

## CHAPTER P-3 CHARACTERISTIC (FUNCTIONAL) GROUPS

- P-30 Introduction
- P-31 Modification of the degree of hydrogenation of parent hydrides
- P-32 Prefixes for substituent groups derived from parent hydrides with a modified degree of hydrogenation
- P-33 Suffixes
- P-34 Parent structures other than parent hydrides and corresponding prefixes for substituent groups
- P-35 Prefixes denoting characteristic groups

### P-30 Introduction

The prefixes and/or suffixes attached to a parent name specify a particular molecular structure and usually represent **substituents** of various types, which are considered to take the place of hydrogen atoms of the parent hydride or parent structure. It has been customary to regard such substituents as **characteristic** (or **functional**) when the link between substituent and parent is not a carbon-carbon bond, for example,  $-\text{OH}$ ,  $=\text{O}$  and  $-\text{NH}_2$ , but exceptions are recognized, such as  $-\text{COOH}$  and  $-\text{CN}$ . It seems appropriate to retain the general view of **functionality** as implying the presence of heteroatoms, but it would not be helpful to attempt to define precisely the limits of application of the term.

Carbon-carbon unsaturation in acyclic and alicyclic compounds is regarded by IUPAC as a special type of functionality and is therefore treated here in Chapter P-3 rather than in Chapter P-2 (Parent hydrides). Its presence here and that of the hydrogenation of parent hydrides having the maximum number of noncumulative double bonds (mancude parent hydrides) is logical for nomenclature, as the unsaturation in acyclic and alicyclic parent hydrides expressed by endings and the saturation of mancude parent hydrides by hydro-dehydro prefixes are essentially equivalent.

This Chapter also deals with **functional parent compounds**, i.e., structures that may be treated as parent structures, having substitutable hydrogen atoms, but possessing characteristics normally associated with functionality, e.g., acetic acid,  $\text{CH}_3\text{-COOH}$  and phosphonic acid  $\text{HP(O)(OH)}_2$ . Functional parent compounds must be distinguished from compounds having a characteristic group systematically introduced as a suffix attached to a parent hydride, for example butanoic acid and ethanol. The latter compounds may be called 'functionalized parent hydrides'.

Although, strictly speaking, **ions** and **radicals** do not fall within the concept of functionality as described above, an ionic center or a radical center is treated like a function and expressed in the same way as characteristic groups, i.e., by suffixes and prefixes. This treatment is introduced in this Chapter and fully discussed in Chapter P-7.

Any characteristic group is expressed in a name either as suffix or as prefix. As prefixes, they are detachable (alphabetizable) prefixes, as are the prefixes derived from parent hydrides discussed in section P-29.

## **P-31 Modification of the degree of hydrogenation of parent hydrides**

- P-31.0 Introduction
- P-31.1 The endings 'ene' and 'yne'
- P-31.2 Hydro prefixes
- P-31.3 Dehydro prefixes

### **P-31.0 Introduction**

Parent hydrides are divided into two groups, fully saturated or fully unsaturated. Fully unsaturated cyclic parent hydrides are, by convention, defined as having the maximum number of noncumulative double bonds, also called 'mancude' compounds (an acronym for MAXimum Number of nonCUmulated Double bonds). Thus a degree of hydrogenation different from those denoting these two groups must be expressed by an additive or subtractive operation corresponding to the addition or the subtraction of hydrogen atoms. Specific rules are devised for compounds having saturated and unsaturated parts, such as cyclophanes, spiro compounds, etc.

The state of hydrogenation of parent hydrides is modified in two ways: (a) by a subtractive operation (subtraction of two or more hydrogen atoms) denoted by the 'ene' and 'yne' endings or by the prefix 'dehydro'; or (b) by an additive operation (addition of two or more hydrogen atoms) denoted by the prefix 'hydro'.

It is important to take note that endings 'ene' and 'yne' and 'hydro' and 'dehydro' prefixes are detachable. When used to modify parent hydrides, they are regulated by the principle of lowest locants, in accord with the numbering of the parent hydride and after priority has been given to indicated hydrogen, added hydrogen, and suffixes, when present, as specified in the general rules for numbering (P-14.4).

### **P-31.1 The endings 'ene' or 'yne'**

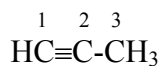
#### **P-31.1.1 General methodology**

**P-31.1.1.1** The presence of one or more double or triple bonds in an otherwise saturated parent hydride (except for parent hydrides with Hantzsch-Widman names or retained names denoting partial hydrogenation as indicated later) is denoted by changing the ending 'ane' of the name of a saturated parent hydride to 'ene' or 'yne'. Locants as low as possible are given to multiple bonds as a set, even though this may at times give 'yne' endings lower locants than 'ene' endings. If a choice remains, preference for low locants is given to the double bonds. In names, the ending 'ene' always precedes 'yne', with elision of the final letter 'e' in 'ene'. Only the lower locant for a multiple bond is cited except when the numerical difference between the two locants is greater than one, in which case the higher locant is enclosed in parentheses.

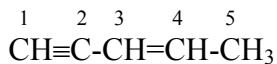
Examples:



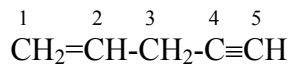
but-1-ene (PIN)



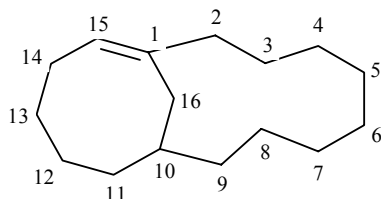
prop-1-yne (PIN)



pent-3-en-1-yne (PIN)



pent-1-en-4-yne (PIN)



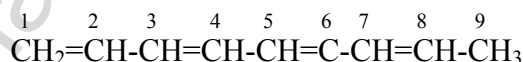
bicyclo[8.5.1]hexadec-1(15)-ene (PIN)

**P-31.1.1.2** The multiplying prefixes ‘di’, ‘tri’, etc., are placed before endings denoting unsaturation to indicate the number of multiple bonds of each kind, as required, for example ‘diene’ and ‘triyne’. For euphonic reasons, when the endings ‘ene’ and ‘yne’ are preceded by a multiplying prefix and a locant, the letter ‘a’ is inserted. There is no elision of the final letter ‘a’ of a multiplying prefix before ‘ene’ or ‘yne’, for example, ‘tetraene’ and ‘pentayne’.

Examples:



buta-1,3-diene (PIN)



nona-1,3,5,7-tetraene (PIN)

The method of P-31.1.1 is applicable to the following saturated hydrocarbon parent hydrides and to the corresponding hydrides modified by skeletal replacement (‘a’) nomenclature that are described in Chapter 2.

- P-31.1.2 Acyclic parent hydrides
- P-31.1.3 Monocyclic parent hydrides
- P-31.1.4 Bi- and polycyclic von Baeyer parent hydrides
- P-31.1.5 Spiro parent hydrides composed of monocyclic rings
- P-31.1.6 Phane parent hydrides
- P-31.1.7 Ring assembly parent hydrides (under specific conditions)

The method is not used to modify Hantzsch-Widman names for saturated heterocyclic compounds or totally or partially hydrogenated mancade compounds having retained names (indane, imidazolidine, indoline, isoindoline, morpholine, piperazine, piperidine, pyrazolidine, pyrrolidine, quinuclidine, and also chromane, isochromane, and their chalcogen analogues).

When necessary, the corresponding mancude compounds are modified by using prefixes 'hydro' or 'dehydro', as indicated in P-31.2, below.

**P-31.1.2** Acyclic parent hydrides

**P-31.1.2.1** Retained names

The name acetylene is retained for the compound  $\text{HC}\equiv\text{CH}$ . It is the preferred IUPAC name, but substitution of any kind is not allowed. Substitution is allowed in general nomenclature, but not by alkyl groups or any other group that extends the carbon chain, or by characteristic groups expressed by suffixes.

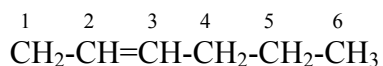
The name allene, for  $\text{CH}_2=\text{C}=\text{CH}_2$ , is retained for general use only. Substitution is allowed, but not by alkyl or any other group that extends the carbon chain, or characteristic groups expressed by suffixes.

The name isoprene, for  $\text{CH}_2=\text{C}(\text{CH}_3)\text{-CH}=\text{CH}_2$ , is retained but only for general nomenclature. No substitution of any kind is allowed.

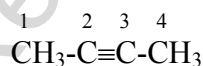
**P-31.1.2.2** Systematic names

**P-31.1.2.2.1** Homogeneous acyclic parent hydrides and acyclic parent hydrides composed of alternating heteroatoms are modified by the general method of P-31.1.1.

Examples:

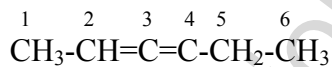


hex-2-ene (PIN)



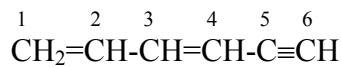
but-2-yne (PIN)

(not dimethylacetylene)

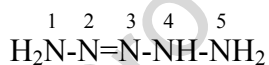


hexa-2,3-diene (PIN)

(not 1-ethyl-3-methylallene)

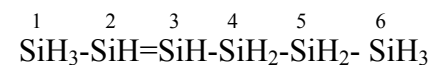


hexa-1,3-dien-5-yne (PIN)



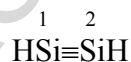
pentaaz-2-ene

(preselected name, see P-12.2)



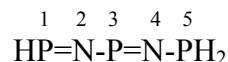
hexasil-2-ene

(preselected name, see P-12.2)



disilyne

(preselected name, see P-12.2)



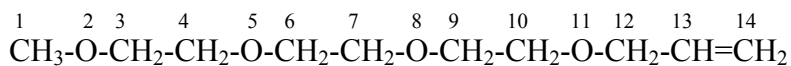
triphosphaza-1,3-diene

(preselected name, see P-12.2)

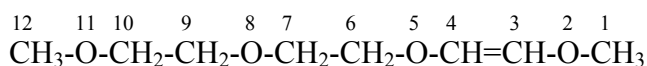
**P-31.1.2.2.2** Acyclic parent hydrides modified by skeletal replacement ('a') nomenclature

Locants are assigned to unsaturation sites in chains in accordance with the fixed numbering of the hetero chain. If a choice remains, then lowest locants are assigned to unsaturated sites.

Examples:



2,5,8,11-tetraoxatetradec-13-ene (PIN)

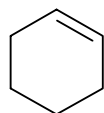


2,5,8,11-tetraoxadodec-3-ene (PIN)

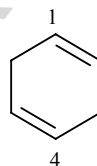
**P-31.1.3** Monocyclic parent hydrides

**P-31.1.3.1** In monocyclic homogeneous unsaturated compounds, one double or triple bond is always allocated the locant '1'. When alone, locant '1' is omitted in names.

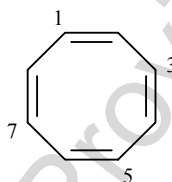
Examples:



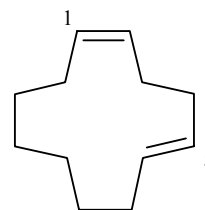
cyclohexene (PIN)



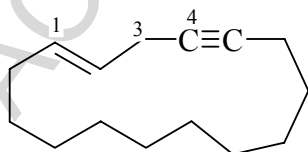
cyclohexa-1,4-diene (PIN)



cycloocta-1,3,5,7-tetraene (PIN)



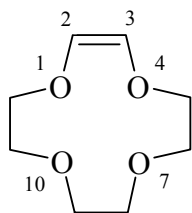
cyclododeca-1,5-diene (PIN)



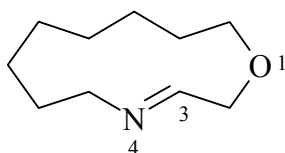
cyclopentadec-1-en-4-yne (PIN)

**P-31.1.3.2** In rings modified by skeletal replacement ('a') nomenclature, low locants are assigned first to heteroatoms and then to unsaturated sites.

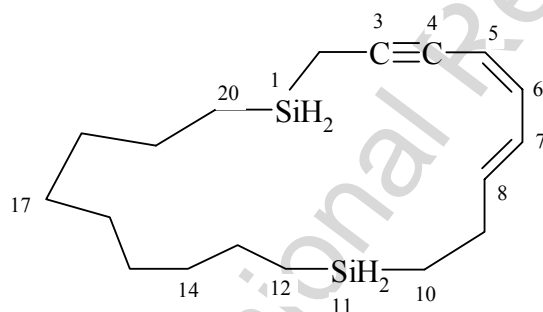
Examples:



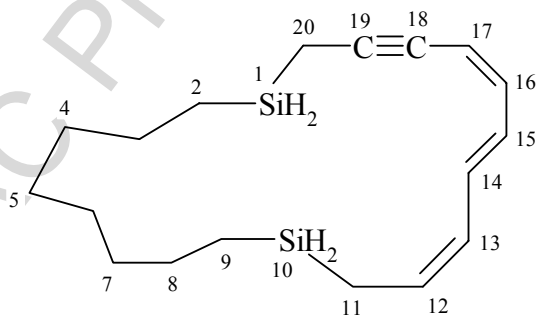
1,4,7,10-tetraoxacyclododec-2-ene (PIN)



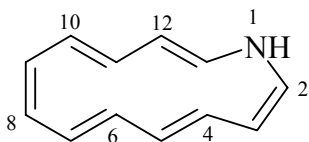
1-oxa-4-azacyclododec-3-ene (PIN)



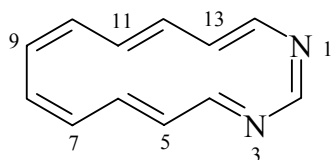
1,11-disilacycloicosa-5,7-dien-3-yne (PIN)  
(not 1,11-disilacycloicosa-4,6-dien-8-yne; the locant set '3,5,7' is lower than '4,6,8')



1,10-disilacycloicosa-12,14,16-trien-18-yne (PIN)



1-azacyclotrideca-2,4,6,8,10,12-hexaene (PIN)  
1*H*-1-aza[13]annulene



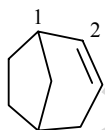
1,3-diazacyclotetradeca-1,3,5,7,9,11,13-heptaene (PIN)  
1,3-diaza[14]annulene

#### P-31.1.4 Bi- and polycyclic von Baeyer parent hydrides

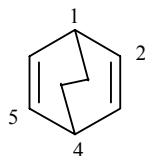
It should be noted that some bi- and polycyclic von Baeyer parent hydrides qualify for phane names as preferred IUPAC names.

**P-31.1.4.1** Low locants are allocated first in accordance with the fixed numbering of the ring system. Low locants are allocated for double bonds when the atoms of each bond have consecutive locants.

Examples:



bicyclo[3.2.1]oct-2-ene (PIN)

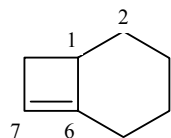


bicyclo[2.2.2]octa-2,5-diene (PIN)

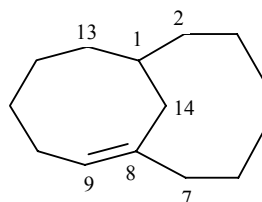
**P-31.1.4.2** If there is a choice of names and numbering, the following criteria are considered in order until a decision is reached.

- (1) Minimum number of compound locants. A compound locant is used for a double bond if the locants of the atoms at each end of the bond do not differ by a value of one. When a compound locant is required, the higher locant is cited in parentheses. A benzene ring is shown and described as a cyclohexatriene corresponding to the Kekulé structure. Other aromatic rings are treated similarly, when required.

