

## CHAPTER 5 CONSTRUCTING PREFERRED IUPAC NAMES

- P-50 Introduction
- P-51 Selecting the preferred type of nomenclature
- P-52 Selecting preferred IUPAC names and preselected names (see P-12) for parent hydride names
- P-53 Selecting the preferred method for modifying the degree of hydrogenation for parent hydrides
- P-54 Selecting the preferred suffix (the principal group)
- P-55 Selecting preferred retained names
- P-56 Selecting preferred substituent group names
- P-57 Selecting preferred names for tautomeric compounds
- P-58 Name Construction

### P-50 Introduction

Many compounds can have multiple names in accordance with two or more methods recommended by IUPAC for their formation, one of which is recommended herein as the preferred IUPAC name (PIN). Preferred IUPAC names are part of a systematic approach to nomenclature based on a minimum of principles, rules and conventions that are actually applied. Thus, preferred IUPAC names are not new names, although the continued rationalization of nomenclature has led to some recommended changes. Preferred IUPAC names are essential today to communicate precisely in legal situations with manifestations in patents, and for export-import regulations, health and safety information, etc.

This Chapter summarizes the selection rules that are recommended for generation of preferred IUPAC names.

### P-51 Selecting the preferred method of nomenclature

Substitutive nomenclature is by far the preferred method of nomenclature for naming organic compounds. Other methods are used to enhance substitutive nomenclature or to simplify substitutive names.

- P-51.1 Functional class nomenclature
- P-51.2 Multiplicative nomenclature
- P-51.3 Skeletal replacement ('a') nomenclature
- P-51.4 Phane nomenclature

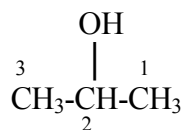
#### P-51.1 Functional class nomenclature

Substitutive nomenclature is preferred to functional class nomenclature for generating preferred IUPAC names, except for naming esters (see P-65.3.3.1), acyl halides and pseudohalides (see P-65.2), and oximes (see P-68.3.1.2).

Examples:



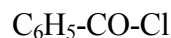
bromomethane (PIN)  
methyl bromide



propan-2-ol (PIN)  
isopropyl alcohol



methyl acetate (PIN)



benzoyl chloride (PIN)



acetyl cyanide (PIN)

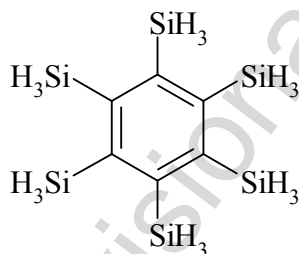


butanal oxime (PIN)

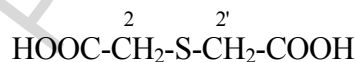
### P-51.2 Multiplicative nomenclature

Multiplicative nomenclature (P-15.3) is preferred to simple substitutive nomenclature for generating preferred IUPAC names to express multiple occurrences of parent hydrides, other than alkanes, functional parents, or functionalized parent hydrides in names.

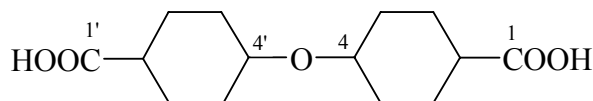
Examples:



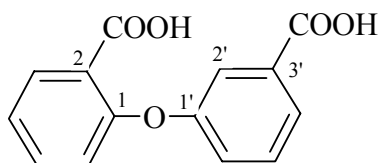
benzenehexaylhexasilane (PIN, multiplicative name)  
(2,3,4,5,6-pentasilylphenyl)silane (simple substitutive name)



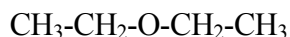
2,2'-sulfanediylodiacetic acid (PIN, multiplicative name)  
2-[(carboxymethyl)sulfanyl]acetic acid (simple substitutive name)



4,4'-oxydi(cyclohexane-1-carboxylic acid) (PIN, multiplicative name)  
4-[(4-carboxycyclohexyl)oxy]cyclohexane-1-carboxylic acid (simple substitutive name)



2,3'-oxydibenzoic acid (PIN, multiplicative name; see P-15.3)  
2-(3-carboxyphenoxy)benzoic acid (simple substitutive name)



ethoxyethane (PIN, simple substitutive name)  
(not 1,1'-oxydiethane; carbon chains are not allowed as  
parent hydrides in multiplicative nomenclature)

### P-51.3 Skeletal replacement ('a') nomenclature

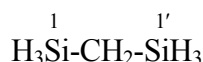
Skeletal replacement ('a') nomenclature is used in two ways to generate preferred IUPAC names:

- (1) it is the only recommended method to generate names for certain heterocyclic compounds;
- (2) it is used to simplify substitutive nomenclature or multiplicative nomenclature when heteroatoms are present in chains.

