CHAPTER P-1 NOMENCLATURE OF ORGANIC COMPOUNDS

P-10 Introduction

For nomenclature purposes, a structure containing at least one carbon atom is considered to be an organic compound. The formation of a systematic name for an organic compound requires selection and then naming of a parent structure. This basic name may then be modified by prefixes, infixes, and, in the case of a parent hydride, suffixes, which convey precisely the structural changes required to generate the compound in question from the parent structure. In contrast to such systematic names, there are traditional names which are widely used in industry and academic circles. Examples are acetic acid, benzene and pyridine. Therefore, when they meet the requirements of utility and when they fit into the general pattern of systematic nomenclature, these traditional names are retained.

A major new principle is elaborated in these Recommendations. The concept of ‘preferred IUPAC names’ is developed and systematically applied. Up to now, the nomenclature developed and recommended by IUPAC has emphasized the generation of unambiguous names in accord with the historical development of the subject. In 1993, due to the explosion in the circulation of information and the globalization of human activities, it was deemed necessary to have a common language that will prove important in legal situations, with manifestations in patents, export-import regulations, environmental and health and safety information, etc. However, rather than recommend only a single ‘unique name’ for each structure, we have developed rules for assigning ‘preferred IUPAC names’, while continuing to allow alternatives in order to preserve the diversity and adaptability of the nomenclature to daily activities in chemistry and in science in general.

Thus, the existence of preferred IUPAC names does not prevent the use of other names to take into account a specific context or to emphasize structural features common to a series of compounds. Preferred IUPAC names belong to ‘**preferred IUPAC nomenclature’** Any name other than a preferred IUPAC name, as long as it is unambiguous and follows the principles of the IUPAC recommendations herein, is acceptable as a ‘general’ IUPAC name, in the context of **‘general’ IUPAC nomenclature**.

The concept of preferred IUPAC names is developed as a contribution to the continuing evolution of the IUPAC nomenclature of organic compounds. This book (Recommendations 2004) covers and extends the principles, rules and conventions described in two former publications: *Nomenclature of Organic Chemistry*, 1979 Edition (ref. 1) and *A Guide to IUPAC Nomenclature of Organic Compounds, Recommendations 1993* (ref. 2). In a few instances, the 1979 rules and the 1993 recommendations have been modified to achieve consistency within the entire system. In case of divergence among the various recommendations, Recommendations 2004 prevail.

P-11 Scope of nomenclature for organic compounds

For nomenclature purposes we consider all compounds containing carbon as organic compounds. Oxygen and nitrogen are two elements usually associated with carbon to form the system of functions or characteristic groups. Other elements, among them the halogens and sulfur, complete the basic core of elements found in organic compounds. Substitutive nomenclature was first applied to compounds containing this set of atoms. The success of this type of nomenclature was such that it was extended to all elements of Groups 14, 15, 16, 17 and, in Group 13, to boron; it is now fully extended to all elements of Group 13.

Table 1.1 Elements included in these recommendations

Groups	13	14	15	16	17
	B boron	C carbon	N nitrogen	O oxygen	F fluorine
	Al aluminium	Si silicon	P phosphorus	S sulfur	Cl chlorine
	Ga gallium	Ge germanium	As arsenic	Se selenium	Br bromine
	In indium	Sn tin	Sb antimony	Te tellurium	I iodine
	Tl thallium	Pb lead	Bi bismuth	Po polonium	As astatine

The ending 'ane', characteristic of alkanes, was borrowed from methane, ethane, etc., and glued to terms forming the roots of the names of the various elements, for example sulfane, H_2S; phosphane, PH_3; silane, SiH_4; alumane, AlH_3. The resulting names constitute the basis of substitutive nomenclature; this treatment of parent hydrides is called **generalized 'ane' nomenclature** because all the rules applicable to alkanes are applicable to all hydrides of the elements of Groups 13, 14, 15, 16 and 17. The nomenclature of hydrides of carbon may be conveniently termed **'carbane nomenclature'**; whereas the term **'heterane nomenclature'** covers the hydrides of elements other than carbon. Names of mononuclear parent hydrides are listed in Table 2.1 in Chapter 2.

Organometallic compounds, i.e., compounds in which one or more carbon atom(s) is (are) directly attached to a metal atom, were always regarded as organic compounds for nomenclature purposes. This association is maintained in these recommendations (see P-69), for the metals, semimetals, and nonmetals included in Groups 13, 14, 15, 16, and 17. The nomenclature for other organic derivatives of the elements in Groups 1 through 12 is considered as part of the nomenclature of inorganic compounds.

The construction of systematic names is based on general nomenclature operations and rules, and on operations and rules specific to different types of nomenclature. These aspects are discussed in the following sections.

P-12 Preferred, preselected and retained IUPAC names

P-12.1 'Preferred IUPAC names' are names that are preferred among two or more names for the same structure generated from two or more recommended IUPAC rules or the many synonyms that have been coined and used over the years.

Preferred IUPAC names, or PINs, for short, are names selected according to the set of principles, conventions, and rules given herein. They originate from the strict application of the rules; in this sense, they can be referred to as 'single names'. All preferred IUPAC names are identified by the parenthetical abbreviation '(PIN)' following the name. Names used in the past, but now discarded or no longer recommended, are sometimes mentioned as a link to past rules and recommendations and are identified by words such as 'not' or 'formerly' or phrases like 'no longer recommended'.

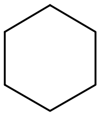
It is necessary to select a preferred alternative in many instances in the construction of the names of organic compounds. Preferred IUPAC names are given to parent structures and to characteristic groups denoted by prefixes and suffixes. They also result from the choice to be made among the different types of nomenclature, for example, substitutive nomenclature, functional class nomenclature and multiplicative nomenclature; and among the different types of operations, for example substitutive, additive and subtractive.

Most commonly, a **parent structure** is a **parent hydride**, i.e., a structure containing, in addition to one or more hydrogen atoms, a single atom of an element, for example, methane; or a number of atoms (alike or different) linked together to form an unbranched chain, for example, pentane; or a monocyclic or polycyclic ring system, for example, cyclohexane and quinoline. Methane is a retained name (see P-12.3) that is preferred to the systematic name 'carbane', a name never recommended to replace methane, but used to derive the names 'carbene' and carbyne for the radicals **:**CH_2 and **:**$CH\cdot$, respectively. The name 'pentane' is formed by application of P-21.2.1 and is marked as the preferred IUPAC name, or PIN, even though no rule has been cited giving an alternative name. The same reasoning applies to cyclohexane, a IUPAC name resulting from the application of P-22.1.1. The name 'quinoline' is a retained name that is preferred to the systematic alternative fusion names '1-benzopyridine' and 'benzo[*b*]pyridine'.

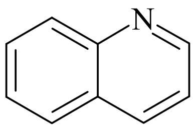
Examples:

CH_4 methane (preferred IUPAC name or PIN, a retained name)
carbane

CH_3-CH_2-CH_2-CH_2-CH_3 pentane (preferred IUPAC name or PIN)

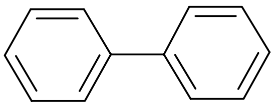


cyclohexane (PIN)

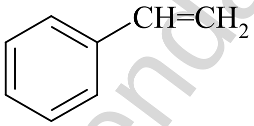


quinoline (PIN, a retained name)
1-benzopyridine (a systematic fusion name)
benzo[*b*]pyridine (a systematic fusion name)

It is sometimes convenient to employ parent hydrides of more complex structure, such as ring or ring-chain assemblies, for example biphenyl and styrene. The name ‘1,1′-biphenyl’ results from the application of Rule P-28.2.1; it is the preferred IUPAC name and the locants 1,1′ are compulsory; the name ‘biphenyl’, without locants, can be used in general IUPAC nomenclature. The name ‘styrene’ is a retained name and is preferred to the systematic substitutive names ‘vinylbenzene’, ‘ethenylbenzene’, ‘phenylethene’ and ‘phenylethylene’, that are acceptable in general IUPAC nomenclature as being clear and unambiguous.



1,1′-biphenyl (PIN)
biphenyl

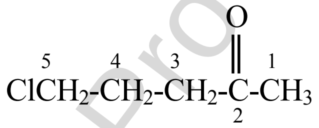


styrene (PIN, a retained name)
vinylbenzene
ethenylbenzene
phenylethene
phenylethylene

A special class of parent structures having retained names (see P-12.3) is called **functional parents**, for example acetone and acetic acid. These two names are preferred IUPAC names; the corresponding systematic alternatives, propan-2-one and ethanoic acid, may be used in general IUPAC nomenclature.

CH_3-CO-CH_3	CH_3-COOH
acetone (PIN) propan-2-one	acetic acid (PIN) ethanoic acid

In order to generate the parent structure from a compound to be named, various formal **operations** must be carried out. For example, in naming the structure below, the parent hydride ‘pentane’ is formally derived by replacing the oxygen and chlorine atoms by the appropriate number



$$\overset{5}{\mathrm{ClCH_2}}\text{-}\overset{4}{\mathrm{CH_2}}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\underset{2}{\overset{\overset{\mathrm{O}}{\|}}{\mathrm{C}}}\text{-}\overset{1}{\mathrm{CH_3}}$$

of hydrogen atoms. For constructing the name, the formal operation is reversed; the suffix ‘one’ and the prefix ‘chloro’, indicating **substitution** of the hydrogen atoms of pentane, are attached to the name of the parent hydride to give the name ‘5-chloropentan-2-one’. Suffixes and prefixes can represent a number of different types of formal operations on the parent structure. Frequently, the suffix or prefix denotes the attachment of a characteristic group (functional group), for example, ‘one’ or ‘oxo’ for =O. A prefix may also describe a group derived from a parent hydride, for example ‘pentyl’, from pentane, for CH_3-CH_2-CH_2-CH_2-CH_2–.

The **substitutive operation**, described in P-13.1, is the operation used most extensively in organic nomenclature. Indeed, the comprehensive nomenclature system based largely on the application of this operation to parent structures is, for convenience, termed **substitutive nomenclature**, although this nomenclature also involves many of the other types of operations described in P-13. Substitutive nomenclature is the set of **substitutive names and principles, conventions, and rules used for name construction**. Examples of substitutive and other nomenclature operations are shown in Table 1.2

Another type of nomenclature expresses the principal characteristic group not as a suffix but as a term denoting the functional class cited in a name as a separate word; in Table 1.2, the name 'ethyl propyl ether' is a typical **functional class name** based on the functional class name 'ether'. The corresponding substitutive name '1-ethoxypropane' is constructed by using the prefix 'ethoxy' and the parent hydride name 'propane'.

Substitutive and functional class names are written differently. Generally, substitutive names are unitary names that combine prefixes, names of parent hydrides, endings and suffixes in one word. On the contrary, a functional class name is written as separate words, even though the part describing the parent hydride or the modified parent hydride is the result of the same operations used to construct substitutive names.

The great majority, if not all, of organic compounds can be named in accordance with the principles of substitutive and functional class operations. However, in these recommendations, where there is a choice, names obtained by the substitutive operation are preferred IUPAC names. In Table 1.2, examples 1, 2 and 3 illustrates this preference. The substitutive names ethoxypropane and 2-chloropentan-2-one are preferred to the functional class names based on the names of the corresponding class, ether and ketone, ethyl propyl ether and 2-chloropropyl methyl ketone. On the contrary, a functional class name is preferred for the ester trimethyl phosphite over the substitutive name trimethoxyphosphane. Esters, along with acid halides and anhydrides are preferably named by using functional class nomenclature; substitutive nomenclature is not adapted to naming these classes.

Other types of operations are widely used, alone or along with substitutive nomenclature. **The skeletal replacement operation** (often referred to as 'a' replacement) is used as a necessary complement in order to introduce heteroatoms into cyclic hydrocarbons and to avoid the proliferation of prefixes in names for acyclic systems. For example, the name formed by skeletal replacement '2,5,8,11-tetraoxatridecane' is preferred to the substitutive name '1-ethoxy-2-[2-(methoxyethoxy)ethoxy]ethane'. **Additive** and **subtractive operations** have been extended for naming radicals and ions. They are the sole method for modification of the degree of hydrogenation, by adding or subtracting pairs of hydrogen atoms. Examples 5 and 6 illustrate the preference for substitutive operations over additive or subtractive operations. **The conjunctive operation** eliminates hydrogen atoms from two different compounds and then combines them; this method is used to name parent hydrides composed of repeated identical units or to link rings and chains under specific conditions. Example 7 in Table 1.2 illustrates such an operation; in IUPAC nomenclature,
however, a substitutive name is always preferred to a conjunctive name, for example '1*H*-indol-1-ylacetic acid' is preferred to '1*H*-indole-1-acetic acid'.

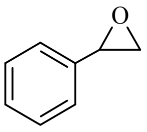
Table 1.2 Nomenclature operations

CH_3-CH_2-O-CH_2-CH_2-CH_3 CH_3-CHCl-CH_2-CO-CH_3 $P(OCH_3)_3$

1 2 3

CH_3-O-CH_2-CH_2-O-CH_2-CH_2-O-CH_2-CH_2-O-CH_2-CH_3

4



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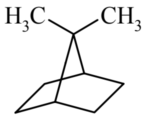

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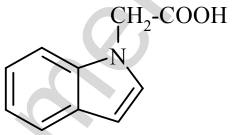

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Formula	Parent Structure (Class Name)	Operation	Name	Reference
1	propane (ether)	substitutive functional class	1-ethoxypropane (PIN) ethyl propyl ether	P-13.1 P-13.3.3.2
2	pentane (ketone)	substitutive functional class	4-choropentan-2-one (PIN) 2-chloropropyl methyl ketone	P-13.1 P-13.3.3.2
3	phosphane (phosphite)	substitutive functional class	trimethoxyphosphane trimethyl phosphite (PIN)	P-13.1 P-13.3.3.2
4	ethane tridecane	substitutive skeletal (‘a’) replacement	1-ethoxy-2-[2-(methoxyethoxy)ethoxy]ethane 2,5,8,11-tetraoxatridecane (PIN)	P-13.1 P-13.2.1
5	oxirane styrene + oxide	substitutive additive	2-phenyloxirane (PIN) styrene oxide	P-13.1 P-13.3.3.1
6	bornane bicycloheptane	substitutive substitutive	10-norbornane 7,7-dimethylbicyclo[2.2.1]heptane (PIN)	P-13.4.4.3 P-13.1
7	acetic acid acetic acid + indole	substitutive conjunctive	1*H*-indol-1-ylacetic acid (PIN) 1*H*-indole-1-acetic acid	P-13.2 P-13.5.2

A nomenclature embraces the major operations along with the principles, conventions and rules necessary to construct names of a particular type. Substitutive nomenclature and functional class nomenclature have been discussed above. Replacement nomenclature and conjunctive nomenclature also require specific principles, conventions and rules. On the contrary, additive and subtractive operations do not correspond to nomenclatures in their own right, but are necessary complements to other nomenclatures.

It is very important to recognize that, in general, the rules of the nomenclature of organic compounds are written in terms of classical valence bonding and do not imply electronic configurations of any kind.

Principles and general rules are described in this Chapter. Substitutive nomenclature is then elaborated in Chapter 2 (parent hydride names), in Chapter 3 (endings, suffixes and prefixes), and in Chapter 4 (rules for name construction). Chapter 5 describes the construction of preferred IUPAC names. In Chapter 6 the naming of compounds arranged in classes and groups is described. In Chapter 7, nomenclature for radicals, ions and related species is discussed. Chapter 8 describes isotopic modifications of organic compounds. Chapter 9 deals with configuration and conformation specification and Chapter 10 covers natural products.

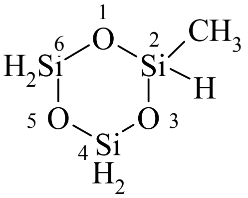
Several topics discussed in these recommendations have been published recently as fully comprehensive documents: radicals and ions (ref. 3), fused and bridged fused ring systems (ref. 4), phane nomenclature (refs. 5,6), the von Baeyer system for polycyclic compounds (ref. 7), spiro compounds (ref. 8), natural products (ref. 9), and fullerenes (ref. 10). They are not reproduced *in extenso* in these recommendations. Rather, the principles, conventions and rules are discussed in a less rigorous manner. Readers should use the full publications to deal with more complex cases; these publications are not superseded unless specifically noted in boxed comments. Again, all modifications made to achieve consistency are clearly signaled in these Recommendations and prevail over any former rules or interpretations.

P-12.2 ‘Preselected names‘ are names chosen among two or more names for noncarbon-containing (inorganic) parents to be used as the basis for preferred IUPAC names for organic derivatives in the nomenclature of organic compounds.

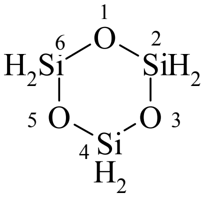
In the context of substitutive organic nomenclature, we need to select names for parent hydrides or other parent structures that do not contain carbon, in order to name organic derivatives. The names chosen here for this purpose are termed 'preselected'. Each non-carbon-containing parent capable of substitution or functionalization by carbon-containing groups is assigned a unique 'preselected' name to be used as the basis for deriving a preferred IUPAC name. Parent names identified here as 'preselected' may not necessarily emerge as preferred IUPAC names in the context of inorganic chemical nomenclature.

All names listed in Table 2.1, with the exception of methane (carbane), are preselected names, and the concept is illustrated by the following two examples.

$CH_3\text{-}SnH_2\text{-}[SnH_2]_{11}\text{-}SnH_3$	$SnH_3\text{-}[SnH_2]_{11}\text{-}SnH_3$
1-methyltridecastannane (PIN)	tridecastannane (preselected name)
$(CH_3\text{-}O)_3PO$	$(HO)_2P(O)\text{-}OH$
trimethyl phosphate (PIN)	phosphoric acid (preselected name)



2-methyl-1,3,5,2,4,6-trioxatrisilinane (PIN)
2-methylcyclotrisiloxane



1,3,5,2,4,6-trioxatrisilinane (preselected name;
see P-22.2.2.1.6)
cyclotrisiloxane (P-22.2.5)

P-12.3 'Retained names' are traditional or common well-established names that may be used either as preferred IUPAC name or as an allowed alternatives in general nomenclature, for example, naphthalene, benzoic acid and pyridine.

P-12.4 Methodology

In this book, names of parent structures, characteristic groups and their prefixes, and organic compounds are systematically identified as preferred IUPAC names or preselected IUPAC names; preferred IUPAC stereodescriptors are described and used in Chapter 9. To facilitate the construction of the names of organic compounds, preferred prefixes for use in generating preferred IUPAC names are listed in Appendix 2 along with other recommended prefixes to be used in general nomenclature.

P-13 Operations in nomenclature of organic compounds

The operations described in this section all involve structural modifications, and are classified first according to the type of modification, for example 'replacement'; and then according to the way in which the modification is expressed, for example 'by use of replacement infixes'. The structures to which the various modifications are applied can be regarded as parent structures, and the modifications are expressed by suffixes, affixes, infixes and prefixes, or by a change of the endings.

P-13.1 The substitutive operation
P-13.2 The replacement operation
P-13.3 The additive operation
P-13.4 The subtractive operation
P-13.5 The conjunctive operation
P-13.6 The multiplicative operation
P-13.7 The fusion operation
P-13.8 Operations used only in the nomenclature of natural products

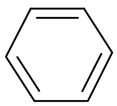
P-13.1 The substitutive operation

The substitutive operation involves the exchange of one or more hydrogen atoms for another atom or group of atoms. This process is expressed by a suffix or a prefix denoting the atom or group being introduced.

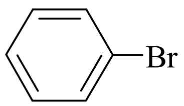
Examples:

CH_3-CH_3 ⟶ CH_3-CH_2-SH

ethane (PIN) ethanethiol (PIN)
(substitutive suffix = ‘thiol’)



benzene (PIN)



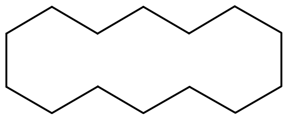
bromobenzene (PIN)
(substitutive prefix = ‘bromo’)

P-13.2 The replacement operation

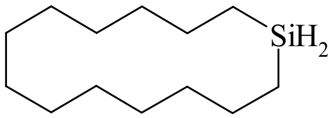
The replacement operation involves the exchange of one group of atoms or a single nonhydrogen atom for another. This can be expressed in several ways, as shown in the following subsections.

P-13.2.1 By replacement (‘a’) prefixes that represent the element being introduced. This type of replacement is called ‘skeletal replacement’. The most important type in the nomenclature of organic compounds is replacement of carbon atoms by O, S, Se, Te, N, P, As, Sb, Bi, Si, Ge, Sn, Pb, B, Al, Ga, In, or Tl.

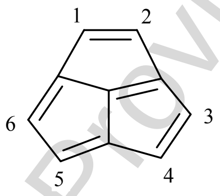
Examples:



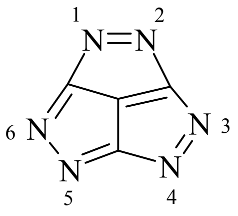
cyclotetradecane (PIN)



silacyclotetradecane (PIN)
(replacement prefix = ‘sila’)



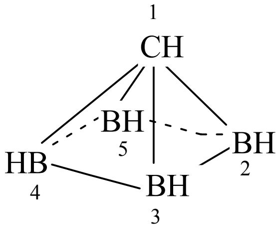
cyclopenta[*cd*]pentalene (PIN)



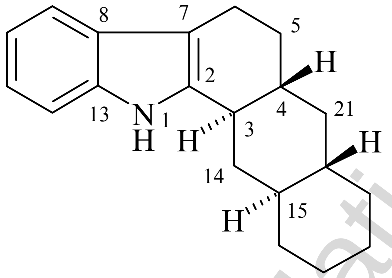
1,2,3,4,5,6-hexaazacyclopenta[*cd*]pentalene (PIN)
(replacement prefix = ‘aza’)

In specific instances, a heteroatom may be replaced by a carbon atom or another heteroatom. The former is exemplified in the nomenclature of cyclic polyboranes (see I-11.4.3.2, ref. 11) and both are found in natural products (see RF-5, ref. 9 and P-101.4) and must be applied only when specifically prescribed because the nomenclature of organic compounds is normally based on carbon atoms.

Examples:



1-carba-*nido*-pentaborane(5) (PIN)
(replacement prefix = 'carba';
carbon replacing boron)



(4β)-1*H*-4-carbayohimban (PIN)
(replacement prefix = 'carba'; carbon
replacing nitrogen; see P-94.2)

P-13.2.2 By prefixes or infixes signifying replacement of oxygen atoms or oxygen-containing groups. This type of replacement is called 'functional replacement'. The affixes represent the group(s) being introduced. Functional replacement nomenclature is described in P-15.5.

Examples:

$(CH_3)_2P(O)\text{-}OCH_3 \longrightarrow (CH_3)_2P(=NH)\text{-}OCH_3$

methyl dimethylphosphinate (PIN)

methyl *P*,*P*-dimethylphosphinimidate (PIN)
methyl *P*,*P*-dimethyl(imidophosphinate)
(replacement infix = 'imid(o)';
=NH replacing =O)

$C_6H_5\text{-}P(O)(OH)_2 \longrightarrow C_6H_5\text{-}P(\equiv N)\text{-}OH$

phenylphosphonic acid (PIN)

phenylphosphononitridic acid (PIN)
phenyl(nitridodophosphonic acid)
(replacement infix = 'nitrid(o)';
≡N replacing both =O and −OH)

The affixes 'thio', 'seleno', and 'telluro' indicate replacement of an oxygen atom of a characteristic group by another chalcogen atom.

Examples:

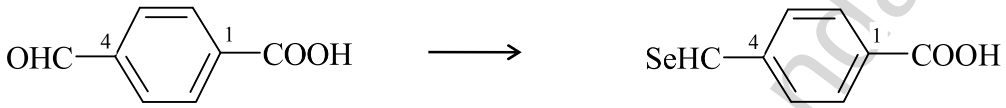
$C_6H_5\text{-}COOH \longrightarrow C_6H_5\text{-}C\{O,Se\}H$

benzoic acid

benzenecarboselenoic acid (PIN)
selenobenzoic acid
(replacement prefix = 'selen(o)';
selenium replacing either =O or −O−)

$$CH_3\text{-}[CH_2]_4\text{-}COOH \longrightarrow CH_3\text{-}[CH_2]_4\text{-}C(S)SH$$

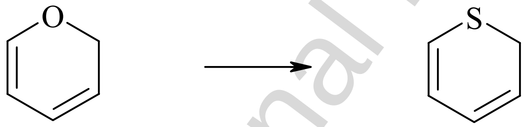
hexanoic acid (PIN)	hexanedithioic acid (PIN) hexane(dithioic) acid (replacement infix = ‘thi(o)’; S replaces both =O and −O−)



4-formylbenzoic acid (PIN)	4-methaneselenoylbenzoic acid (PIN) 4-(selenoformyl)benzoic acid (replacement prefix = ‘selen(o)’; Se replaces =O)

In specific instances, the prefixes ‘thio’, ‘seleno’, and ‘telluro’, indicate a skeletal modification. This replacement occurs with the cyclic parent hydrides having retained names, i.e., morpholine (see Table 2.3), pyran (see Table 2.2), chromene, isochromene, and xanthene (see Table 2.7), chromane and isochromane (see Table 3.1).

Example:



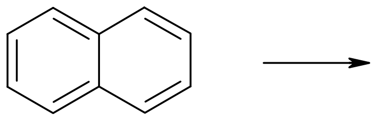
2*H*-pyran (PIN) 2*H*-oxine	2*H*-thiopyran (PIN) 2*H*-thiine (replacement prefix = ‘thio’; S replacing O)

P-13.3 The additive operation

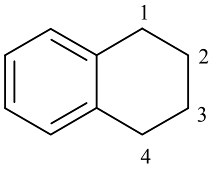
The additive operation involves the formal assembly of a structure from its component parts without loss of any atoms or groups. This operation can be expressed in several ways, as shown in the following subsections.