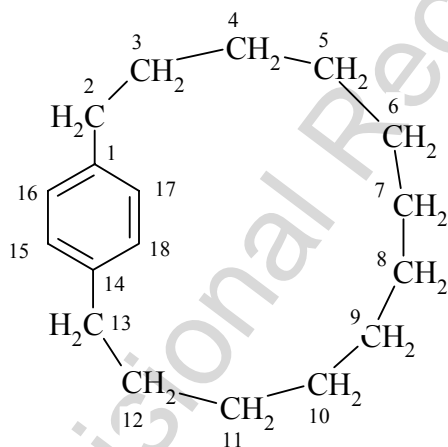
Examples:



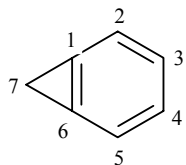
bicyclo[4.2.0]oct-6-ene (PIN)  
[not bicyclo[4.2.0]oct-1(8)-ene]



bicyclo[6.5.1]tetradec-8-ene (PIN)  
[not bicyclo[6.5.1]tetradec-1(13)-decene;  
this is a change from R-3.1.1 in the Guide(ref. 2)]



bicyclo[12.2.2]octadeca-1(16),14,17-triene  
[not bicyclo[12.2.2]octadeca-1(17),14(18),15-triene]  
1(1,4)-benzenacyclotridecaphane (PIN, see P-52.5.2.2)

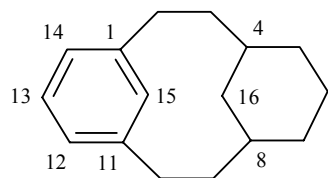


bicyclo[4.1.0]hepta-1,3,5-triene (PIN)  
[not bicyclo[4.1.0]hepta-1(6),2,4-triene]

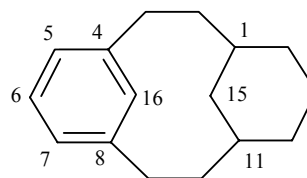
- (2) When comparing double bond locants including compound locants any number in parentheses is ignored.



Examples:

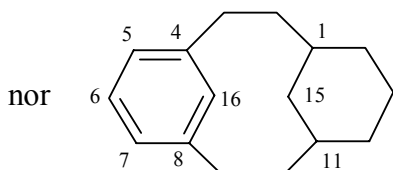


not



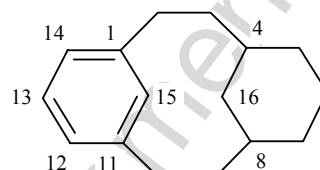
**(I)**

**(II)**



nor

nor



**(III)**

**(IV)**

tricyclo[9.3.1.1<sup>4,8</sup>]hexadeca-1(15),11,13-triene **(I)**

[not tricyclo[9.3.1.1<sup>4,8</sup>]hexadeca-4(16),5,7-triene **(II)**;

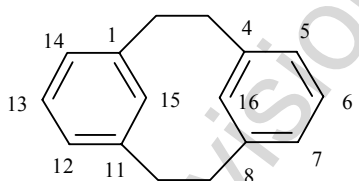
nor tricyclo[9.3.1.1<sup>4,8</sup>]hexadeca-4,6,8(16)-triene **(III)**;

nor tricyclo[9.3.1.1<sup>4,8</sup>]hexadeca-1(14),11(15),12-triene **(IV)**]

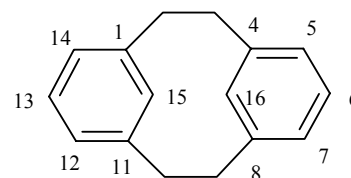
[the set of locants 1,11,13 in **(I)** is lower than 4,5,7 in **(II)** and 4,6,8 in **(III)**;

**(IV)** has two compound locants whereas **(I)** has only one compound locant]

1(1,3)-cyclohexana-4(1,3)-benzenacyclohexaphane (PIN, see P-52.5.2.2)

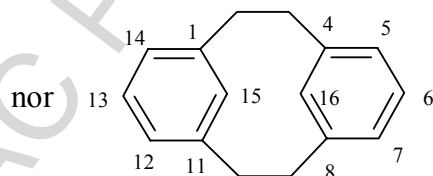


not



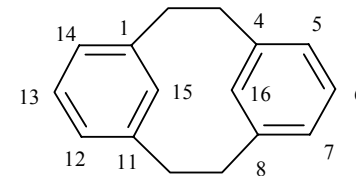
**(I)**

**(II)**



nor

nor



**(III)**

**(IV)**

tricyclo[9.3.1.1<sup>4,8</sup>]hexadeca-1(15),4(16),5,7,11,13-hexaene **(I)** (PIN)

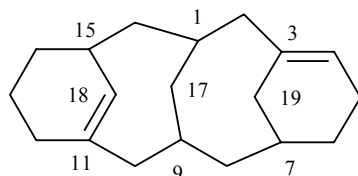
[not tricyclo[9.3.1.1<sup>4,8</sup>]hexadeca-1(15),4,6,8(16),11,13-hexaene **(II)**;

nor tricyclo[9.3.1.1<sup>4,4</sup>]hexadeca-1(14),4,6,8(16),11(15),12-hexaene (**III**);  
nor tricyclo[9.3.1.1<sup>4,8</sup>]hexadeca-1(14),4(16)5,7,11(15)12-hexaene (**IV**)  
[the set of locants in (**I**), '1,4,5,7,11,13' is lower than '1,4,6,8,11,13' in (**II**);  
and also name (**I**) has two compound locants compared to three in names  
(**III**) and (**IV**)]

1,4(1,3)-dibenzenecyclohexaphane (PIN, see P-52.5.2.2)

(3) if there is still a choice, low locants are selected considering all locants as a set.

Example:



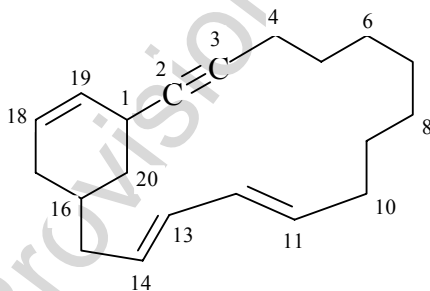
tetracyclo[7.7.1.1<sup>3,7</sup>.1<sup>11,15</sup>]nonadeca-3,11(18)-diene (PIN)  
[not tetracyclo[7.7.1.1<sup>3,7</sup>.1<sup>11,15</sup>]nonadeca-3(19),11-diene;  
the locant set 3,11,18 is lower than 3,11,19]

### P-31.1.4.3 Bi- and polycyclic von Baeyer structures with both double and triple bonds

If there are double and triple bonds present, the following criteria for numbering are considered, in order, until a decision is reached.

(1) Lower locants are assigned to multiple bonds as a set.

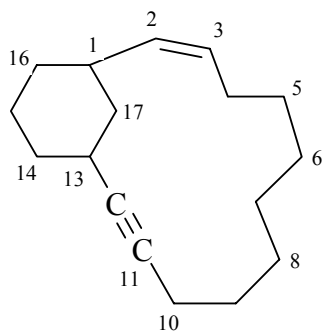
Example:



bicyclo[14.3.1]icosa-11,13,18-trien-2-yne (PIN)  
(not bicyclo[14.3.1]icosa-3,5,17-trien-14-yne;  
the locant set 2,11,13,18 is lower than 3,5,14,17)

(2) Lower locants are assigned to double bonds.

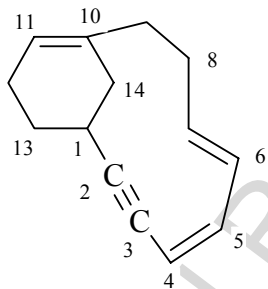
Example:



bicyclo[11.3.1]heptadec-2-en-11-yne (PIN)  
(not bicyclo[11.3.1]heptadec-11-en-2-yne)

(3) Compound locants are kept to a minimum.

Example:

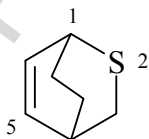


bicyclo[8.3.1]tetradeca-4,6,10-trien-2-yne (PIN)  
(not bicyclo[8.3.1]tetradeca-1(13),4,6-trien-8-yne)

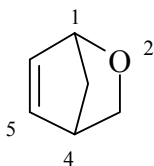
**P-31.1.4.4** Bi- and polycyclic von Baeyer heterocycles names by skeletal replacement ('a') nomenclature

In heterocyclic compounds formed by using skeletal replacement ('a') nomenclature, low locants are assigned to heteroatoms, in accord with the fixed numbering of the system, then to unsaturated sites.

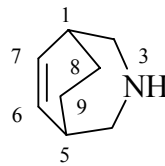
Examples:



2-thiabicyclo[2.2.2]oct-5-ene (PIN)



2-oxabicyclo[2.2.1]hept-5-ene (PIN)



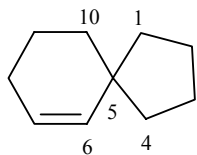
3-azabicyclo[3.2.2]non-6-ene (PIN)

### P-31.1.5 Spiro compounds

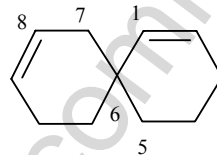
#### P-31.1.5.1 Spiro compounds composed of saturated rings

**P-31.1.5.1.1** Low locants are assigned to double bonds in accordance with the fixed numbering of the spiro compound.

Examples:



spiro[4.5]dec-6-ene (PIN)

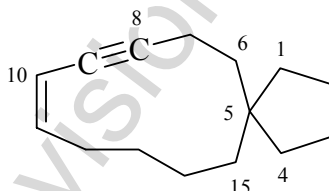


spiro[5.5]undeca-1,8-diene (PIN)

**P-31.1.5.1.2** If there are double and triple bonds present, the following criteria are considered, in order, until a decision is reached.

- (1) Lower locants are assigned to multiple bonds as a set..

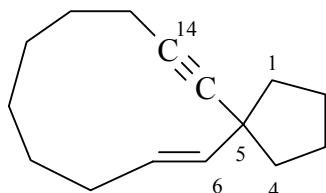
Example:



spiro[4.10]pentadec-10-en-8-yne (PIN)

- (2) If there is still a choice, low locants are assigned to double bonds.

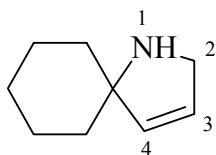
Example:



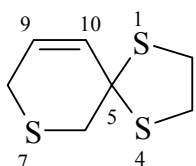
spiro[4.10]pentadec-6-en-14-yne (PIN)

**P-31.1.5.1.3** Heteroatoms in spiro compounds consisting of monocyclic rings denoted by skeletal replacement ('a') nomenclature have priority for low locants.

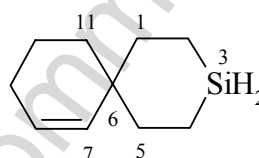
Example:



1-azaspiro[4.5]dec-3-ene (PIN)



1,4,7-trithiaspiro[4.5]dec-9-ene (PIN)

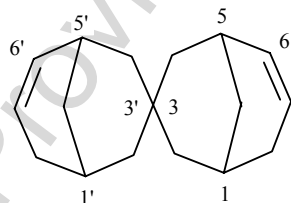


3-silaspiro[5.5]undec-7-ene (PIN)

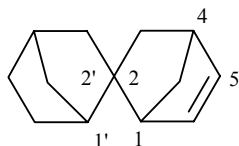
**P-31.1.5.2** Spiro compounds composed of identical polycyclic von Baeyer components

Unsaturation in a spiro ring system with one or more components named by the von Baeyer system is indicated by the endings 'ene', 'diene', etc. They are cited after the last bracket of the spiro name; only the final letter 'e' of the saturated hydrocarbon name is elided if followed by a vowel. If there is a choice, low locants are assigned, in order, to spiro junction(s), heteroatoms and double bonds. This is a change from the Guide (ref. 2; see ref. 7)

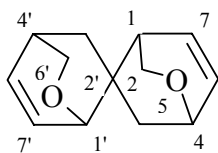
Examples:



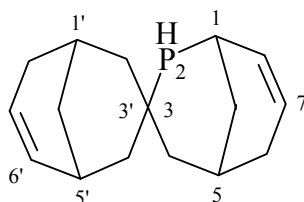
3,3'-spirobi[bicyclo[3.3.1]nonane]-6,6'-diene (PIN)



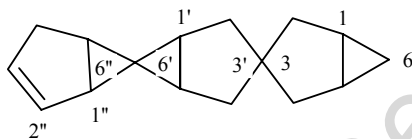
2,2'-spirobi[bicyclo[2.2.1]heptan]-5-ene (PIN)



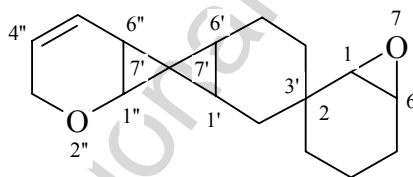
5,6'-dioxo-2,2'-spirobi[bicyclo[2.2.2]octane]-7,7'-diene (PIN)



2-phospha-3,3'-spirobi[bicyclo[3.3.1]nonane]-6',7'-diene (PIN)



3,3':6',6''-dispiroter[bicyclo[3.1.0]hex]-2''-ene (PIN)



2'',7'-dioxo-2,3':7',7''-dispiroter[bicyclo[4.1.0]hexan]-4''-ene (PIN)  
[not 5'',7'-dioxo-2,3':7',7''-dispiroter[bicyclo[4.1.0]hexan]-2''-ene; the locant set '2'',7' is lower than '5'',7' for the 'oxa' prefixes]

### P-31.1.6 Phane parent hydrides

#### P-31.1.6.1 Double bonds in amplificants and in simplified phane skeletons

The presence of one or more double or triple bonds in an otherwise saturated phane parent hydride, except in amplificants with Hantzsch-Widman names, is denoted by changing the final letter 'e' of the phane parent hydride name to 'ene' or 'yne', with appropriate multiplying prefixes to indicate the multiplicity of each kind of unsaturated site.

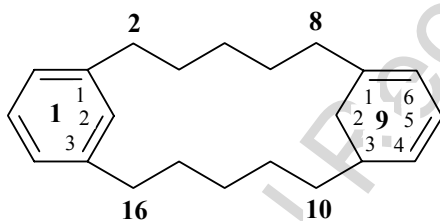
Low locants are allocated for double or triple bonds in accordance with the fixed numbering of the phane parent hydride and of phane parent hydrides that are modified by skeletal replacement ('a') nomenclature. Three types of locants are used to fully describe compounds derived from phane parent hydrides:

- (1) primary locants, i.e. arabic number locants that denote the atoms and superatoms of the phane parent skeleton;
- (2) composite locants, i.e. primary locants with a superscript arabic number locant denoting positions in amplificants (see P-26.4.3);
- (3) compound locants, which are primary or composite locants followed by another locant in parentheses, indicating that a double bond is not located between two consecutive locants.

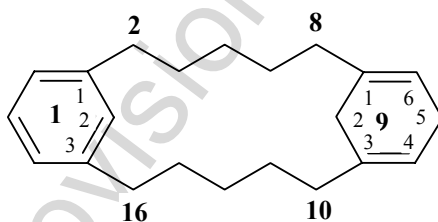
In phane nomenclature, double and triple bonds are denoted in two ways:

- (1) by the lowest locant of a double or triple bond when two consecutive locants are:
  - (a) primary locants; or
  - (b) composite locants, neither of which is adjacent to a primary locant;
- (2) by a compound locant, when one locant is a composite locant adjacent to a primary locant.