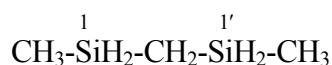
**P-51.3.1** Skeletal replacement ('a') nomenclature is used to derive preferred IUPAC names for heteromonocyclic compounds having more than ten ring atoms (see P-22.2.3), heterocyclic von Baeyer ring systems (see P-23.3.1), heterocyclic spiro parent hydrides consisting of two or more saturated monocyclic rings (see P-24.2.4.1.1), heteropolycyclic ring systems for which fusion nomenclature based on heterocyclic parent rings is not applicable (see P-25.5.1), heterophane ring systems (see P-26.5), and for heterofullerenes (see P-27.5).

**P-51.3.2** Skeletal replacement ('a') nomenclature is used to generate preferred IUPAC names in place of substitutive or multiplicative names for acyclic structures when four and more heterounits are present (see P-15.4.3.2).

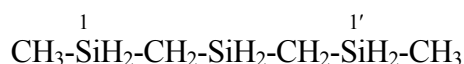
Example 1:



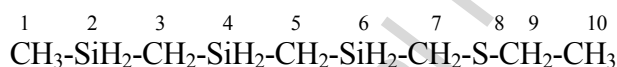
1,1'-methylenebis(silane) (PIN, multiplicative name)  
(silylmethyl)silane (simple substitutive name)



1,1'-methylenebis(methylsilane) (PIN, multiplicative name)  
methyl[(methylsilyl)methyl]silane (simple substitutive name)

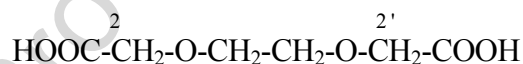


1,1'-[silanediylbis(methylene)]bis(methylsilane) (PIN), multiplicative name  
(treats two silane groups as parent hydrides)  
bis[(methylsilyl)methyl]silane  
(treats only one silane group as a parent hydride; two silane groups as  
substituents)

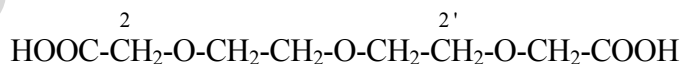


8-thia-2,4,6-trisiladecane (PIN, skeletal replacement ('a') name)  
1-[(ethylsulfanyl)methyl]-1'-methyl-1,1'-[silanediylbis(methylene)]bis(silane)  
(multiplicative name)  
({[(ethylsulfanyl)methyl]silyl}methyl)[(methylsilyl)methyl]silane  
(simple substitutive name)

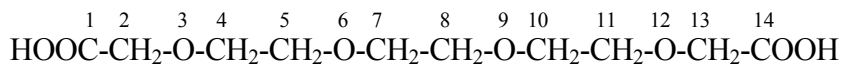
Example 2:



2,2'-[ethane-1,2-diylbis(oxy)]diacetic acid (PIN, multiplicative name)  
2-[2-(carboxymethoxy)ethoxy]acetic acid (simple substitutive name)



2,2'-[oxybis(ethane-2,1-diyloxy)]diacetic acid (PIN, multiplicative name)  
2-{2-[2-(carboxymethoxy)ethoxy]ethoxy}acetic acid (simple substitutive name)

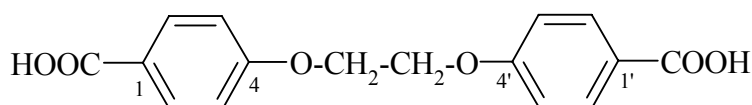


3,6,9,12-tetraoxatetradecane-1,14-dioic acid [PIN, skeletal replacement ('a') name]

2,2'-{ethane-1,2-diylbis[(oxyethane-2,1-diyl)oxy]}diacetic acid (multiplicative name)

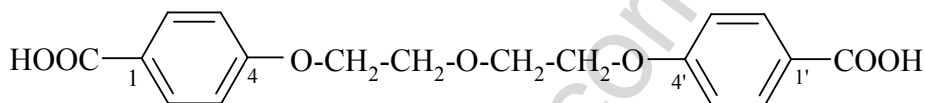
2-(2-{2-[2-(carboxymethoxy)ethoxy]ethoxy}ethoxy)acetic acid (simple substitutive name)