P-13.3.1 By an additive prefix

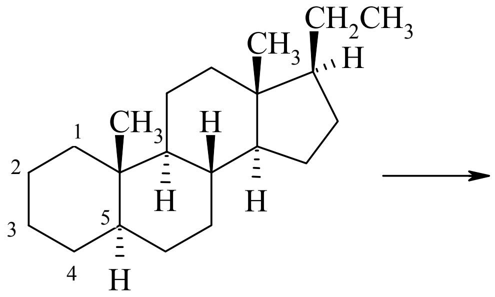
Examples:



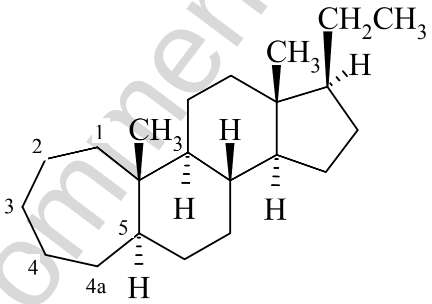
naphthalene (PIN)



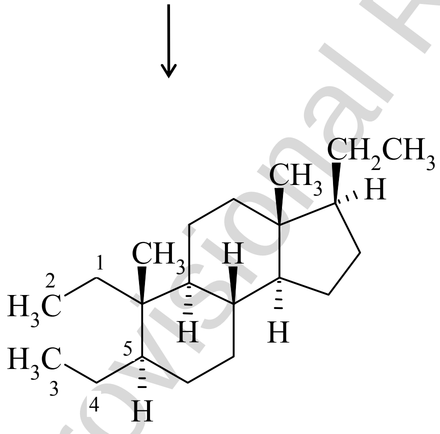
1,2,3,4-tetrahydronaphthalene (PIN)
('hydro' = prefix designating addition of one hydrogen atom)



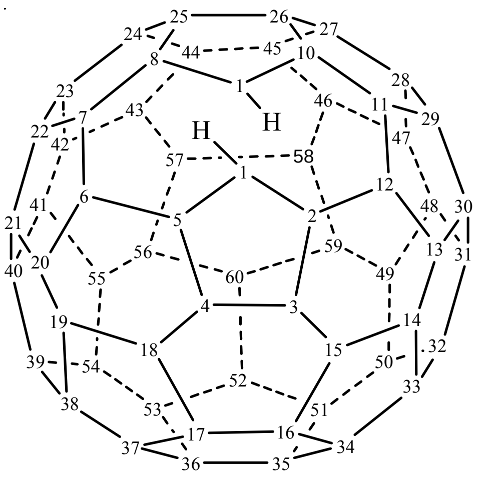
5α -pregnane (PIN)



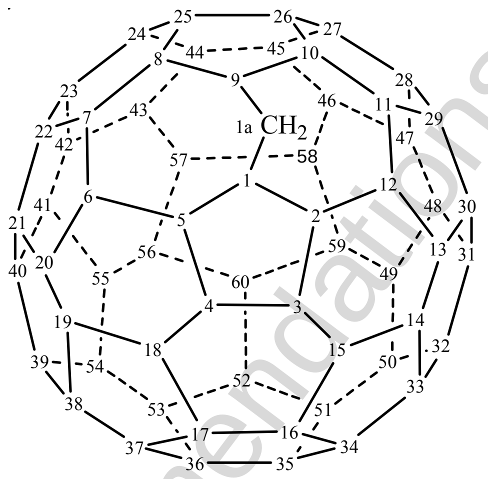
4a-homo-5α -pregnane (PIN)
('homo' = addition of a methylene, CH_2, group, which in this case expands a ring, see P-101.3.2.1)



2,3-seco-5α -pregnane (PIN)
('seco' = addition of two hydrogen atoms following the cleavage of a bond)



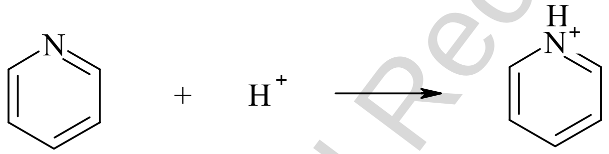
1,9-seco(C_{60}-I_h)[5,6]fullerene (PIN)



1a*H*-1(9)a-homo(C_{60}-I_h)[5,6]fullerene (PIN)

P-13.3.2 By an additive suffix

Examples:



pyridine (PIN)

pyridinium (PIN)
(‘ium’ = suffix designating the addition of one H^+)

$BH_3 + H^- \longrightarrow BH_4^-$

borane (preselected name)

boranuide (preselected name)
(‘uide’ = suffix designating the addition of one H^-)

P-13.3.3 By a separate word

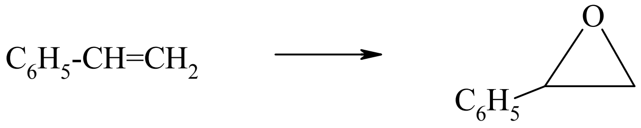
P-13.3.3.1 With the name of a neutral parent structure

Examples:

$CH_3\text{-}C{\equiv}N \longrightarrow CH_3\text{-}C{\equiv}NO$

acetonitrile (PIN)

acetonitrile oxide (PIN)



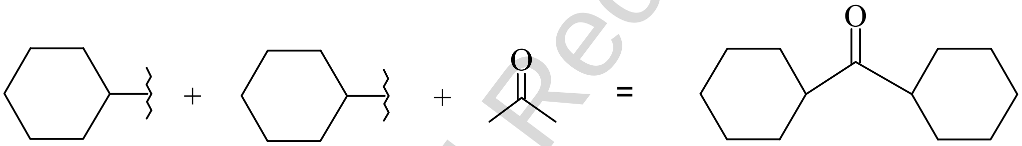
styrene ethenylbenzene (PIN)	styrene oxide 2-phenyloxirane (PIN)

P-13.3.3.2 With one or more substituent prefix name(s)

Here the separate word is a class or subclass name representing the characteristic group or the kind of characteristic group to which the substituents are linked (see also functional class nomenclature, P-15.2).

Examples:

$CH_3–$	+	$–OH$	→	CH_3-OH
methyl (PIN)		alcohol		methyl alcohol methanol (PIN)



cyclohexyl (PIN)	cyclohexyl (PIN)	ketone	dicyclohexyl ketone dicyclohexylmethanone (PIN)

$CH_3–$	+	$C_6H_5–$	+	–O–	→	CH_3-O-C_6H_5
methyl (PIN)		phenyl (PIN)		ether		methyl phenyl ether anisole (PIN) methoxybenzene

C_6H_5-$CH_2–$	+	–CN	→	C_6H_5-CH_2-CN
benzyl (PIN)		cyanide		benzyl cyanide phenylacetonitrile (PIN)

P-13.3.4 By adding substituent groups, in an operation called 'concatenation'

Examples:

CH_3-CH_2-CH_2-CH_2-$CH_2–$	+	–O–	→	CH_3-CH_2-CH_2-CH_2-CH_2-O–
pentyl (PIN)		oxy		pentyloxy (PIN)

$Cl–$	+	$–CO–$	$\longrightarrow$	$Cl\text{-}CO–$
chloro (preselected name)		carbonyl (PIN)		chlorocarbonyl carbonochloridoyl (PIN)

$–NH–$	+	$–CH_2\text{-}CH_2–$	+	$–NH–$	$\longrightarrow$	$–NH\text{-}CH_2\text{-}CH_2\text{-}NH–$
azanediyl (preselected name)		ethane-1,2-diyl (PIN)		azanediyl (preselected name)		ethane-1,2-diylbis(azanediyl) (PIN)

P-13.3.5 By adding molecular entities together

Chemical species AB in which two molecular entities A and B are combined directly with no loss of atoms from either A or B can be named by citing the names of A and B linked with an 'em' dash.

Example:

CO	+	BH_3	$\longrightarrow$	$CO \bullet BH_3$
carbon monoxide (PIN)		borane (preselected name)		carbon monoxide—borane (PIN)

P-13.4 The subtractive operation

The subtractive operation involves the removal of an atom or group implicit in a name. This operation can occur with no other change, with introduction of unsaturation, or with formation of substituent groups, radicals, or ions. Several prefixes are used to indicate subtractive operations of many kinds in natural products. Subtraction can be expressed in several ways as shown in the following subsections.

P-13.4.1 By a suffix

Examples:

CH_4	–	$H^\bullet$	$\longrightarrow$	$CH_3^\bullet$ or $CH_3–$
methane (PIN)		monohydrogen		methyl (PIN; a radical or substituent group; the suffix 'yl' indicates loss of one hydrogen atom)
$CH_3\text{-}CH_3$	–	H^+	$\longrightarrow$	$CH_3\text{-}CH_2^-$
ethane (PIN)		hydron		ethanide (PIN: the suffix 'ide' indicates loss of a hydron, i.e., a hydrogen cation)
$CH_3\text{-}CH_2\text{-}CH_2\text{-}CH_3$	–	H^-	$\longrightarrow$	$CH_3\text{-}CH_2\text{-}\overset{2}{C}H^+\text{-}\overset{1}{C}H_3$
butane (PIN)		hydride		butan-2-ylium (PIN; the suffix 'ylium' indicates loss of a hydride ion)

P-13.4.2 By a change in ending

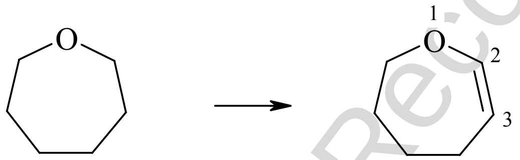
Examples:

$C_6H_5\text{-}SO_2\text{-}OH$	–	H^+	$\longrightarrow$	$C_6H_5\text{-}SO_2\text{-}O^-$
benzenesulfonic acid (PIN)		hydron		benzenesulfonate (PIN;the ending -ate indicates loss of a hydron, i.e., a hydrogen cation, from an ‘ic acid’)

$CH_3\text{-}CH_2\text{-}CH_3$	–	H_2	$\longrightarrow$	$CH_3\text{-}\overset{2}{C}H\text{=}\overset{1}{C}H_2$
Propane (PIN)		hydrogen		prop-1-ene (PIN;the ending ‘ene’ indicates loss of 2 hydrogen atoms)

P-13.4.3 By a prefix

Example:



oxepane (PIN) 2,3-didehydrooxepane (PIN; the prefix ‘didehydro’ indicates loss of 2 hydrogen atoms)

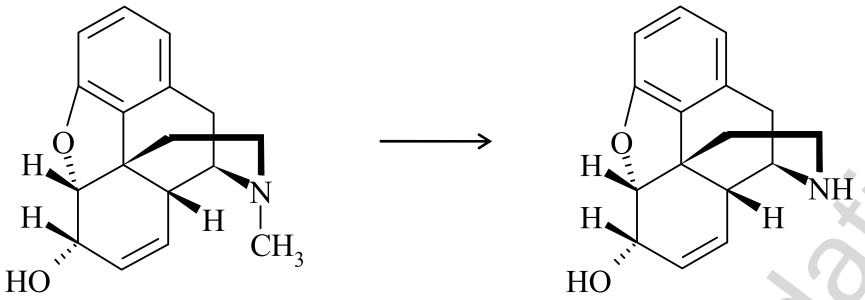
P-13.4.4 Prefixes used only in the nomenclature of natural products

In the nomenclature of natural products several prefixes are used to indicate the loss of a group, i.e., the exchange of a group for hydrogen. The subtraction of the elements of water with concomitant bond formation can also be regarded as a subtractive operation. Subtraction can be expressed as illustrated in the following subsections.

P-13.4.4.1 By the prefixes ‘de’ and ‘des’

P-13.4.4.1.1 The prefix ‘de’ (not ‘des’), followed by the name of a group or atom (other than hydrogen), denotes removal (or loss) of that group and addition of the necessary hydrogen atoms, i.e., exchange of that group with hydrogen atoms.

Example:

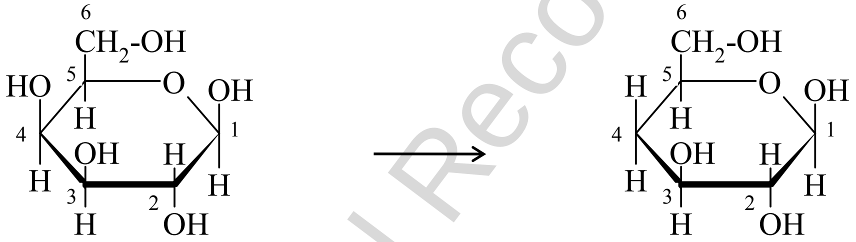


morphine (PIN)

demethylmorphine
(exchange of methyl for H)
17-normorphine (PIN)

As an exception, ‘deoxy’, when applied to hydroxy compounds, denotes the removal of an oxygen atom. ‘Deoxy’ is extensively used as a subtractive prefix in carbohydrate nomenclature (see P-93.6).

Example:



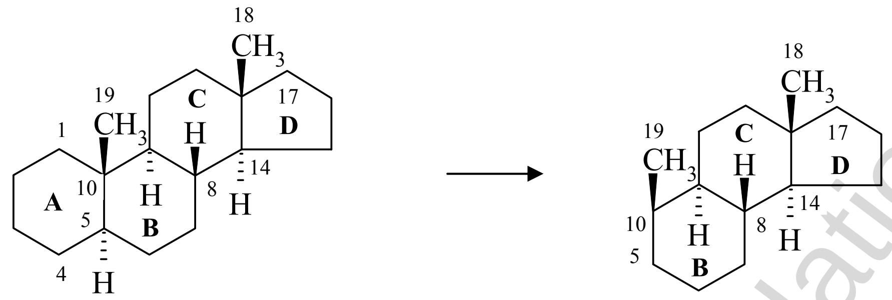
β-D-galactopyranose (PIN)

4-deoxy-β-D-*xylo*-hexopyranose (PIN)
(not 4-deoxy-β-D-galactopyranose)

P-13.4.4.1.2 The prefix ‘des’ signifies removal of an amino acid residue of a polypeptide, with rejoining of the chain (see P-103.5) or the removal of a terminal ring of a stereoparent (see P-101.3.6).

Examples:

oxytocin (PIN) ⟶ des-7-proline-oxytocin (PIN)
(removal of the proline residue at position 7)



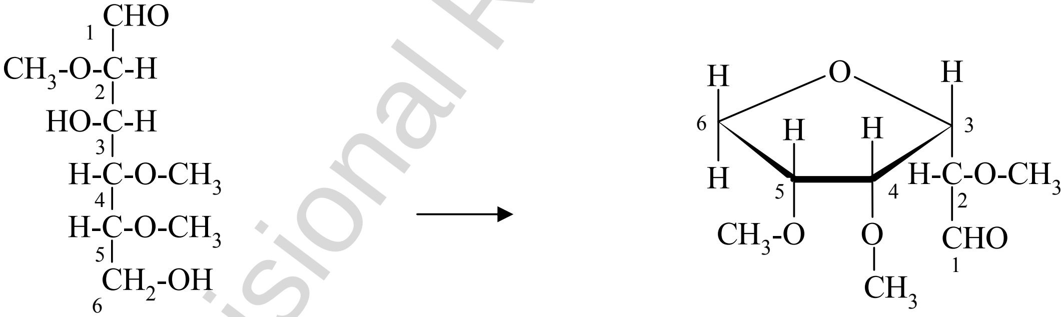
5α-androstane (PIN)

des-*A*-androstane
(3a*S*,5a*R*,6*R*,9a*R*,9b*S*)-3a,6-dimethyldodeca-hydrocyclopenta[*a*]naphthalene (PIN)

P-13.4.4.2 By the prefix ‘anhydro’

Intramolecular ethers, formally arising by elimination of water from two hydroxy groups of a single molecule of a monosaccharide (aldose or ketose) or monosaccharide derivative, is indicated by the detachable prefix ‘anhydro’ preceded by a pair of locants identifying the two hydroxy groups involved. The prefix ‘anhydro’ is placed in a name in accordance with the principles of alphabetical order (see P-102.5.5.7.1).

Example:



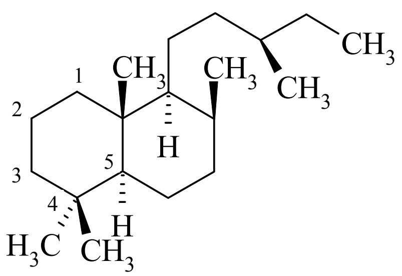
2,4,5-tri-*O*-methyl-D-mannitol (PIN)

3,6-anhydro-2,4,5-tri-*O*-methyl-D-mannitol (PIN)
(the prefix ‘anhydro’ describes removal of water from 2 ‘OH’ groups in the same molecule)

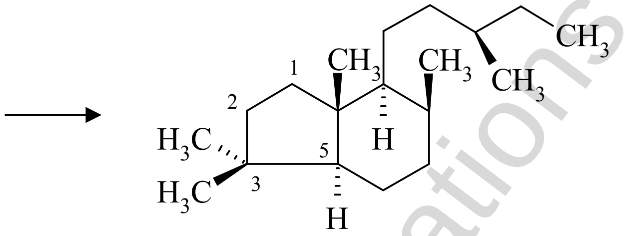
P-13.4.4.3 By the prefix ‘nor’

The prefix ‘nor’ is used to indicate removal of an unsubstituted saturated skeletal atom from a ring or a chain of a stereoparent parent structure with its attached hydrogen atom(s). It can also indicate the loss of a –CH= group from a mancude ring in a stereoparent parent structure (see P-101.3.1).

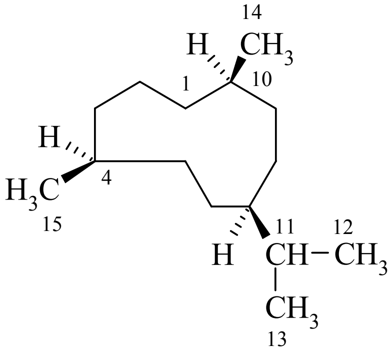
Examples:



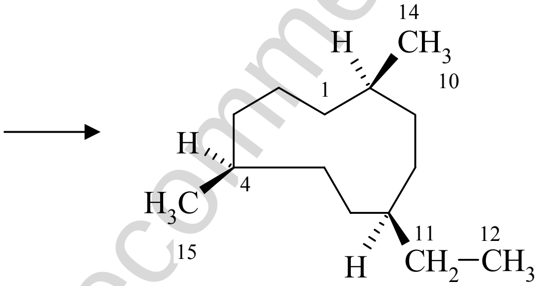
labdane (PIN)



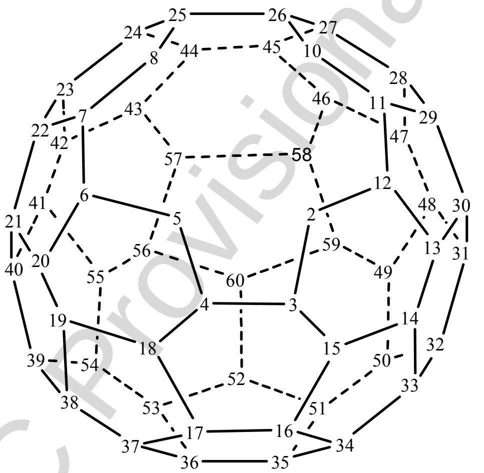
3-norlabdane (PIN; ring contraction by removal of a methylene, $-CH_2-$, group)



germacrane (PIN)



13-norgermacrane (removal of a side chain methylene, $-CH_2-$, group)
(1*R*,4*s*,7*S*)-1-ethyl-4,7-dimethylcyclodecane (PIN, see P-101.3.1.1)



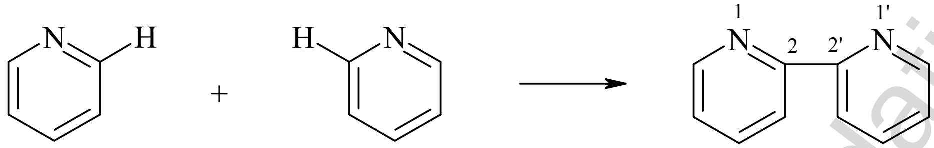
1,9-dinor(C_{60}-*I*$_h$)[5,6]fullerene (PIN)

P-13.5 The conjunctive operation

The conjunctive operation involves the formal construction of a name for a compound from the names of its components with subtraction of the same number of hydrogen atoms from each component at each site of the junction. This operation is expressed as noted in the following subsections.

P-13.5.1 By placing a multiplicative prefix ‘bi’, ‘ter’, ‘quater’, etc., before the name of the corresponding parent hydride.

Example:

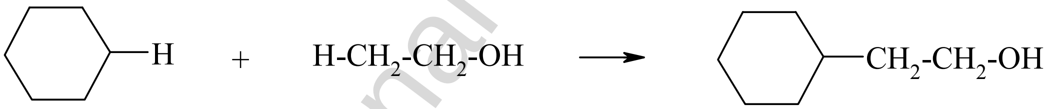


pyridine (PIN) pyridine (PIN) 2,2′-bipyridine (PIN)

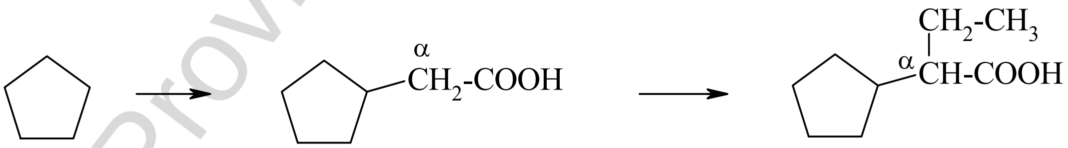
P-13.5.2 By juxtaposition of component names (conjunctive nomenclature)

This method is used by Chemical Abstracts Service. It is not recommended for constructing preferred IUPAC names; substitutive nomenclature is the recommended operation. This method is most commonly used when the two components to be joined are a ring or a ring system and a carbon chain (or chains) substituted by the principal characteristic group of the compound. In this method, both the principal characteristic group and the ring, or ring system, must terminate the chain; the rest of the structure attached to the chain, if any, is described by substituent prefixes, the location of which is indicated by Greek letter locants, α, β, etc. (α designates the atom next to the principal characteristic group).

Examples:



cyclohexane (PIN) ethanol (PIN) cyclohexaneethanol
2-cyclohexylethanol (PIN)

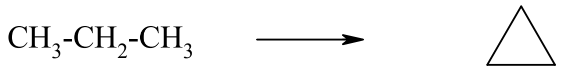


cyclopentane (PIN) cyclopentaneacetic acid
2-cyclopentylacetic acid (PIN)
α-ethylcyclopentaneacetic acid
2-cyclopentylbutanoic acid (PIN)

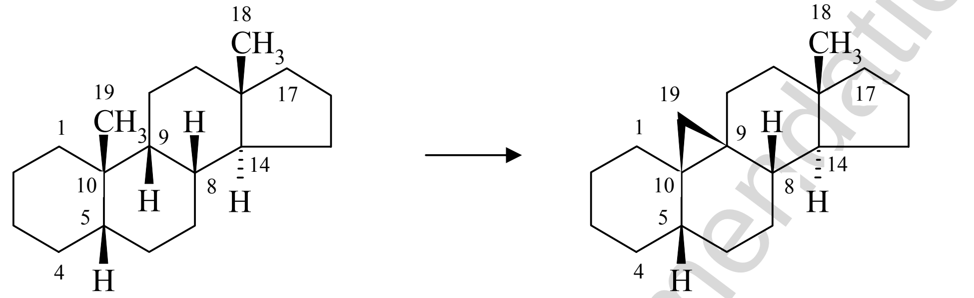
P-13.5.3 Ring formation

The formation of a ring by means of a direct link between any two atoms of a parent structure with loss of one hydrogen atom from each is indicated by the prefix ‘cyclo’.

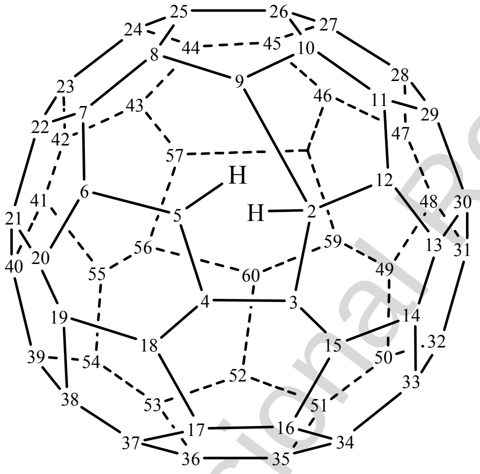
Examples:



propane (PIN) cyclopropane (PIN)



5β,9β-androstane (PIN) 9,19-cyclo-5β,9β-androstane (PIN; see P-101.3.3)

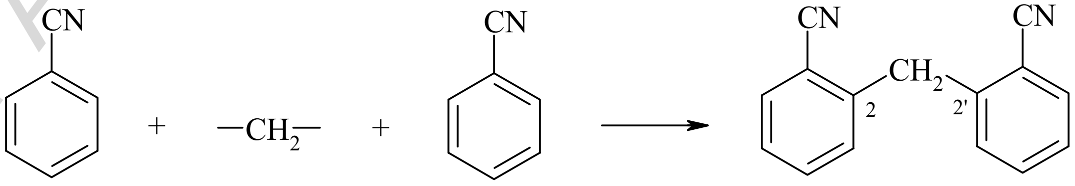


2H-2,9-cyclo-1-nor(C_{60}-I_h)[5,6]fullerene (PIN)

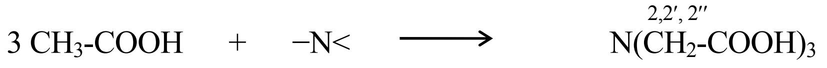
P-13.6 The multiplicative operation

This operation is used to name assemblies of identical units linked by di- or polyvalent substituent groups. Identical units are functionalized parent hydrides, functional parents and rings or ring systems. It is in fact substitutive nomenclature in which identical parent compounds are interconnected by a substituent group.

Examples:

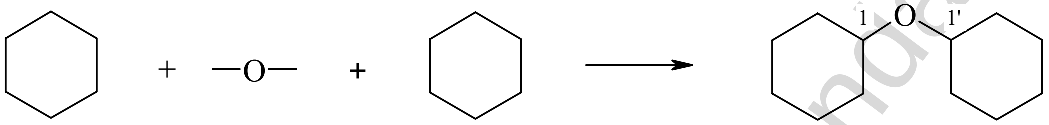


benzonitrile (PIN) methylene (PIN) benzonitrile (PIN) 2,2′-methylenedibenzonitrile (PIN)



$$3\ CH_3\text{-}COOH \quad + \quad -N< \quad \longrightarrow \quad \overset{2,2',2''}{N(CH_2\text{-}COOH)_3}$$

acetic acid (PIN) nitrilo (PIN) 2,2′,2″-nitrilotriacetic acid
N,*N*-bis(carboxymethyl)glycine (PIN)

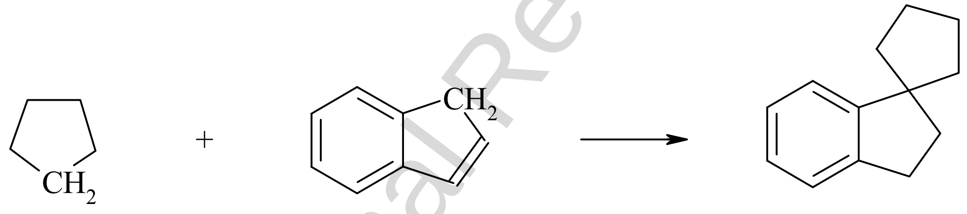


cyclohexane (PIN) oxy (PIN) cyclohexane (PIN) 1,1′-oxydicyclohexane (PIN)

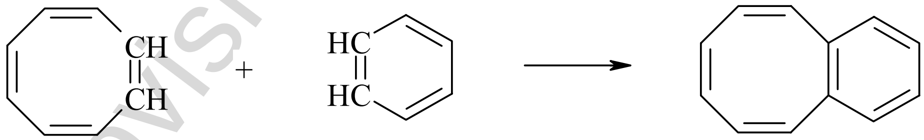
P-13.7 The fusion operation

The fusion operation involves the union of two rings or ring systems so that atoms or atoms and bonds are common to each. Spiro systems have one atom in common; fused ring systems have both atoms and bonds in common,

Examples:



cyclopentane (PIN) indene (PIN) spiro[cyclopentane-1,1′-indene] (PIN)



[8]annulene
cyclooctatetraene (PIN) benzene (PIN) benzo[8]annulene (PIN)

P-13.8 Operations used only in the nomenclature of natural products

The nomenclature of natural products and related compounds, described in Chapter 9, has its own principles, conventions and rules. In addition to the replacement, additive, subtractive, and conjunctive operations shared with systematic nomenclature, other operations are used only to modify parent structures, most of which are cyclic systems. These operations involve rearrangement of single bonds, and moving double bonds, and are denoted by the nondetachable prefixes ‘abeo*’* and ‘*retro’* respectively. The use of these prefixes and others is described and exemplified in Chapter 10.