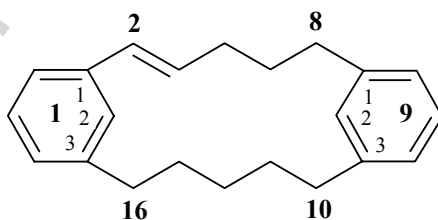
Examples:



1(1,3)-benzena-9(1,3)-cyclohexanacyclohexadecaphane-9<sup>1</sup>(9<sup>6</sup>),9<sup>4</sup>-diene (PIN)



1(1,3)-benzena-9(1,3)-cyclohexanacyclohexadecaphane-9<sup>1</sup>(9<sup>6</sup>),9<sup>3</sup>(9<sup>4</sup>)-diene (PIN)

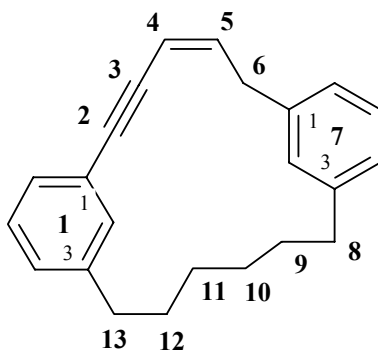


1,9(1,3)-dibenzenacyclohexadecaphan-2-ene (PIN)

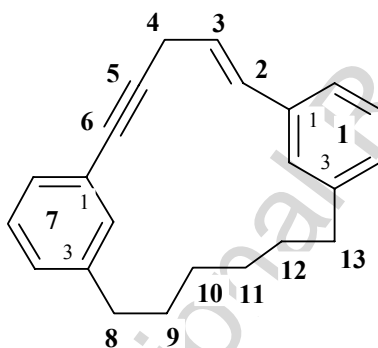
**P-31.1.6.2** Phane structures with both double and triple bonds

Double and triple bonds in a phane structure are described by the method of P-31.1.4.4. Low locants are allocated to double and triple bonds first when considered together as a set in ascending order and, if a choice is still needed, to double bonds.

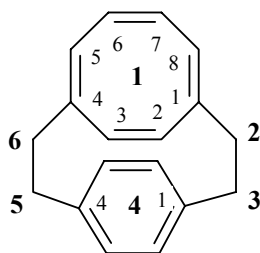
Examples:



1,7(1,3)-dibenzenacyclotridecaphan-4-en-2-yne (PIN)



1,7(1,3)-dibenzenacyclotridecaphan-2-en-5-yne (PIN)



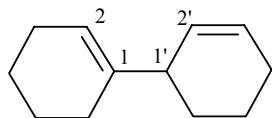
1(1,4)-cyclooctana-4(1,4)-benzenacyclohexaphane-1<sup>1</sup>(1<sup>8</sup>),2,4,6-tetraene (PIN)

**P-31.1.7** Ring assemblies of unsaturated components. Names identified by (1) and (2) are formed according to the two methods given in P-28.2.1. The numbering method is indicated by the letters (a) or (b) according to the two methods given in P-28.3.1.

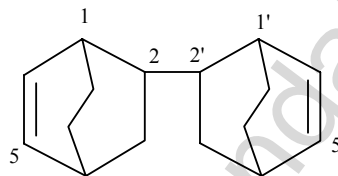


**P-31.1.7.1** Ring assemblies composed of saturated components, monocyclic or alicyclic, are modified by 'ene' endings ('yne' endings, and any combination of 'ene' and 'yne' endings are also used when appropriate, in accordance with the general rule P-31.1.1). Low locants are assigned, in order, to ring junctions, heteroatoms and multiple bonds.

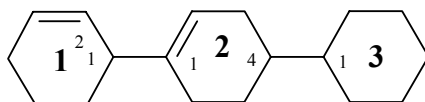
Examples:



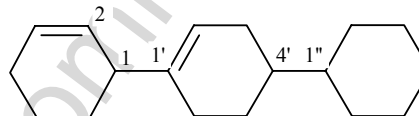
[1,1'-bicyclohexane]-1,2'-diene (PIN)



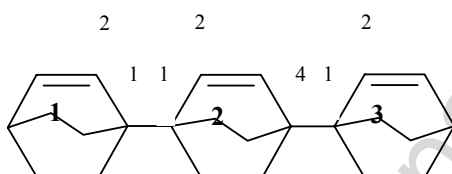
[2,2'-bibicyclo[2.2.2]octane]-5,5'-diene (PIN)



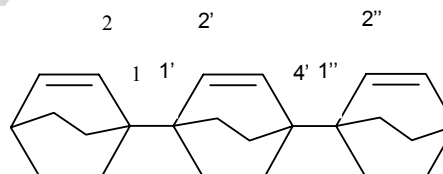
(1a) [1<sup>1</sup>,2<sup>1</sup>:2<sup>4</sup>,3<sup>1</sup>-tercyclohexane]-1<sup>2</sup>,2<sup>1</sup>-diene (PIN)  
(see P-28.2.1; P-28.3.1)



(1b) [1,1':4',1''-tercyclohexane]-1',2-diene  
(see P-28.2.1; P-28.3.1)



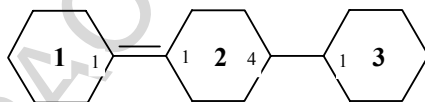
(1a) [1<sup>1</sup>,2<sup>1</sup>:2<sup>4</sup>,3<sup>1</sup>-terbicyclo[2.2.2]octane]-1<sup>2</sup>,2<sup>2</sup>,3<sup>2</sup>-triene (PIN) (see P-28.2.1; P-28.3.1)



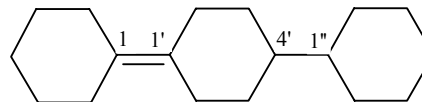
(1b) [1,1':4',1''-terbicyclo[2.2.2]octane]-2,2',2''-triene (see P-28.2.1; P-28.3.1)

**P-31.1.7.2** Double bonds linking two rings or ring systems are named in the same way in assemblies composed of three or more identical saturated components. Locants for the terminal position of such bonds are enclosed in parentheses (compound locants).

Examples:



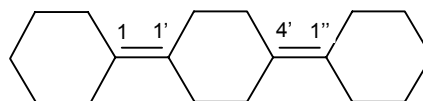
(1a) [1<sup>1</sup>,2<sup>1</sup>:2<sup>4</sup>,3<sup>1</sup>-tercyclohexan]-1<sup>1</sup>(2<sup>1</sup>)-ene (PIN)  
(see P-28.2.1; P-28.3.1)



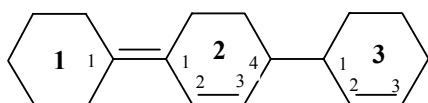
(1b) [1,1':4',1''-tercyclohexan]-1(1')-ene  
(see P-28.2.1; P-28.3.1)



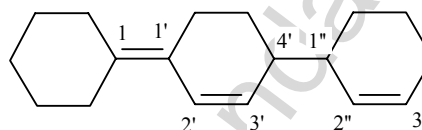
(1a) [1<sup>1</sup>,2<sup>1</sup>:2<sup>4</sup>,3<sup>1</sup>-tercyclohexane]-1<sup>1</sup>(2<sup>1</sup>),2<sup>4</sup>(3<sup>1</sup>)-  
-diene (PIN)  
(see also P-28.2.1; P-28.3.1)



(1b) [1,1':4',1''-tercyclohexane]-  
1(1'),4'(1'')-diene (see also  
P-28.2.1; P-28.3.1)



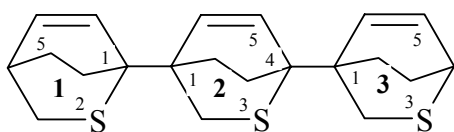
(1a) [1<sup>1</sup>,2<sup>1</sup>:2<sup>4</sup>,3<sup>1</sup>-tercyclohexane]-1<sup>1</sup>(2<sup>1</sup>),2<sup>2</sup>,3<sup>2</sup>-  
-triene (PIN)  
(see also P-28.2.1; P-28.3.1)



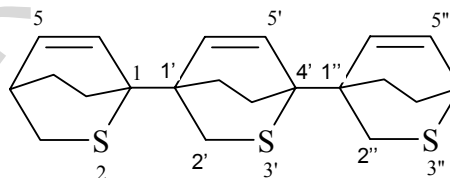
(1b) [1,1':4',1''-tercyclohexane]-  
1(1'),2',2''-triene (see also  
P-28.2.1; P-28.3.1)

**P-31.1.6.3** When heterocyclic ring assemblies consisting of monocyclic or bi- or polycyclic alicyclic components are named by skeletal replacement ('a') nomenclature, low locants are assigned, in order, to ring junctions, heteroatoms and then unsaturation sites.

Example:



(1a) 1<sup>2</sup>,2<sup>3</sup>,3<sup>3</sup>-trithia[1<sup>1</sup>,2<sup>1</sup>:2<sup>4</sup>,3<sup>1</sup>-terbicyclo-  
[2.2.2]octane]-1<sup>5</sup>,2<sup>5</sup>,3<sup>5</sup>-triene (PIN)  
(see also P-28.2.1; P-28.3.1)



(1b) 2,3',3''-trithia-[1,1':4',1''-terbicyclo-  
[2.2.2]octane]-5,5',5''-triene  
(see P-28.2.1; P-28.3.1)

## P-31.2 'Hydro/dehydro' prefixes

**P-31.2.1** The prefixes 'hydro/dehydro' are used to indicate addition and subtraction, respectively, of hydrogen atoms to or from mancude compounds.

It is recommended that 'hydro/dehydro' prefixes be considered as detachable prefixes but not included in those prefixes that are cited in alphanumerical order. In names, they are cited immediately at the front of the name of the parent hydride, after alphabetized prefixes and before nondetachable prefixes.

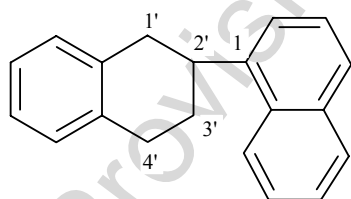
The starting point and direction of numbering of a compound are chosen so as to give lowest locants to the following structural features (if present) considered successively in the order listed until a decision can be made.

- (a) fixed numbering of a polycyclic ring system, as in naphthalene, quinoline, etc.
- (b) heteroatoms in heterocycles; and heteroatoms in chains modified by skeletal replacement ('a') nomenclature
- (c) indicated hydrogen [for unsubstituted compounds; a higher locant may be needed at another position to provide for a substituent suffix in accordance with structural feature (d)].
- (d) principal group named as suffix and cumulative suffixes denoting free valences and radical or ionic sites
- (e) added hydrogen (consistent with the structure of the compound and in accordance with further substitution)
- (f) unsaturation-saturation ('ene/yne' endings, and 'hydro/dehydro' prefixes)
- (g) substituents named as prefixes (low locants are allocated for substituents regardless of kind; then, if necessary, in the order of citation in the name).

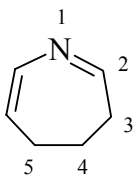
#### P-31.2.2 General methodology

'Hydro' and 'dehydro' prefixes are associated with the hydrogenation and the dehydrogenation, respectively, of a double bond; thus, multiplying prefixes of even values, as 'di', 'tetra', etc. are used to indicate the saturation of double bond(s), for example 'dihydro', 'tetrahydro', or creation of double bonds, as 'didehydro', etc.. In names, they are placed immediately in front of the name of the parent hydride and any nondetachable prefixes. Indicated hydrogen atoms have priority over 'hydro' prefixes for low locants. If indicated hydrogen atoms are present in a name, the 'hydro' prefixes precede them.

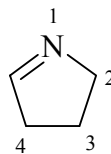
Examples:



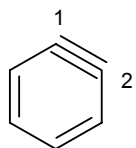
1',2',3',4'-tetrahydro-1,2'-binaphthalene (PIN)



4,5-dihydro-3*H*-azepine (PIN)



3,4-dihydro-2*H*-pyrrole (PIN)



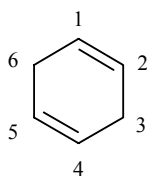
1,2-didehydrobenzene (PIN, see P-31.4.1)  
cyclohexa-1,3-dien-5-yne  
(not benzyne)

### P-31.2.3 The prefix 'hydro'

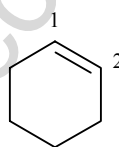
#### P-31.2.3 Saturation of double bonds in monocyclic mancade compounds

**P-31.2.3.1** 'Hydro' prefixes are used to modify the degree of hydrogenation of monocyclic mancade compounds having retained or systematic names, except for benzene, for which the traditional names 'cyclohexene' and 'cyclohexadiene' are recommended.

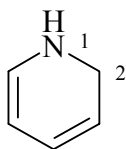
Examples:



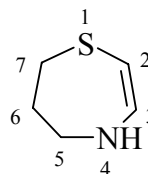
cyclohexa-1,4-diene (PIN)  
(not 1,4-dihydrobenzene)



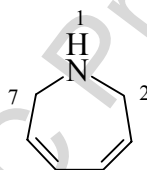
cyclohexene (PIN)  
(not 1,2,3,4-tetrahydrobenzene)



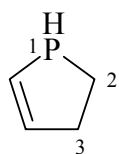
1,2-dihydropyridine (PIN)



4,5,6,7-tetrahydro-1,4-thiazepine (PIN)



2,7-dihydro-1*H*-azepine (PIN)



2,3-dihydro-1*H*-phosphole (PIN)

#### P-31.2.3.2 Retained names for fully hydrogenated monocyclic parent hydrides

Names listed in Table 2.3 (P-22.2.1) are retained names used as preferred IUPAC names and in general nomenclature. They are treated as parent hydrides in all respects, except for the use of suffixes such as '-ene' or '-yne'.

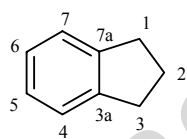
**P-31.2.3.3 Saturation of double bonds in polycyclic mancude compounds**

- P-31.2.3.3.1 Retained names of partially saturated mancude compounds
- P-31.2.3.3.2 Polycyclic mancude compounds
- P-31.2.3.3.3 Spiro compounds
- P-31.2.3.3.4 Phane compounds
- P-31.2.3.3.5 Ring assemblies

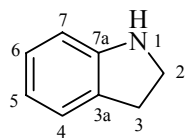
**P-31.2.3.3.1 Retained names of partially saturated mancude compounds**

Names listed in Table 3.1 are retained names that are not used as preferred IUPAC names. They are, however acceptable in general nomenclature with full substitution, including characteristic groups expressed as suffixes, but not as fusion components nor as amplificants in Phane Nomenclature.

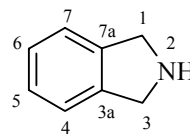
**Table 3.1 Retained names of partially saturated polycyclic parent hydrides**



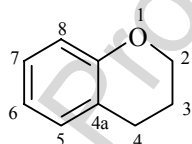
indane  
(formerly indan)  
2,3-dihydro-1*H*-indene (PIN)



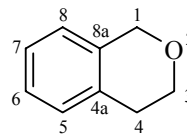
indoline  
2,3-dihydro-1*H*-indole (PIN)



isoindoline  
2,3-dihydro-1*H*-isoindole (PIN)



chromane  
3,4-dihydro-2*H*-1-benzopyran (PIN)  
thiochromane (S instead of O)  
3,4-dihydro-2*H*-1-benzothiopyran (PIN)  
selenochromane (Se instead of O)  
3,4-dihydro-2*H*-1-benzoselenopyran (PIN)  
tellurochromane (Te instead of O)  
3,4-dihydro-2*H*-1-benzotelluopyran (PIN)

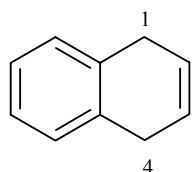


isochromane  
3,4-dihydro-1*H*-2-benzopyran (PIN)  
isothiochromane (S instead of O)  
3,4-dihydro-1*H*-2-benzothiopyran (PIN)  
isoselenochromane (Se instead of O)  
3,4-dihydro-1*H*-2-benzoselenopyran (PIN)  
isotellurochromane (Te instead of O)  
3,4-dihydro-1*H*-2-benzotelluopyran (PIN)

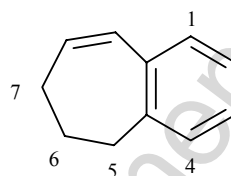
### P-31.2.3.3.2 Polycyclic mancude compounds

The degree of hydrogenation of individual mancude ring systems, carbocyclic or heterocyclic, is given by 'hydro' prefixes, in accordance with the general methodology described in P-31.2.2. Total hydrogenation is indicated by the appropriate multiplicative prefixes indicating the total number of hydrogen atoms attached, but locants are omitted [see P-14.3.3 (c)].