Example 3:



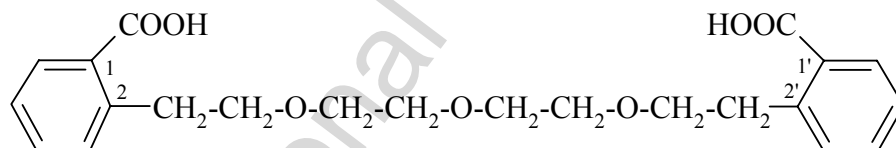
4,4'-[ethane-1,2-diylbis(oxy)]dibenzoic acid (PIN, multiplicative name)

4-[2-(4-carboxyphenoxy)ethoxy]benzoic acid (simple substitutive name)



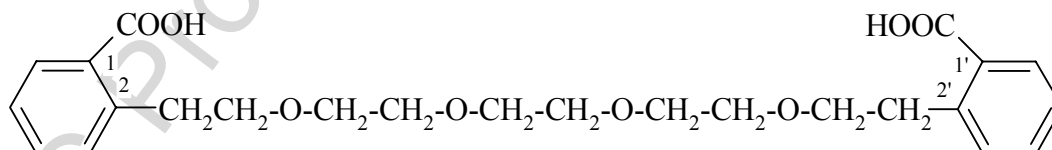
4,4'-[oxybis(ethane-2,1-diyloxy)]dibenzoic acid (PIN, multiplicative name)

4-{2-[2-(4-carboxyphenoxy)ethoxy]ethoxy}benzoic acid (simple substitutive name)



2,2'-{oxybis[(ethane-2,1-diyloxy)ethane-2,1-diyl]}dibenzoic acid (PIN, multiplicative name)

2-[2-(2-{2-[2-(2-carboxyphenyl)ethoxy]ethoxy}ethoxy)ethyl]benzoic acid  
(simple substitutive name)



2,2'-(3,6,9,12-tetraoxatetradecane-1,9-diyl)dibenzoic acid (PIN, multiplicative name  
using the skeletal replacement ('a') name for the multiplying substituent group)

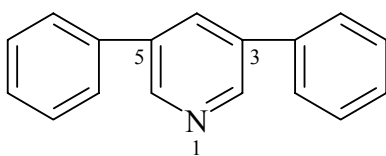
2,2'-{[ethane-1,2-diylbis(oxy)]bis(ethane-2,1-diyloxyethane-2,1-diyl)}dibenzoic acid  
(multiplicative name using simple substitutive nomenclature)

2-{2-[2-(2-{2-[2-(2-carboxyphenyl)ethoxy]ethoxy}ethoxy)ethoxy]ethyl}benzoic acid  
(simple substitutive name)

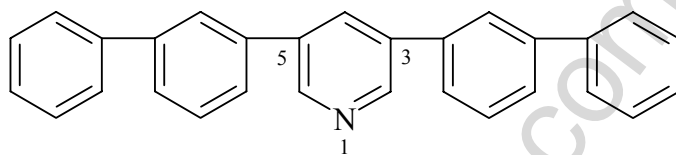
### P-51.4 Phane nomenclature

**P-51.4.1** Phane nomenclature is used to generate preferred IUPAC names for linear acyclic/cyclic compounds that include a minimum of seven nodes including four rings or ring systems, two of which are terminal, even though these compounds can also be named by substitutive or multiplicative nomenclature.

Example 1:



3,5-diphenylpyridine (PIN, substitutive name)



3,5-bis([biphenyl]-3-yl)pyridine (PIN, substitutive name)

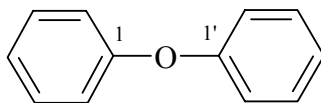


4(3,5)-pyridina-1,7(1),2,3,5,6(1,3)-hexabenzenaheptaphane (PIN, phane name)

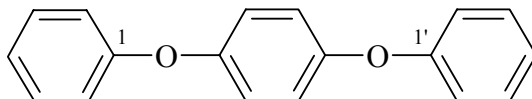
3,5-bis([1<sup>1</sup>,2<sup>1</sup>:2<sup>3</sup>,3<sup>1</sup>-terphenyl]-1<sup>3</sup>-yl)pyridine (simple substitutive name, see P-28.2.1 and P-28.3.1)

