> ] <sub>2</sub> -cH <sub>2</sub>	isohexyl***	4-methylpentyl (RC-81.1.1) 4-methylpentan-1-yl (RC-81.1.2)
2.	С, сн₂	salicyl (Rule A- 13.3; C-201.4 <sup>1</sup> )	<pre>(2-hydroxyphenyl)methyl   (RC-81.1.1) 2-hydroxybenzyl (see entry   A-17, above)</pre>
3.	но СН₂	vanillyl (cf. Rule A-13.3; C-201.4; C-411.1 <sup>1</sup> )	<pre>(4-hydroxy-3-methoxyphenyl)-   methyl (RC-81.1.1) (4-hydroxy-3-methoxy)benzyl   (see entry A-17, above)</pre>

\* Where appropriate, the suffixes "-ylidene" and "-ylidyne" are used with the trivial and abbreviated names given here (see RC-81.1.3.2).

\*\* This name is included in "A Guide to the Use of IUPAC Nomenclature of Organic Compounds", Recommendations, 1993 (in press)<sup>5</sup>, but substitution is allowed only on the ring.

\*\*\* This name is used for unsubstituted structures only; see Rule A-2.251.

	Structure	Trivial Name*	Systematic Name(s) According to the Recommendations Herein*
4.	н₃с—о СН₂ о—сн₃	veratryl (cf. Rules A-13.3; C-201.4; C-411.1 <sup>1</sup> )	<pre>(3,4-dimethoxyphenyl)methyl (RC-81.1.1) 3,4-dimethoxybenzyl (see entry A-17, above)</pre>
5.	C CH2	piperonyl (cf. Rule C-411.1 <sup>1</sup> )	<pre>(benzo[d][1,3]dioxol-5-yl)-   methyl (RC-81.1.1) (1,3-benzodioxol-5-yl)-   methyl<sup>3h</sup> (RC-81.1.1)</pre>
6.	CH O	phthalidyl (Rule B-5.11; C-473.1 <sup>1</sup> )	3-oxo-1,3-dihydroisobenzo- furan-1-yl (RC-81.1.2)
7.	H <sub>3</sub> C	xylyl (Rule A-13.1 <sup>1</sup> ) (2,3-isomer shown)	dimethylphenyl (RC-81.1.2) (2,3-isomer shown)
8.	(CH <sub>3</sub> )₂CH-	cumenyl (Rule A-13.1 <sup>1</sup> ) (3-isomer shown)	<pre>isopropylphenyl (RC-81.1.2 and entry A-1 above) (1-methylethyl)phenyl (RC- 81.1.1 and RC-81.1.2) propan-2-ylphenyl (RC- 81.1.2)</pre>
9.		picryl (Rule C-202.2 <sup>1</sup> )	2,4,6-trinitrophenyl (RC-81.1.2)

Trivial	and Abbreviated Name	s for Compound	B With Radical	Centers on Carbon
Atoms.	List B (cont'd.)			