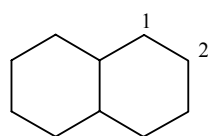
Examples:



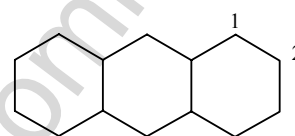
1,4-dihydronaphthalene (PIN)



6,7-dihydro-5*H*-benzo[7]annulene (PIN)



decahydronaphthalene (PIN)

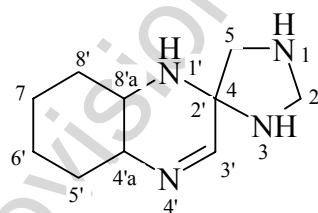


dodecahydroanthracene (PIN)

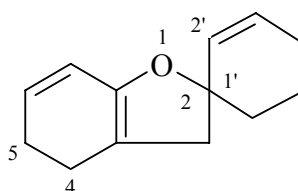
### P-31.2.3.3.3 Spiro compounds

Spiro compounds including mancude components are modified in accordance with the general methodology described in P-31.2.2.

Examples:



4'*a*,5',6',7',8',8'*a*-hexahydro-1'*H*-spiro[imidazolidine-4,2'-quinoxaline] (PIN)



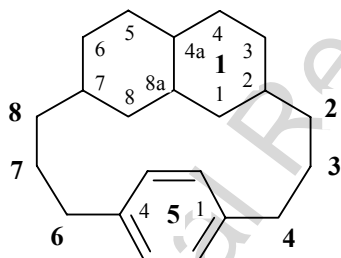
4,5-dihydro-3*H*-spiro[1-benzofuran-2,1'-cyclohexan]-2'-ene (PIN)

#### P-31.2.3.3.4 Phane compounds

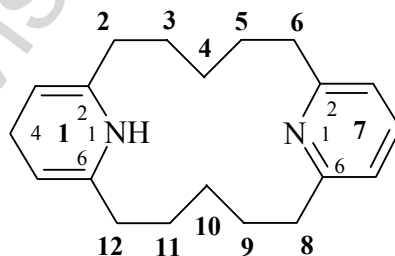
When the name of an amplificant implies the presence of a maximum number of noncumulated double bonds, other states of hydrogenation are indicated by use of the prefix 'hydro'. This method is applied as follows:

- (1) 'Hydro' prefixes are used to modify mancude heteromonocycles having retained names or named in accordance with the extended Hantzsch-Widman system. However, names for the fully saturated heteromonocycles that have retained names or Hantzsch-Widman names are preferred to those expressed by 'hydro' prefixes, for example, oxolane and piperidine are preferred to tetrahydrofuran and hexahydropyridine, respectively.
- (2) 'Hydro' prefixes are used to indicate all modifications of the degree of unsaturation of carbocyclic or heterocyclic mancude parent hydrides, except for benzene. Retained names of partially hydrogenated parent hydrides, such as indane and chromane (see P-31.2.3.3.1), are not recommended as amplificants in phane nomenclature.

Examples:



1<sup>1</sup>,1<sup>2</sup>,1<sup>3</sup>,1<sup>4</sup>,1<sup>4a</sup>,1<sup>5</sup>,1<sup>6</sup>,1<sup>7</sup>,1<sup>8</sup>,1<sup>8a</sup>-decahydro-1(2,7)-naphthalena-5(1,4)-benzenacyclooctaphane (PIN)



1<sup>1</sup>,1<sup>4</sup>-dihydro-1,7(2,6)-dipyridinacyclododecaphane (PIN)

#### P-31.2.3.5 Ring assemblies

The degree of hydrogenation of ring assemblies composed of mancude components is given by 'hydro' prefixes, in accordance with the general methodology described in P-31.2.2. Since assemblies are considered as parent hydrides, the degree of hydrogenation of the different components can be modified, to a certain extent, in a way that is not allowed for the individual component. This is the case of assemblies composed of monocyclic components, in which the

names are different for the mancude and the saturated component. Thus, assemblies composed of monocyclic components and those composed of ring systems are treated differently. In the examples that follow, names identified by (1) and (2) are formed according to the two methods given in P-28.2.1; the numbering method is indicated by the letter (a) or (b) according to the two methods given in P-28.3.1.

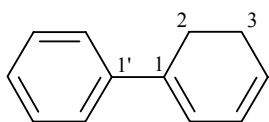
P-31.2.3.3.5.1 Ring assemblies composed of monocyclic components

P-31.2.3.3.5.2 Ring assemblies composed of ring systems

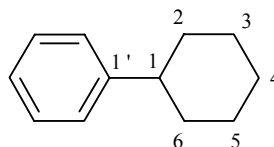
**P-31.2.3.3.5.1** Ring assemblies composed of monocyclic components

(a) Ring assemblies composed of monocyclic mancude or saturated hydrocarbons. Low locants are assigned to 'hydro' prefixes in accordance with the fixed numbering of each assembly. In biphenyl and polyphenyl assemblies, one benzene ring must remain in the assembly; otherwise, the starting point is the saturated assembly and the ending 'ene' is used to denote unsaturation (see P-31.1.6). Furthermore, when the modified ring assembly is composed of benzene rings and saturated rings, substitutive nomenclature is preferred (see Chapter 5).

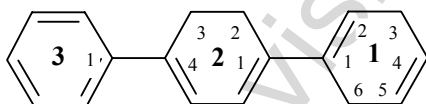
Examples:



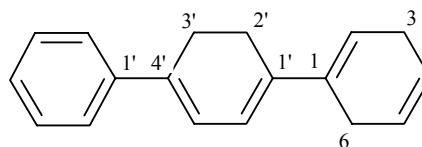
2,3-dihydro-1,1'-biphenyl (PIN)  
(numbering shown)  
1-(cyclohexa-1,3-dien-1-yl)benzene



cyclohexylbenzene (PIN)  
1,2,3,4,5,6-hexahydro-1,1'-biphenyl  
(numbering shown)



(2a) 1<sup>3</sup>,1<sup>6</sup>,2<sup>2</sup>,2<sup>3</sup>-tetrahydro-1<sup>1</sup>,2<sup>1</sup>:2<sup>4</sup>,3<sup>1</sup>-terphenyl  
(PIN; see also P-28.2.1 and P-28.3.1)

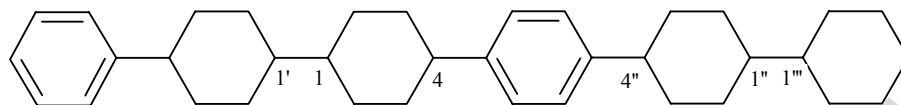


(2b) 2',3,3',6-tetrahydro-1,1':4',1''-terphenyl  
(see also P-28.2.1 and P-28.3.1)

[4-(cyclohexa-1,4-dien-1-yl)cyclohexa-1,3-dien-1-yl]benzene (substitutive name)



For the following example, the phane name is the preferred IUPAC name (see P-26.4.1.2)

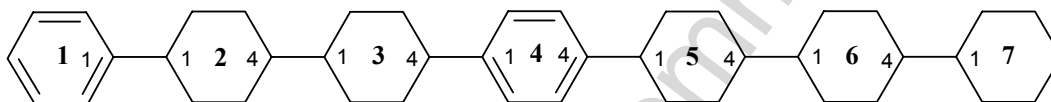


4'-phenyl-4,4''-(1,4-phenylene)di(1,1'-bicyclohexane)

(substitutive name: numbering shown)

(2a) 1<sup>1</sup>,1<sup>2</sup>,1<sup>3</sup>,1<sup>4</sup>,1<sup>5</sup>,1<sup>6</sup>,2<sup>1</sup>,2<sup>2</sup>,2<sup>3</sup>,2<sup>4</sup>,2<sup>5</sup>,2<sup>6</sup>,4<sup>1</sup>,4<sup>2</sup>,4<sup>3</sup>,4<sup>4</sup>,4<sup>5</sup>,4<sup>6</sup>,5<sup>1</sup>,5<sup>2</sup>,5<sup>3</sup>,5<sup>4</sup>,5<sup>5</sup>,5<sup>6</sup>-tetracosahydro-1<sup>1</sup>,2<sup>1</sup>,2<sup>4</sup>,3<sup>1</sup>,3<sup>4</sup>,4<sup>1</sup>,4<sup>4</sup>,5<sup>1</sup>,5<sup>4</sup>,6<sup>1</sup>-sexiphenyl (see also P-28.2.1 and P-28.3.1)

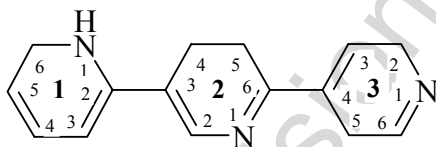
(2b) 1,1',1'',1''',2,2',2'',2''',3,3',3''',3''',4,4',4'',4''',5,5',5'',5''',6,6',6'',6'''-tetracosahydro-1,1':4',1'':4'',1''':4''',1''':4''',1''''-sexiphenyl (see also P-28.2.1 and P-28.3.1)



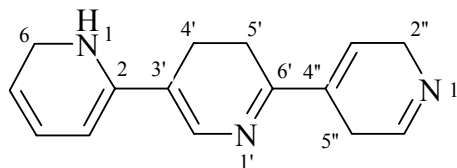
1(1),4(1,4)-dibenzena-2,3,5,6(1,4),7(1)-pentacyclohexanaheptaphane (PIN)

(b) Ring assemblies composed of heteromonocycles. Low locants are assigned to the junctions between rings, then to indicated hydrogen, if any, and finally to 'hydro' prefixes.

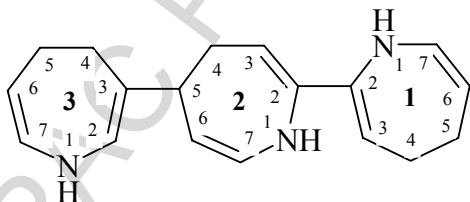
Examples:



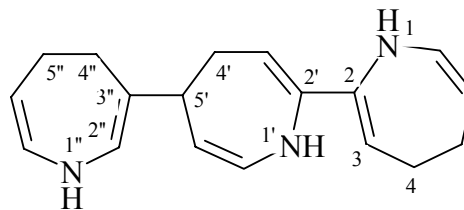
(1a) 1<sup>1</sup>,1<sup>6</sup>,2<sup>4</sup>,2<sup>5</sup>,3<sup>2</sup>,3<sup>5</sup>-hexahydro-1<sup>2</sup>,2<sup>3</sup>:2<sup>6</sup>,3<sup>4</sup>-terpyridine (PIN, see also P-28.2.1 and P-28.3.1)



(1b) 1,2'',4',5',5'',6-hexahydro-2,3':6',4''-terpyridine (see also P-28.2.1 and P-28.3.1)



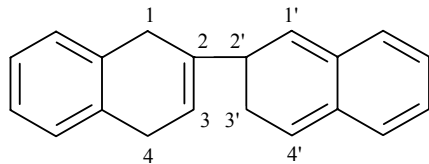
(1a) 1<sup>4</sup>,1<sup>5</sup>,2<sup>4</sup>,2<sup>5</sup>,3<sup>4</sup>,3<sup>5</sup>-hexahydro-1<sup>1</sup>H,2<sup>1</sup>H,3<sup>1</sup>H-1<sup>2</sup>,2<sup>2</sup>:2<sup>5</sup>,3<sup>3</sup>-terazepine (PIN, see also P-28.2.1 and P-28.3.1)



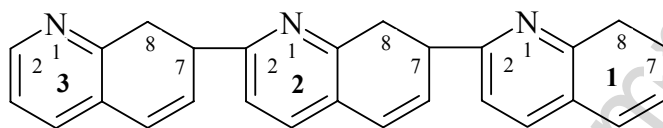
(1b) 4,4',4'',5,5',5''-hexahydro-1H,1'H,1''H-2,2':5':3''-terazepine (see also P-28.2.1 and P-28.3.1)

**P-31.2.3.3.5.2** Ring assemblies composed of polycyclic compounds Low locants are assigned to the junctions between components, then to indicated hydrogen atoms, if any, and finally to 'hydro' prefixes.

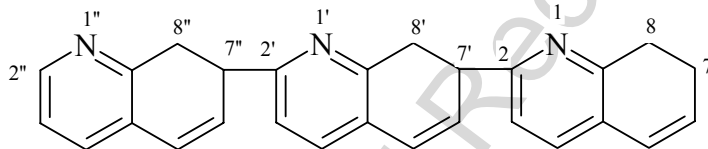
Examples:



1,2',3',4-tetrahydro-2,2'-binaphthalene (PIN)



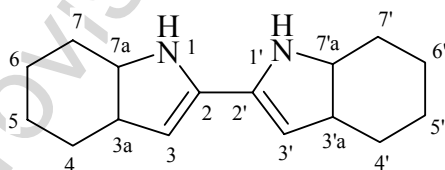
(1a)



(1b)

(1a) 1',1',2',2',3',3'-hexahydro-1,2':2',3'-terquinoline (PIN, see also P-28.2.1 and P-28.3.1)

(1b) 7,7',7'',8,8',8''-hexahydro-2,7':2',7''-terquinoline (see also P-28.2.1 and P-28.3.1)

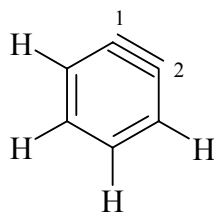


3a,3'a,4,4'a,5,5',6,6',7,7a,7',7'a-dodecahydro-1H,1'H-2,2'-biindole (PIN)

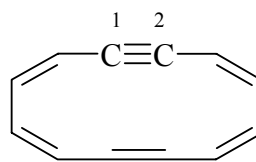
### P-31.3 The 'dehydro' prefix

**P-31.3.1** The subtractive prefix 'dehydro' is used to denote the removal of hydrogen atoms and the formation of multiple bonds. Its use is very limited in systematic nomenclature of organic compounds. Applied to benzene, it leads to the name '1,2-didehydrobenzene', that must be used in place of 'benzyne' that was formerly used. Applied to annulenes, it leads to didehydro[*n*]annulenes not used in preferred IUPAC names, but acceptable for use in general nomenclature.

Examples:



1,2-didehydrobenzene (PIN)  
cyclohexa-1,3-dien-5-yne  
(formerly called 'benzyne')

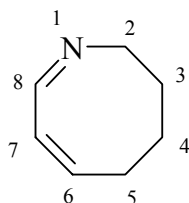


1,2-didehydro[12]annulene  
cyclododeca-1,3,5,7,9-pentaen-11-yne (PIN)

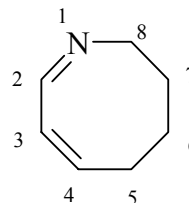
**P-31.3.2** The 'dehydro' prefix is more widely used in natural product nomenclature in order to preserve semisystematic names of stereoparents (see P-101.6.6). It is also used in the nomenclature of carbohydrates (ref. 22).

**P-31.3.3** The use of the 'dehydro' prefix is not recommended to denote double bond unsaturation in heterocyclic rings having Hantzsch-Widman names. Names must be formed by using the 'hydro' prefix, as shown in the following examples.