P-14 General rules

P-14.0 Introduction

Rules described in this section are of general application for naming types of compounds and individual compounds. They must be closely followed to construct preferred IUPAC names as well as names for general use.

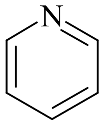
P-14.1 Bonding number

The concept of a standard valence state is fundamental to organic nomenclature. Since most organic names are derived by formal exchange of atoms or groups for hydrogen atoms of a parent structure, it is necessary to know exactly how many hydrogen atoms are implied by the name of the parent structure. For example, does the name phosphane refer to PH_3 or PH_5? This is a problem when an element can occur in more than one valence state; in such cases, the standard state is normally not specified, but any other valence state is noted by citation of an appropriate **bonding number**. More details are given in the publication 'Treatment of Variable Valence in Organic Nomenclature (Lambda Convention)' (ref. 12). In these Recommendations, this convention is called simply the 'λ-convention'.

P-14.1.1 Definition.

The bonding number '*n*' of a skeletal atom is the sum of the total number of bonding equivalents (valence bonds) of that skeletal atom to adjacent skeletal atoms if any in a parent hydride and the number of hydrogen atoms.

Examples:

H_2S	for S, $n = 2$
H_6S	for S, $n = 6$
$(C_6H_5)_3PH_2$	for P, $n = 5$
	for N, $n = 3$

P-14.1.2 Standard bonding numbers. The bonding number of a skeletal atom is standard when it has the value given in Table 1.3.

Table 1.3 Standard bonding numbers for the elements of Groups 13, 14, 15, 16, and 17

Standard bonding number (*n*)	Elements				
3	B	Al	Ga	In	Tl
4	C	Si	Ge	Sn	Pb
3	N	P	As	Sb	Bi
2	O	S	Se	Te	Po
1	F	Cl	Br	I	At

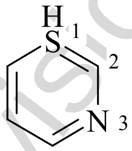
P-14.1.3 Nonstandard bonding numbers

A nonstandard bonding number of a **neutral** skeletal atom in a parent hydride is indicated by the symbol λ^n, cited in conjunction with an appropriate locant. Note that the '*n*' in the symbol 'λ^n ' is italicized but the numbers in a specific symbol, e.g., λ^4, are not (for the use of italicized '*n*' in λ^n see the General rules for symbols in physical quantities, Section 1.3 in ref. 13).

Examples:

CH_3-SH_5
methyl-λ^6-sulfane (PIN)

$(C_6H_5)_3PH_2$
triphenyl-λ^5-phosphane (PIN)



1λ^4,3-thiazine (PIN)

P-14.2 Multiplying prefixes

Three types of multiplying prefixes are used in names to denote multiplicity of identical features in structures (characteristic groups, substituent groups or terms) and correspondingly of affixes (suffixes and prefixes) in names. They are always placed before the part of the name to which they relate.

P-14.2.1 Basic multiplying prefixes denote simple features and, in general, are the first choice among prefixes to specify multiplicity (ref. 14). They are listed in Table 1.4.

Table 1.4 Basic numerical terms (multiplying prefixes)

Number	Numerical Term	Number	Numerical Term	Number	Numerical Term	Number	Numerical Term
1	mono, hen	11	hendeca	101	henhecta	1001	henkilia
2	di, do	20	icosa	200	dicta-	2000	dilia
3	tri	30	triaconta	300	tricta-	3000	trilia
4	tetra	40	tetraconta	400	tetracta	4000	tetralia
5	penta	50	pentaconta	500	pentacta	5000	pentalia
6	hexa	60	hexaconta	600	hexacta	6000	hexalia
7	hepta	70	heptaconta	700	heptacta	7000	heptalia
8	octa	80	octaconta	800	octacta	8000	octalia
9	nona	90	nonaconta	900	nonacta	9000	nonalia
10	deca	100	hecta	9000	nonalia		

P-14.2.1.1 The prefix mono

P-14.2.1.1.1 When alone, the numerical term for the number 1 is 'mono' and that for 2 is 'di'. In association with other numerical terms, the number 1 is represented by 'hen' (except in the case of 'undeca') and the number 2 by 'do' (except in the cases of 'dicta' and 'dilia'). The numerical term for the number 11 is 'undeca'.

P-14.2.1.1.2 The prefix 'mono' is not used in systematically formed names to indicate the presence of one nomenclatural feature, for example suffixes, prefixes, endings. It is used in functional class nomenclature to designate a monoester of a diacid, for example phthalic acid monomethyl ester, and in terminology, to emphazise singleness, for example, monocyclic and mononuclear in contrast to bicyclic and polynuclear.

P-14.2.1.2 Derivation of basic numerical terms

After 'undeca-' (number eleven), composite numerical terms are formed systematically by citing the basic terms in the order opposite to that of the constituent digits in the arabic numbers. The composite terms are formed by direct joining of the basic terms, without hyphen(s). The letter 'i' in 'icosa' is elided after a vowel.

Examples:

486 hexaoctacontatetracta
| 6 | 80 | 400 |

14	tetradeca	21	henicosa	22	docosa
23	tricosa	24	tetracosa	41	hentetraconta
52	dopentaconta	111	undecahecta		
363	trihexacontatricta				

P-14.2.2 Numerical terms for complex features

Multiplying prefixes for complex entities, such as substituted substituents, are formed by adding the ending ‘kis’ to the basic multiplying prefix ending in ‘a’, ‘tetrakis’, ‘pentakis’, etc. (ref. 14). The prefixes ‘bis’ and ‘tris’ correspond to ‘di’ and ‘tri’. The basic prefix ‘mono’ has no counterpart in this series.

Examples:

2	bis	3	tris	4	tetrakis
231	hentriacontadictakis				

P-14.2.3 Multiplying prefixes for naming assemblies of identical units

Latin based prefixes are used to denote the number of repeated identical units in unbranched assemblies: ‘bi’, ‘ter’, ‘quater’,

2	bi	5	quinque	8	octi
3	ter	6	sexi	9	novi
4	quater	7	septi	10	deci

The list has been completed from 11 to 9999. The prefixes are formed by changing the ending ‘a’ of basic numerical prefixes into ‘i’, for example, ‘undeci’ for 11, ‘hexadeci’ for 16, ‘tetraconti’ for 40.

P-14.3 Locants and numbering

P-14.3.1 Types of locants

Traditional types of locants are arabic numbers, i.e., 1, 2, 3; primed locants, i.e., 1′, 1‴, 2″; locants including a lower case Roman letter, i.e., 3a, 3b; italicized Roman letters, i.e., *O*, *N*, *P*; Greek letters, i.e., α, β, γ; and compound locants, i.e., 1(10), 5(17).

Composite locants, for example, 3^2 and $2a^1$, have been developed in recent years for various purposes and are included in these recommendations. They are used in Phane Nomenclature to indicate positions in amplificants (see P-26.4.3); for numbering in ring assemblies, (see P-29.3); for numbering polyanhydrides (see P-65.4.7.1.2); to denote interior positions in fused ring systems (see P-25.3.3.3); in von Baeyer descriptors for spiro ring systems (see P-24.2.2); and in numbering natural products, for example, amino acids (see P-103.2.2). Although not included in these recommendations, they are also used in steroid and tetrapyrrole nomenclature.

Primes are added to differentiate between the same locant in the same or different parts of the structure, for example, 1′, 2″, *N*′, and α′. In locants consisting of two or more characters, primes are generally added to the primary character. For example, in locants including a lower case Roman letter, used in fused rings, primes are added following the arabic number, for example, 3′a and 2′a^1; this format follows the principle that in locants for fusion positions in a fused ring system a letter follows the previous peripheral locant. For composite locants used in phane nomenclature, the prime follows the superatom locant, as in $2'^3$ and $2'^{4a}$.

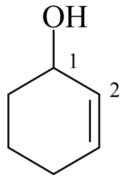
P-14.3.2 Position of locants

Locants (numerals and/or letters) are placed immediately before that part of the name to which they relate, except in the case of the traditional contracted names when locants are added at the front of their names.

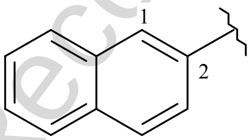
Examples:

$$\overset{6}{CH_3}\text{-}\overset{5}{CH_2}\text{-}\overset{4}{CH_2}\text{-}\overset{3}{CH}\text{=}\overset{2}{CH}\text{-}\overset{1}{CH_3}$$

hex-2-ene (PIN)
(not 2-hexene)



cyclohex-2-en-1-ol (PIN)
(not 2-cyclohexen-1-ol)



naphthalen-2-yl (PIN)
2-naphthyl
(not naphth-2-yl)

P-14.3.3 Omission of locants

The practice of omitting locants when there is no ambiguity is widespread. However for designating preferred IUPAC names it is necessary to be prescriptive about when omission of locants is permissible. Thus, in preferred IUPAC names, if any locants are essential for defining the structure, then all locants should be cited. For example, the omission of the locant ‘1’ in 2-chloroethanol, while permissible in general usage, is not allowed in the preferred IUPAC name 2-chloroethan-1-ol. Also, in preferred IUPAC multiplicative names and in preferred IUPAC names for ring assemblies locants are always cited, e.g., 1,1′-oxydibenzene and 1,1′-biphenyl.

Locants are omitted in preferred IUPAC names in the following cases.

P-14.3.3.1 Terminal locants in names for mono- and dicarboxylic acids derived from acyclic hydrocarbons and their corresponding acyl halides, amides, nitriles, and aldehydes are never cited (however, see P-15.4.3.1).

Examples:

HOOC-CH_2-CH_2-COOH	butanedioic acid (PIN)
CH_3-CH_2-CH_2-CH_2-CO-	pentanoyl (PIN)

P-14.3.3.2 The locant ‘1’ is omitted:

(a) in substituted mononuclear parent hydrides;

Examples:

CH_3Cl	SiH_2Cl_2	$(CH_3)_3Al$
chloromethane (PIN)	dichlorosilane (preselected name)	trimethylalumane (PIN)

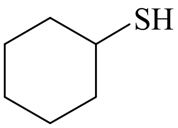
(b) in monosubstituted homogeneous chains consisting of only two identical atoms;

Examples:

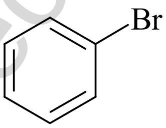
CH_3-CH_2-OH	NH_2−NH-Cl
ethanol (PIN)	chlorohydrazine (preselected name)

(c) in monosubstituted homogeneous monocyclic rings;

Examples:



cyclohexanethiol (PIN)

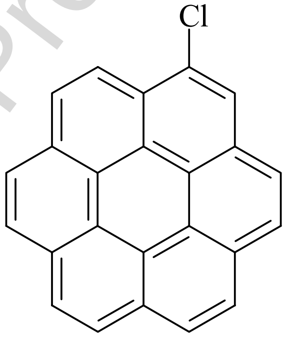


bromobenzene (PIN)

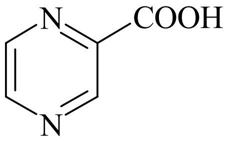
(d) in monosubstituted symmetrical parent hydrides or parent compounds where there is only one kind of substitutable hydrogen;

Examples:

CH_3-NH_2-CO-NH_2	Cl-SiH_2-O-SiH_3
methylurea (PIN)	chlorodisiloxane (preselected name)



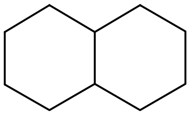
chlorocoronene (PIN)



pyrazinecarboxylic acid (PIN)

P-14.3.3.3 All locants are omitted in compounds in which all substitutable positions are completely substituted or modified in the same way. The prefix ‘per-’ is no longer recommended. In case of partial substitution or modification, all numerical prefixes must be indicated.

Examples:



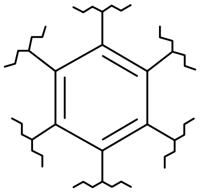
decahydronaphthalene (PIN)

CF_3-CF_2-CF_2-COOH

heptafluorobutanoic acid (PIN)

$\overset{3}{C}F_3$-$\overset{2}{C}F_2$-$\overset{1}{C}H_2$-OH

2,2,3,3,3-pentafluoropropan-1-ol (PIN)



benzenehexayl (PIN)

P-14.3.4 Lowest set of locants

The lowest set of locants is defined as the set that, when compared term by term with other locant sets, each cited in order of increasing value, has the lowest term at the first point of difference; for example, the locant set ‘2,3,5,8’ is lower than ‘3,4,6,8’ and ‘2,4,5,7’.

Primed locants are placed immediately after the corresponding unprimed locants in a set arranged in ascending order; locants consisting of a number and a lower-case letter are placed immediately after the corresponding numeric locant with or without prime and are followed by locants having superscripts.

Examples:

2 is lower than 2′

3 is lower than 3a

8a is lower than 8b

4′ is lower than 4a

4′a is lower than 4″a

1^2 is lower than 1^3

1^4 is lower than 2′

3a is lower than $3a^1$

Italic capital and lower-case letter locants are lower than Greek letter locants, which, in turn, are lower than numerals.

Example:

'*N*, α,1,2' is lower than '1,2,4,6'

P-14.4 Numbering

When several structural features appear in cyclic and acyclic compounds, low locants are assigned to them in the following decreasing order of seniority.

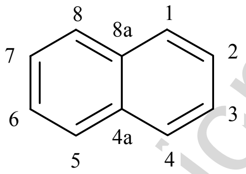
Two important changes have been made to the 1979 recommendations (ref 1).

(1) heteroatoms in chains are now considered as part of the parent hydride; as such, they have seniority over suffixes for numbering;

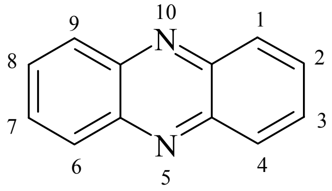
(2 hydro/dehydro prefixes are now classified as detachable prefixes, but are not included in the category of alphabetized detachable prefixes.

(a) fixed numbering of a ring or ring system;

Examples:



naphthalene (PIN)



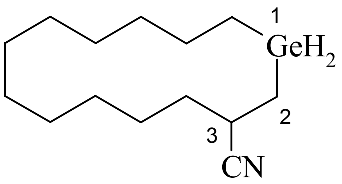
phenazine (PIN)

(b) heteroatoms in chains and in rings and ring systems;

Examples:

$$\overset{1}{C}H_3\text{-}\overset{2}{S}\text{-}\overset{3}{C}H_2\text{-}\overset{4}{C}H_2\text{-}\overset{5}{O}\text{-}\overset{6}{C}H_2\text{-}\overset{7}{C}H_2\text{-}\overset{8}{S}\text{-}\overset{9}{C}H_2\text{-}\overset{10}{C}H_2\text{-}\overset{11}{Si}H_2\text{-}\overset{12}{C}H_2\text{-}\overset{13}{C}H_2\text{-}\overset{14}{C}OOH$$

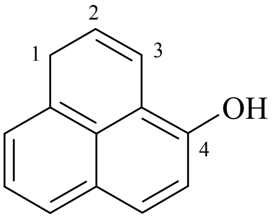
5-oxa-2,8-dithia-11-silatetradecan-14-oic acid (PIN)

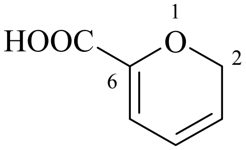


1-germacyclotetradecane-3-carbonitrile (PIN)

(c) indicated hydrogen;

Examples:

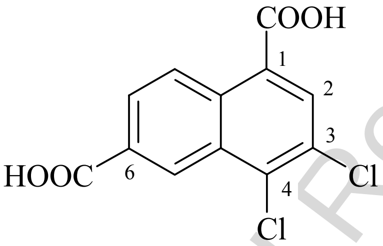




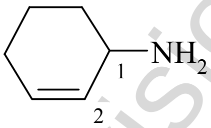
1*H*-phenalen-4-ol (PIN) 2*H*-pyran-6-carboxylic acid (PIN)

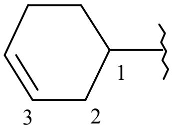
(d) principal characteristic groups and free valences (suffixes);

Examples:



3,4-dichloronaphthalene-1,6-dicarboxylic acid (PIN)

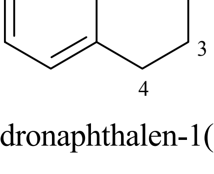




cyclohex-2-en-1-amine (PIN) cyclohex-3-en-1-yl (PIN)

(e) added hydrogen;

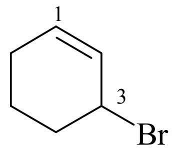
Example:



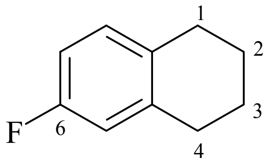
3,4-dihydronaphthalen-1(2*H*)-one (PIN)

(f) saturation/unsaturation (hydro/dehydro prefixes and ‘ene’ and ‘yne’ endings);

Examples:



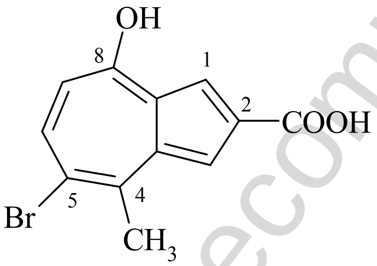
3-bromocyclohex-1-ene (PIN)



6-fluoro-1,2,3,4-tetrahydronaphthalene (PIN)

(g) detachable alphabetized prefixes, all considered together in a series of increasing numerical order;

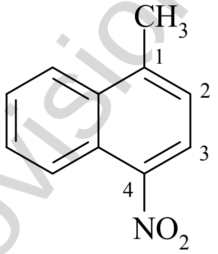
Example:



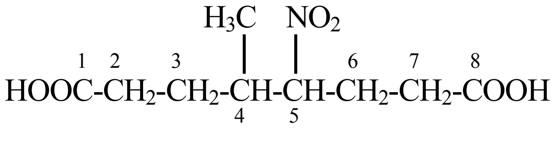
5-bromo-8-hydroxy-4-methylazulene-2-carboxylic acid (PIN)

(h) lowest locants for the substituent cited first as a prefix in the name;

Examples:



1-methyl-4-nitronaphthalene (PIN)

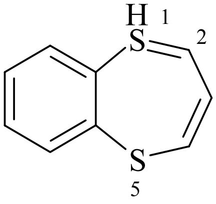


$$\mathrm{HOOC\text{-}CH_2\text{-}CH_2\text{-}\overset{\overset{H_3C}{|}}{CH}\text{-}\overset{\overset{NO_2}{|}}{CH}\text{-}CH_2\text{-}CH_2\text{-}COOH}$$

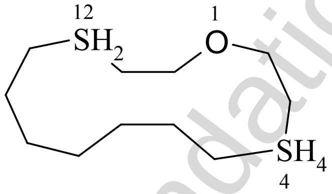
4-methyl-5-nitrooctanedioic acid (PIN)

(i) When a choice is needed between the same skeletal atom in different valence states, the one in a nonstandard valence state is assigned the lower locant. If a further choice is needed between the same skeletal atom in two or more nonstandard valence states, the one in the higher valence state is assigned the lower locant;

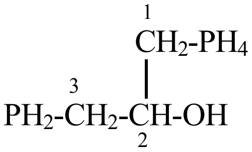
Examples:



1λ⁴,5-benzodithiepine (PIN)



1-oxa-4λ⁶,12λ⁴-dithiacyclotetradecane (PIN)



$$\begin{array}{r} \overset{1}{C}H_2\text{-}PH_4 \\ | \quad\quad\; \\ PH_2\text{-}\overset{3}{C}H_2\text{-}\underset{2}{C}H\text{-}OH \end{array}$$

1-(λ^5-phosphanyl)-3-phosphanylpropan-2-ol (PIN)
(λ^5-phosphanyl is cited before phosphanyl and
is given the lower locant)

(j) When there is a choice between equivalent numberings in an isotopically unmodified compound, the starting point and the direction of numbering of the analogous isotopically substituted compound are chosen so as to give lowest locants to the modified atoms or groups considered together in one series in increasing numerical order. If a choice still remains, the lower locant is given to the nuclide of higher atomic number. In the case of different nuclides of the same element, the lower locant is assigned to the nuclide of higher mass number.

Examples:

$\overset{1}{C}H_3\text{-}{}^{14}\overset{2}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{4}{C}H_3$

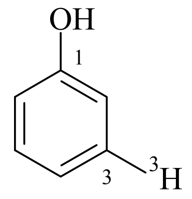
(2-^{14}C)butane (PIN)
[not (3-^{14}C)butane]

$\overset{1}{C}H_3\text{-}\overset{2}{C}{}^{2}H_2\text{-}{}^{14}\overset{3}{C}H_2\text{-}\overset{4}{C}H_3$

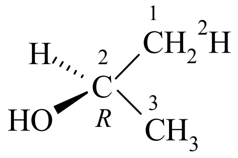
(3-^{14}C,2,2-$^{2}H_2$)butane (PIN)
[not (2-^{14}C,3,3-$^{2}H_2$)butane]

$\overset{1}{C}H_3\text{-}{}^{14}\overset{2}{C}H_2\text{-}\overset{3}{C}H{}^{2}H\text{-}\overset{4}{C}H_3$

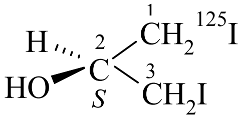
(2-^{14}C,3-$^{2}H_1$)butane (PIN)
[not (3-^{14}C,2-$^{2}H_1$)butane]



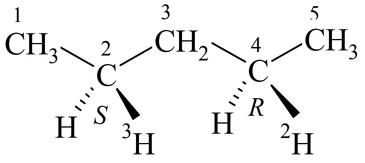
(3-^{3}H)phenol (PIN)



(*R*)-(1-$^{2}\mathrm{H}_{1}$)propan-2-ol (PIN)



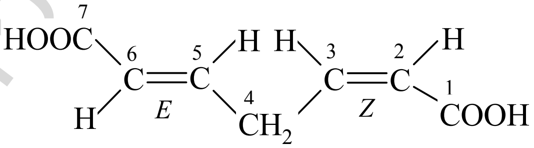
(*S*)-1,3-(1-^{125}I)diiodopropan-2-ol (PIN)



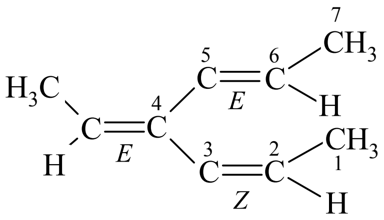
(2*S*,4*R*)-(4-$^{2}\mathrm{H}_{1}$,2-$^{3}\mathrm{H}_{1}$)pentane (PIN)
[not (2*R*,4*S*)-(2-$^{2}\mathrm{H}_{1}$,4-$^{3}\mathrm{H}_{1}$)pentane; isotopic modifications have seniority for low locants over stereodescriptors described in (k) below]

(k) When there is a choice for lower locants related to the presence of stereogenic centers or stereoisomers, the lower locant is assigned to CIP stereodescriptors *Z*, *R*, R_{a}, R_{p}, *M* , and *r* CIP stereodescriptors, that are preferred to non-CIP stereodescriptors *cis* or *r*, *c* (see P-92 for CIP and non-CIP stereodescriptors).

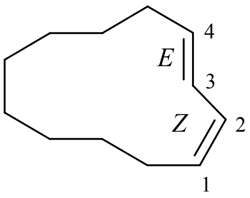
Examples:



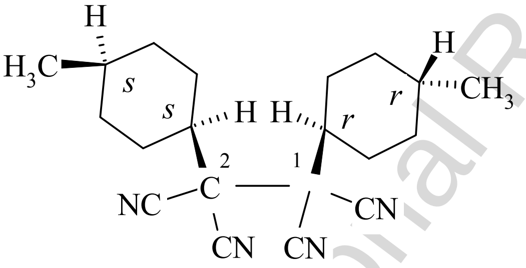
(2*Z*,5*E*)-hepta-2,5-dienedioic acid (PIN)
(the chain is numbered by assigning the low locant to the '*Z*' double bond)



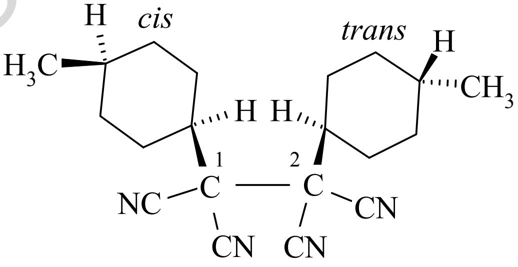
(2*Z*,4*E*,5*E*)-4-ethylidenehepta-2,5-diene (PIN)
(low locants are assigned to the longest chain, then to the ‘*Z*’ double bond)



(1*Z*,3*E*)-cyclododeca-1,3-diene (PIN)



I

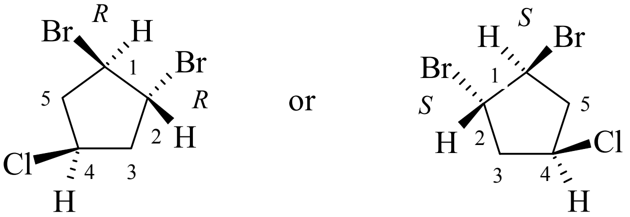


II

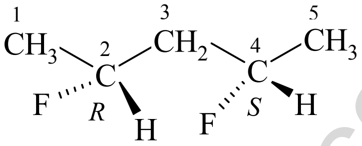
1-[(1*r*4*r*)-4-methylcyclohexyl-2-[(1*s*,4*s*)-4-methylcyclohexyl]ethane-1,1,2,2-tetracarbonitrile **(I)** (PIN)
(the substituent denoted by the ‘*r*’ stereodescriptor receives the lowest locant, ‘1’; the use of CIP stereodescriptor generates the preferred IUPAC name)

1-(*cis*-4-methylcyclohexyl)-2-(*trans*-4-methylcyclohexyl)ethane-1,1,2,2-tetracarbonitrile **(II)**
(the ‘*cis*’ substituent receives the lowest locant, ‘1’)

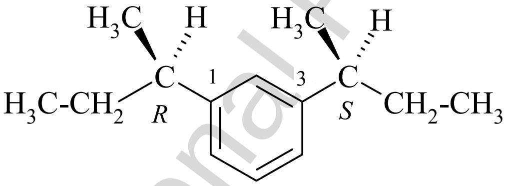
.