3,5-bis([1,1':3',1''-terphenyl]-3-yl)pyridine (simple substitutive name, see P-28.2.1 and P-28.3.1)

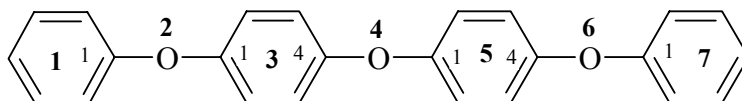
Example 2:



1,1'-oxydibenzene (PIN, multiplicative name)  
phenoxybenzene (simple substitutive name)  
(not diphenyl ether)

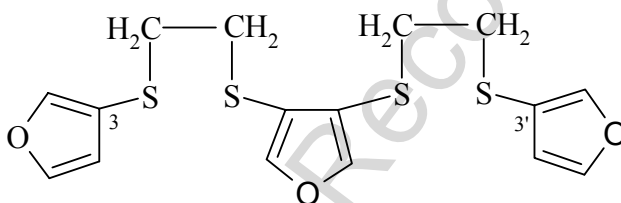


1,1'-[1,4-phenylenebis(oxy)]dibenzene (PIN, multiplicative name)  
1,4-diphenoxybenzene (simple substitutive name)

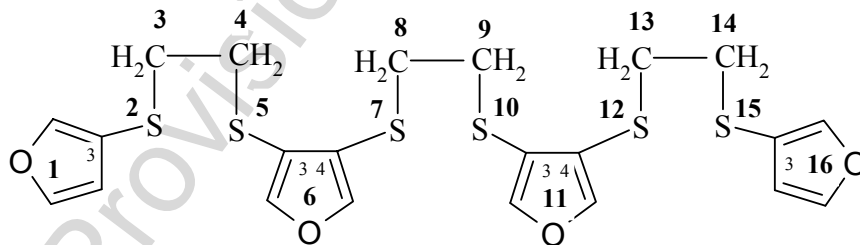


2,4,6-trioxa-1,7(1),3,5(1,4)-tetrabenzenaheptaphane (PIN, phane name)  
1,1'-oxybis(4-phenoxybenzene) (multiplicative name)  
1-phenoxy-4-(4-phenoxyphenoxy)benzene (simple substitutive name)

Example 3:



3,3'-{furan-3,4-diylbis[(sulfanedylethane-2,1-diyl)sulfaneyl]}difuran  
(PIN, multiplicative name)  
3,4-bis{[2-(furan-3-ylsulfanyl)ethyl]sulfanyl}furan (simple substitutive name)



2,5,7,10,12,15-hexathia-1,16(3),6,11(3,4)-tetrafuranahexadecaphane (PIN, phane name)  
3,3'-[ethane-1,2-diylbis(sulfaneyl)]bis({4-[2-(furan-3-ylsulfanyl)ethyl]sulfanyl}furan)  
(multiplicative name)  
3-{[2-(furan-3-ylsulfanyl)ethyl]sulfanyl}-4-({2-[(4-{[2-(furan-3-ylsulfanyl)ethyl]sulfanyl}furan-3-yl)sulfanyl]ethyl}sulfanyl)furan  
(a simple substitutive name)

**P-52 Selecting preferred IUPAC names and preselected names (see P-12) for parent hydrides**

For naming the parent hydrides described in Chapter 2, when only one method is described, the resulting single names are naturally preferred IUPAC names. When more than one method is recommended for generating the names of parent hydrides, preferred IUPAC names, and in some cases, preselected names, must be chosen. Some retained names are used as preferred IUPAC names and as names for use in general nomenclature.

P-52.1 Selecting preselected names

P-52.2 Selecting preferred IUPAC names

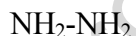
**P-52.1** Selecting preselected names

**P-52.1.1** Preselected mononuclear parent hydride names (see P-21.1.1)

fluorane	HF	azane	NH <sub>3</sub>	borane	BH <sub>3</sub>
chlorane	HCl	phosphane	PH <sub>3</sub>	alumane	AlH <sub>3</sub>
bromane	HBr	arsane	AsH <sub>3</sub>	indigane	InH <sub>3</sub>
iodane	HI	stibane	SbH <sub>3</sub>	gallane	GaH <sub>3</sub>
astatane	HAt	bismuthane	BiH <sub>3</sub>	thallane	TlH <sub>3</sub>
oxidane	H <sub>2</sub> O	silane	SiH <sub>4</sub>		
selane	H <sub>2</sub> Se	germane	GeH <sub>4</sub>		
sulfane	H <sub>2</sub> S	stannane	SnH <sub>4</sub>		
tellane	H <sub>2</sub> Te	plumbane	PbH <sub>4</sub>		
polane	H <sub>2</sub> Po				