Example:



2,3,4,5-tetrahydroazocine (PIN) not



1,2,3,4-tetrahydroazocane

## P-32 Substituent prefixes for substituents derived from parent hydrides with a modified degree of hydrogenation

P-32.0 Introduction

P-32.1 Substituent groups denoted by 'ene' or 'yne' endings

P-32.2 Substituent groups denoted by the prefix 'hydro'

P-32.3 Retained names

### P-32.0 Introduction

Names of substituents derived from the names of the corresponding unsaturated compounds described in Section P-31 are formed by using the appropriate suffixes 'yl', 'ylidene' or 'ylidyne', as described for the formation of substituent prefixes in Section P-29. These names of substituents may contain the endings 'ene' or 'yne', or the prefixes 'hydro' or 'dehydro' in the case of mancude compounds.

**P-32.1** Substituent groups derived from parent hydrides with 'ene' or 'yne' endings

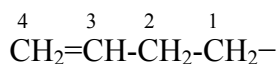
**P-32.1.1** Substituents derived from unsaturated acyclic compounds are named in two ways.

- (1) As suffixes have priority for low locants, the position(s) of multiple bonds must be selected in accord with low locants assigned to free valences. These free valences can be in any position of modified parent structure(s). Accordingly, for acyclic parent structures, all locants for the free valences, including '1', must be cited. All locants must be cited for acyclic and cyclic parent structures.
- (2) Names can also be formed by substituting simple substituents into larger ones, in a manner similar to saturated prefixes described in Section 29.

A major change is now recommended to this traditional method. The longest chain must be chosen as the principal chain, not the most unsaturated one. The following examples illustrate this methodology (for preferred IUPAC names see also Chapter 5).

Method (1) leads to preferred IUPAC names

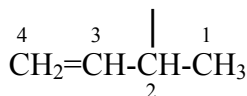
Examples:



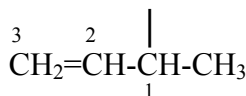
(1) but-3-en-1-yl (PIN)



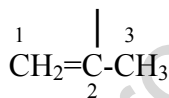
(1) prop-2-en-1-yl (PIN)



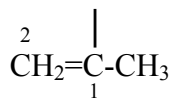
(1) but-3-en-2-yl (PIN)



(2) 1-methylprop-2-en-1-yl

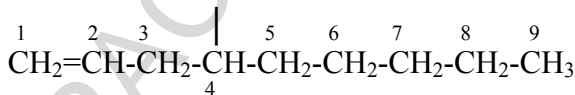


(1) prop-1-en-2-yl (PIN)

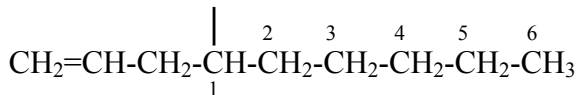


(2) 1-methyleth-1-en-1-yl

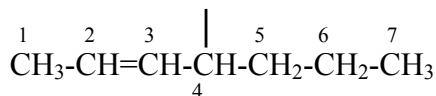
isopropenyl (retained name, but not substitutable, see P-32.3)



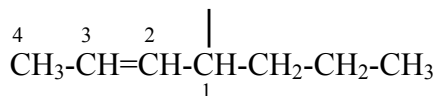
(1) non-1-en-4-yl (PIN)



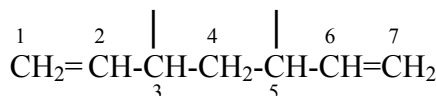
(2) 1-(prop-2-en-1-yl)hexyl  
(not 1-pentylbut-3-en-1-yl)



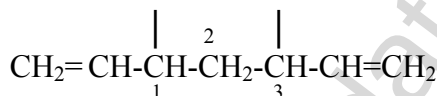
(1) hept-2-en-4-yl (PIN)



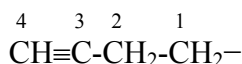
(2) 1-propylbut-2-en-1-yl



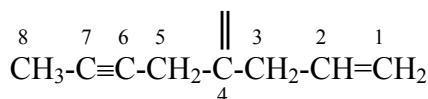
(1) hepta-1,6-diene-3,5-diyl (PIN)



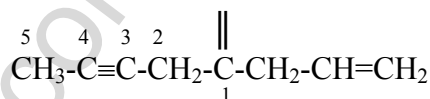
(2) 1,3-diethenylpropane-1,3-diyl



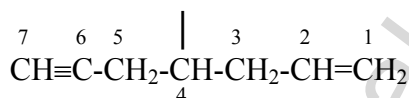
(1) but-3-yn-1-yl (PIN)



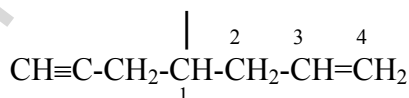
(1) oct-1-en-6-yn-4-ylidene (PIN)



(2) 1-(prop-2-en-1-yl)pent-3-yn-1-ylidene

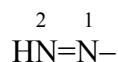


(1) hept-1-en-6-yn-4-yl (PIN)

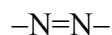


(2) 1-(prop-2-yn-1-yl)but-3-en-1-yl

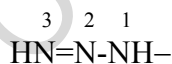
[In (1) lowest locants are assigned to the double bond;  
in (2) the principal chain includes the double bond]



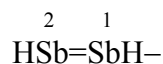
(1) diazenyl  
(preselected name, see P-12.2)



(1) diazenediyl  
(preselected name, see P-12.2)



(1) triaz-2-en-1-yl  
(preselected name, see P-12.2)

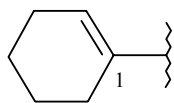


(1) distibenyl  
(preselected name, see P-12.2)

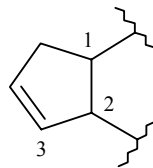
**P-32.1.2** Monocyclic substituent groups

Method (1) described in P-32.1.1 is used to name monocyclic substituent groups.

Examples:



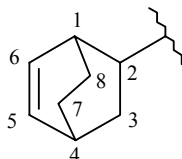
cyclohex-1-en-1-yl (PIN)



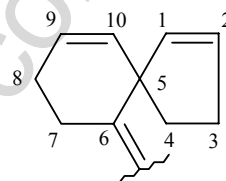
cyclopent-3-ene-1,2-diyl (PIN)

**P-32.1.3** Substituent groups derived from parent hydrides having a fixed numbering. Lowest possible locants are assigned first to free valence(s), then to unsaturated sites, in accordance with the fixed numbering of the parent hydride.

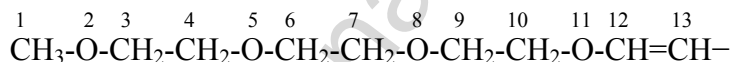
Examples:



bicyclo[2.2.2]oct-5-en-2-yl (PIN)



spiro[4.5]deca-1,9-dien-6-ylidene (PIN)



2,5,8,11-tetraoxatridec-12-en-13-yl (PIN)

(not 3,6,9,12-tetraoxatridec-1-en-1-yl; the suffix '-yl' is added to the parent hydride name 2,5,8,11-tetraoxatridecane)

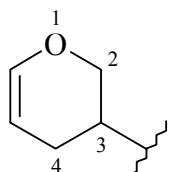
**P-32.2** Substituent groups derived from partially hydrogenated mancude parent hydrides

Names of substituent groups are formed in accord with the following order of seniority (see P-14.4) for assigning lowest possible locants. Indicated and added hydrogen atoms must be cited in names.

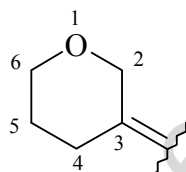
- fixed numbering (naphthalene, bicyclo[2.2.2]octane, etc.)
- heteroatoms in heterocycles
- indicated hydrogen [for unsubstituted compounds; a higher locant may be needed at another position to provide for a substituent suffix in accordance with the structural feature (d)]
- free valence suffix

- (e) added hydrogen (consistent with the structure of the compound and in accordance with further substitution)
- (f) saturation ('hydro'/'dehydro' prefixes) or unsaturation ('ene', 'yne' endings)
- (g) substituents named as prefixes (low locants are allocated for substituents regardless of kind; then, if necessary, in the order of citation).

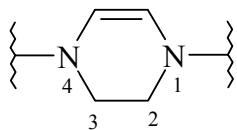
Examples:



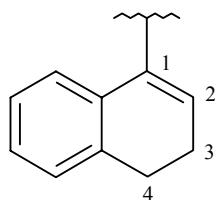
3,4-dihydro-2*H*-pyran-3-yl (PIN)



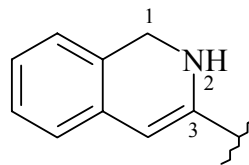
5,6-dihydro-2*H*-pyran-3(4*H*)-ylidene (PIN)



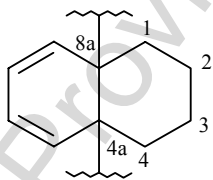
2,3-dihydropyrazine-1,4-diyl (PIN)



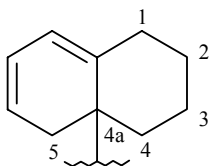
3,4-dihydronaphthalen-1-yl (PIN)



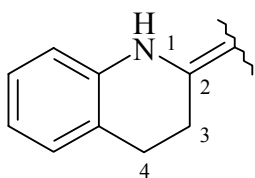
1,2-dihydroisoquinolin-3-yl (PIN)



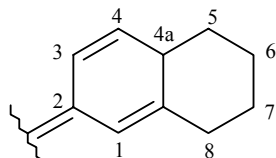
1,2,3,4-tetrahydronaphthalene-4a,8a-diyl (PIN)



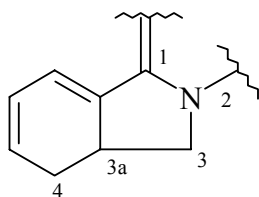
1,3,4,5-tetrahydronaphthalen-4a(2*H*)-yl (PIN)



3,4-dihydroquinolin-2(1*H*)-ylidene (PIN)



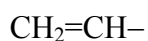
5,6,7,8-tetrahydronaphthalen-2(4a*H*)-ylidene (PIN)



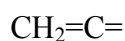
3a,4-dihydro-1*H*-isoindol-2(3*H*)-yl-1-ylidene (PIN)

### P-32.3 Retained names for prefixes derived from unsaturated acyclic parent hydrides

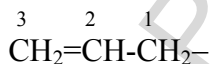
The following names are retained but are not used as preferred IUPAC names, which are formed systematically; these names are acceptable for general use, with substitution as defined in P-29.6.



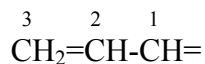
vinyl  
ethenyl (PIN)



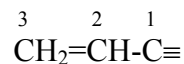
vinylidene  
ethenylidene (PIN)



allyl  
prop-2-en-1-yl (PIN)



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



allylidyne  
prop-2-en-1-ylidyne (PIN)

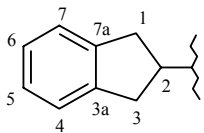
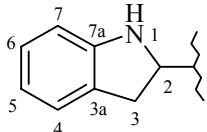
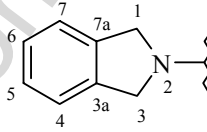
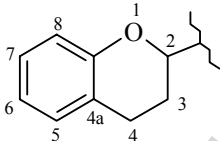
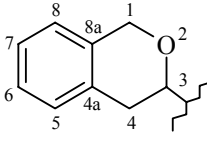
The retained name isopropenyl, for  $\text{CH}_2=\text{C}(\text{CH}_3)-$ , is not used as a preferred IUPAC name. It is acceptable for general use, but no substitution is allowed. The preferred IUPAC name is prop-1-en-2-yl.



**P-32.4 Retained names for prefixes derived from partially saturated mancude parent hydrides.**

The names in Table 3.2 are retained but are not used as preferred IUPAC names, which are formed systematically; these names are acceptable for general use, with full substitution.

**Table 3.2 Retained names of prefixes for partially saturated polycyclic parent hydrides**

 <p>indan-2-yl (also 1-, 4-, and 5- isomers) 2,3-dihydro-1<i>H</i>-inden-2-yl (PIN) (also, 1-, 4-, and 5- isomers)</p>	
 <p>indolin-2-yl (also 1-, 3-, 4-, 5-, 6-, and 7- isomers) 2,3-dihydro-1<i>H</i>-indol-2-yl (PIN) (also, 1-, 3-, 4-, 5-, 6-, and 7- isomers)</p>	 <p>isoindolin-2-yl (also 1-, 4-, and 5- isomers) 2,3-dihydro-1<i>H</i>-isoindol-2-yl (PIN) (also, 1-, 4-, and 5- isomers)</p>
 <p>chroman-2-yl (also 3-, 4-, 5-, 6-, 7-, and 8- isomers) 3,4-dihydro-2<i>H</i>-1-benzopyran-2-yl (PIN) (also 3-, 4-, 5-, 6-, 7-, and 8- isomers)  thiochroman-2-yl (S instead of O) (also 3-, 4-, 5-, 6-, 7-, and 8- isomers) 3,4-dihydro-2<i>H</i>-1-benzothiopyran-2-yl (PIN) (also 3-, 4-, 5-, 6-, 7-, and 8- isomers)  selenochroman-2-yl (Se instead of O) (also 3-, 4-, 5-, 6-, 7-, and 8- isomers) 3,4-dihydro-2<i>H</i>-1-benzoselenopyran-2-yl (PIN) (also 3-, 4-, 5-, 6-, 7-, and 8- isomers)  tellurochroman-2-yl (Te instead of O) (also 3-, 4-, 5-, 6-, 7-, and 8- isomers) 3,4-dihydro-2<i>H</i>-1-benzotelluropyran (PIN) (also 3-, 4-, 5-, 6-, 7-, and 8- isomers)</p>	 <p>isochroman-3-yl (also 1-, 4-, 5-, 6-, 7-, and 8- isomers) 3,4-dihydro-1<i>H</i>-2-benzopyran-3-yl (PIN) (also 1-, 4-, 5-, 6-, 7-, and 8- isomers)  isothiochroman-3-yl (S instead of O) (also 1-, 4-, 5-, 6-, 7-, and 8- isomers) 3,4-dihydro-1<i>H</i>-2-benzothiopyran-3-yl (PIN) (also 1-, 4-, 5-, 6-, 7-, and 8- isomers)  isoselenochroman-3-yl (Se instead of O) (also 1-, 4-, 5-, 6-, 7-, and 8- isomers) 3,4-dihydro-1<i>H</i>-2-benzoselenopyran-3-yl (PIN) (also 1-, 4-, 5-, 6-, 7-, and 8- isomers)  tellurochroman-2-yl (Te instead of O) (also 1-, 4-, 5-, 6-, 7-, and 8- isomers) 3,4-dihydro-1<i>H</i>-2-benzotelluropyran (PIN) (also 1-, 4-, 5-, 6-, 7-, and 8- isomers)</p>

### P-33 Suffixes

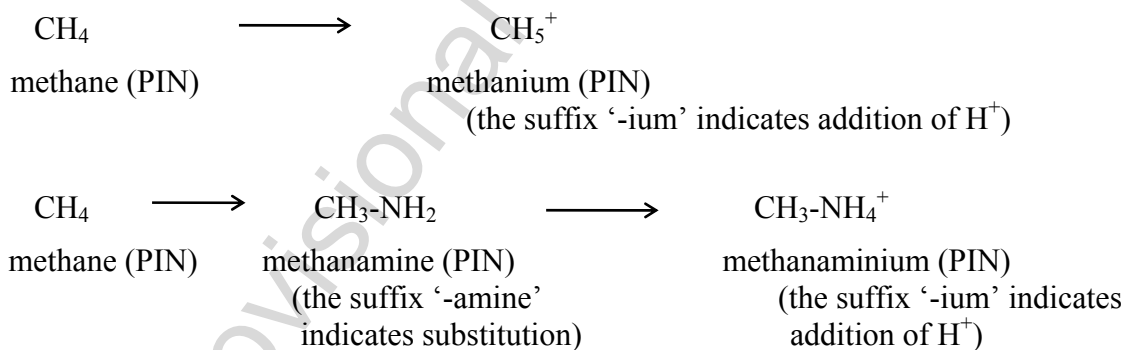
- P-33.0 Introduction
- P-33.1 Functional suffixes
- P-33.2 Cumulative suffixes

#### P-33.0 Introduction

This Section includes names of substituents denoting characteristic groups expressed as suffixes. These characteristic groups are essentially those having free valence(s) on atoms such as the chalcogens (O, S, Se, Te) and nitrogen. The concept is extended to carbon atoms linked to halogens, chalcogens and nitrogen, such as  $-\text{CO}-\text{Cl}$ ,  $-\text{CO}-\text{OH}$ ,  $-\text{CS}-\text{SH}$ ,  $-\text{CHO}$ ,  $-\text{CN}$ . Radicals and ions are expressed by suffixes in substitutive nomenclature although they are not classified as characteristic groups.