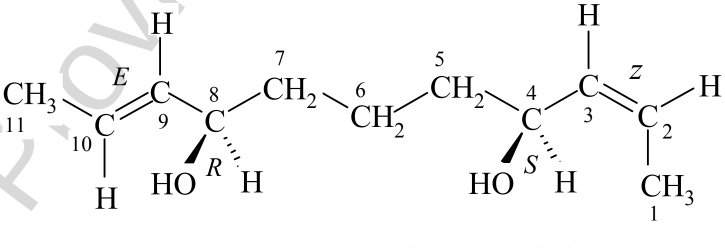
rel-(1*R*,2*R*)-1,2-dibromo-4-chlorocyclopentane (PIN)
1*r*,2*t*-dibromo-4-*c*-chlorocyclopentane
(the preferred IUPAC name is denoted by CIP stereodescriptors; in the second name, the relative configuration is expressed by the non CIP stereodescriptors 1*r*,2*t*,4*c* rather than 1*r*,2*t*,4*t*, because a '*cis*' arrangement, denoted by '*c*', has priority over a '*trans*' arrangement, denoted by '*t*', in position '4')



(2*R*,4*S*)-2,4-difluoropentane (PIN)



1-[(2*R*)-butan-2-yl]-3-[(2S)-butan-2-yl]benzene (PIN)



(2*Z*,4*S*,8*R*,9*E*)-undeca-2,9-diene-4,8-diol (PIN)
(the choice is between '*E*' and '*Z*' for position '2', not between '*R*' and '*S*' for position '4')

P-14.5 Alphanumerical order

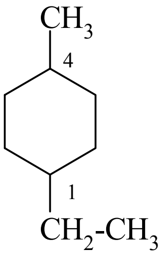
> Alphanumerical order has been commonly called ‘alphabetical order’. As it does imply ordering both letters and numbers, in a strict sense it is best called ‘alphanumerical order’ in order to convey the message that both letters and numbers are involved.

Alphanumerical order is used to establish the order of citation of detachable prefixes and the numbering of a chain, ring, or ring system by giving the lowest possible locants to nondetachable prefixes.

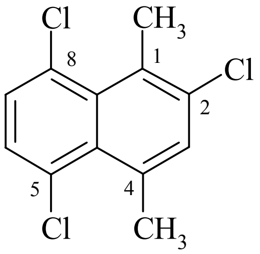
Alphanumerical order is applied as follows in organic nomenclature. Letters are considered first (all Roman letters before any italic letters), unless used as locants or part of a compound or composite locant, for example, ‘*N*-‘ or ‘4a’). If there is a further choice, numerical locants are considered in order from lowest to highest

P-14.5.1 Simple prefixes (i.e., those describing atoms and unsubstituted substituents) are arranged alphabetically; multiplying prefixes, if necessary, are then inserted and do not alter the alphabetical order already established.

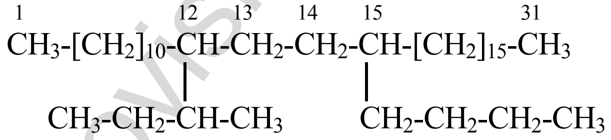
Examples:



1-ethyl-4-methylcyclohexane (PIN)



2,5,8-trichloro-1,4-dimethylnaphthalene (PIN)

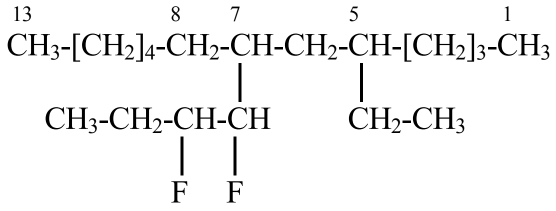


$$\mathrm{\overset{1}{CH_3}\text{-}[CH_2]_{10}\text{-}\underset{\displaystyle CH_3\text{-}CH_2\text{-}CH\text{-}CH_3}{\overset{12}{CH}}\text{-}\overset{13}{CH_2}\text{-}\overset{14}{CH_2}\text{-}\underset{\displaystyle CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_3}{\overset{15}{CH}}\text{-}[CH_2]_{15}\text{-}\overset{31}{CH_3}}$$

12-(butan-2-yl)-15-butylhentriacontane (PIN)
(butyl is not treated as butan-1-yl; see also P-56.2.2)

P-14.5.2 The name of a prefix for a substituted substituent is considered to begin with the first letter of its complete name.

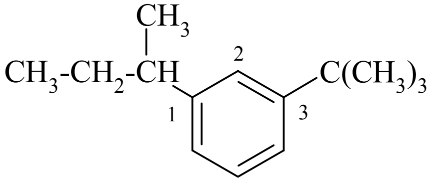
Example:



7-(1,2-difluorobutyl)-5-ethyltridecane (PIN)

P-14.5.3 When an alphanumerical ordering is required and Roman letters do not permit a decision for the order of citation, italicized letters are considered.

Example:

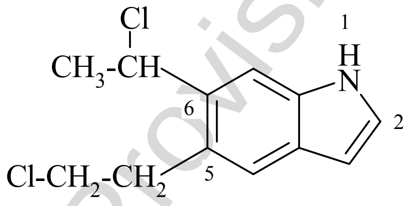


1-*sec*-butyl-3-*tert*-butylbenzene
1-(butan-2-yl)-3-*tert*-butylbenzene (PIN)

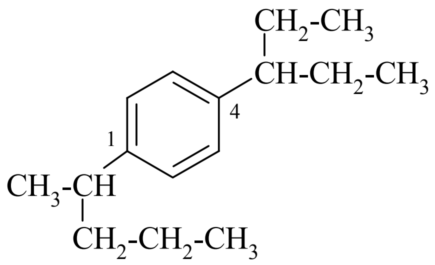
Similarly, *as*-indacen-1-yl is senior to *s*-indacen-1-yl and naphtho[1,2-*f*]quinolin-2-yl is senior to naphtho[1,2-*g*]quinolin-1-yl (‘*f*’ before ‘*g*’).

P-14.5.4 When two or more prefixes consist of identical Roman letters, priority for order of citation is given to the group that contains the lowest locant at the first point of difference.

Examples:



6-(1-chloroethyl)-5-(2-chloroethyl)indole (PIN)

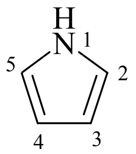


1-(pentan-2-yl)-4-(pentan-3-yl)benzene (PIN)

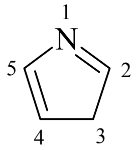
P-14.6 Indicated and added hydrogen

Under certain circumstances it is necessary to indicate in the name of a mancude ring or ring system, i.e., one that contains the maximum number of noncumulative double bonds, one or more positions where no multiple bond is attached. This is done by specifying the presence of an ‘extra’ hydrogen atom at such positions by citation of the appropriate numerical locant followed by an italicized capital ‘*H*’.

Examples:



1*H*-pyrrole (PIN)
pyrrole

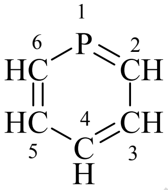


3*H*-pyrrole (PIN)

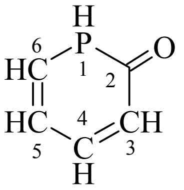
In the first example, the ‘indicated hydrogen’ locates one hydrogen atom in position '1' of the pyrrole ring; and in the second, the ‘indicated hydrogen’ indicates an ‘extra’ hydrogen’ atom at position '3' , i.e., one hydrogen atom more than the number present if there were a double bond in the ring at that position. Indicated hydrogen of this type normally precedes the name of a parent hydride. Indicated hydrogen may be omitted (see P-25-7-1.3). 1*H*-Pyrrole is usually called just ‘pyrrole’. However, when locants are present in a preferred IUPAC name, indicated hydrogen atoms must be cited.

A second type of indicated hydrogen, called ‘added hydrogen’ describes hydrogen atoms added to a specified structure as the consequence of the addition of a suffix or a prefix describing a structural modification. ‘Added hydrogen’ is normally cited in parentheses after the locant of the structural feature to which it refers.

Example:



phosphinine (PIN)

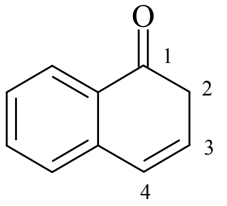


phosphinin-2(1*H*)-one (PIN)

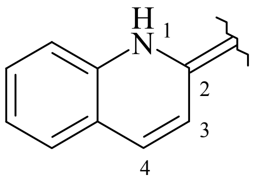
‘Added hydrogen’ is used to introduce a free valence, a radical or an ionic center, or a principal characteristic group into a fully unsaturated heteromonocyclic compound or fused polycyclic system in the absence of, or lack of sufficient hydrogen atoms, to accommodate the operation at the site of the operation. Such substituted compounds are named by using a suffix to denote an operation on either a –CH= group or a =C< atom, or on equivalent heteroatoms such as –N= or =Si<, or groups such as –SiH=.

Detailed procedures for using both ‘indicated hydrogen’ and ‘added hydrogen’ are discussed in P-58.3.3.3.

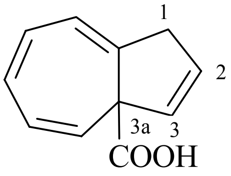
Examples:



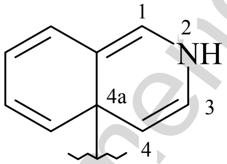
naphthalene-1(2*H*)-one (PIN)



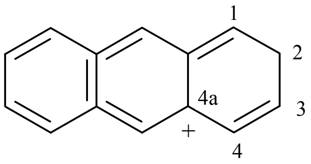
quinolin-2(1*H*)-ylidene (PIN)



azulene-3a(1*H*)-carboxylic acid (PIN)



isoquinolin-4a(2*H*)-yl (PIN)



anthracen-4a(2*H*)-ylium (PIN)

P-15 Types of nomenclature

P-15.0 Introduction

‘Nomenclature’, in chemistry, is a system by which names are formed using various nomenclatural operations in accordance with a set of principles, rules and conventions. There are fundamentally two types of nomenclature: (1) substitutive nomenclature, the principal nomenclature used in organic chemistry and is the basis of IUPAC preferred organic names; and (2) additive nomenclature used in inorganic chemistry for generating binary and coordination names. These two types are applied to name organic compounds and inorganic compounds, thus making nomenclature a matter of choice between these two types of compounds. For example, $SiCl_4$ can be named silicon tetrachloride (binary name), tetrachloridosilicon (coordination name), and tetrachlorosilane (substitutive name). Although coordination nomenclature is not discussed in these recommendations, it is used in the nomenclature of organometallic compounds belonging to Groups 1 and 2, for example dimethylmagnesium. Binary names are used for salts composed of an anionic or cationic organic part, for example sodium acetate and methanaminium chloride. Preferred IUPAC names (PINs) are recommended when there is a choice within the limits of the nomenclature of organic compounds, but not between coordination and/or binary names and substitutive names.

The nomenclature of organic compounds is considered as the set of different types of nomenclature based on the various operations described in P-13. The term nomenclature is usually associated with more than one operation. **Substitutive nomenclature** may be regarded as based on substitutive, additive, and subtractive operations. **Functional class nomenclature** is essentially based on additive operations, but includes substituent groups formed by substitutive nomenclature. **Multiplicative nomenclature** is a subtype of substitutive nomenclature based on cyclic parent structures, functionalized or not; functionalized acyclic parent structures; or heteroacyclic parent structures. **Skeletal replacement nomenclature** usually refers to replacement by 'a' terms and is thus often called just **'a' nomenclature**. Similarly, **conjunctive nomenclature** is restricted to conjunction operations involving rings or ring systems substituted by a principal group named substitutively or having a retained name.

The term nomenclature is not associated with one operation. In this case, names are formed by simply describing the type of operation, for example subtractive operation in the formation of double bonds and functional replacement operation in the replacement of oxygen atoms by chalcogen or nitrogen atoms.

The term nomenclature also applies to families or classes of compounds, for instance **Nomenclature of Radicals and Ions**, **Phane Nomenclature** for naming compounds composed of chains and/or ring systems and **Fullerene Nomenclature** to describe all operations necessary to name polycyclic carbon cage compounds and their derivatives. This term is also used to describe families of compounds of natural origin, for example **Nomenclature of Natural Products** is based on the concept of stereoparents. The nomenclature of carbohydrates, of α-amino-acids, peptides, lipids, and of some other compounds of biochemical significance, is generally considered to be **Biochemical Nomenclature** and, as such, is published comprehensively separately.

P-15.1 Substitutive nomenclature

Substitutive nomenclature is based on the choice of a compound having substitutable hydrogen atoms, called a parent hydride, and its substitution by structural fragments represented by suffixes and prefixes to generate names can be represented as follows:

prefixes—parent hydride—suffixes

A complete substitutive name is indicated schematically in **Fig. 1**. It includes the parent hydride, the different kinds of suffixes, prefixes, and endings, and the order in which they are placed in a name.

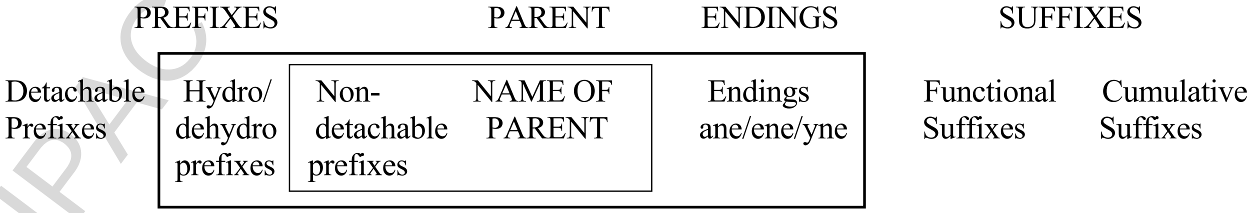


Fig. 1 Order of components in substitutive names

P-15.1.1 Order of suffixes

Suffixes are of two kinds depending on the operation used to generate them. **Functional suffixes** are used for characteristic groups expressing classes, for example ketones, acids, amines, etc.. **Cumulative suffixes** designate radicals, ions, radical ions, and related species, as well as substituent groups.

Functional suffixes are **exclusive suffixes**, as the presence of one denoting the principal characteristic group excludes all other functional suffixes; the modifications normally signaled by those suffixes must be designated as prefixes. To the contrary, cumulative suffixes can be present in any number and kind in a name and can even be associated with functional suffixes.

Functional suffixes are attached only to the name of the parent hydride. Cumulative suffixes are attached to the name of the parent hydride or to a functional suffix, if present.

Examples:

CH_4	$\longrightarrow$	$CH_4^{+\bullet}$
methane (PIN) (parent hydride)		methaniumyl (PIN) ('iumyl' is a cumulative suffix)

CH_3-CH_3	$\longrightarrow$	CH_3-CH_2-NH_2	$\longrightarrow$	CH_3-CH_2-NH_3^+
ethane (PIN) (parent hydride)		ethanamine (PIN) ('amine' is a functional suffix)		ethanaminium (PIN) ('ium' is a cumulative suffix)

P-15.1.2 Position of endings

The modification of the ending 'ane' to 'ene' or 'yne' in acyclic, cyclic and polycyclic parent hydrides is used to describe the subtractive operation that forms double and triple bonds.

P-15.1.3 Prefixes and their order in names

There are different kinds of prefixes in substitutive names:

P-15.1.3.1	Nondetachable prefixes
P-15.1.3.2	Hydro/dehydro prefixes
P-15.1.3.3	Detachable or alphabetized prefixes

Nondetachable, hydro/dehydro, and detachable prefixes are cited in names as indicated in Fig. 1.

P-15.1.3.1 Nondetachable prefixes

Nondetachable prefixes are permanently attached to the name of the parent structure in a given order, which normally matches the order of operations used to modify the parent structure. Prefixes describing the first operation are attached directly to the name of the parent structure; those resulting from a second operation are placed in front of those already introduced, and so on (this technique may be termed 'advancing backwards' from the name of the parent structure). The order is precisely prescribed for each category, as indicated below:

P-15.1.3.1.1 Nondetachable prefixes creating new parent structures:

(a) alicyclic rings and ring systems: ‘cyclo’, ‘bicyclo’, ‘tricyclo’, etc.; ‘spiro’, ‘dispiro’, etc.

(b) fused ring systems by fusion prefixes: ‘benzo’, ‘naphtho’, ‘imidazo’, etc.

(c) bridged fused ring systems by addition of bridge prefixes: ‘methano’, ‘epoxy’, etc.

(d) spiro compounds formed by combining cyclic compounds (a), (b), and/or (c).

P-15.1.3.1.2 Replacement of atoms other than hydrogen by other atoms.

This type of replacement, called ‘skeletal replacement’, is essentially the replacement of carbon atoms by heteroatoms; it takes place with cyclic and acyclic hydrocarbons and generates new parent compounds by using ‘a’ prefixes, i.e., ‘oxa’, ‘aza’, ‘thia’, etc.

P-15.1.3.1.3 Indicated hydrogen

Under certain circumstances it is necessary to indicate in the name of a ring or ring system that contains the maximum number of noncumulative double bonds one or more positions where no double bond is attached. This is done by specifying the presence of an ‘extra’ hydrogen atom at such positions by citation of the appropriate numerical locant followed by an italicized capital *H*. Indicated hydrogen is considered a nondetachable prefix and is introduced last, that is, last before the detachable prefixes.

P-15.1.3.2 ‘Hydro’ and ‘dehydro’ prefixes

These two prefixes are considered as detachable but are not included in the category of alphabetized detachable prefixes described in P-15.1.3.3. In names, they occupy a place between nondetachable prefixes and alphabetized detachable prefixes. These prefixes are used to express modifications of the degree of hydrogenation and are treated like the endings ‘ene’ and ‘yne’, which fulfill the same function. In names, the prefix ‘dehydro’ precedes the prefix ‘hydro’, when both are present. Simple numerical terms, such as ‘di-’‘tetra-’, etc., are used with ‘dehydro’

P-15.1.3.3 Detachable (alphabetized) prefixes

These prefixes describe substituent groups denoting characteristic groups or groups derived from parent hydrides and are cited before ‘hydro-dehydro’ prefixes, if present (see P-15.1.3.2), or nondetachable prefixes, if present, as indicated in Fig. 1. They are alphabetized in accordance with P-14.5.

P-15.1.4 Other components of substitutive names

In addition to the components described above, the following nomenclatural indicators are added, as required:

P-15.1.4.1 Multiplying prefixes placed before suffixes and prefixes to indicate multiple occurrence;

P-15.1.4.2 Locants used to indicate positions of the parent structure at which modifications represented by suffixes, prefixes, and endings occur;

P-15.1.4.3 Stereodescriptors placed at the front of the complete name or name fragment.

P-15.1.5 Construction of substitutive names

This subsection describes the formation of substitutive names and the application of four general rules: numbering, locants, multiplying prefixes, and alphanumerical order. These four rules are applied in constructing names of most organic compounds. In the first set of examples, alkanes and branched alkanes are used. In the second set, the general rule of numbering is exemplified by saturated and unsaturated acyclic compounds denoted by suffixes. The full question of name construction is considered in P-46.

P-15.1.5.1 Naming alkanes and branched alkanes

(a) The names of alkanes are either retained names, which are methane, ethane, propane, and butane; or are formed systematically by adding the ending ‘ane’ to a basic multiplying prefix, with elision of the final letter ‘a’ of the multiplicative term (See Chapter 2).

Examples:

CH_4
methane (PIN)

CH_3-CH_3
ethane (PIN)

CH_3-CH_2-CH_3
propane (PIN)

CH_3-CH_2-CH_2-CH_3
butane (PIN)

CH_3-CH_2-CH_2-CH_2-CH_3
pentane (PIN)

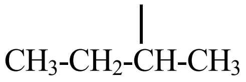
CH_3-$[CH_2]_8$-CH_3
decane (PIN)

(b) Monovalent substituent groups derived from unbranched acyclic hydrocarbons (alkanes) by the removal of one hydrogen atom from a terminal carbon atom (subtractive operation) are named by replacing the ending ‘ane’ of the name of the hydrocarbon by ‘yl’ (see P-19-3.2.1) or, if one hydrogen atom is removed from a nonterminal carbon atom of a chain, by replacing the final ‘e’ of the name of the hydrocarbon by ‘yl’ (see P-29-3.2.2) (‘yl’ is a cumulative suffix, see P-15.1).

Examples:

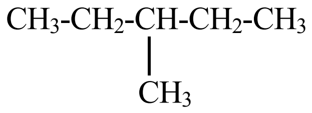
CH_3-CH_2-CH_2-CH_2–
butyl (PIN)

CH_3-CH_2-CH_2-CH_2-CH_2–
pentyl (PIN)


$CH_3\text{-}CH_2\text{-}\overset{|}{C}H\text{-}CH_3$
butan-2-yl (PIN)

(c) A saturated branched acyclic hydrocarbon is formed by substituting one or more substituent groups, formed as described in (b), into the longest chain present in the formula (substitutive operation); it is named by prefixing the designations of the side chains, as formed in (b), to the name of the longest chain [see (d) for numbering].

Example:

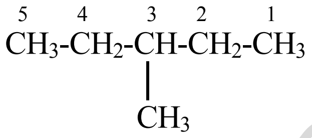


$CH_3\text{-}CH_2\text{-}\underset{\displaystyle CH_3}{CH}\text{-}CH_2\text{-}CH_3$

3-methylpentane (PIN)

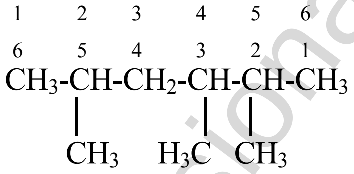
(d) The longest chain is numbered from one end to the other by arabic numbers, the direction being so chosen as to give the lower locants possible to the substituent groups (side chains) [see P-14.4(g)]. The lower set of locants is defined as the set that, when compared term by term with other locant sets cited in order of increasing magnitude, has the lower term at the first point of difference (see P-14.3.4). The locants are placed immediately in front of the part of the name to which they refer. Identical substituent groups are indicated by the appropriate multiplying prefix ‘di’, ‘tri’, etc. (see P-14.2). This rule is applied regardless of the nature of the substituent groups.

Examples:



$\overset{5}{CH_3}\text{-}\overset{4}{CH_2}\text{-}\underset{\displaystyle CH_3}{\overset{3}{CH}}\text{-}\overset{2}{CH_2}\text{-}\overset{1}{CH_3}$

3-methylpentane (PIN)



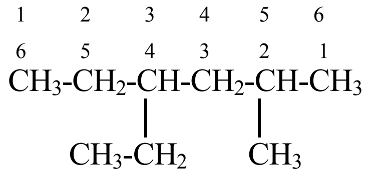
$\overset{\overset{1}{6}}{CH_3}\text{-}\underset{\displaystyle CH_3}{\overset{\overset{2}{5}}{CH}}\text{-}\overset{\overset{3}{4}}{CH_2}\text{-}\underset{\displaystyle H_3C}{\overset{\overset{4}{3}}{CH}}\text{-}\underset{\displaystyle CH_3}{\overset{\overset{5}{2}}{CH}}\text{-}\overset{\overset{6}{1}}{CH_3}$

incorrect numbering
correct numbering

2,3,5-trimethylhexane (PIN)
(not 2,4,5-trimethylhexane; the locant set 2,3,5 is lower than 2,4,5)

(e) If two or more different substituent groups are present, they are cited in names in alphanumerical order (see P-14.4). When two or more substituent groups occupy equivalent positions, the one to be assigned the lower locant is that one cited first in the name.

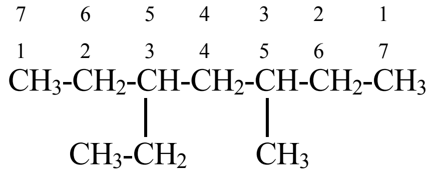
Examples:



$CH_3\text{-}CH_2\text{-}CH(CH_2\text{-}CH_3)\text{-}CH_2\text{-}CH(CH_3)\text{-}CH_3$

incorrect numbering
correct numbering

4-ethyl-2-methylhexane (PIN)
(not 3-ethyl-5-methylhexane; the locant set 2,4 is lower than 3,5)



$CH_3\text{-}CH_2\text{-}CH(CH_2\text{-}CH_3)\text{-}CH_2\text{-}CH(CH_3)\text{-}CH_2\text{-}CH_3$

incorrect numbering
correct numbering

3-ethyl-5-methylheptane (PIN)
(not 5-ethyl-3-methylheptane; the lower locant must be assigned to the substituent group that is cited first)

P-15.1.5.2 The numbering rule

The following examples illustrate the rule for numbering described in P-14.4. This rule establishes an order of priority among different nomenclatural features for assignment of the lowest possible locants.

(a) Alcohols are named by attaching the suffix ‘ol’ to the name of the parent hydride, with elision of the final letter ‘e’ in the parent hydride, if present. When alone in the structure, the characteristic group(s) must receive the lowest locant(s) possible, which is (are) cited immediately in front of the suffix (see P-14.3.2).

Example:

3 2 1
$CH_3\text{-}CH_2\text{-}CH_2\text{-}OH$

propan-1-ol (PIN)

(b) Alkenes are acyclic branched or unbranched hydrocarbons having one double bond. When one double bond is present, an unbranched alkene is named by changing the ending ‘ane’ in the name of the alkane having the same number of carbon atoms to the ending ‘ene’ (see P-31). The double bond is assigned the lower locant possible, which is placed immediately in front of the ending ‘ene’ (see P-14.3.2)

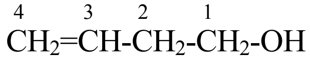
Example:

1 2 3 4
$CH_2{=}CH\text{-}CH_2\text{-}CH_3$

but-1-ene (PIN)

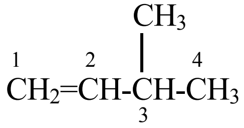
(c) When several nomenclatural features are present in a structure, lowest locants are assigned in accordance with P-14.4. For example, in a cyclic unsaturated alcohol having one substituent group, lowest locants are assigned in the order: (i) characteristic group cited as suffix (-ol); (ii) unsaturation (‘ene’ ending, for example); (iii) detachable alphabetized prefixes (a methyl group, for instance). The following examples illustrate the application of the rule.

Examples:



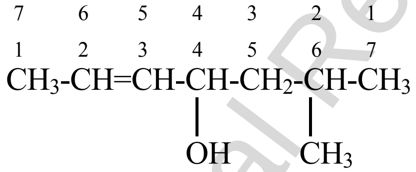
$\overset{4}{C}H_2=\overset{3}{C}H-\overset{2}{C}H_2-\overset{1}{C}H_2-OH$

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



$\overset{1}{C}H_2=\overset{2}{C}H-\underset{3}{\overset{CH_3}{\overset{|}{C}}}H-\overset{4}{C}H_3$

3-methylbut-1-ene (PIN)



$\overset{\overset{7}{1}}{C}H_3-\overset{\overset{6}{2}}{C}H=\overset{\overset{5}{3}}{C}H-\underset{\underset{OH}{|}}{\overset{\overset{4}{4}}{C}}H-\overset{\overset{3}{5}}{C}H_2-\underset{\underset{CH_3}{|}}{\overset{\overset{2}{6}}{C}}H-\overset{\overset{1}{7}}{C}H_3$

incorrect numbering
correct numbering

6-methylhept-2-en-4-ol (PIN)
(not 2-methylhept-5-en-4-ol)

P-15.2 Functional class nomenclature

P-15.2.0 Introduction

Functional class nomenclature was quite important in early days of organic chemistry when many compounds were named using class names. The procedures were identical with those of substitutive nomenclature except that suffixes were never used. Substituent groups, called ‘radicals’ in early nomenclature, were used in association with a name denoting the class; this nomenclature was called ‘radicofunctional nomenclature’. With time, substitutive nomenclature replaced functional class nomenclature in all but a few instances. In the context of IUPAC preferred names, substitutive nomenclature is the primary way for naming organic compounds; functional class nomenclature is reduced to a strict minimum.