**P-52.1.2** Preselected names for homogeneous acyclic polynuclear parent hydrides (see P-21.2.2)

Examples:



hydrazine (preselected name)



nonaazane (preselected name)



pentasilane (preselected name)



trisulfane (preselected name)

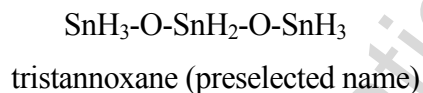
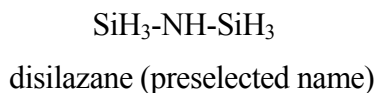


triphosphane (preselected name)



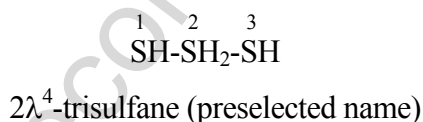
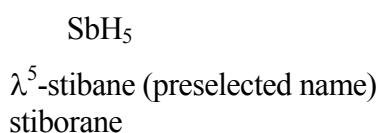
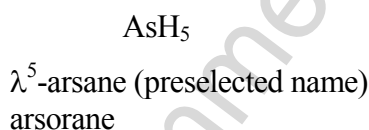
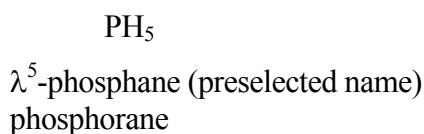
**P-52.1.3** Heterogeneous acyclic parent hydrides composed of alternating atoms [a(ba)<sub>n</sub> hydrides], excluding carbon (see P-21.2.3.1)

Examples:



**P-52.1.4** Parent hydrides with nonstandard bonding numbers

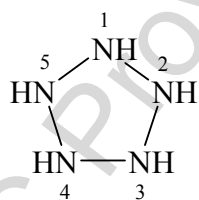
Examples:



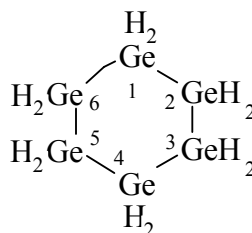
**P-52.1.5** Homogeneous heteromonocyclic parent hydrides

Preselected names for homogeneous heteromonocyclic parent hydrides are Hantzsch-Widman names (see P-22.2.2) for rings composed of ten or fewer ring members. Skeletal replacement ('a') names (see P-22.2.3) are preselected names for heterogeneous monoheterocyclic parent hydrides with alternating heteroatoms with more than ten ring members. Alternative names are those formed by using the prefix 'cyclo' (see P-22.2.5).

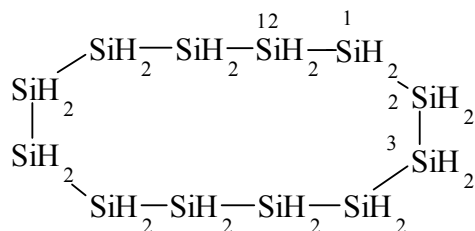
Examples:



pentazolane (preselected name)  
cyclopentaazane



hexagerminane (preselected name)  
cyclohexagermane

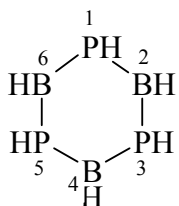


dodecasilacyclododecane (preselected name)  
cyclododecasilane

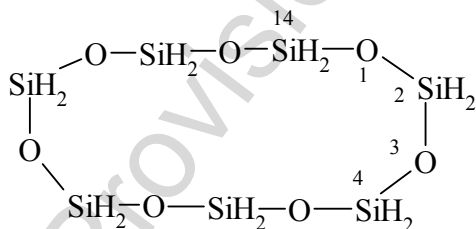
**P-52.1.6** Heterogeneous heteromonocyclic parent hydrides consisting of alternating heteroatoms

Preselected names for heterogeneous heteromonocyclic parent hydrides with ten or fewer ring members composed of alternating heteroatoms are Hantzsch-Widman names (see P-22.2.2). Skeletal replacement ('a') names (see P-22.2.3) are preselected names for heterogeneous monoheterocyclic parent hydrides with alternating heteroatoms with more than ten ring members. Alternative names are those formed by using the prefix 'cyclo' (see P-22.2.5).