Suffixes describing characteristic groups are divided into 'functional suffixes' and 'cumulative suffixes'. Functional suffixes are used to denote characteristic groups; they are exclusive because only one of them can be placed at the end of a name to represent the principal characteristic group or function. Suffixes designating radicals and ions, on the other hand, can be used in association with each other and also in association with functional suffixes. In names, functional suffixes are always attached to the name of the parent hydride. Cumulative suffixes can be attached directly to the names of parent hydrides; but when functional suffixes are present, cumulative suffixes are attached to them.

Examples:



#### P-33.1 Functional suffixes

Functional suffixes are classified as 'basic suffixes' and 'derived suffixes'.

##### P-33.1.1 Basic suffixes

Basic suffixes are those composed only of oxygen and/or nitrogen, with or without association with carbon, as in the case of carboxylic acids, amides, nitriles and aldehydes, and also with sulfur to denote sulfonic acids and sulfinic acids, and the corresponding amides and hydrazides. They are listed in Table 3.3

The suffix 'peroxol', for  $-OOH$ , has been added to the list of basic suffixes. It is modified by functional replacement generating the suffixes ' $-OS$ -thioperoxol' for  $-OSH$ , and ' $-SO$ -thioperoxol' for  $-SOH$ . The suffix 'sulfenic acid', for  $-SOH$ , was abandoned in the 1993 Recommendations.

**Table 3.3 Basic suffixes, in decreasing order of seniority for citation as the principal characteristic group**

Formula	Basic suffix	Formula	Basic suffix
(1) $-CO-OH$	carboxylic acid (PIN)	(9) $-CN$	carbonitrile (PIN)
(2) $-(C)O-OH$	oic acid (PIN)	(10) $-(C)N$	nitrile (PIN)
(3) $-SO_2-OH$	sulfonic acid (PIN)	(11) $-CHO$	carbaldehyde (PIN)
(4) $-SO-OH$	sulfinic acid (PIN)	(12) $-(C)HO$	al (PIN)
(5) $-CO-NH_2$	carboxamide (PIN)	(13) $=O$	one (PIN)
(6) $-(C)O-NH_2$	amide (PIN)	(14) $-OH$	ol (PIN)
(7) $-CO-NNH_2$	carbohydrazide (PIN)	(15) $-OOH$	peroxol (PIN)
(8) $-(C)O-NNH_2$	hydrazide (PIN)	(16) $-NH_2$	amine (PIN)
		(17) $=NH$	imine (PIN)

### P-33.1.2 Derived suffixes

Derived suffixes are formed in various ways by modifying basic suffixes.

- (1) Suffixes including a carbon atom are modified by functional replacement by using infixes to indicate the replacement of oxygen atoms by  $-OO-$ ,  $-S-$ ,  $=S$ ,  $-Se-$ ,  $=Se$ ,  $-Te-$ ,  $=Te$ ,  $=NH$  and  $=NNH_2$ , as indicated in P-15.5; it is to be noted that the letter 'x' of 'carboxylic' is maintained before a vowel and that the letter 'o' is not elided before amide and aldehyde.

Examples:

$-CO-OH$	carboxylic acid (PIN)	$-C(O)-OOH$	carboperoxoic acid (PIN)
		$-C(O)-SH$	carbothioic <i>S</i> -acid (PIN)
		$-C(Se)-OH$	carbosenoic <i>O</i> -acid (PIN)
		$-C(=NH)-OH$	carboximidic acid (PIN)
		$-C(=NNH_2)-OH$	carbohydrazonic acid (PIN)
		$-C(=NH)-SH$	carboximidithioic acid (PIN)
$-CO-NH_2$	carboxamide (PIN)	$-C(Te)-NH_2$	carbotelluroamide (PIN)
$-CO-NHNNH_2$	carbohydrazide (PIN)	$-C(S)-NHNH_2$	carbothiohydrazide (PIN)
$-CHO$	carbaldehyde (PIN)	$-CHS$	carbothioaldehyde (PIN)

- (2) Suffixes not including a carbon atom are modified by functional replacement, by using prefixes to indicate the replacement of oxygen atoms by  $-\text{OO}-$ ,  $-\text{S}-$ ,  $=\text{S}$ ,  $-\text{Se}-$ ,  $=\text{Se}$ ,  $-\text{Te}-$ ,  $=\text{Te}$ ,  $=\text{NH}$  and  $=\text{NNH}_2$ , as indicated in P-15.5; it is to be noted that the letter 'o' is not elided before amide and that an additional 'o' is elided from 'imido' before 'oic' for euphonic reasons.

Examples:

$-(\text{C})\text{O}-\text{OH}$	oic acid (PIN)	$-(\text{C})\text{O}-\text{OOH}$	peroxoic acid (PIN)
		$-(\text{C})\text{O}-\text{SH}$	thioic <i>S</i> -acid (PIN)
		$-(\text{C})\text{Te}-\text{OH}$	telluroic <i>O</i> -acid (PIN)
		$-(\text{C})(=\text{NH})-\text{OH}$	imidic acid (PIN) (not imidoic acid)
		$-(\text{C})(=\text{NNH}_2)-\text{OH}$	hydrazonic acid (PIN)
		$-(\text{C})(=\text{NH})-\text{SeH}$	imidoselenoic acid (PIN)
$-(\text{C})\text{O}-\text{NH}_2$	amide (PIN)	$-(\text{C})\text{S}-\text{NH}_2$	thioamide (PIN)
$-(\text{C})\text{O}-\text{NHNH}_2$	hydrazide (PIN)	$-(\text{C})\text{S}-\text{NHNH}_2$	thiohydrazide (PIN)
$-(\text{C})\text{HO}$	al (PIN)	$-(\text{C})\text{HSe}$	selenal (PIN)
$=\text{O}$	one (PIN)	$=\text{S}$	thione (PIN)
		$=\text{Se}$	selone (PIN) (not selenone)
		$=\text{Te}$	tellone (PIN) (not tellurone)
$-\text{OH}$	ol (PIN)	$-\text{SH}$	thiol (PIN)
$-\text{OOH}$	peroxol (PIN)	$-\text{OSH}$	<i>OS</i> -thioperoxol (PIN)

- (3) The stem 'sulf' is replaced by 'selen' and 'tellur' to generate the selenium and tellurium analogues of sulfonic and sulfinic acids.

Examples:

$-\text{SO}_2-\text{OH}$	sulfonic acid (PIN)	$-\text{SeO}_2-\text{OH}$	selenonic acid (PIN)
$-\text{SO}-\text{OH}$	sulfinic acid (PIN)	$-\text{TeO}-\text{OH}$	tellurinic acid (PIN)

- (4) Suffixes of the type 'sulfonic acid' and analogues are modified by functional replacement by using infixes to indicate the replacement of oxygen atoms by  $-\text{OO}-$ ,  $-\text{S}-$ ,  $=\text{S}$ ,  $-\text{Se}-$ ,  $=\text{Se}$ ,  $-\text{Te}-$ ,  $=\text{Te}$ ,  $=\text{NH}$  and  $=\text{NNH}_2$ , as indicated in P-15.5.

Examples:

$-\text{SO}_2\text{-OH}$	sulfonic acid (PIN)	$-\text{SO}_2\text{-OOH}$	sulfonoperoxoic acid (PIN)
$-\text{SeO-OH}$	seleninic acid (PIN)	$-\text{S(=NNH)}_2\text{-OH}$	sulfonodihydrazonic acid (PIN)
$-\text{TeO}_2\text{-OH}$	telluronic acid (PIN)	$-\text{SeO-SH}$	seleninothioic <i>S</i> -acid (PIN)
$-\text{SO-OH}$	sulfinic acid (PIN)	$-\text{Te(=NH)-OH}$	telluronimidic acid (PIN)
		$-\text{SO(=NNH}_2\text{)-OH}$	sulfinohydrazonic acid (PIN)

- (5) Names of amides and hydrazides are formed by replacing the 'ic acid' ending in suffixes by 'amide' or 'hydrazide', respectively ; a euphonic letter 'o' is added as required:

Examples:

$-\text{C(=NH)-OH}$	imidic acid (PIN)
$-\text{C(=NH)-NH}_2$	imidamide (PIN)
$-\text{C(=NH)-OH}$	carboximidic acid (PIN)
$-\text{C(=NH)-NH}_2$	carboximidamide (PIN)
$-\text{C(=NNH}_2\text{)-OH}$	hydrazonic acid (PIN)
$-\text{C(=NNH}_2\text{)-NHNH}_2$	hydrazonohydrazide (PIN)
$-\text{SO}_2\text{-OH}$	sulfonic acid (PIN)
$-\text{SO}_2\text{-NH}_2$	sulfonamide (PIN)
$-\text{SeO-OH}$	seleninic acid (PIN)
$-\text{SeO-NHNH}_2$	seleninohydrazide (PIN)

- (6) Suffixes with  $-\text{NH}_2$  and  $=\text{NH}$  groups substituted by an  $-\text{OH}$  group are no longer named by using the 'carbohydroxamic acid' and 'carbohydroximic acid' suffixes. They are now named as *N*-hydroxy derivatives of amides or imides.

Examples:

$\text{CH}_3\text{-CH}_2\text{-CO-NH}_2$ propanamide (PIN)	$\text{CH}_3\text{-CH}_2\text{-CO-NH-OH}$ <i>N</i> -hydroxypropanamide (PIN) (formerly propanehydroxamic acid)
$\text{CH}_3\text{-CH}_2\text{-C(=NH)-OH}$ propanimidic acid (PIN)	$\text{CH}_3\text{-CH}_2\text{-C(=N-OH)-OH}$ <i>N</i> -hydroxypropanamidic acid (PIN) (formerly propanehydroximic acid)

### P-33.2 Cumulative suffixes

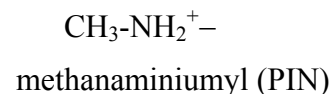
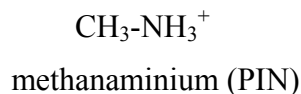
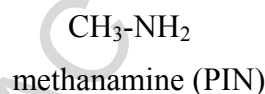
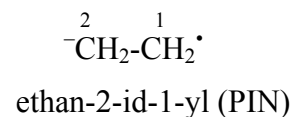
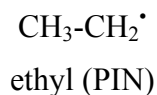
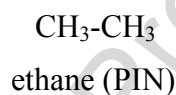
Suffixes used to denote radical and ionic centres in a parent structure are given in Table 3.4. They are classified in decreasing order of seniority, radicals > anions > cations.

Suffixes are added to the name of a parent hydride in the customary manner, or to suffixes expressing another type of radical or ion, or to suffixes denoting characteristic groups. Names of radicals are formed in the same manner as substituent groups (see P-29.2), with the exception that di- and trivalent radicals centered on a single atom are denoted by the suffixes 'ylidene' and 'ylidyne', respectively, and never by 'diyl' or 'triyl'.

**Table 3.4 Affixes for radical and ionic centers in parent structures**

	Operation	Suffix
Radicals	Loss of H <sup>•</sup>	yl
	Loss of 2 H <sup>•</sup> from one atom from different atoms	ylidene
		diyl
	Loss of 3H <sup>•</sup> from one atom from different atoms	ylidyne
		triyl or ylylidene
etc.		
Anions	Loss of H <sup>+</sup>	ide
		ate
	Addition of H <sup>-</sup>	uide
Cations	Loss of H <sup>-</sup>	ylum
	Addition of H <sup>+</sup>	ium

Examples:



## P-34 Functional parent structures

- P-34.0 Introduction
- P-34.1 Definitions
- P-34.2 Types of parent structures
- P-34.3 Parent structures and corresponding prefixes

### P-34.0 Introduction

Many trivial and semisystematic names have been used in organic chemistry. As systematic names have increasingly been preferred, the number of trivial and semisystematic names has been gradually reduced, in the 1979 Rules and again in the 1993 Recommendations. This Section describes the 2005 codification for parent compounds with an implied characteristic group or class.

### P-34.1 Definitions

A functional parent is a structure whose name implies the presence of one or more characteristic groups and that has one or more hydrogen atoms attached to at least one of its skeletal atoms or one of its characteristic groups, or in which at least one of its characteristic groups can form at least one kind of functional modification.

Examples:

- CH<sub>3</sub>-COOH acetic acid (PIN) (see P-34.4.1)
- C<sub>6</sub>H<sub>5</sub>-NH<sub>2</sub> aniline (PIN) (see P-34.5)
- HP(O)(OH)<sub>2</sub> phosphonic acid (preselected name, see P-12.2; see Section P-67 for oxo acids of Groups 13, 14, 15, 16 and 17)

A parent hydride bearing a characteristic group denoted by a suffix, for example cyclohexanol, is not considered to be a functional parent compound but may be described as a 'functionalized parent hydride'.

In these Recommendations, parent hydrides whose degree of hydrogenation has been modified are broadly classified as functional parents, for example acetylene and allene (see P-31.1.2.1 and P-32.3), and partially hydrogenated mancude ring systems, for example, indane and indoline (see P- P-31.2.3.3.1 and P-32.4)

**P-34.1.1** Functional parents with substitutable hydrogen atoms, i.e., the structure has one or more substitutable hydrogen atoms attached to at least one skeletal atom or one characteristic group

Examples of functional parents and substituent groups:

- CH<sub>3</sub>-COOH acetic acid (PIN)      Cl-CH<sub>2</sub>-COOH 2-chloroacetic acid (PIN)
- H<sub>2</sub>N-CO-NH<sub>2</sub> urea (PIN)              NH<sub>2</sub>-CO-NH-CH<sub>3</sub> methylurea (PIN)
- HP(O)(OH)<sub>2</sub> phosphonic acid (preselected name; see P-12.2)

$C_6H_5-P(O)(OH)_2$  phenylphosphonic acid (PIN)

**P-34.1.2** Functional parents having no substitutable hydrogen atoms, i.e., their structure has at least one characteristic group that can form at least one kind of functional modification, for example, formation of esters. These are given preselected names (see P-12).

Examples:

$P(O)(OH)_3$	phosphoric acid (preselected name, see P-12.2)	$P(O)(OCH_3)_3$	trimethyl phosphate (PIN)
$N(O)-OH$	nitrous acid (preselected name, see P-12.2)	$N(O)-O-[CH_2]_4-CH_3$	pentyl nitrite (PIN)

### **P-34.2** Types of retained names for functional parent structures

Parent structures are divided into types related to their substitutability, which may differ according to whether the name is required for a preferred IUPAC name or for general nomenclature (see P-46).