The notion of functional class nomenclature is also applied to compounds that are named using a class name, but not necessarily preceded by a substituent group name. To that purpose, ‘functional modifiers’ are used to indicate a functional change, for example the change of acid to anhydride, as acetic anhydride, or the formation of derivatives of ketones, for example, butan-2-one oxime.

It is convenient to classify the main operation involved in functional class nomenclature as an additive one, as is done in P-13.3.3.2. However it is also possible (and probably more relevant from a historical point of view) to regard the process as one of specifying the substituent groups ('radicals') present in compounds for which a class name is given. For instance, the name 'methyl alcohol' (for CH_3-OH) consists of the name 'methyl' for the substituent group CH_3– and the class name 'alcohol' (for R-OH).

Functional class nomenclature is discussed in relation to the traditional use of substituent group names and the use of functional modifiers. Some names are formed on the basis of a class name, but are not considered as belonging to the functional class nomenclature. They are called 'descriptive' names and are never considered as IUPAC preferred names. The order of seniority of classes is discussed in the context of IUPAC preferred names.

P-15.2.1 Functional class nomenclature using substituent group names

P-15.2.1.1 Names are formed by expressing the functional class name of the compound as one word and the remainder of the molecule, a monovalent substituent or acyl group as separate word, placed in front of the class name.

Examples:

CH_3-CH_2-CO-O-CH_3	methyl propanoate (PIN)
CH_3-CO-Cl	acetyl chloride (PIN)
C_6H_5-CO-CN	benzoyl cyanide (PIN)
C_6H_5-CH_2-NCS	benzyl isothiocyanate (isothiocyanatomethyl)benzene (PIN)
C_6H_5-NC	phenyl isocyanide isocyanobenzene (PIN)
CH_3-OH	methyl alcohol methanol (PIN)
C_6H_5-N_3	phenyl azide azidobenzene (PIN)

P-15.2.1.2 When the functional class name refers to a characteristic group that is divalent, the two substituent groups attached to it are each named. When different, they are written as separate words, being in alphanumerical order.

Examples:

CH_3-CH_2-CO-CH_2-CH_3	diethyl ketone pentan-3-one (PIN)
CH_3-CH_2-CO-CH_3	ethyl methyl ketone (not methyl ethyl ketone) butan-2-one (PIN)

P-15.2.2 Functional class nomenclature using functional modifiers

Many derivatives of principal characteristic groups or functional parent compounds (see P-34) may be named by modifiers consisting of one or more separate words placed after the name of the parent structure. This method is most useful in an indexing environment, but it is the sole method used for naming acyclic anhydrides in the context of IUPAC preferred names.

P-15.2.2.1 For IUPAC preferred names, functional class modifiers are used to generate IUPAC preferred names for acyclic anhydrides. Substitutive nomenclature is preferred to the use of other modifiers.

Examples:

CH_3-CO-O-CO-CH_3	acetic anhydride (PIN) (the term ‘acid’ is replaced by ‘anhydride’)
CH_3-CH_2-CH=N-OH	propanal oxime (the term ‘oxime’ is added to the name of the carbonyl compound) *N*-propylidenehydroxylamine (PIN)

P-15.2.2.2 Functional modifers are still acceptable for general nomenclature purposes, but substitutive names are preferred IUPAC names for azines, hydrazones, semicarbazones, carbohydrazones, acetals, and hemiacetals.

Examples:

CH_3-CH_2-CH=N-NH_2	propanal hydrazone propylidenehydrazine (PIN)
$(CH_3)_2$C=N-NH-CO-NH_2	acetone semicarbazone 2-(propan-2-ylidene)hydrazinecarboxamide (PIN)
CH_3-CH_2-CH(O-CH_3)$_2$	propanal dimethyl acetal 1,1-dimethoxypropane (PIN)
CH_3-CH_2-CH_2-CO-OCH_3	butanoic acid methyl ester methyl butanoate (PIN)

P-15.2.3 Rules for functional class nomenclature

Functional class nomenclature is used in place of substitutive nomenclature to name acyclic anhydrides. When two classes are present and both named by functional class nomenclature, the senior class must be chosen in accordance with the seniority order of classes (see P-41). The relevant order for acid functional classes is acids, anhydrides, esters, acyl halides. The senior class is expressed by functional class nomenclature and the lower ranking classes are expressed by prefixes, as usual, in that part of the name that is constructed by substitutive nomenclature.

Examples:

$$\mathrm{Cl\text{-}\overset{4}{C}O\text{-}CH_2\text{-}CH_2\text{-}\overset{1}{C}OOH}$$

4-chloro-4-oxobutanoic acid (PIN)
4-(chlorocarbonyl)propanoic acid
4-carbonochloridoylpropanoic acid
(acid senior to acyl halide)

$$\mathrm{Cl\text{-}\overset{4}{C}O\text{-}CH_2\text{-}CH_2\text{-}\overset{1}{C}OO\text{-}CH_3}$$

methyl 4-chloro-4-oxobutanoate (PIN)
methyl 4-(chlorocarbonyl)propanoate
methyl 4-carbonochloridoylpropanoate
(ester senior to acyl halide)

$$\mathrm{NC\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}O\text{-}Cl}$$

2-cyanoacetyl chloride (PIN)
(acyl chloride senior to nitrile)

$$\mathrm{CH_3O\text{-}\overset{4}{C}H_2\text{-}CH_2\text{-}CH_2\text{-}\overset{1}{C}O\text{-}OCH_3}$$

methyl 4-methoxybutanoate (PIN)
(ester senior to ether)

Functional class names for polyfunctional compounds are not recommended. Substitutive nomenclature is preferred.

Example:

$$\mathrm{HO\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}O\text{-}\overset{1}{C}H_3}$$

4-hydroxybutan-2-one (PIN; substitutive name)
2-hydroxyethyl methyl ketone (functional class name)

P-15.3 Multiplicative nomenclature

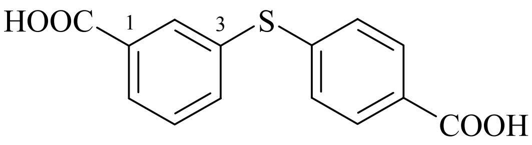
P-15.3.0 Introduction

Assemblies involving two or more identical parent structures linked by di- or polyvalent substituent groups can be named in two ways:

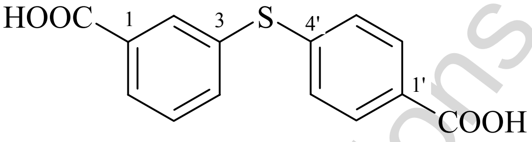
(a) by regular substitutive nomenclature in which one of the parent structures is chosen and the remainder of the structure is substituted into it; and,

(b) by multiplicative nomenclature, a form of substitutive nomenclature through which a multiplicity of parent structures can be recognized.

The following compound can be named 3-[(4-carboxyphenyl)sulfanyl]benzoic acid by simple substitutive nomenclature [numbering shown in **(I)**], a name that recognizes only one benzoic acid group as the parent structure.



(I)



(II)

Alternatively, it can be named 3,4′-sulfanediyldibenzoic acid (PIN) [numbering shown in **(II)**] using multiplicative nomenclature, a name that recognizes both benzoic acid groups in the parent structure.

This method was reserved for naming compounds having characteristic groups expressed as suffixes or implied by a retained name and heteroacyclic parent hydrides. It is now recommended that it be extended to cyclic structures with or without characteristic groups. Chains composed only of carbon atoms are excluded from this type of nomenclature; the traditional approach, based on substitutive nomenclature, is recommended. The system has also been expanded by allowing substitution on the central unit of a multiplying group and the use of nonsymmetrical central units, under specific conditions

P-15.3.1 General methodology

Assemblies of identical units (parent structures) linked by di- or polyvalent substituent groups are named by multiplicative nomenclature when the identical units are:

(a) cyclic parent hydrides, mancude or saturated;

(b) mononuclear or polynuclear acyclic parent hydrides with the exception of acyclic hydrocarbons, saturated or unsaturated; or

(c) cyclic or acyclic parent hydrides substituted by characteristic groups expressed as suffixes.

Names are formed in accordance with the number of occurrences of identical parent structures and the symmetry properties of the linking multiplicative substituent in relation to the parent structures. The resulting multiplicative name must be unambiguous.

P-15.3.2 Assemblies linked by symmetrical substituent groups

P-15.3.2.1 When a compound contains identical units as defined in P-15.3.1 linked by a symmetrical di- or polyvalent substituent group, it may be named by stating successively:

(a) the locants for the positions of substitution of the di- or polyvalent multiplicative substituent substituent group into the identical units (locant 1 is omitted when alone in the name of a mononuclear parent hydride);

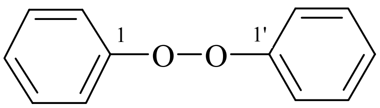
(b) the name of the di- or polyvalent multiplicative substituent group;

(c) the numerical prefix di , tri, etc., with no elision of the final vowel before identical units;

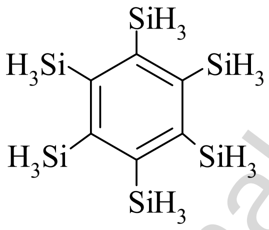
(d) the name of one of the identical units including the principal characteristic group, if any, enclosed in appropriate enclosing marks.

The numbering of the identical units is retained; when there is a choice, the points of substitution by the di- or polyvalent substituent groups on the parent structures are numbered as low as possible. Primes, double primes, etc. are used to distinguish among the locants of the identical units. Retained and systematically formed names are used for the identical units. Unsubstituted parent structures are enclosed in parentheses; parent structures substituted by atoms or groups expressed as prefixes are enclosed in square brackets.

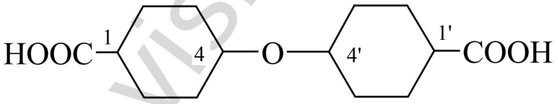
Examples:



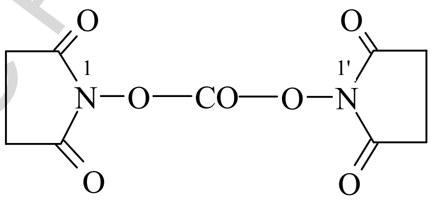
1,1′-peroxydibenzene (PIN)
1,1′-dioxydibenzene



benzenehexaylhexakis(silane) (PIN)

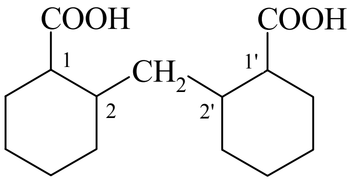


4,4′-oxydi(cyclohexane-1-carboxylic acid) (PIN)

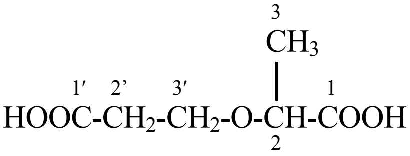


1,1′-[carbonylbis(oxy)]di(pyrrolidine-2,5-dione) (PIN)

P-15.3.2.2 If there is a choice, the greater number of primes is given to the locants of the unit having the higher numbered point of attachment to the di- or polyvalent multiplicative substituent group.
Examples:



2,2′-methylenedi(cyclohexane-1-carboxylic acid) (PIN)



$$\overset{1'}{\mathrm{HOOC}}\text{-}\overset{2'}{\mathrm{CH_2}}\text{-}\overset{3'}{\mathrm{CH_2}}\text{-O-}\underset{2}{\overset{\overset{3}{\mathrm{CH_3}}}{\overset{|}{\mathrm{CH}}}}\text{-}\overset{1}{\mathrm{COOH}}$$

2,3′-oxydipropanoic acid (PIN)

P-15.3.2.3 Simple multiplicative substituent groups.

Any simple polyvalent substituent (see P-29-1 for definitions) may be used as a multiplicative substituent:

$–CH_2–$	methylene (PIN)
–O–	oxy (PIN)
–S–	sulfanediyl (PIN) (thio is no longer recommended)
–OO–	peroxy (PIN) dioxy
–SS–	disulfanediyl (PIN) (dithio is no longer recommended)
–N<	nitrilo (PIN)
$–C_6H_4–$	phenylene (1,2- ;1,3- ;1,4-isomers) (PIN)
$–OC-CH_2-CH_2-CO–$	butanedioyl (PIN) succinyl

The following names derived from the parent hydride name 'azane' are recommended for some multiplicative substituent groups derived from NH_3.

–NH–	azanediyl (PIN; no longer imino; only =NH remains as imino)
–N=	azanylylidene (PIN;no longer nitrilo; only –N< remains as nitrilo)

Examples:

$\overset{2,2',2''}{\mathrm{N(CH_2\text{-}COOH)_3}}$	2,2′,2″-nitrilotriacetic acid (not 2,2′,2″-azanetriyltriacetic acid) *N*,*N*-bis(carboxymethyl)glycine (PIN)
$\overset{3,3'}{\mathrm{O(CH_2\text{-}CH_2\text{-}COOH)_2}}$	3,3′-oxydipropanoic acid (PIN)
$\overset{2,2',2''}{\mathrm{P(CH_2\text{-}COOH)_3}}$	2,2′,2″-phosphanetriyltriacetic acid (PIN)

Substitution is allowed on simple multiplicative substituent groups generating compound multiplicative substituent groups (see P-35.3).

Examples:

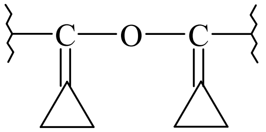
ClCH<	chloromethylene (PIN)
Me-N<	methylazanediyl (PIN) (no longer methylimino)

P-15.3.2.4 Multipart symmetrical di- and polyvalent multiplicative substituent groups

Concatenation is the method used for formation of multipart di- and polyvalent multiplicative substituent groups. In such substituent groups, the central substituent is cited first, then, in order and in the direction of one of the identical units, the successive di- or polyvalent substituent groups are cited.

Examples:

$–O\text{-}CH_2\text{-}O–$	methylenebis(oxy) (PIN) (not methylenedioxy; dioxy is −OO−)
$–CH_2\text{-}O\text{-}CH_2–$	oxybis(methylene) (PIN)
$–H_2C\text{-}NH\text{-}CO\text{-}CH_2\text{-}CO\text{-}NH\text{-}CH_2–$	propanedioylbis(azanediylmethylene) (PIN) malonylbis(azanediylmethylene)

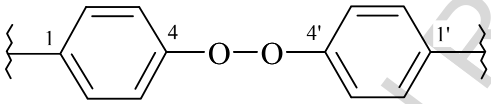


[oxybis(cyclopropylidenemethylene)] (PIN)
(note that if the suffix ‘ylidene’ were not limited to the indication of double bonds, the name given would be ambiguous. It could refer to a structure in which the cyclopropane bonds went to both a CH_2 group and an oxygen atom)

Numbering of the components of a multipart di- or trivalent multiplicative substituent group, when necessary, is achieved by attributing lowest locants to the atoms that are at the end of the component nearest to the parent structure.

Examples:

1 2 2′ 1′
$–CHCl-CH_2–O-CH_2-CHCl–$ oxybis(1-chloroethane-2,1-diyl) (PIN)
oxybis(1-chloroethylene)



peroxydi-4,1-phenylene (PIN)

2 2″
$HOOC-CH_2-O-CH_2-CH_2-O-CH_2-CH_2-O-CH_2-COOH$

2,2′ -[oxybis(ethane-2,1-diyloxy)]diacetic acid (PIN)

14 13 12 11 10 9 8 7 6 5 4 3 2 1
$HOOC-CH_2-O-CH_2-CH_2-O-CH_2-CH_2-O-CH_2-CH_2-O-CH_2-COOH$

2,2′-[ethane-1,2-diylbis(oxyethane-2,1-diyloxy)]diacetic acid (multiplicative name)
3,6,9,12-tetraoxatetradecanedioic acid (PIN; see P-51.4)

P-15.3.2.5 Derivatives of assemblies of identical parent structures

When assemblies named in accordance with Rule P-15.3.2.1 contain substituents on the identical parent structures, whether or not a principal characteristic group is present, these substituent groups are named by prefixes, which are cited in one of two ways.

P-15.3.2.5.1 Substituent groups on the identical parent structures are cited as prefixes associated with the identical parent structures when they fulfill the following two conditions:

(1) the linking bonds (single or multiple) between the central unit of the multiplicative substituent group and all subsequent structural units are identical; and

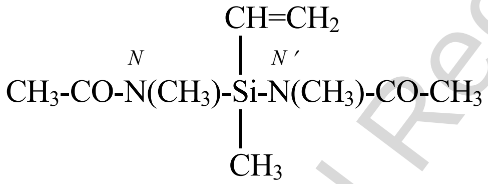
(2) the locants of all substituent groups on the identical parent structures cited as suffixes and prefixes are identical.

The identical parent structures, together with their prefixes and suffix are treated as a complex group, and the multiplicity of occurrences is designated by the appropriate numerical prefixes 'bis', 'tris', tetrakis', etc.

Examples:

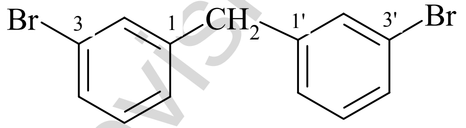
$F_3Si\text{-}\overset{1}{Si}F_2\text{-}CH_2\text{-}\overset{1'}{Si}F_2\text{-}SiF_3$ 1,1′-methylenebis(pentafluorodisilane) (PIN)

$(CH_3)_2\overset{N}{N}\text{-}O\text{-}\overset{N'}{N}(CH_3)_2$ *N*,*N* ′-oxybis(*N*-methylmethanamine)
tetramethyldiazoxane (PIN; see P-21.2.3.1;
diazoxane is a nonfunctional parent hydride)

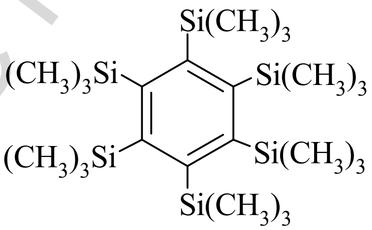


$CH_3\text{-}CO\text{-}\overset{N}{N}(CH_3)\text{-}\underset{\substack{|\\CH_3}}{\overset{\substack{CH=CH_2\\|}}{Si}}\text{-}\overset{N'}{N}(CH_3)\text{-}CO\text{-}CH_3$

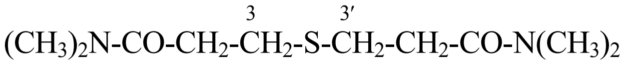
N,N′-[ethenyl(methyl)silanediyl]bis(*N*-methylacetamide)
1,1′-(2-ethenyl-1,2,3-trimethyldisilazane-1,3-diyl)bis(ethan-1-one) (PIN)
(a pseudo ketone; disilazane is a nonfunctional parent hydride)



1,1′-methylenebis(3-bromobenzene) (PIN)

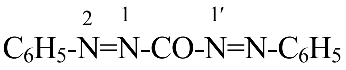


benzenehexaylhexakis(trimethylsilane) (PIN)



$(CH_3)_2N\text{-}CO\text{-}CH_2\text{-}\overset{3}{C}H_2\text{-}S\text{-}\overset{3'}{C}H_2\text{-}CH_2\text{-}CO\text{-}N(CH_3)_2$

3,3′-sulfanediylbis(*N*,*N*-dimethylpropanamide) (PIN)

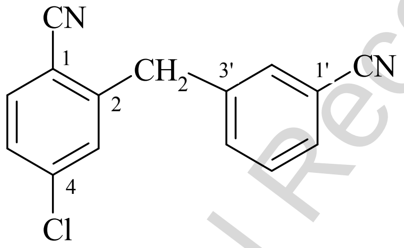


$C_6H_5\text{-}\overset{2}{N}{=}\overset{1}{N}\text{-}CO\text{-}\overset{1'}{N}{=}N\text{-}C_6H_5$

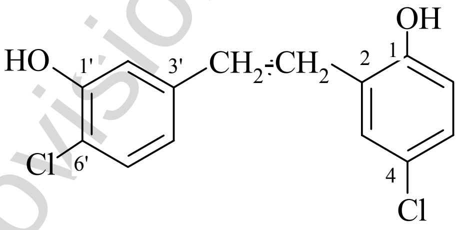
1,1′-carbonylbis(2-phenyldiazene) (PIN)

P-15.3.2.5.2 When the conditions defined in P-15.3.2.5.1 above are not met, the substituent groups other than those identified by suffixes, if present, are cited as prefixes at the front of the name of the assembly. These prefixes are assigned the lowest locants available after priority has been given to the principal characteristic groups, and the linking di- or polyvalent substituent groups.

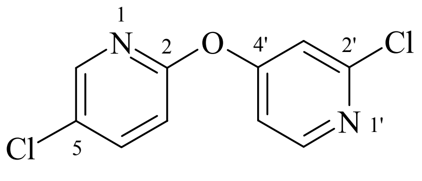
Examples:



4-chloro-2,3′-methylenedibenzonitrile (PIN)



4,6′-dichloro-2,3′-(ethane-1,2-diyl)diphenol (PIN)



2′,5-dichloro-2,4′-oxydipyridine (PIN)

$Cl\text{-}\overset{1}{Si}H_2\text{-}CH_2\text{-}CH_2\text{-}\overset{1'}{Si}H_3$

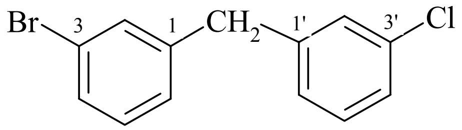
1-chloro-1,1′-(ethane-1,2-diyl)bis(silane) (PIN)

$(CH_3)_3\overset{2}{Si}\text{-}\overset{1}{Si}H_2\text{-}S\text{-}S\text{-}\overset{1'}{Si}H_2\text{-}SiH_3$

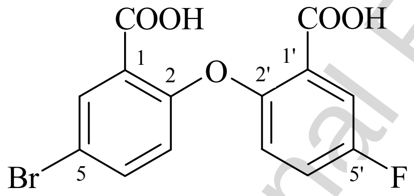
2,2,2-trimethyl-1,1′-(disulfanediyl)bis(disilane) (PIN)

P-15.3.2.5.3 When a choice is possible, unprimed locants are assigned to the identical parent structure having the substituent cited first in alphanumeric order.

Examples:



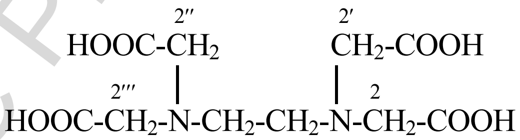
3-bromo-3′-chloro-1,1′-methylenedibenzene (PIN)



5-bromo-5′-fluoro-2,2′-oxydibenzoic acid (PIN)

P-15.3.2.6 When more than two identical parent structures are present, priming is used to distinguish each locant of the identical parent structures located at one end of the multiplying substituent, then at the other end, as required.

Example:

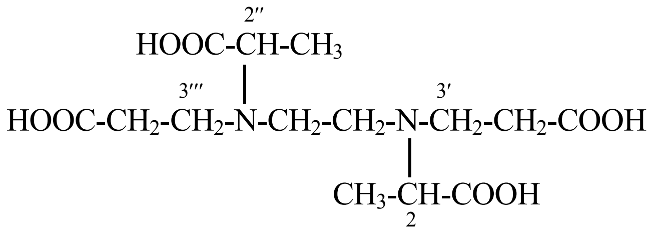


$$\begin{array}{l} \quad\ \ \text{HOOC-}\overset{2''}{\text{CH}_2} \qquad\qquad \overset{2'}{\text{CH}_2}\text{-COOH} \\ \qquad\qquad\quad | \qquad\qquad\qquad | \\ \text{HOOC-}\overset{2'''}{\text{CH}_2}\text{-N-CH}_2\text{-CH}_2\text{-N-}\overset{2}{\text{CH}_2}\text{-COOH} \end{array}$$

2,2′,2′′,2′′′-(ethane-1,2-diyldinitrilo)tetraacetic acid
N,*N*′-ethane-1,2-diylbis[*N*-(carboxymethyl)glycine] (PIN)

If there is a choice, the greater number of primes is given to the locants of the identical parent structure having the higher numbered point of attachment to each end of the polyvalent multiplicative substituent group.

Example:



$$
\begin{array}{l}
\qquad\qquad\qquad HOOC\text{-}\overset{2''}{C}H\text{-}CH_3 \\
\qquad\qquad\qquad\qquad\quad | \\
HOOC\text{-}CH_2\text{-}\overset{3'''}{C}H_2\text{-}N\text{-}CH_2\text{-}CH_2\text{-}N\text{-}\overset{3'}{C}H_2\text{-}CH_2\text{-}COOH \\
\qquad\qquad\qquad\qquad\qquad\qquad\qquad\quad | \\
\qquad\qquad\qquad\qquad\qquad\qquad CH_3\text{-}\underset{2}{C}H\text{-}COOH
\end{array}
$$

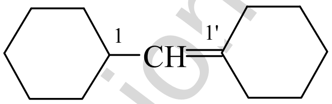
2,2″,3′,3‴-(ethane-1,2-diyldinitrilo)tetrapropanoic acid
N,*N*′-ethane-1,2-diylbis[*N*-(2-carboxyethyl)alanine] (PIN)

P-15.3.3 Assemblies linked by unsymmetrical substituent groups

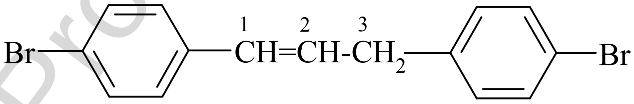
This method constitutes an addition to the nomenclature of assemblies as previously recommended.

P-15.3.3.1 Multiplicative nomenclature can also be used to name assemblies of identical parent structures linked by unsymmetrical substituent groups provided that all parent structures have identical locants assigned to the characteristic groups cited as suffixes and substituent groups cited as prefixes. This method is identical with that described in P-15.3.2.4.1. Unprimed, primed, double primed, etc., locants for attachment points of the unsymmetrical substituent group to the identical parent structures are cited in increasing order of the locants of the unsymmetrical substituent group.