Substitutability of functional parent structures with retained names is classified into three types as follows:

**Type 1.** Unlimited substitution by substituent groups cited as suffixes or prefixes;

**Type 2.** Limited substitution classified as follows:

**Type 2a.** Substitution limited to substituent groups cited as prefixes in recognition of functional groups explicitly expressed or implied in the functional parent compound name;

**Type 2b.** Substitution limited to substituent groups cited as compulsory prefixes;

**Type 2c.** Substitution for parent structures not covered by Type 2a or 2b.

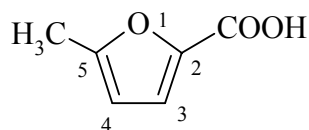
**Type 3.** Substitution of any kind not allowed.

Type 1 substitution is not common for functional parent compounds. It is used mainly for parent hydrides and their derived substituent prefixes (see P-29.6 and P-46)

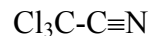
Examples of substituted functional parents:



Type 2a:

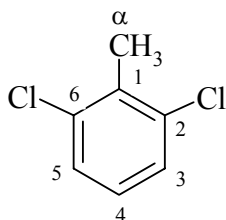


5-methyl-2-furoic acid  
5-methylfuran-2-carboxylic acid (PIN)



trichloroacetonitrile (PIN)

Type 2c



2,6-dichlorotoluene [no substitution by  
principal characteristic groups or  
additional acyclic hydrocarbon  
groups (see P-46.3)]

1,3-dichloro-2-methylbenzene (PIN)

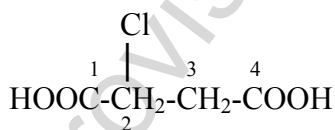


carbonobromidic acid (PIN)  
(not bromoformic acid; formic acid  
cannot be substituted by an atom or  
group used in functional replacement  
nomenclature)

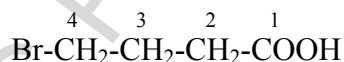


nitroformic acid (PIN, the nitro group is not  
a group used in functional replacement  
nomenclature)

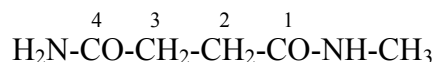
Type 3



2-chlorobutanedioic acid (PIN)  
(not 2-chlorosuccinic acid)



3-bromobutanoic acid (PIN)  
(not 3-bromobutyric acid)



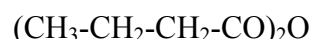
*N*-methylbutanediamide (PIN)  
(not *N*-methylsuccinamide; even  
*N*-substitution is not allowed)

Replacement of the hydrogen atom of a hydroxy group is considered a functionalization rather than a substitution, for instance, in the formation of an ester, and is allowed.

Example:



chloromethyl propanoate (PIN)  
chloromethyl propionate



butanoic anhydride (PIN)  
butyric anhydride

**P-34.3** Retained names for functional parent compounds having implied characteristic groups or classes

Names of functional parents are trivial names identified as ‘retained names’. Some are retained as preferred names and also for use in general nomenclature. Others are not used as preferred names but are acceptable for general use. The complete list of retained names is given in Section P-46. Retained names for unsaturated parent structures and partially saturated parent structures are given in P-31.1.2.1 and P-31.2.3.3.1, respectively. Functional parents are also discussed in Chapter 6 along with systematic names for each class of compounds. The list of names given here is to be considered limiting; however, use of trivial and semisystematic names for compounds covered by special rules, for example amino acids and carbohydrates, is allowed. The substitutability of each structure is indicated by the classification described in P-34.2 above.

For acid names, functionalization, i.e., the formation of esters, salts, and anhydrides, does not constitute substitution. Similarly, for hydroxy compound names, esters and salts do not constitute substitution. Amides, acyl halides and halogenoids, hydrazides, aldehydes, and nitriles derived from retained names for acids follow the same substitution rules as the corresponding acid.

P-34.3.1 Acids

P-34.3.2 Ketones and aldehydes

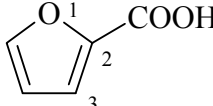
P-34.3.3 Hydroxy compounds and ethers

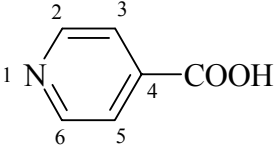
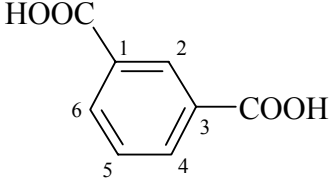
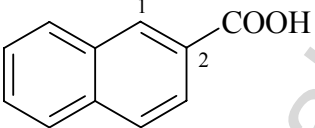
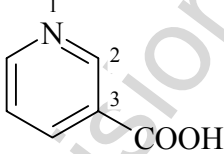
P-34.3.4 Amines, amides and other nitrogen compounds

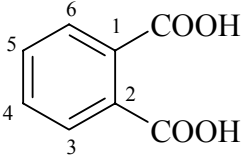
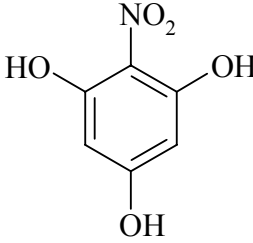
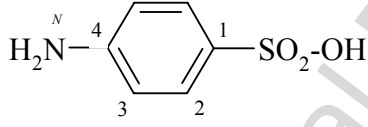
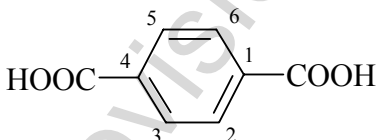
### P-34.3.1 Acids

The names of the following carboxylic acids and related classes (amic acids, amides, and acyl groups, etc.) are used, as indicated, as preferred names or in general nomenclature. They may be used to form the corresponding imidic acids (see P-65.1.1.3.1.1), hydrazonic acids (see P-65.1.1.3.2.1), amic acids (see P-65.1.1.6.1), aldehydic acids (see P-65.1.1.6.3), acyl groups (see P-65.2), salts and esters (see P-65.4), anhydrides (see P-65.5), amides (see P-66.1.1.11), imides (see P-66.2), hydrazides (see P-66.3.1), amidines (see P-66.4.1), amidrazones (see P-66.4.2), hydrazidines (see P-66.4.3), nitriles (see P-66.5), and aldehydes (see P-66.6).

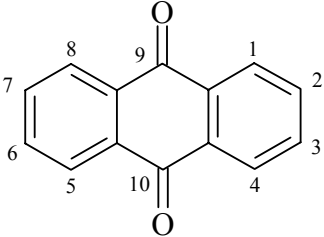
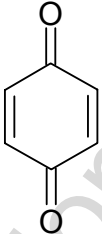
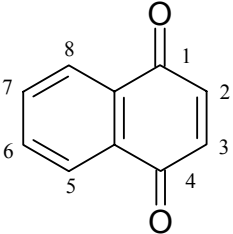
In the following table, ‘NA’ means ‘not applicable’.

Retained Name	Structure	Substitution Type in General Nomenclature	PIN	Substitution Type for PIN
acetic acid	CH <sub>3</sub> -COOH	Type 2a	acetic acid	Type 2a
acrylic acid	CH <sub>2</sub> =CH-COOH	Type 3	prop-2-enoic acid	
adipic acid	HOOC-[CH <sub>2</sub> ] <sub>4</sub> -COOH	Type 3	hexanedioic acid	
benzoic acid	C <sub>6</sub> H <sub>5</sub> -COOH	Type 2a	benzoic acid	Type 2a
butyric acid	CH <sub>3</sub> -CH <sub>2</sub> -CH <sub>2</sub> -COOH	Type 3	butanoic acid	
carbamic acid	H <sub>2</sub> N-COOH	Type 2a	carbamic acid	Type 2a
carbonic acid	HO-CO-OH	NA	carbonic acid	NA
citric acid	$  \begin{array}{c}  \text{CH}_2\text{-COOH} \\    \\  \text{HO-C-COOH} \\    \\  \text{CH}_2\text{-COOH}  \end{array}  $	Type 3	2-hydroxypropane-1,2,3-tricarboxylic acid	
cinnamic acid	C <sub>6</sub> H <sub>5</sub> -CH=CH-COOH	Type 3	3-phenylprop-2-enoic acid	
cyanic acid	NCOH	NA	cyanic acid	NA
formic acid	HCOOH	Type 2c	formic acid	Type 2c
fumaric acid	$  \begin{array}{c}  \text{CH-COOH} \\     \\  \text{HOOC-CH}  \end{array}  $	Type 3	( <i>E</i> )-but-2-enoic acid	
2-furoic acid (also 3- isomer)		Type 2a	furan-2-carboxylic acid	
glutaric acid	HOOC-[CH <sub>2</sub> ] <sub>3</sub> -COOH	Type 3	pentanedioic acid	
glyceric acid	$  \begin{array}{c}  \text{COOH} \\    \\  \text{HO-C-H} \\    \\  \text{CH}_2\text{OH}  \end{array}  $	Type 3	2,3-dihydroxypropanoic acid	

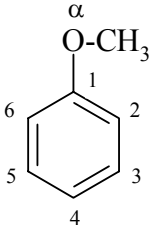
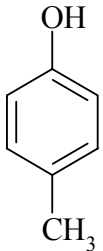
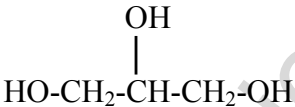
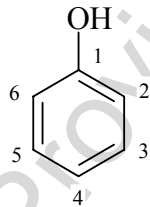
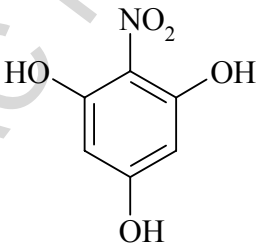
isonicotinic acid		Type 2a	pyridine-4-carboxylic acid	
isophthalic acid		Type 2a	benzene-1,3-dicarboxylic acid	
lactic acid	$\text{CH}_3\text{-CH(OH)-COOH}$	Type 3	2-hydroxypropanoic acid	
maleic acid	$\begin{array}{c} \text{CH-COOH} \\    \\ \text{CH-COOH} \end{array}$	Type 3	(Z)-but-2-enoic acid	
malonic acid	$\text{HOOC-CH}_2\text{-COOH}$	Type 3	propanedioic acid	
methacrylic acid	$\text{CH}_2=\text{C(CH}_3\text{)-COOH}$	Type 3	2-methylprop-2-enoic acid	
2-naphthoic acid (also 1- isomer)		Type 2a	naphthalene-2-carboxylic acid (also 3- isomer)	
nicotinic acid		Type 2a	pyridine-3-carboxylic acid	
oleic acid	$\begin{array}{c} \text{CH}_3\text{-[CH}_2\text{]}_6\text{-CH}_2\text{-C-H} \\   \\ \text{C} \\    \\ \text{C} \\   \\ \text{CH}_3\text{-[CH}_2\text{]}_6\text{-CH}_2\text{-C-H} \end{array}$	Type 3	(Z)-octadec-9-enoic acid	
oxalic acid	$\text{HO-CO-CO-OH}$	NA	oxalic acid	NA
oxaldehydic acid	$\text{HCO-COOH}$	Type 2c	oxaldehydic acid	Type 2a
oxamic acid	$\text{H}_2\text{N-CO-CO-OH}$	Type 2a	oxamic acid	Type 2a
palmitic acid	$\text{CH}_3\text{-[CH}_2\text{]}_{14}\text{-COOH}$	Type 3	hexadecanoic acid	

phthalic acid		Type 2a	benzene-1,2-dicarboxylic acid
picric acid		Type 3	2-nitrobenzene-1,3,5-triol
propionic acid	$\text{CH}_3\text{-CH}_2\text{-COOH}$	Type 3	propanoic acid
pyruvic acid	$\text{CH}_3\text{-CO-COOH}$	Type 3	2-oxopropanoic acid
stearic acid	$\text{CH}_2\text{-[CH}_2\text{]}_{16}\text{-COOH}$	Type 3	octadecanoic acid
succinic acid	$\text{HOOC-CH}_2\text{-CH}_2\text{-COOH}$	Type 3	butanedioic acid
sulfanilic acid ( <i>p</i> -isomer only)		Type 3	4-aminobenzenesulfonic acid
tartaric acid	$\text{HOOC-[CH(OH)]}_2\text{-COOH}$	Type 3	2,3-dihydroxybutanedioic acid
terephthalic acid		Type 2a	benzene-1,4-dicarboxylic acid

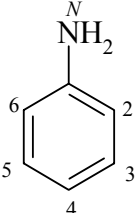
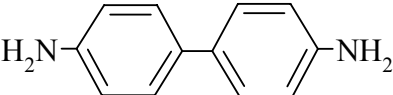
**P-34.3.2 Ketones and Aldehydes**

Retained Name	Structure	Substitution Type in General Nomenclature	PIN	Substitution Type for PIN
acetone	$\text{CH}_3\text{-CO-CH}_3$	Type 2a	propan-2-one	
acetophenone	$\text{C}_6\text{H}_5\text{-CO-CH}_3$	Type 3	1-phenylethan-1-one	
9,10-anthraquinone (also 1,2-, 1,4-, and 2,3- isomers)		Type 2a	anthracene-9,10-dione (also 1,2-, 1,4-, and 2,3- isomers)	
benzophenone	$\text{C}_6\text{H}_5\text{-CO-C}_6\text{H}_5$	Type 3	diphenylmethanone	
1,4-benzoquinone (also 1,2- isomer)		Type 2a	cyclohexa-2,5-diene-1,4-dione (also 3,4-diene-1,2-dione)	
glyceraldehyde	$\begin{array}{c} \text{CHO} \\   \\ \text{H}-\text{C}-\text{OH} \\   \\ \text{CH}_2\text{OH} \end{array}$	Type 3	2,3-dihydroxypropanal	
ketene	$\text{H}_2\text{C=C=O}$	Type 2b	1-ethen-1-one	
1,4-naphthoquinone (also 1,2-, and 2,3- isomers)		Type 2a	naphthalene-1,4-dione (also 1,2-, and 2,3- isomers)	
oxaldehyde	$\text{OCH-CHO}$	Type 2a	oxaldehyde	Type 2a

**P-34.3.3** Hydroxy compounds and ethers

Retained Name	Structure	Substitution Type in General Nomenclature	PIN	Substitution Type for PIN
anisole		Type 2c	anisole	Type 3
<i>p</i> -cresol (also <i>o</i> - and <i>m</i> -isomers)		Type 3	4-methylphenol (also 2- and 3-isomers)	
ethylene glycol	HO-CH <sub>2</sub> -CH <sub>2</sub> -OH	Type 3	ethane-1,2-diol	
glycerol		Type 3	propane-1,2,3-triol	
phenol		Type 2a	phenol	Type 2a
picric acid		Type 3	2-nitrobenzene-1,3,5-triol	

**P-34.3.4 Amines and Other Nitrogen Compounds**

Retained Name	Structure	Substitution Type in General Nomenclature	PIN	Substitution Type for PIN
aniline		Type 2a	aniline	Type 2a
benzidine		Type 3	[1,1'-biphenyl]-4,4'-diamine	
biguanide	$\text{H}_2\text{N}-\text{C}(=\text{NH})-\text{NH}-\text{C}(=\text{NH})-\text{NH}_2$	Type 2b	1,2,3-triimidodicarbonic diamide	
biuret	$\text{H}_2\text{N}-\text{C}(\text{O})-\text{NH}-\text{CO}-\text{NH}_2$	Type 2b	imidodicarbonic diamide	
formazan	$\overset{1}{\text{H}}\text{N}=\overset{2}{\text{N}}-\overset{3}{\text{C}}\text{H}=\overset{4}{\text{N}}-\overset{5}{\text{N}}\text{H}_2$	Type 2b	formazan	Type 2b
guanidine	$\overset{1}{\text{H}_2}\text{N}-\overset{2}{\text{C}}(=\text{NH})-\overset{3}{\text{N}}\text{H}_2$	Type 2b	guanidine	Type 2b
hydroxylamine	$\text{NH}_2-\text{OH}$	Type 2c	hydroxylamine	Type 2c
oxalonitrile	$\text{NC}-\text{CN}$	NA	oxalonitrile	NA
oxamide	$\text{H}_2\text{N}-\text{CO}-\text{CO}-\text{NH}_2$	Type 2b	oxamide	Type 2b
semicarbazide	$\overset{1}{\text{H}_2}\text{N}-\overset{2}{\text{N}}\text{H}-\overset{3}{\text{C}}\text{O}-\overset{4}{\text{N}}\text{H}_2$	Type 2b	hydrazinecarboxamide	
urea	$\overset{1}{\text{H}_2}\text{N}-\overset{2}{\text{C}}\text{O}-\overset{3}{\text{N}}\text{H}_2$	Type 2b	urea	Type 2b



### P-34.4 Prefixes derived from functional parent compounds

P-34.4.0 Introduction

P-34.4.1 Acyl groups

P-34.4.2 Alkoxy groups

P-34.4.3 Carbonyl groups

P-34.4.3 Amines, amides, and other nitrogenous compounds

#### P-34.4.0 Introduction

Names of prefixes derived from functional parent compounds are trivial names identified as 'retained names'. Some are retained as preferred IUPAC names and are also used in general nomenclature. Others are not used as preferred IUPAC names but are acceptable for general use. The complete list of retained names is given in Section P-46. Retained names for prefixes derived from unsaturated parent structures and partially saturated parent structures are given in P-31.1.2.2 and P-31.2.3.3.2, respectively.

#### P-34.4.1 Acyl groups.

Except as given below, the names of prefix groups derived from the acids and related classes. imidic acids, amic acids, hydrazonic acids, and aldehydic acids given in P-34.3.1 are formed by changing the '-ic acid' or '-oic acid' ending of the name of the acid to 'oyl'. They are preferred IUPAC names and may be used in general nomenclature. Substitution follows the type given above for the acid.

Retained Name	Structure	Substitution Type in General Nomenclature	PIN	Substitution Type for PIN
acetyl	CH <sub>3</sub> -CO-	Type 2a	acetyl	Type 2a
butyryl	CH <sub>3</sub> -CH <sub>2</sub> -CH <sub>2</sub> -CO-	Type 3	butanoyl	
carbonyl	-CO-	NA	carbonyl	NA
cyano	NC	NA	cyano	NA
formyl	HCO-	Type 2c	formyl acid	Type 2c
glutaryl	-OC-[CH <sub>2</sub> ] <sub>3</sub> -CO-	Type 3	pentanedioyl	
malonyl	-OC-CH <sub>2</sub> -CO-	Type 3	propanedioyl	
oxalo	HO-CO-CO-	NA	oxalo	NA
oxalyl	-CO-CO-	NA	oxalyl	NA
oxaldehydoyl	OCH-CO-	Type 2c	oxaldehydoyl	Type 2c

oxamoyl	$\text{H}_2\text{N-CO-CO-}$	Type 2a	oxamoyl	Type 2a
propionyl	$\text{CH}_3\text{-CH}_2\text{-CO-}$	Type 3	propanoyl	
succinyl	$\text{-OC-CH}_2\text{-CH}_2\text{-CO-}$	Type 3	butanedioyl	

#### P-34.4.2 Alkoxy groups

Retained Name	Structure	Substitution Type in General Nomenclature	PIN	Substitution Type for PIN
butoxy	$\text{CH}_3\text{-CH}_2\text{-CH}_2\text{-CH}_2\text{-O-}$	Type 2a	butoxy	Type 2a
<i>sec</i> -butoxy	$\text{CH}_3\text{-CH}_2\text{-CH}(\text{CH}_3)\text{-O-}$	Type 3	butan-2-yloxy	
<i>tert</i> -butoxy	$(\text{CH}_3)_3\text{C-O-}$	Type 3	2-(methylpropan-2-yl)oxy	
ethoxy	$\text{CH}_3\text{-CH}_2\text{-O-}$	Type 2a	ethoxy	Type 2a
isopropoxy	$(\text{CH}_3)_2\text{CH-O-}$	Type 3	propan-2-yloxy	
methoxy	$\text{CH}_3\text{-O-}$	Type 2a	methoxy	Type 2a
phenoxy	$\text{C}_6\text{H}_5\text{-O-}$	Type 2a	phenoxy	Type 2a
propoxy	$\text{CH}_3\text{-CH}_2\text{-CH}_2\text{-O-}$	Type 2a	propoxy	Type 2a

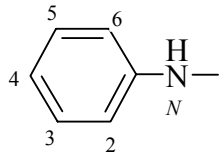
#### P-34.4.3 Carbonyl compounds

The only retained name for prefixes derived from the retained names for aldehydes and ketones (see P-34.3.2) is acetyl,  $\text{CH}_3\text{-CO-CH}_2\text{-}$ . It is not used as a preferred IUPAC name, but can be used in general nomenclature; it belongs to the Type 2 class for substitution. No substituent prefix groups are retained from benzoquinone, naphthoquinone, anthraquinone, acephenone, benzophenone, or ketene for either general nomenclature or as IUPAC preferred names.

**P-34.4.4** Amido, imido, amino, and other nitrogeneous groups

Retained names for amide and imido prefixes derived from the acids given in P-34.3.1 are formed by changing the name of the '...amide or ...imide' ending to '...amido or ...imido', respectively, for example, acetamido, phthalamido, succinimido. These names follow the same substitution rules as the corresponding acid given above.

Other nitrogeneous prefix groups follow.

Retained Name	Structure	Substitution Type in General Nomenclature	PIN	Substitution Type for PIN
anilino		Type 2a	anilino	Type 2a
formazan-1-yl* (also the 3- and 5-yl isomers)	$\begin{array}{ccccccc} & 5 & 4 & 3 & 2 & 1 & \\ & & & & & & \\ \text{H}_2\text{N} & - & \text{N} = & \text{CH} - & \text{N} = & \text{N} - & \end{array}$	Type 2a*	formazan-1-yl* (also the 3- and 5-yl isomers)	Type 2a*

- The -1,5-diyl, the -3,5-diyl, the -1-yl-5-ylidene, the -3-yl-5-ylidene, the -1,3,5-triyl, and the -1,3-diyl-5-ylidene substituent prefix names follow the same pattern.

**P-35** Prefixes corresponding to characteristic groups

P-35.0 Introduction

P-35.1 General methodology

P-35.2 Simple prefixes denoting characteristic groups

P-35.3 Compound substituent prefixes

P-35.4 Complex substituent prefixes

**P-35.0** Introduction

Prefixes used to designate characteristic groups in substitutive nomenclature are those having free valence(s) attached to an atom of Group 17 (F, Cl, Br, and I) or Group 16 (O, S, Se, and Te), or to nitrogen. Oxygen and nitrogen atoms can also be attached to a carbon atom, for example  $-\text{CO}-\text{OH}$ ,  $-\text{CO}-\text{NH}_2$ , and  $-\text{CO}-\text{CH}_2-\text{CH}_3$ , or to a chalcogen atom, for example  $-\text{S}(\text{O}_2)-\text{OH}$ ,  $-\text{Se}(\text{O}_2)-\text{OH}$ . These prefixes correspond to suffixes listed in P-33, for example the prefix 'hydroxy' for  $-\text{OH}$  correspond to the suffix 'ol' for the same group; they also correspond to functionalized parents, for example '2-carboxyethyl' for  $-\text{CH}_2-\text{CH}_2-\text{COOH}$ , derived from propanoic acid,  $\text{CH}_3-\text{CH}_2-\text{COOH}$ . Prefixes are also derived from functional parents as defined in Section P-34, in particular acyl groups such as 'acetyl', for  $-\text{CO}-\text{CH}_3$ , derived from acetic acid.

Prefixes may have both a retained name and a systematic name only one of which can be a preferred name. In order to facilitate the selection of preferred names, clear indications are given in Chapter 6 for each class of compounds. The prefixes are also alphabetically listed in Appendix 2, with indications concerning their status as preferred names as well as their use in substitutive nomenclature and as functional replacement prefixes.

In this Section, the different types of prefixes used in substitutive nomenclature are described.

### P-35.1 General methodology

Substitutive prefixes corresponding to characteristic groups and functional parent compounds may be classified as simple (see P-29.1.1), compound (see P-29.1.2) and complex (see P-29.1.3); mixed substituent groups are complex substituent groups formed by the combination of substitutive and additive operations.

The multiple occurrence of simple prefixes is denoted by the basic multiplying terms 'di', 'tri', etc., or by derived prefixes, 'bis', 'tris', 'tetrakis', etc., in order to distinguish between two simple prefixes and those including a basic multiplying term, for example disulfanyl, '-SSH' and bis(sulfanyl), two -SH groups. Compound and mixed substituent prefixes require the derived multiplying terms, 'bis', 'tris', 'tetrakis', etc., to designate their multiplicity in substitutive nomenclature..

Simple prefixes are either retained or systematically formed as follows:

- (1) by subtraction of hydrogen atom(s) from parent hydrides (described as substituent groups derived from parent hydrides in Section 29), for example, 'sulfanyl', -SH, and 'diselanyl', -SeSeH; from functional parents, for example, acetyl, CH<sub>3</sub>-CO-CH<sub>2</sub>-; or from a contracted name, for example, 'phenoxy', C<sub>6</sub>H<sub>5</sub>-O-;
- (2) acyl groups are formed by subtraction of all -OH groups from oxo acids for example, 'acetyl', CH<sub>3</sub>-CO- and 'carbonyl', >C=O.

### P-35.2 Simple prefixes denoting characteristic groups

#### P-35.2.1 Retained traditional prefixes

Examples:

-F  
fluoro (preselected name)

-Cl  
chloro (preselected name)

-Br  
bromo (preselected name)

-I  
iodo (preselected name)

-OH  
hydroxy (preselected name)

=O  
oxo (preselected name)

-O-  
oxy (preselected name)

–COOH  
carboxy (PIN)

–SO<sub>2</sub>-OH  
sulfo (preselected name)  
selenono (Se instead of S; preselected name)  
tellurono (Te instead of S)

–SO-OH  
sulfino (preselected name)  
selenino (Se instead of S)  
tellurino (Te instead of S)

–NH<sub>2</sub>  
amino (preselected name)

=NH  
imino (to the same atom; preselected name)

–N<  
nitrilo (to different atoms; preselected name)

=N<sub>2</sub>  
dialo (preselected name)

–N<sub>3</sub>  
azido (preselected name)

–CN  
cyano (PIN)

–NC  
isociano (PIN)

–NCO  
isocianato (PIN)  
isotiocianato (S instead of O; PIN)  
isoselenocianato (Se instead of O; PIN)  
isotellurocianato (Te instead of O; PIN)

**P-35.2.2** Substituents formed by the subtraction of one or more hydrogen atoms from mono- and dinuclear parent hydrides (see P-21). Systematic names are formed by the general methodology described in P-28.2.

Examples:

–IH<sub>2</sub>  
 $\lambda^3$ -iodanyl (preselected name)

–SH  
sulfanyl (preselected name)  
(not mercapto-)

–S–  
sulfanediyl (preselected name)  
thio



disulfanediyyl (preselected name)  
dithio



azanediyl (preselected name)  
(to different atoms)



azanylylidene (preselected name)  
(to different atoms)



azanylidyne (to the same atom)

### P-35.2.3 Simple prefixes derived from functional parents

A few simple prefixes are derived from functional parents. They are described in Section P-34.

Examples:



carbonyl (PIN; see P-65.1.1.5.1.5)



phosphoryl (preselected name;  
see P-67.1.4.1.2)



sulfonyl (preselected name;  
sulfuryl  
(see P-65.3.2.3.1)



sulfinyl (preselected name;  
thionyl  
(see P-65.3.2.3.1)



selenonyl (preselected name;  
(see P-65.3.2.3.1)



seleninyl (preselected name;  
(see P-65.3.2.3.1)



telluronyl (preselected name;  
(see P-65.3.2.3.1)



tellurinyll (preselected name;  
(see P-65.3.2.3.1)

### P-35.3 Compound substituent prefixes

**P-35.3.1** Names of compound prefixes derived from suffixes or functional parent compounds may be formed by substituting simple prefixes into other simple prefixes.

Examples:

-SSeH	selanylsulfanyl (preselected name)
-NH-Cl	chloroamino (preselected name)
-NH-CH <sub>3</sub>	methylamino (PIN)

**P-35.3.2** Names of compound prefixes derived from suffixes or functional parent compounds may be formed by the additive operation called concatenation. It is used to assemble simple mono-, di-, tri-, and tetravalent prefixes. Hydrocarbyl divalent substituents can be attached to prefixes expressing characteristic groups.

Examples:

-O-CH <sub>2</sub> -CH <sub>2</sub> -CH <sub>2</sub> -CH <sub>2</sub> -CH <sub>3</sub>	pentyloxy (PIN)
-O-CH <sub>2</sub> -C <sub>6</sub> H <sub>5</sub>	benzyloxy (PIN)
-CO-Cl	carbonochloridoyl (PIN) chlorocarbonyl
-C(=NH)-OH	C-hydroxycarbonimidoyl (PIN)
-C(=N-NH <sub>2</sub> )-OH	C-hydroxycarbonohydrazonyl (PIN)
-CO-NH-NH <sub>2</sub>	hydrazinylcarbonyl (PIN)
-O-CH <sub>2</sub> -CH <sub>2</sub> -O-	ethane-1,2-diylbis(oxy) (PIN)
>N-CH <sub>2</sub> -N<	methylenedinitrilo (PIN)

**P-35.3.3** Mixed substituent prefix names are formed by combining substitutive and additive operations.

Examples:

CH <sub>3</sub> -CH <sub>2</sub> -O-SO-NH-	(ethoxysulfinyl)amino (PIN)
CH <sub>3</sub> -CO-S-CO-	(acetylsulfanyl)carbonyl (PIN)
CH <sub>3</sub> -CO-O-NH-SO-O-	{[(acetyloxy)amino]sulfinyl}oxy (PIN)

#### **P-35.4** Complex substituent prefixes

**P-35.4.1** Names of complex substituent prefixes may be formed by substituting a simple or compound substituent prefix into a compound substituent prefix.

Examples:

–NH-S-SeH (selanylsulfanyl)amino (preselected name)

–CH<sub>2</sub>-NH-Cl (chloroamino)methyl (PIN)

**P-35.4.2** Names of complex substituent prefixes may be formed by adding simple or compound substituent prefixes to a compound substituent prefix by the process called 'concatenation'.

Examples:

–CO-O-CH<sub>2</sub>-C<sub>6</sub>H<sub>5</sub> (benzyloxy)carbonyl (PIN)

–O-CO-NHNH<sub>2</sub> (hydrazinylcarbonyl)oxy (PIN)

**P-35.4.3** Complex mixed substituent prefix names are formed by combining the substitutive and additive operations. .

Examples:

CH<sub>3</sub>-CH<sub>2</sub>-O-SO-NH– (ethoxysulfinyl)amino (PIN)

CH<sub>3</sub>-CO-S-CO– (acetylsulfanyl)carbonyl (PIN)

CH<sub>3</sub>-CO-O-NH-SO-O– {[ (acetyloxy)amino]sulfinyl}oxy (PIN)