Examples:



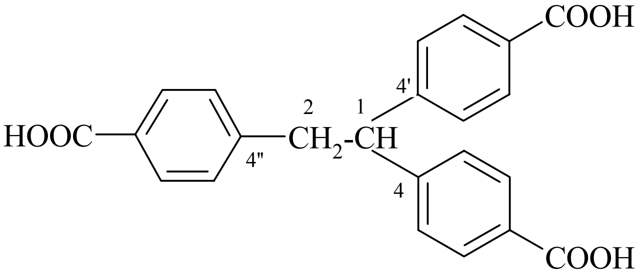
1,1′-methanylylidenedicyclohexane (PIN)



1,1′-(prop-1-en-1,3-diyl)bis(4-bromobenzene) (PIN)

$(CH_3)_3Si\text{-}\overset{2}{C}H(CH_3)\text{-}\overset{1}{C}H_2\text{-}Si(CH_3)_3$

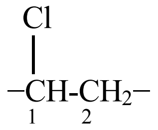
(propane-1,2-diyl)bis(trimethylsilane) (PIN)



4,4′,4′′-ethane-1,1,2-triyltribenzoic acid (PIN)

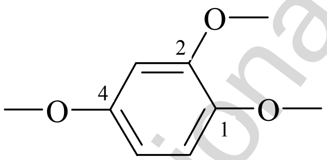
P-15.3.3.2 Unsymmetrical central substituent groups are allowed if they are formed from a basic multivalent substituent group to which subsequent groups are attached by identical bonds (single or multiple). There is no limit to the number of individual groups in the full central substituent used as a multiplier.

P-15.3.3.2.1 Examples of allowed unsymmetrical multiplicative substituent groups:

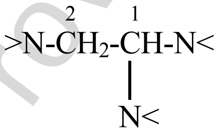


$$\underset{1}{-\overset{\text{Cl}}{\overset{|}{\text{CH}}}}\text{-}\underset{2}{\text{CH}_2}-$$

(1-chloroethane-1,2-diyl) (PIN)



[1,2,4-benzenetriyltris(oxy)] (PIN)



$$>\text{N-}\overset{2}{\text{CH}_2}\text{-}\underset{\underset{\text{N}<}{|}}{\overset{1}{\text{CH}}}\text{-N}<$$

(ethane-1,1,2-triyltrinitrilo) (PIN)

P-15.3.3.2.2 Disallowed unsymmetrical multiplicative substituent groups:

(a) Unsymmetrical substituent groups consisting of two different components:

Examples: $-\text{CH}_2\text{-OO}-$ $-\text{CH}_2\text{-NH}-$

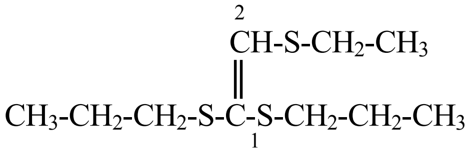
(b) Unsymmetrical substituent groups having terminal atoms with different bonding orders:

Example: $-CH\text{-}CH{=}N\text{-}CH_2\text{-}CH{=}$

(c) Unsymmetrical multipart substituent groups;

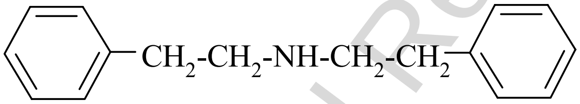
Example: $-O\text{-}CH_2\text{-}CH_2\text{-}S-$

P-15.3.4 Examples of multiplicative names that are not allowed



$$CH_3\text{-}CH_2\text{-}CH_2\text{-}S\text{-}\underset{1}{\overset{\overset{2}{C}H\text{-}S\text{-}CH_2\text{-}CH_3}{\overset{\|}{C}}}\text{-}S\text{-}CH_2\text{-}CH_2\text{-}CH_3$$

2-(ethylsulfanyl)-1,1-bis(propylsulfanyl)ethene (PIN; substitutive name)
(not 1,1′-{[(2-ethylsulfanyl)ethene-1,1-diyl]bis(sulfanyl)}dipropane; multiplication of alkanes is not allowed; see P-15.1.2.1)



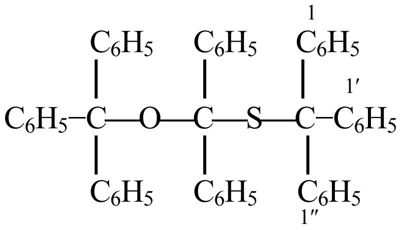
2-phenyl-*N*-(2-phenylethyl)ethan-1-amine (PIN)
(functionality expressed by a suffix is senior to a multiplicative name based on a parent cyclic hydrocarbon)

P-15.3.5 Multiple occurrences of identical parent structures

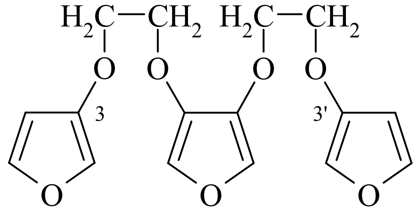
When more than two identical parent structures occur in the whole structure, the following rules are to be followed. It should be noted that preferred IUPAC names are formed by using Phane Nomenclature when four rings are present, two being terminal, in a system containing a minimum of seven nodes (see P-52.5.3.2) and that skeletal replacement (‘a’) nomenclature is used when the conditions for its use are met (see P-15.4.3.2).

P-15.3.5.1 A maximum number of parent structures must be expressed

Example:



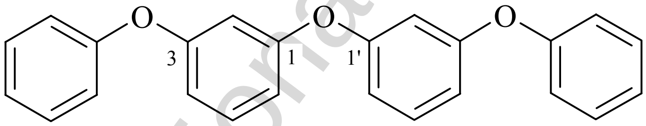
1,1′,1″-({[diphenyl(triphenylmethoxy)methyl]sulfanyl}methanetriyl)tribenzene (PIN)



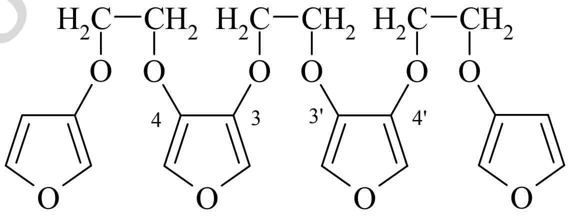
3,3′-[furan-3,4-diylbis(oxyethane-2,1-diyloxy)]difuran (PIN)

P-15.3.5.2 When the parent structure occurs more than three times in the whole structure, the two parent structures to be multiplied are those nearer to the central unit of the multiplicative substituent group; the other parent structures are substituted into the multiplied structure.

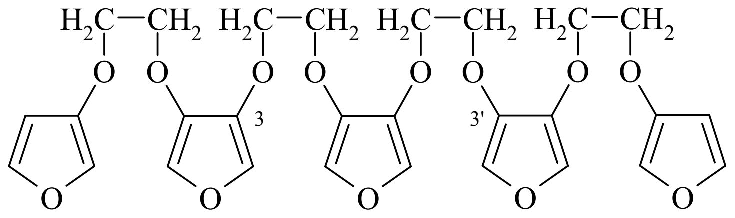
Examples:



1,1′-oxybis(3-phenoxybenzene) (multiplicative name)
2,4,6-trioxa-1,7(1),3,5(1,3)-tetrabenzenaheptaphane (PIN; phane name, see P-51.4)



3,3′-[ethane-1,2-diylbis(oxy)]bis{4-[2-(furan-3-yloxy)ethoxy]furan} (multiplicative name)
2,5,7,10,12,15-hexaoxa-1,16(3),6,11(3,4)-tetrafuranahexadecaphane (PIN; phane name, see P-51.4)



3,3′-[furan-3,4-diylbis(oxyethane-2,1-diyloxy)]bis{4-[2-(furan-3-yloxy)ethoxy]furan} (multiplicative name)

2,5,7,10,12,15,17,20-octaoxa-1,21(3), 6,11,16,21(3,4)-pentafuranahenicosaphane (PIN; phane name, see P-51.4)

P-15.4 Skeletal replacement (‘a’) nomenclature

P-15.4.0 Introduction.

Skeletal replacement nomenclature is a subset of the replacement operation that also includes functional replacement nomenclature (see P-13.2). Functional replacement nomenclature is discussed in P-15.5. Just as functional replacement is considered a nomenclature, skeletal replacement is also considered a nomenclature.

In the nomenclature of organic compounds, skeletal replacement based on the replacement of carbon atoms by other atoms included in the general scope of the nomenclature of organic compounds is described under the title of skeletal replacement (‘a’) nomenclature, because the heteroatoms replacing carbon atoms are denoted by nondetachable prefixes ending in ‘a’. Skeletal replacement (‘a’) nomenclature also includes replacement of boron atoms by other atoms, including carbon, (see P-68.1.1.3.4) and the replacement of heteroatoms by other atoms, including carbon, to modify fundamental structures of natural products as described in P-101.4. Skeletal replacement denoted by methods other than ‘a’ prefixes is described for the replacement of nitrogen atoms by phosphorus and arsenic atoms in certain heterocycles (see Table 2.7) and oxygen atoms by sulfur, selenium and tellurium atoms in other specific heterocycles (see Table 2.6).

This section deals primarily with skeletal replacement in hydrocarbon parent hydrides. Skeletal replacement (‘a’) nomenclature is used in two ways:

(a) to generate names for heterocyclic parent hydrides by replacing carbon atoms in corresponding cyclic hydrocarbons; and

(b) to generate simpler names for heteroacyclic structures than those formed by substitutive nomenclature when four or more heterounits (usually heteroatoms) are present, for example, in naming polyamines, polyethers, etc.

P-15.4.1 General rules

P-15.4.1.1 Nondetachable prefixes, called ‘a’ prefixes, are used to designate replacing skeletal atoms with their standard bonding number. Those related to these recommendations are listed in Table 1.5.

Table 1.5 Skeletal replacement ‘a’ prefixes

Standard Bonding Numbers	3		4		3		2		1	
	B	bora	C	carba	N	aza	O	oxa	F	fluora
	Al	alumina	Si	sila	P	phospha	S	thia	Cl	chlora
	Ga	galla	Ge	germa	As	arsa	Se	selena	Br	broma
	In	inda	Sn	stanna	Sb	stiba	Te	tellura	I	ioda
	Tl	thalla	Pb	plumba	Bi	bisma	Po	polona	At	astata

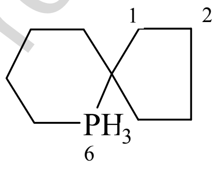
P-15.4.1.2 For naming and numbering purposes, the following decreasing order of seniority is followed: F > Cl > Br > I > At > O > S > Se > Te > Po > N > P > As > Sb > Bi > C > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl.

P-15.4.1.3 Names are formed by citing the ‘a’ terms (see Table 1.5) as prefixes to the name of the parent structure with the same number of skeletal atoms in the order given in P-15.4.1.2. The numerical prefixes ‘di’, ‘tri’, ‘tetra’, etc., are used to indicate a multiplicity of identical replacing atoms. The final letter ‘a’ of the ‘a’ term and the final letters ‘a’ and ‘i’ of a multiplying prefix are not elided when followed by a vowel.

P-15.4.1.4 Numbering is based first on the numbering of the acyclic or cyclic parent structure, and then low locants are assigned on the basis of the seniority order of the ‘a’ prefixes given in P-15.4.1.2. Once a structure modified by skeletal replacement (‘a’) prefixes has been named and numbered, it is considered to be a new parent hydride.

P-15.4.1.5 The symbol λ^n is used to describe heteroatoms having nonstandard bonding numbers (P-14.1.3). In names, it is placed immediately after the locant (without an intervening hyphen) denoting the heteroatom.

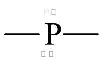
Example:



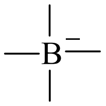
6λ^5-phosphaspiro[4.5]decane (PIN)

P-15.4.1.6 Derived skeletal replacement (‘a’) prefixes are used to designate anionic and cationic heteroatoms.

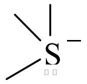
Examples:



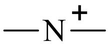
posphanida (PIN)



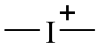
boranuida (PIN)



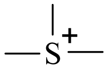
sulfanuida (PIN)
λ^4-sulfanida



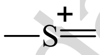
azanylia (PIN)



iodonia (PIN)



or



thionia (PIN)

These prefixes are used when skeletal replacement ('a') nomenclature is recommended to name ionic parent structures. This question and the selection of preferred IUPAC names are fully discussed in P-73.4.

P-15.4.2 Skeletal replacement ('a') nomenclature for rings and ring systems

Skeletal replacement ('a') nomenclature is used to modify rings and ring systems. Such rings and ring systems differ in the modalities of application of the general rules for naming and numbering parent hydrides; therefore, these rings and ring systems are described at the end of each section that describes their naming and numbering before the replacement operation occurs.

(a) cycloalkanes having more than ten skeletal carbon atoms, in P-22.2.3;

(b) di- and polycycloalkanes of the von Baeyer type, in P-23.2;

(c) spiro compounds, in P-24.2.4;

(d) fusion systems, in P-25.5.1;

(e) phane parent hydrides, in P-26.5;

(f) fullerenes, in P-27.

P-15.4.3 Skeletal replacement ('a') nomenclature for chains

> A major modification to Rule C-0.6 (ref. 1) has been made to skeletal replacement ('a') nomenclature as applied to chains. In these recommendations, skeletal replacement ('a') nomenclature generates new acyclic parent hydrides whose numbering is fixed as it is for rings and ring systems. Then suffixes, endings, and prefixes are added in accordance with this fixed numbering.

P-15.4.3.1 Name formation

P-15.4.3.1.1 Names are formed by placing 'a' prefixes in front of the name of the unbranched parent structure formed in accord with their seniority order given in P-15.4.1.2. Multiplicative prefixes 'di', 'tri', 'tetra', etc, indicate a multiplicity of identical heteroatoms, and locants are used to designate their positions.

Unbranched chains are numbered continuously from one end to the other so as to give a lower set of locants to heteroatoms considered together as a set without regard to kind, and then, if there is a choice, to heteroatoms cited first in the seniority order given in P-15.4.1.2.

Examples:

1 2 3 4 5 6 7 8 9 10
$\mathrm{CH_3\text{-}SiH_2\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}S\text{-}CH_2\text{-}CH_3}$

8-thia-2,4,6-trisiladecane (PIN)
(the locant set' 2,4,6,8' is lower than '3,5,7,9')

9 8 7 6 5 4 3 2 1
$\mathrm{CH_3\text{-}SiH_2\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}O\text{-}CH_3}$

2-oxa-4,6,8-trisilanonane (PIN)
(the heteroatom locant sets, '2,4,6,8', are identical;
therefore, the low locant is given to 'O' over 'Si')

P-15.4.3.1.2 Free valences of substituent groups receive locants according to the fixed numbering of the heterochain.

Example:

1 2 3 4 5 6 7 8 9 10
$\mathrm{CH_3\text{-}\ SiH_2\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}CH_2}$–

2,4,6,8-tetrasiladecan-10-yl (PIN)
(Note: 'decan-10-yl' not 'dec-10-yl'; see P-29.2.1)


$\mathrm{\overset{1}{CH_3}\text{-}\ \overset{2}{Si}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{4}{Si}H_2\text{-}\underset{5}{\overset{|}{C}}H\text{-}\overset{6}{Si}H_2\text{-}\overset{7}{C}H_2\text{-}\overset{8}{Si}H_2\text{-}\overset{9}{C}H_2\text{-}\overset{10}{C}H_3}$

2,4,6,8-tetrasiladecan-5-yl (PIN)

P-15.4.3.1.3 Characteristic groups cited as suffixes are given locants in accordance with the fixed numbering of the heterochain.

Examples:

9 8 7 6 5 4 3 2 1
$\mathrm{CH_3\text{-}\ SiH_2\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}SiH_2\text{-}COOH}$

2,4,6,8-tetrasilanonanoic acid (PIN)
(locant 1 is omitted; see P-14.3.3.1)

1 2 3 4 5 6 7 8 9 10
$\mathrm{CH_3\text{-}\ SiH_2\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}CH_2\text{-}OH}$

2,4,6,8-tetrasiladecan-10-ol (PIN)

$$\overset{1}{\mathrm{CH_3}}\text{-}\ \overset{2}{\mathrm{SiH_2}}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\overset{4}{\mathrm{SiH_2}}\text{-}\overset{5}{\mathrm{CH_2}}\text{-}\overset{6}{\mathrm{SiH_2}}\text{-}\overset{7}{\mathrm{CH_2}}\text{-}\overset{8}{\mathrm{SiH_2}}\text{-}\overset{9}{\mathrm{CH_2}}\text{-}\overset{10}{\mathrm{COOH}}$$

2,4,6,8-tetrasiladecan-10-oic acid (PIN)

P-15.4.3.1.4 Double and triple bonds are given locants in accordance with the fixed numbering of the heterochain, and, if there is a choice, according to the general priorities for multiple bonds (see P-31.1.2).

Example:

$$\overset{1}{\mathrm{CH_3}}\text{-}\ \overset{2}{\mathrm{SiH_2}}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\overset{4}{\mathrm{SiH_2}}\text{-}\overset{5}{\mathrm{CH_2}}\text{-}\overset{6}{\mathrm{SiH_2}}\text{-}\overset{7}{\mathrm{CH_2}}\text{-}\overset{8}{\mathrm{SiH_2}}\text{-}\overset{9}{\mathrm{CH}}\text{=}\overset{10}{\mathrm{CH_2}}$$

2,4,6,8-tetrasiladec-9-ene (PIN)

P-15.4.3.1.5 Heteroatoms with nonstandard valences

(a) A nonstandard bonding number of a neutral skeletal heteroatom in a parent hydride is indicated by the symbol λ^n, where '*n*' is the bonding number following the appropriate locant (see P-14.1.3).

Example:

$$\overset{1}{\mathrm{CH_3}}\text{-}\overset{2}{\mathrm{O}}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\overset{4}{\mathrm{CH_2}}\text{-}\overset{5}{\mathrm{O}}\text{-}\overset{6}{\mathrm{CH_2}}\text{-}\overset{7}{\mathrm{CH_2}}\text{-}\overset{8}{\mathrm{O}}\text{-}\overset{9}{\mathrm{CH_2}}\text{-}\overset{10}{\mathrm{CH_2}}\text{-}\overset{11}{\mathrm{SH_2}}\text{-}\overset{12}{\mathrm{CH_3}}$$

2,5,8-trioxa-11λ^4-thiadodecane (PIN)
('O' is preferred to 'S' for low locant)

(b) When there is a choice, low locants are assigned to heteroatoms having a higher bonding number.

Example:

$$\overset{1}{\mathrm{CH_3}}\text{-}\overset{2}{\mathrm{SH_2}}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\overset{4}{\mathrm{CH_2}}\text{-}\overset{5}{\mathrm{S}}\text{-}\overset{6}{\mathrm{CH_2}}\text{-}\overset{7}{\mathrm{CH_2}}\text{-}\overset{8}{\mathrm{S}}\text{-}\overset{9}{\mathrm{CH_2}}\text{-}\overset{10}{\mathrm{CH_2}}\text{-}\overset{11}{\mathrm{S}}\text{-}\overset{12}{\mathrm{CH_3}}$$

2λ^4,5,8,11-tetrathiadodecane (PIN)

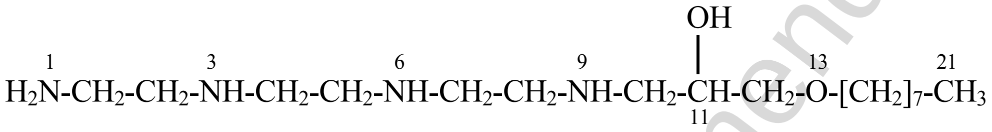
P-15.4.3.1.6 The use of anionic and cationic skeletal replacement ('a') prefixes is discussed in P-72.4 and P-73.4, respectively.

P-15.4.3.2 General conditions for use of skeletal replacement ('a') nomenclature

Skeletal replacement ('a') nomenclature is used in place of substitutive or multiplicative nomenclature when the following conditions are fulfilled.

P-15.4.3.2.1 Skeletal replacement ('a') nomenclature must be used when at least four heteroatoms or units are present in a unbranched chain containing at least one carbon atom and none of the heteroatoms constitute all or part of the principal characteristic group of the compound. A heterounit is a set of heteroatoms having a name of its own as, −SS−, disulfanediyl; $SiH_2SiOSiH_2$−, disiloxane-1,3-diyl; –SOS–, dithioxanediyl; but not –$OSiH_2O$–, nor _–OSO– that correspond to three consecutive units ‘oxysilanediyloxy’ and ‘oxysulfanesiyloxy’, respectively. Acids such as carbonic acid or phosphorus, arsenic and antimony acids, when representing the parent compound or the principal group, are not considered as units. In presence of a characteristic group having seniority for citation as a suffix, the group –O-P(O)(OCH_3)-O– is composed of three units (see third example below).

Examples:

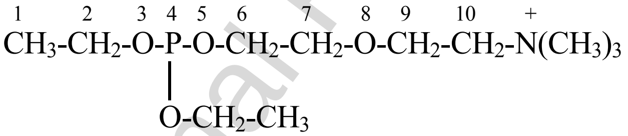


$$\overset{1}{H_2N}\text{-}CH_2\text{-}CH_2\text{-}\overset{3}{N}H\text{-}CH_2\text{-}CH_2\text{-}\overset{6}{N}H\text{-}CH_2\text{-}CH_2\text{-}\overset{9}{N}H\text{-}CH_2\text{-}\underset{11}{\overset{OH}{\overset{|}{C}}}H\text{-}CH_2\text{-}\overset{13}{O}\text{-}[CH_2]_7\text{-}\overset{21}{CH_3}$$

1-amino-13-oxa-3,6,9-triazahenicosan-11-ol (PIN)

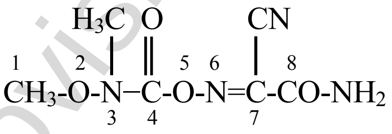
$$\overset{1}{F}\text{-}CO\text{-}\overset{2}{N}H\text{-}\overset{3}{S}\text{-}\overset{4}{N}H\text{-}CH_2\text{-}\overset{6}{O}\text{-}\overset{7}{N}\text{=}CH\text{-}\overset{9}{C}H\text{=}\overset{10}{N}\text{-}\overset{11}{O}\text{-}CH_2\text{-}\overset{13}{N}H\text{-}\overset{14}{S}\text{-}\overset{15}{N}H\text{-}\overset{16}{C}O\text{-}F$$

6,11-dioxa-3,14-dithia-2,4,7,10,13,15-hexaazahexadeca-7,9-dienedioyl difluoride (PIN)
(an acyclic dioyl fluoride is preferred to a multiplied carbamoyl difluoride)



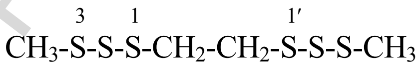
$$\overset{1}{CH_3}\text{-}\overset{2}{CH_2}\text{-}\overset{3}{O}\text{-}\underset{\underset{O\text{-}CH_2\text{-}CH_3}{|}}{\overset{4}{P}}\text{-}\overset{5}{O}\text{-}\overset{6}{CH_2}\text{-}\overset{7}{CH_2}\text{-}\overset{8}{O}\text{-}\overset{9}{CH_2}\text{-}\overset{10}{CH_2}\text{-}\overset{+}{N}(CH_3)_3$$

4-ethoxy-*N*,*N*,*N*-trimethyl-3,5,8-trioxa-4-phosphadecan-10-aminium (PIN)



$$\overset{1}{CH_3}\text{-}\overset{2}{O}\text{-}\underset{3}{\overset{H_3C}{\overset{|}{N}}}{-}\underset{4}{\overset{O}{\overset{\|}{C}}}\text{-}\overset{5}{O}\text{-}\overset{6}{N}\text{=}\underset{7}{\overset{CN}{\overset{|}{C}}}\text{-}\overset{8}{C}O\text{-}NH_2$$

7-cyano-3-methyl-4-oxo-2,5-dioxa-3,6-diazaoct-6-en-8-amide (PIN)



$$\overset{3}{CH_3}\text{-}S\text{-}S\text{-}\overset{1}{S}\text{-}CH_2\text{-}CH_2\text{-}\overset{1'}{S}\text{-}S\text{-}S\text{-}CH_3$$

1,1′-(ethane-1,2-diyl)bis(3-methyltrisulfane) (PIN)
(not 2,3,4,7,8,9-hexathiadecane; trisulfane, HS-S-SH, is a parent hydride and is not allowed to be a heterounit)

$\mathrm{(CH_3)_3C\text{-}OO\text{-}Si(CH_3)_2\text{-}O\text{-}CO\text{-}CH_2\text{-}CH_3}$

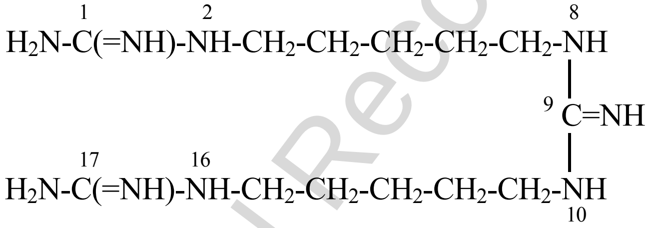
(*tert*-butylperoxy)dimethylsilyl propanoate (PIN)
(not 3,4,6-trioxa-5-silaoctan-7-one; only two heterounits are present: –OO– and –Si–; the principal characteristic group is an ester and the –O– is a part of it)

$\mathrm{CH_3\text{-}O\text{-}PH(O)\text{-}O\text{-}CH_2\text{-}O\text{-}CH_3}$

methoxymethyl methyl phosphonate (PIN)
(not 2,4,6-trioxa-3λ^5-phosphan-3-one; the principal characteristic group, an ester, must be expressed, leaving only one heterounit, −O−)

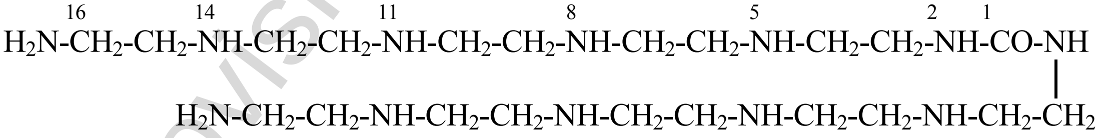
P-15.4.3.2.2 The same number of characteristic groups that would be expressed as suffixes in substitutive names must be present in skeletal replacement ('a') names.

Examples:



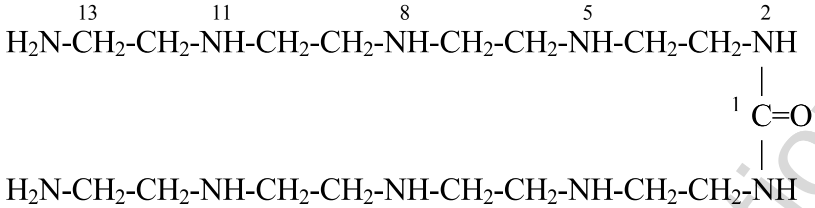
$$\begin{array}{l} \mathrm{H_2N\text{-}\overset{1}{C}(=NH)\text{-}\overset{2}{N}H\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}\overset{8}{N}H} \\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\quad | \\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\quad\ {}^{9}\mathrm{C{=}NH} \\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\quad | \\ \mathrm{H_2N\text{-}\overset{17}{C}(=NH)\text{-}\overset{16}{N}H\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}\underset{10}{N}H} \end{array}$$

9-imino-2,8,10,16-tetraazaheptadecanediimidamide (PIN)
(a diimidamide expressed as a principal characteristic group is senior to a carbonimidic diamide)



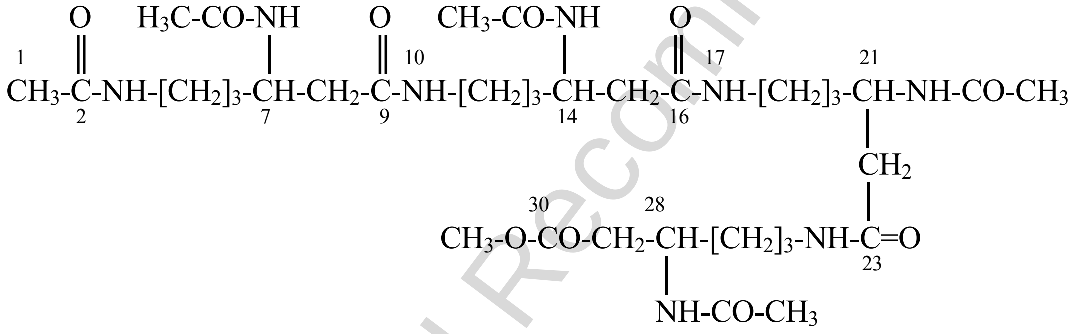
$$\begin{array}{r} \mathrm{H_2N\text{-}\overset{16}{C}H_2\text{-}CH_2\text{-}\overset{14}{N}H\text{-}CH_2\text{-}CH_2\text{-}\overset{11}{N}H\text{-}CH_2\text{-}CH_2\text{-}\overset{8}{N}H\text{-}CH_2\text{-}CH_2\text{-}\overset{5}{N}H\text{-}CH_2\text{-}CH_2\text{-}\overset{2}{N}H\text{-}\overset{1}{C}O\text{-}NH} \\ | \\ \mathrm{H_2N\text{-}CH_2\text{-}CH_2\text{-}NH\text{-}CH_2\text{-}CH_2\text{-}NH\text{-}CH_2\text{-}CH_2\text{-}NH\text{-}CH_2\text{-}CH_2\text{-}NH\text{-}CH_2\text{-}CH_2} \end{array}$$

16-amino-*N*-(14-amino-3,6,9,12-tetraazatetradecan-1-yl)-2,5,8,11,14-pentaazahexadecanamide (PIN)
[an amide expressed as a principal characteristic group is senior to urea, a carbonic diamide, or an amine expressed as a principal characteristic group; since four heteroatoms are also present in the *N*-substituent group, it must also be named by skeletal replacement ('a') nomenclature]



$$\begin{array}{r} \overset{13}{H_2N}\text{-}CH_2\text{-}\overset{11}{CH_2}\text{-}NH\text{-}CH_2\text{-}\overset{8}{CH_2}\text{-}NH\text{-}CH_2\text{-}\overset{5}{CH_2}\text{-}NH\text{-}CH_2\text{-}CH_2\text{-}\overset{2}{NH} \\ | \\ {}^{1}\,C{=}O \\ | \\ H_2N\text{-}CH_2\text{-}CH_2\text{-}NH\text{-}CH_2\text{-}CH_2\text{-}NH\text{-}CH_2\text{-}CH_2\text{-}NH\text{-}CH_2\text{-}CH_2\text{-}NH \end{array}$$

13-amino-*N*-(2-{2-[(2-{[2-(2-aminoethyl)amino]ethyl}amino)ethyl]amino}ethyl)-2,5,8,11-tetraazatridecanamide (PIN)
(an amide expressed as a characteristic group is senior to urea, a carbonic diamide, and to an amine expressed as a characteristic group; since only three heteroatoms are present in the *N*-substituent group, it must be named substitutively)



$$\overset{1}{CH_3}\text{-}\underset{2}{\overset{O}{\overset{\|}{C}}}\text{-}NH\text{-}[CH_2]_3\text{-}\underset{7}{\overset{H_3C\text{-}CO\text{-}NH}{\overset{|}{CH}}}\text{-}CH_2\text{-}\underset{9}{\overset{O}{\overset{\|}{C}}}\text{-}\overset{10}{NH}\text{-}[CH_2]_3\text{-}\underset{14}{\overset{CH_3\text{-}CO\text{-}NH}{\overset{|}{CH}}}\text{-}CH_2\text{-}\underset{16}{\overset{O}{\overset{\|}{C}}}\text{-}\overset{17}{NH}\text{-}[CH_2]_3\text{-}\overset{21}{CH}\text{-}NH\text{-}CO\text{-}CH_3$$

$$\overset{30}{CH_3}\text{-}O\text{-}CO\text{-}CH_2\text{-}\underset{NH\text{-}CO\text{-}CH_3}{\underset{|}{\overset{28}{CH}}}\text{-}[CH_2]_3\text{-}NH\text{-}\underset{23}{C}{=}O \;\;(\text{C-23 bonded via } CH_2 \text{ to C-21})$$

methyl 7,14,21,28-tetrakis(acetamido)-2,9,16,23-tetraoxo-3,10,17,24-tetraazatriacontan-30-oate
(PIN; an ester is senior to an amide or a ketone)

P-15.4.3.2.3 The chain must be terminated by C or one of the following heteroatoms: P, As, Sb, Bi, Si, Ge, Sn, Pb, B, Al, Ga, In, or Tl.

Examples:

$$\overset{1}{H_3Si}\text{-}\overset{2}{O}\text{-}CH_2\text{-}\overset{4}{S}\text{-}\overset{5}{SiH_3}$$

2-oxa-4-thia-1,5-disilapentane (PIN)

P-15.5 Functional replacement nomenclature

P-15.5.1 Definition

Functional replacement nomenclature is a method by which oxygen atoms of characteristic groups and in functional parent compounds are replaced by halogen, chalcogen and/or nitrogen atoms.

P-15.5.2 General methodology

The replacement of oxygen atoms or hydroxy groups by other atoms or groups can be described by prefixes attached to, or infixes inserted into, names of characteristic groups, parent hydrides and functional parent compounds having retained or systematic names. A list of prefixes and infixes is given in Table 1.6. Prefixes and infixes are used for designating the replacing atom(s) −OO−, S, Se, and Te. For example, thio indicates the replacement of oxygen atoms by sulfur in the suffixes sulfonothioyl and carbothioyl and in the functional parent thioacetic acid. Similarly, peroxo or peroxy indicates the replacement of an oxygen atom by a −OO− group in the suffix peroxoic acid and in the name peroxyacetic acid.

Table 1.6 Prefixes and infixes in functional replacement nomenclature

Prefix	Infix	Replaced atom or group	Replacing atom or group
amido	amido	–OH	$–NH_2$
azido	azido	–OH	$–N_3$
bromo	bromido	–OH	–Br
chloro	chlorido	–OH	–Cl
cyanato	cyanatido	–OH	–OCN
cyano	cyanido	–OH	–CN
dithioperoxy*	dithioperoxo*	–O–	–S-S–
fluoro	fluorido	–OH	–F
hydrazido	hydrazido	–OH	$–NH-NH_2$
hydrazono	hydrazono	=O	$=N-NH_2$
imido	imido	=O	=NH
iodo	iodido	–OH	–I
isocyanato	isocyanatido	–OH	–NCO
isocyano	isocyanido	–OH	–NC
isothiocyanato*	isothiocyanatido*	–OH	–NCS
nitrido	nitrido	=O and –OH	≡N
peroxy	peroxo	–O–	–O-O–
seleno	seleno	=O or –OH	=Se or –SeH

telluro	telluro	=O or –OH	=Te or –TeH
thio	thio	=O or –OH	=S or –S–
thiocyanato*	thiocyanatido*	–OH	–SCN
thioperoxy*	thioperoxo*	–O–	–OS– or –SO–

* Selenium and tellurium analogues are named using ‘seleno’ and ‘telluro’ instead of ‘thio’.

P-15.5.3 Scope of functional replacement nomenclature

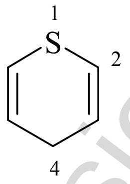
Prefixes and infixes are used in accordance with specific rules describing replacement in:

P-15.5.3.1 Heterocyclic parent hydrides
P-15.5.3.2 Characteristic groups expressed as suffixes in substitutive nomenclature
P-15.5.3.3 Characteristic groups expressed as prefixes in substitutive nomenclature
P-15.5.3.4 Functional parents

P-15.5.3.1 Replacement in heterocyclic parent hydrides

Prefixes are used to modify a limited group of parent hydrides as follows. See Table 2.3 for pyran, Table 2.4 for morpholine, Table 2.11 for chromene, isochromene and xanthene, and Table 3.2 for chromane and isochromane.

Example:



4*H*-thiopyran (PIN)
4*H*-thiine

P-15.5.3.2 Replacement in characteristic groups expressed as suffixes

Replacement in suffixes is limited to –OO–, =S and –S–, =Se and –Se–, =Te and –Te–, =NH and $=NNH_2$ and any combination of these affixes. Suffixes including a carbon atom and those corresponding to sulfonic and sulfinic acids and their analogues are modified by infixes. Other suffixes are modified by prefixes. For examples and the order of seniority of suffixes modified by functional replacement see Tables 4.4 and 4.5 and Appendix 2.

Examples:

–CO-OOH	carboperoxoic acid
–CO-SH	carbothioic *S*-acid

−CS-OH	carbothioic *O*-acid
−C(=NH)-OH	carboximidic acid
−SO-OOH	sulfinoperoxoic acid
$-S(=NNH_2)$-OH	sulfinohydrazonic acid
−(C)O-SH	thioic acid
$-(C)S-NH_2$	thioamide (no contraction to thiamide)
=S	thione
−SeH	selenol

P-15.5.3.3 Functional replacement in prefixes

Functional replacement is used to modify prefixes containing oxygen atoms by the prefixes ‘thio’, ‘seleno’, and ‘telluro’. Prefixes are described in appropriate sections of Chapter 6 and listed in Appendix 1.

Examples:

−C{O/S}H	thiocarboxy (PIN)
=S	thioxo sulfanylidene (PIN)

P-15.5.3.4 Functional replacement in functional parents

Functional replacement is used to modify carboxylic acids and oxoacids, by prefixes and suffixes according to specific rules given in P-15.5.3.4.1 and P-15.5.3.4.2 below. It is also used to modify two retained names expressing functional parent structures, urea and semicarbazone, as described in P-15.5.3.4.3 below. Functional replacement is not used to replace oxygen atoms in ketones, alcohols, and derivatives such as acetals and ketals, etc.; systematic names are recommended instead.

Examples:

CH_3-CS-CH_3	propane-2-thione (PIN) (not thioacetone)
C_6H_5-SH	benzenethiol (PIN) (not thiophenol)

P-15.5.3.4.1 In general nomenclature, retained names of monocarboxylic acids may be modified by the prefixes peroxy, thio, seleno and telluro to indicate the replacement of an oxygen atom by the replacing atom(s) –OO–, –S– or =S, –Se– or =Se, and –Te– or =Te (see P-65.1.1.4.2.2).

Examples:

CH_3-CO-SH	CH_3-CH_2-CS-OH
thioacetic *S*-acid ethanethioic *S*-acid (PIN)	thiopropionic *O*-acid propanethioic *O*-acid (PIN)
C_6H_5-CS-SH	
dithiobenzoic acid benzenecarbodithioic acid (PIN)	

P-15.5.3.4.2 Names of mononuclear and polynuclear oxoacids are modified by prefixes and infixes listed in Table 1.6 according to the rules described in P-67.

Example:

CH_3-P(=NH)(OH)(SH)

methylphosphonimidothioic acid (PIN)

P-15.5.3.4.3 Retained names of acyclic polynitrogen functional parent compounds described in P-68.3.1 are modified by prefixes thio, seleno and telluro.

Examples:

H_2N-CS-NH_2	H_2N-NH-CS-NH_2
thiourea (PIN) carbonothioic diamide	thiosemicarbazide hydrazinecarbothioamide (PIN)

P-15.6 Conjunctive nomenclature

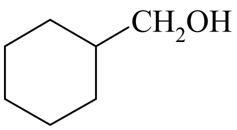
P-15.6.0 Introduction

Conjunctive nomenclature is based essentially on the conjunctive operation, by which a compound is formally constructed by subtracting the same number of hydrogen atoms from each component at each site where joined. It is traditionally reserved for naming compounds having a principal group attached to an acyclic component that is also directly attached by a carbon-carbon bond to a cyclic component. This method can be used in general nomenclature as an alternative to substitutive nomenclature, but it is not recommended for generating preferred IUPAC names. Its principles, conventions and rules have been established for Chemical Abstracts index nomenclature They are briefly discussed in this section. Its limitations are dealt with in P-15.6.2.

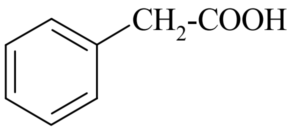
P-15.6.1 Name formation

P-15.6.1.1 Names are formed by juxtaposition of component names. The name of the cyclic component is cited first followed by the systematic or retained name of the component to which the principal characteristic group is attached.

Examples:



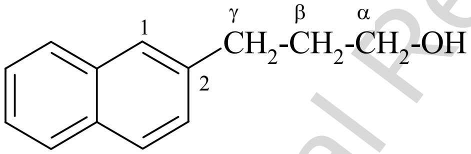
cyclohexanemethanol
cyclohexylmethanol (PIN)



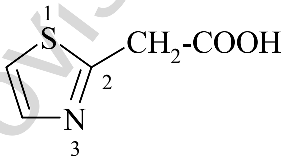
benzeneacetic acid
phenylacetic acid (PIN)

P-15.6.1.2 When necessary, the position of attachment of the side chain to the cyclic component is given by the appropriate locant placed before the name of the cyclic component, unless locants for structural features referring to the cyclic component, such as heteroatoms and indicated hydrogen, are already there; in this case the locant follows the name of the cyclic component chain. Since the acyclic component must terminate at the cyclic component, it is not necessary to give its locant of attachment. Carbon atoms of the side chain are indicated by Greek letters proceeding from the principal characteristic group to the cyclic component; these locants are used in the name only to locate other substituents on the side chain. The carbon atom of the characteristic group (in acids, aldehydes, nitriles, etc.) is omitted when allocating Greek letter locants.

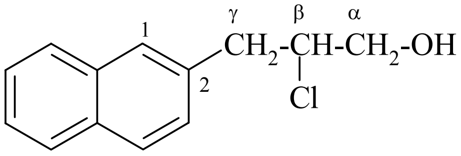
Examples:



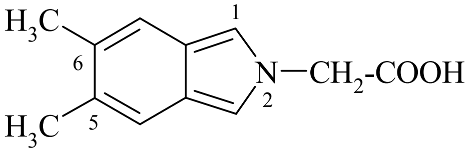
2-naphthalenepropanol
3-(naphthalen-2-yl)propan-1-ol (PIN)
3-(2-naphthyl)propan-1-ol



1,3-thiazole-2-acetic acid
1,3-thiazol-2-ylacetic acid (PIN)



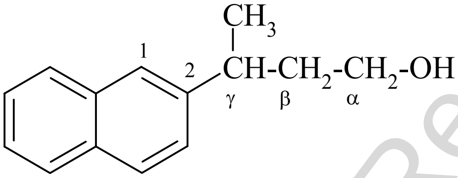
β-chloro-2-naphthalenepropanol
2-chloro-3-(naphthalen-2-yl)propan-1-ol (PIN)



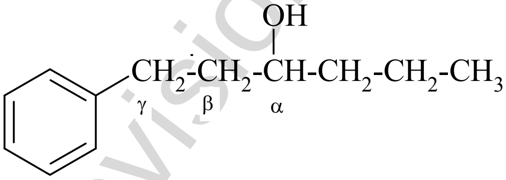
5,6-dimethyl-2*H*-isoindole-2-acetic acid
(5,6-dimethyl-2*H*-isoindol-2-yl)acetic acid (PIN)

P-15.6.1.3 For all purposes in conjunctive nomenclature the side chain is considered to extend only from the principal group to the cyclic component. Any other chain members, even those extending the side chain terminally, are named as substituents, appropriate prefixes and locants being placed before the name of the cyclic component.

Examples:



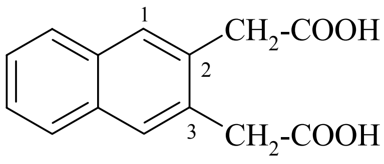
γ-methyl-2-naphthalenepropanol
3-(naphthalen-2-yl)butan-2-ol (PIN)
3-(2-naphthyl)butan-2-ol



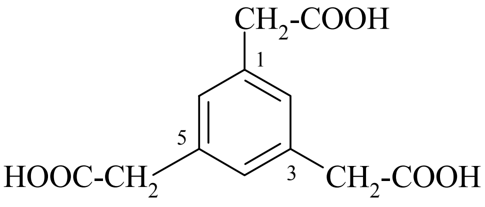
α-propylbenzenepropanol
1-phenylhexan-3-ol (PIN)

P-15.6.1.4 When a cyclic component carries at least two identical side chains, multiplying prefixes ‘di’, ‘tri’, etc. are used to indicate their number; these prefixes are placed before the name of the side chain.

Examples:



2,3-naphthalenediacetic acid
2,2′-naphthalene-2,3-diyldiacetic acid (PIN)



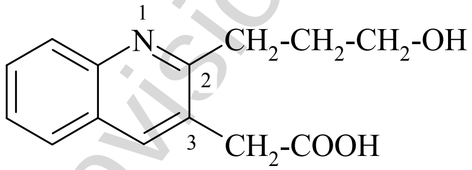
1,3,5-benzenetriacetic acid
benzene-1,3,5-triyltriacetic acid (PIN)

P-15.6.1.5 When different side chains are attached to a cyclic component:

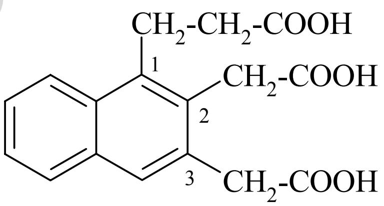
(a) the chain that contains the principal characteristic group is chosen for naming by the conjunctive method; or

(b) if there is more than one side chain containing the principal characteristic group, the conjunctive name that expresses the greater number of the principal characteristic group is chosen. When necessary, side chains are selected by applying the seniority order for selecting the principal chain (see P-44.3).

Examples:



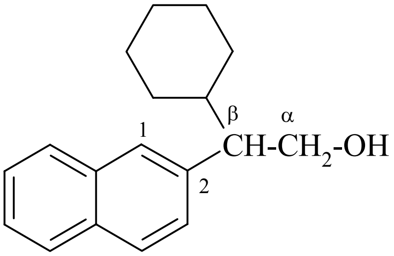
2-(3-hydroxypropyl)-3-quinolineacetic acid
[2-(3-hydroxypropyl)quinolin-3-yl]acetic acid (PIN)
(a carboxylic acid is senior to an alcohol)



1-(2-carboxyethyl)-2,3-naphthalenediacetic acid
[1-(2-carboxyethyl)naphthalen-2,3-diyl]diacetic acid (PIN)

P-15.6.1.6 When the side chain is linked to two different cyclic components, the senior ring or ring system is selected in accord with the seniority order of rings and ring systems (see P-44.2).

Example:



β-cyclohexyl-2-naphthaleneethanol
2-cyclohexyl-2-(naphthalen-2-yl)ethan-1-ol (PIN)
(naphthalene is senior to cyclohexane)

P-15.6.2 Limitations of conjunctive nomenclature

Conjunctive nomenclature is not used when:

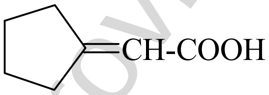
(a) a double bond links the acyclic component and a ring system;

(b) a double bond or a heteroatom is present in the side chain;

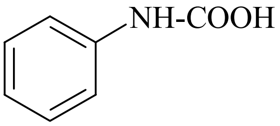
(c) two identical characteristic groups are located on the side chain;

(d) characteristic groups having priority for citation as principal groups are located on the cyclic component or when two or more characteristic groups of the same kind are located on the ring or ring system. In such cases, substitutive nomenclature is used.

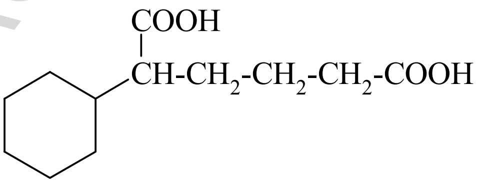
Examples:



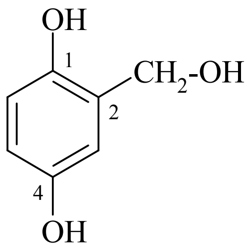
cyclopentylideneacetic acid (PIN)



phenylcarbamic acid (PIN)



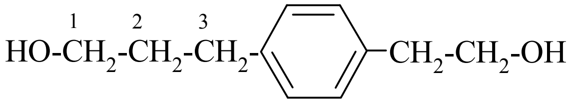
2-cyclohexylhexanedioic acid (PIN)



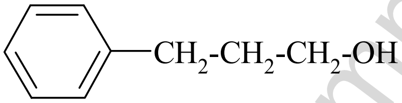
2-(hydroxymethyl)benzene-1,4-diol (PIN)

P-15.6.3 Analysis for construction of conjunctive names

Example 1:



Principal group	–OH	ol
Parent:		
ring:	C_6H_6	benzene
chain:	$CH_3\text{-}CH_2\text{-}CH_3$	propane
Parent including suffix		



benzenepropanol

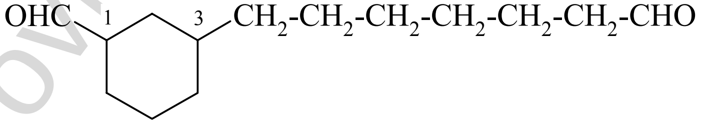
Prefix:	$\text{–}CH_2\text{-}CH_2\text{-}OH$	
Prefix components:	–OH	hydroxy
	$\text{–}CH_2\text{-}CH_3$	ethyl

Prefix name: 2-hydroxyethyl

Together with other rules, this analysis leads to the conjunctive and substitutive names:

4-(2-hydroxyethyl)benzenepropanol
3-[4-(2-hydroxyethyl)phenyl]propan-1-ol (PIN)

Example 2



Principal group:	–CHO	carbaldehyde or al
Parent:	ring	cyclohexane
	chain	heptane
Parent including suffix	ring + chain	cyclohexaneheptanal (a conjunctive name)
Prefix:	–CHO	formyl

Together with other rules this analysis leads to the names:

3-formylcyclohexaneheptanal
7-(3-formylcyclohexyl)heptanal (PIN)

P-16 Name writing

P-16.0 Introduction

Names are written in accordance with a symbolism specific to the nomenclature of organic compounds in order to avoid ambiguity and to establish an unequivocal relationship between a name and the corresponding structure. The recommended symbolism is particularly important in the formation of IUPAC preferred names. As usual, IUPAC recognizes the needs of other languages to introduce modifications specific to a particular language, but it is hoped that, whenever possible, the following conventions will be applied to construct IUPAC names for general use as well as for IUPAC preferred names.

In the 1979 and 1993 recommendations, names were written with a capital initial letter. This practice has been abandoned in recent publications in order to ensure that names of organic compounds are not considered as proper nouns; the usual practice to capitalize letters at the beginning of a sentence must however be respected.

P-16.1 Spelling

The spelling of elements is that given in the IUPAC *Nomenclature of Inorganic Chemistry* (ref. 11), for example, sulfur not sulphur, aluminium not aluminum, and caesium not cesium.

P-16.2 Punctuation

P-16.2.1 Commas are used:

(a) to separate locants, numerals, or italicized letters;

Examples: 1,2-dibromoethane (PIN, P-61.3.1)

N,*N*-diethylfuran-2-carboxamide (PIN, P-66.1.1.3.1.1)

(b) to separate numbers, as well as italicized letters, in fusion descriptors when they indicate the presence of separate attached components; however, italicized letters denoting *peri*-fused junctions are not separated by commas.

Examples: dibenzo[*a*,*j*]anthracene (PIN, P-25.3.3.1.1)

6*H*-pyrrolo[3,2,1-*de*]acridine (PIN, P-25.3.1.3)

P-16.2.2 Full stops

Full stops are used to separate numbers that denote lengths of bridges in polyalicyclic names constructed according to the von Baeyer system (see P-23.2.5.1) and of chain lengths between spiro atoms in von Baeyer spiro names (see P-24.2.1).

Examples: bicyclo[3.2.1]octane (PIN, P-23.2.3)

6-oxaspiro[4.5]decane (PIN, P-24.2.4.1.1)

P-16.2.3 Colons and semicolons

Colons separate related sets of locants; if a higher level of separation is required, semicolons are used.

Examples: benzo[1′′,2′′:3,4;4′′,5′′:3′,4′]dicyclobuta[1,2-*b*:1′,2′-*c*′]difuran (PIN, P-25.3.7.3)

1^1,2^1:2^2,3^1-tercyclopropane (PIN, P-28.3.1)

P-16.2.4 Hyphens

P-16.2.4.1 Hyphens are used in substitutive names:

(a) to separate locants from words or word fragments;

Example: 2-chloro-2-methylpropane (PIN, P-61.3.1)

(b) after parentheses, if the final parenthesis is followed by a locant;

Examples: 1-(chloromethyl)-4-nitrobenzene (PIN, P-61.5.1)

N-(2-aminomethyl)-*N*,*N*′,*N*′-trimethylethane-1,2-diamine (P-62.2.1.3)

(c) to separate adjacent locants from a subsequent opening enclosing mark:

Examples: 1-(1,2,3,4-tetrahydroquinolin-1-yl)ethan-1-one (PIN, P-64.3.2)

N-acetyl-*N*-(3-chloropropanoyl)benzamide (PIN, P-66.1.2.1)

P-16.2.4.2 No hyphen is placed before a numerical prefix cited in front of a compound substituent enclosed by parentheses, even if that substituent begins with locants;

Example: *N*,1-bis(4-chlorophenyl)methanimine (PIN, P-62.3.1.2)

P-16.2.4.3 Hyphens in fusion names. Hyphens separate the two parts of a fusion descriptor, i.e., numbers and italicized letters.

Example: naphtho[1,2-*a*]azulene (PIN, P-25.3.1.3)

P-16.2.4.4 Hyphens related to stereodescriptors

Hyphens separate stereodescriptors from the rest of the name or the part of a name to which they relate.

Example: (2*E*)-but-2-ene (PIN, P-92.1.7.2)

P-16.2.5 A long hyphen (em dash)

An em dash is used to separate the names of components in adducts;

Example: carbon monoxide—borane (PIN, P-13.3.5)

P-16.2.6 Spaces are a very important type of punctuation for many kinds of names in the English language. If a space is required in a name, it must be used. On the other hand, the use of spaces where they are not required, for example, in substitutive names that must be written continuously from one end to the other using hyphens to connect the different parts, may be misleading. Spaces are used in:

(a) names of acids and salts:

Examples: acetic acid (PIN, P-65.1.1.1)

calcium diacetate (PIN, P-65.6.2.1)

(b) functional class names,

Examples: ethyl acetate (PIN, P-65.6.3.2.1)

2-(chlorocarbonothioyl)benzoyl cyanide (PIN, P-65.5.3)

butyl ethyl sulfoxide (P-63.6)
[ethanesulfonylbutane (PIN)]

(c) names formed using a class modifier,

Examples: cyclohexanone ethyl methyl ketal (P-66.6.5.1.1)
[1-ethoxy-1-methoxycyclohexane (PIN)]

pentan-2-one oxime (P-68.3.1.1.2)
[*N*-pentan-2-ylidenehydroxylamine (PIN)]

(d) additive names

Examples:

ethylene oxide (P-63.5)
[oxirane (PIN)]

trimethylphosphane oxide (PIN, P-74.2.1.4)

P-16.3 Numerical (multiplicative) prefixes

Numerical prefixes are derived from Greek and Latin number names (see P-14.3) and are the principal method for describing a multiplicity of identical features of a structure in chemical names.

P-16.3.1 The basic numerical prefixes ‘di’, ‘tri’, ‘tetra’, etc. are used to indicate a multiplicity of substituent suffixes, conjunctive components, replacement affixes, simple (i.e., unsubstituted) substituent prefixes, and simple (i.e., unsubstituted) functional modification terms provided that there is no ambiguity (see also P-16.3.2).

Examples:

diol

dicarboxylic acid

tricyclohexyl

di(tridecyl)

diamido

diaza

di(propan-2-yl)

di(tetradecane-1,14-diyl)

tetra(2-naphthyl)
[tetra(naphthalen-2-yl) (PIN)]

dioxime

dibenzenesulfonate

di(isoxazol-3-yl)
[di([1,2-oxazol-3-yl) (PIN)]

benzene-1,3,5-triacetic acid (P-15.6.1.4)
[benzene-1,3,5-triyltriacetic acid (PIN)]

di(cyclohexane-1-carboxylic acid)

P-16.3.2 The numerical prefixes ‘bis’, ‘tris’, ‘tetrakis’, etc., are used to indicate a multiplicity of complex (i.e., substituted) substituent prefixes or functional modifiers.

Examples:

bis(2-aminoethyl) (PIN)

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

bis(2-chloropropan-2-yl) (PIN)

bis(phenylhydrazone)
[bis(phenylhydrazinylidene)(PIN)]

These prefixes are also used when the use of ‘di’, ‘tri’, etc.:

(a) indicates another structure; or,

(b) is (or could be) ambiguous; this usually happens when an analogue of the term being multiplied begins with a basic numerical prefix.

Examples:

(a) tris(methylene) (PIN) indicates three methylene ($-CH_2-$) groups;. trimethylene [propane-1,3-diyl (PIN)] describes the multiplicative substitutive group $-[CH_2]_3-$;

(b) tris(decyl) (PIN) indicates three decyl ($C_{10}H_{11}$–) groups; tridecyl (PIN) describes the $C_{13}H_{14}$– substitutive group;

(c) bisoxy) (PIN) indicates two oxy (–O–) groups; dioxy has been used to mean both a –OO– group (peroxy, PIN) and two oxy (–O–) (PIN) groups

(d) bis(benzo[*a*]anthracen-1-yl) (PIN)

(e) benzo[1,2-*c*:3,4-*c*′]bis[1,2,5]oxadiazole (PIN)

(f) ethane-1,2-diylbis(azanediyl) (PIN)

P-16.3.3 The numerical prefixes ‘bi’, ‘ter’, ‘quater’, etc. are used mainly in naming ring assemblies (see P-28).

Examples: 1,1′-biphenyl (PIN, P-28.2.3)

$1^2,2^2:2^6,3^2:3^6,4^2$-quaterpyridine (PIN, P-28.3.1)

P-16.3.4 The prefix ‘mono’ is usually omitted in names of organic compounds. However, it is used to indicate that only one characteristic group of a parent structure has been modified. The ending ‘kis’ is never associated with ‘mono’.

Example: monoperoxyphthalic acid (P-65.1.4.2)
2-carboxybenzenecarboperoxoic acid (PIN)

P-16.4 Enclosing marks

Parentheses, ( ), (also called ‘curves’ or ‘round brackets’), brackets, [ ], (also called ‘square brackets’), and braces { }, (also called ‘curly brackets’) are used in chemical nomenclature to set off parts of a name dealing with specific structural features in order to convey the structure of a compound as clearly as possible. It is important to note that they are used differently in names of organic and inorganic compounds.

All enclosing marks is recommended in preferred IUPAC names. In general nomenclature, when there is no possible ambiguity, enclosing marks may be omitted to simplify a name.

P-16.4.1 Parentheses (also called curves or round brackets)

P-16.4.1.1 Parentheses are used around complex (substituted) prefixes; after the numerical multiplicative prefixes ‘bis’, ‘tris’, etc.; and to enclose a multiplied parent structure consisting of a parent hydride and a substituent suffix even though preceded by a simple prefix, such as ‘di‘, ‘tri‘, etc..

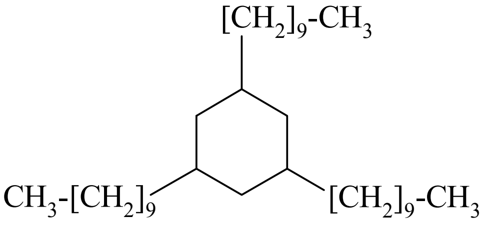
Examples:

$Cl\text{-}CH_2\text{-}SiH_3$

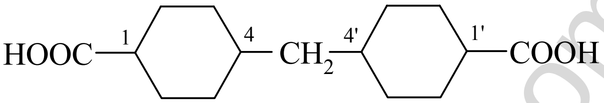
(chloromethyl)silane (PIN)

$(HO\text{-}CH_2\text{-}CH_2\text{-}O)_2CH\text{-}COOH$

bis(2-hydroxyethoxy)acetic acid (PIN)



1,3,5-tris(decyl)cyclohexane (PIN)
(not 1,3,5-tridecylcyclohexane)



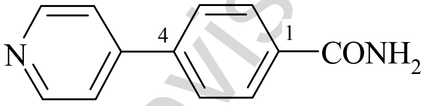
4,4′-methylenedi(cyclohexane-1-carboxylic acid) (PIN)

$H\{S/O\}C\text{-}CH_2\text{-}CH_2\text{-}C\{O/S\}H$

butanebis(thioic acid) (PIN)

P-16.4.1.2 Parentheses are used around simple substituent prefixes to separate locants of the same type referring to different structural elements, even though only one may be expressed.

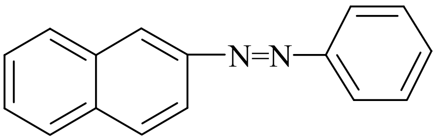
Example:



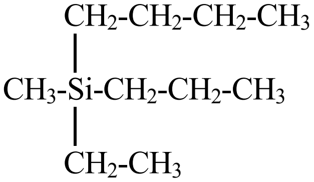
4-(pyridin-4-yl)benzamide (PIN)
4-(4-pyridyl)benzamide

P-16.4.1.3 Parentheses are placed around prefixes denoting simple substituent groups in front of parent hydrides when no locants are necessary and around prefixes defining simple substituent groups qualified by locants. A minimum of parentheses must be used. Enclosing marks are never used around the name of the first cited simple substituent group.

Examples:



naphthalen-2-yl(phenyl)diazene (PIN)
2-naphthyl(phenyl)diazene

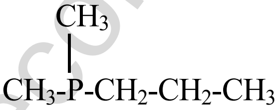


$$\begin{array}{l} \quad CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_3 \\ \quad | \\ CH_3\text{-}Si\text{-}CH_2\text{-}CH_2\text{-}CH_3 \\ \quad | \\ \quad CH_2\text{-}CH_3 \end{array}$$

butyl(ethyl)methyl(propyl)silane (PIN)

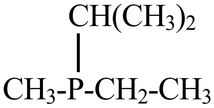
$CH_3\text{-}SiH_2Cl$

chloro(methyl)silane (PIN)



$$\begin{array}{l} \quad CH_3 \\ \quad | \\ CH_3\text{-}P\text{-}CH_2\text{-}CH_2\text{-}CH_3 \end{array}$$

ethyl(methyl)propylphosphane (PIN)



$$\begin{array}{l} \quad CH(CH_3)_2 \\ \quad | \\ CH_3\text{-}P\text{-}CH_2\text{-}CH_3 \end{array}$$

ethyl(methyl)propan-2-ylphosphane (PIN)
ethyl(isopropyl)methylphosphane

P-16.4.1.4 Parentheses are placed around the prefix denoting simple hydrocarbyl substituents adjacent to the name ‘amine’ in amines named by using the parent structure ‘amine’, when several different substituent groups are present. This requirement is necessary to insure the specificity of this kind of names of amines and to distinguish them from older names. Other parentheses are used as needed.

Examples: (2-chloroethyl)(propyl)amine (P-62.2.1.2.1)
[*N*-(2-chloroethyl)propan-1-amine (PIN)]

butyl(ethyl)(propyl)amine (P-62.2.1.2.1)
[*N*-ethyl-*N*-propylbutan-1-amine (PIN)]

butyl(ethyl)(methyl)amine (P-62.2.1.2.1)
[*N*-ethyl-*N*-methylbutan-1-amine (PIN)]

P-16.4.1.5 Parentheses are used to isolate the second locant of a compound locant, around locants denoting ring numbering in phane nomenclature, and to enclose fullerene identifiers.

Examples: bicyclo[8.5.1]hexadec-1(15)-ene (PIN, P-31.1.1.1)

1(1,3),4(1,4)-dibenzenacycloheptaphane (PIN, P-26.4.2.2)

(C_{60}-I_h)[5,6]fullerene (PIN, P-27.2.2)

P-16.4.1.6 Parentheses are used to enclose 'added hydrogen' and its locant, stereodescriptors such as '*E*', '*Z*', '*R*', '*S*', '*cis*', '*trans*', etc., and descriptors for isotopically substituted compounds;

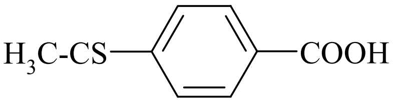
Examples: phosphinin-2(1*H*)-one (PIN, P-14.6)

(2*E*)-but-2-ene (PIN, P-92.1.7.2)

(^{13}C)methane (PIN, P-82.2.1)

P-16.4.1.7 Parentheses are used to avoid ambiguity.

Example:



4-(thioacetyl)benzoic acid
[4-ethanethioylbenzoic acid (PIN)]

P-16.4.1.8 Parentheses are used to enclose groups attached to a chain in linear formulas.

Examples:

CH_3-CH(SH)-CH_3 propane-2-thiol (PIN, P-63.1.5)

CH_3-CH(OH)-CO-CH_3 3-hydroxybutan-2-one (PIN, P-64.8)

P-16.4.2 Brackets (also called square brackets)

P-16.4.2.1 Brackets enclose descriptors denoting fusion sites in fused ring systems and enclose numbers denoting the length of bridges and chains connecting spiro atoms in names of polyalicyclic ring systems constructed according to von Baeyer methods. They also enclose ring assembly names when these are followed by a principal group suffix or a cumulative suffix and enclose names of components in von Baeyer spiro names.

Examples: naphtho[2,1-*a*]azulene (PIN, P-25.3.1.3)

bicyclo[3.2.1]octane (PIN, P-23.2.2)

spiro[4.5]decane (PIN, P-24.2.1)

[2,2′-bipyridin]-4-yl (PIN, P-29.3.5)

spiro[cyclohexane-1,1′-indene] (PIN, P-24.5.1)

P-16.4.2.2 Brackets enclose locants that describe structural features of components, such as double bonds in bridges and heteroatoms of component rings in names of fused ring systems.

Examples: 6,7-(prop[1]en[1]yl[3]ylidene)benzo[*a*]cyclohepta[*e*][8]annulene (PIN, P-25.4.3.3)

5*H*-pyrido[2,3-*d*][1,2]oxazine (PIN, P-25.3.2.4)

P-16.4.2.3 Brackets enclose the numerals that describe ring size in annulenes and fullerenes.

Examples: [10]annulene (P-22.1.2)
[cyclodeca-1,3,5,7,9-pentaene (PIN)]

(C_{60}-I_h)[5,6]fullerene (PIN, P-27.2.2)

P-16.4.2.4 Brackets enclose substituent prefixes in which parentheses have already been used.

Example: 4-[(hydroxyselanyl)methyl]benzoic acid (PIN, P-63.4.2,2)

P-16.4.2.5 Brackets are used to enclose descriptors for isotopically labeled compounds.

Example: [^{13}C]methane (PIN, P-83.1.3)

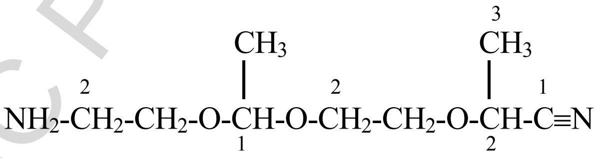
P-16.4.2.6 Brackets are employed in formulae to indicate repetition of a group in a chain.

Example: $CH_3\text{-}[CH_2]_{68}\text{-}CH_3$ heptacontane (PIN, P-21.2.1)

P-16.4.3 Braces (also called curly brackets)

P-16.4.3.1 Braces are used to enclose substituent prefixes in which brackets and parentheses have already been used.

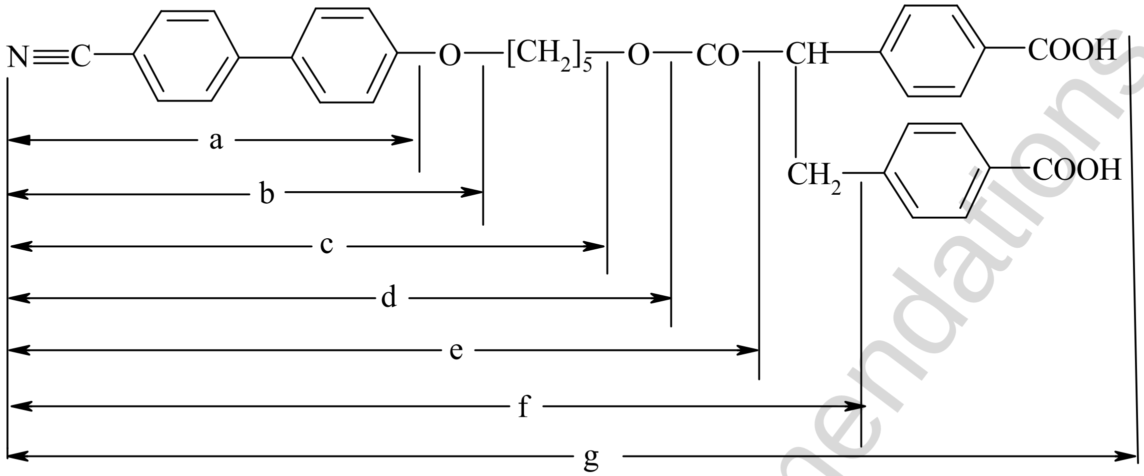
Example:



$$NH_2\text{-}\overset{2}{C}H_2\text{-}CH_2\text{-}O\text{-}\underset{1}{\overset{\overset{CH_3}{|}}{C}}H\text{-}O\text{-}\overset{2}{C}H_2\text{-}CH_2\text{-}O\text{-}\underset{2}{\overset{\overset{\overset{3}{CH_3}}{|}}{C}}H\text{-}\overset{1}{C}{\equiv}N$$

2-{2-[1-(2-aminoethoxy)ethoxy]ethoxy}propanenitrile (PIN)

P-16.4.3.2 When additional enclosing marks are required, the nesting order is {[({[( )]})]}, etc., as illustrated in Fig. 1.2.



(a) = 4′-cyanobiphenyl-4-yl

(b) = (4′-cyanobiphenyl-4-yl)oxy

(c) = 5-[(4′-cyanobiphenyl-4-yl)oxy]pentyl

(d) = {5-[(4′-cyanobiphenyl-4-yl)oxy]pentyl}oxy

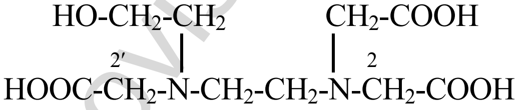
(e) = ({5-[(4′-cyanobiphenyl-4-yl)oxy]pentyl}oxy)carbonyl

(f) = 1-[({5-[(4′-cyanobiphenyl-4-yl)oxy]pentyl}oxy)carbonyl]ethane-1,2-diyl

(g) = 4,4′-{1-[({5-[(4′-cyanobiphenyl-4-yl)oxy]pentyl}oxy)carbonyl]ethane-1,2-diyl}dibenzoic acid (PIN)

FIG. 1.2 Nesting order of enclosing marks

Example:



$$\begin{array}{l} \quad\;\; \text{HO-CH}_2\text{-CH}_2 \qquad\qquad \text{CH}_2\text{-COOH} \\ \qquad\qquad\quad {}^{2'}\;| \qquad\qquad\qquad | \;{}^{2} \\ \text{HOOC-CH}_2\text{-N-CH}_2\text{-CH}_2\text{-N-CH}_2\text{-COOH} \end{array}$$

2,2′-({2-[(carboxymethyl)(2-hydroxyethyl)amino]ethyl}azanediyl)diacetic acid
[*N*-(carboxymethyl)-*N*′-(2-hydroxyethyl)-*N*,*N*′-ethane-1,2-diyldiglycine (PIN)]

P-16.5 Italicization

Italicizing marks letters that are not involved in the primary stage of alphanumerical ordering. In manuscripts, italics are conventionally indicated by underlining when an italic font is not available.

P-16.5.1 Lower case italic letters are used in descriptors for fusion sites in names of fused ring systems.

Example: selenopheno[2,3-*b*]selenophene (PIN, P-25.3.1.3)

The letters *o*, *m*, and *p* have been used in place of *ortho*, *meta*, and *para*, respectively, to designate the 1,2- 1,3-, and 1,4- isomers of disubstituted benzene. This usage is strongly discouraged and is not used in preferred IUPAC names.

Examples: *o*-xylene (P-61.2.3)
[1,2-xylene (PIN)]

p-dinitrosobenzene (P-61.5.1)
[1,4-dinitrosobenzene (PIN)]

P-16.5.2 Italicized elements symbols, such as *O*, *N*, *As*, are locants indicating attachment of a substituent to these heteroatoms

Examples: *N*,*N*-diethylethanamine (PIN, P-62.2.1.2.1)

O-ethyl hexaneselenoate (PIN, P-65.6.3.2.4)

The italic element symbol *H* denotes indicated or added hydrogen.

Examples: 1*H*-azepine (PIN, P-22.2.2.1.4)

quinolin-2(1*H*)-one (PIN, P-64.3.1)

P-16.5.3 Italic terms, syllables and capital Roman letters are used in some structural descriptors and stereodescriptors, such as '*cis*', '*trans*', '*R*', '*S*', '*E*', '*Z*', '*r*', '*c*', '*t*', and '*retro*'.

Examples: *tert*-, but not 'iso' (P-29.6.3)

'*E*' and '*Z*' (P-92.1.7.1); '*cis*', and '*trans*' (P-92.2.1.1); '*r*', '*c*', and '*t*' (P-92.2.1.1); '*r*' and '*s*' (P-91.4)

'*R*' and '*S*' (P-92.1.1), '*R**' (spoken R-star), '*S**' (spoken S-star), '*rel*' (P-92.1.2)

'*meso*' (P-92.2.2.6), '*ambo*' (P-92.2.2.7), '*rac*' (P-92.1.3)

'*M*' and '*P*', 'R_a' and 'S_a', 'R_p' and 'S_p' (P-982.1.5)

'*TPY*-3', '*TS*-3', '*SS*-4', '*TBPY*', '*SPY*', and '*OC*' (P-92.1.9)

'*retro*', but not 'abeo', 'apo', 'cyclo', 'de', 'des', 'homo', 'nor' or 'seco' (P-101.3.1 through P-101.3.7)

P-16.6 Elision of vowels

P-16.6.1 Vowels are systematically elided as follows:

(a) the terminal letter 'e' in names of parent hydrides or endings 'ene' and 'yne' when followed by a suffix or 'en' ending beginning with 'a', 'e', 'i', 'o', 'u' or 'y';

Examples: pentanal (PIN, P-6.6.2.1)

cyclopentadec-1-en-4-yne (PIN, P-31.1.3.1)

methanium (PIN, P-73.1.1.2)

butan-2-one (PIN, P-64.2.2.1)

tetramethylboranuide (PIN, P-72.3)

sulfanyl (PIN, P-29.3.1)

(b) in Hantszch-Widman names, the final letter ‘a’ of an ‘a’ prefix when followed by a vowel;

Examples: 1,3-thiazole (PIN, P-22.2.2.1.2)
(not 1,3-thiaazaole)

1,6,2-dioxazepane (PIN, P-22.2.2.1.2)
(not 1,6,2-dioxaazaepane)

(c) the terminal letter ‘a’ in the names of numerical multiplicative affixes when followed by a suffix beginning with ‘a’ or ‘o’;

Examples: [1,1′-biphenyl]-3,3′,4,4′-tetramine (PIN, P-62.2.1.1.2)
(not [1,1′-biphenyl]-3,3′,4,4′-tetraamine)

benzenehexol (PIN, P-63.1.2)
(not benzenehexaol)

(d) the terminal letter ‘a’ of an element ‘a’ prefix in ‘a(ba)$_n$’ repeating unit names when followed by a vowel;

Examples: disilazane (preselected name, P-21.2.3.1)
(not disilaazane)

tetrastannoxane (preselected name, P-21.2.3.1)
(not tetrastannaoxane)

(e) the terminal letter ‘o’ of a functional replacement infix when followed by a vowel;

Example: *P*-phenylphosphonamidimidic acid (PIN, P-67.1.2.1)
(not *P*-phenylphosphonoamidoimidic acid)

(f) the terminal letter ‘o’ of ‘benzo’ in names of ‘benzoheterocycles’ formed by fusion of a benzene ring to a heteromonocycle whose name begins with a vowel [an exception to P-16.6.6(f)].

Examples: 3-benzoxepine (PIN, P-25.2.2.4)

4*H*-3,1-benzoxazine (PIN, P-25.2.2.4)

P-16.6.2 There is no elision of terminal vowels in the following cases:

(a) in conjunctive names

Example: benzeneacetic acid (P-15.6.1.1)
[phenylacetic acid (PIN)]

(b) from replacement or numerical multiplicative prefixes in skeletal replacement (‘a’) nomenclature;

Example: 2,4,6,8-tetrasilaundecane (PIN, P-15.4.1.3)

(c) from numerical multiplicative prefixes in multiplying parent compounds;

Example: 2,2′,2″,2‴-(ethane-1,2-diyldinitrilo)tetraacetic acid (P-15.3.2.6)
[*N*,*N*′-ethane-1,2-diylbis[*N*-(carboxymethyl)glycine (PIN)]

(d) from numerical multiplicative prefixes before substituent prefix names;

Example: 5,6,7,8-tetraiodo-1,2,3,4-tetrahydroanthracene-9-carboxylic acid (PIN, P-65.1.2.4)

(e) from component prefixes of compound and complex prefixes before following prefixes beginning with a vowel;

Examples: chloroamino (preselected name, P-34.3.1)

aminooxy (preselected name, P-68.3.1.1.1.5)

(f)) from prefixes designating attached components in fusion nomenclature; for example, the terminal letter ‘o’ of acenaphtho, benzo, perylo, phenanthro, and the terminal letter ‘a’ of anthra, cyclopropa, cyclobuta, are not elided before a vowel [see P-16.6.1(f) for an exception involving 'benzo'].

This recommendation is in accordance with P-25.3.1.3 (see below) and Rule R-2.4.1.1 in the 1993 Recommendations (ref. 2). Rule A-21.4 that recommended the elision in the 1979 Recommendations (ref. 1) is abrogated.

Examples: cyclopropa[*de*]anthracene (PIN, P-25.3.8.1)

naphtho[1,2-*a*]azulene (PIN, P-25.3.1.3)

P-16.7 Addition of vowels

P-16.7.1 For euphonic reasons, in functional replacement nomenclature the vowel ‘o’ is inserted between consonants.

Examples: ethanesulfonodiimidic acid (PIN, P-65.3.1.4)
(not ethanesulfondiimidic acid)

phenylphosphononitridic acid (PIN, P-67.1.1.2.2)
(not phenylphosphonnitridic acid)

P-16.7.2 For euphonic reasons, the letter ‘a’ is inserted between the root of the name for polyenes, polyynes, and polyenynes, and the numerical multiplying prefix ‘di’, ‘tri’, etc., preceding the ending ‘ene’ or ‘yne

Examples: buta-1,2-diene (PIN, P-31.1.1.2)
(not but-1,2-diene)

hexa-1,3-dien-5-yne (PIN, P-31.1.2.2.1)
(not hex-1,3-dien-5-yne)

P-16.8 Primes

P-16.8.1 Primes (′), double primes (″), triple primes (‴), etc., are used to differentiate identical locants, for example *N*,*N*′, 1,1′,1″. Such usage occurs:

(a) in multiplicative nomenclature to denote multiplied units and modify locants accordingly;

Example:

2,2′,2″-nitrilotriethanol (PIN, P-15.3.2.3)

(b) in spiro-fused compounds, to denote positions in polycyclic systems, identical or different;

Examples:

7,7′-spsirobi[bicycle[4.1.0]heptane] (PIN, P-24.3.1)

1*H*,1′*H*,1″*H*,3′*H*-2,2′:7,2″-dispiroter[naphthalene] (PIN, P-24.4.1)

spiro[cyclohexane-1,1′-indene] (PIN, P-24.5.1)

(c) in ring assemblies, to number identical ring components;

Examples:

1,1′-bi(cyclopropane) (PIN, P-28.2.1)

1,1′-biphenyl (PIN, P-28.2.3)

P-16.8.2 Primes also occur:

(a) in fusion nomenclature, to identify first and higher attached components, identical attached components and multiparent names;

Examples:

pyrido[1″,2″:1,2′]imidazo[4′,5′:5,6]pyrazino[2,3-*b*]phenazine (PIN, P-25.3.4.1.1)

difuro[3,2-*b*;2′,3′-*e*]pyridine (PIN, P-25.3.4.1.2)

cyclopenta[1,2-*b*:5,1-*b*′]bis[1,4]oxathiazine (PIN, P-25.3.4.1.3)

(b) in fullerenes *ortho*-fused to organic ring or ring systems, to identify positions in the nonfullerene component;

Example:

3′*H*-cyclopropa[1,9](C_{60}-I_h)[5,6}fullerene (PIN, P-27.6.1)

(c) in natural product nomenclature, to identify positions in ring(s) fused to a fundamental parent hydride;

Example:

benzo[2,3]-5α-androstane (PIN, P-101.5.1.1)