Examples:



1,3,5,2,4,6-triphosphatriborinane (preselected name)  
cyclotriboraphosphane

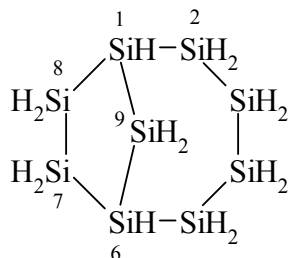


1,3,5,7,9,11,13-heptaoxa-2,4,6,8,10,12,14-heptasilacyclotetradecane (preselected name)  
cycloheptasiloxane

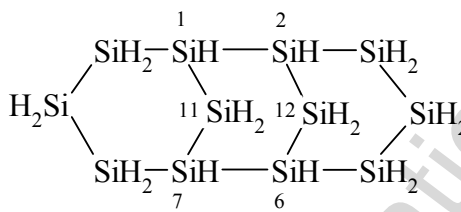
**P-52.1.7** Homogeneous heterocyclic von Baeyer systems and spiro compounds

Preselected names for von Baeyer systems and spiro compounds composed entirely of heteroatoms of the same kind, are names formed by using the total number of heteroatoms expressed as mononuclear parent hydrides; alternative names are those formed by skeletal replacement ('a') nomenclature (see P-23.3 and P-2.4.2)

Examples:



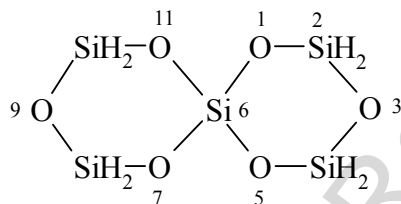
bicyclo[4.2.1]nonasilane (preselected name)  
nonasilabicyclo[4.2.1]nonane



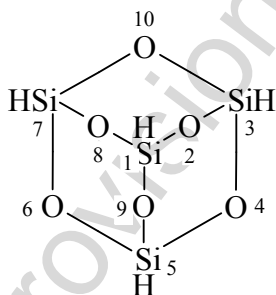
tricyclo[5.3.1.1<sup>2,6</sup>]dodecasilane (preselected name)  
dodecasilatricyclo[5.3.1.1<sup>2,6</sup>]dodecane

**P-52.1.8** Preselected names for bi- and polyalicyclic ring systems (von Baeyer ring systems) and spiro compounds having only monocyclic components composed of alternating heteroatoms are formed by citing the number and the names of the alternating atoms (see P-23.5); alternative names are those formed by skeletal replacement ('a') nomenclature.

Examples:



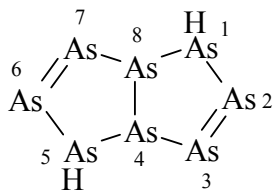
spiro[5.5]pentasiloxane (preselected name)  
1,3,5,7,9,11-hexaoxa-2,4,6,8,10-pentasilaspiro[5.5]undecane



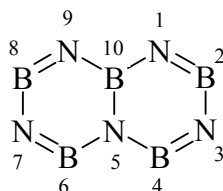
tricyclo[3.3.1.1<sup>3,7</sup>]tetrasiloxane (preselected name)  
2,4,6,8,9,10-hexaoxa-1,3,5,7-tetrasilabicyclo[3.3.1.1<sup>3,7</sup>]decane

**P-52.1.9** Preselected names for homogeneous and heterogeneous heterobi- and polycyclic fused ring systems are appropriate fusion names

Examples:



1*H*,5*H*-pentarsolopentarsole (preselected name)



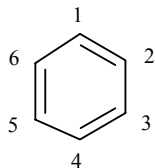
[1,3,5,2,4,6]triazatriborino[1,2-*a*][1,3,5,2,4,6]triazatriborine (preselected name)

## P-52.2 Selecting preferred IUPAC names

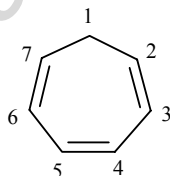
### P-52.2.1 Monocyclic hydrocarbons

The name [*n*]annulene is used in preferred IUPAC fusion names as a parent component (see P-25.3.2.1.1) and may be used in general nomenclature as a parent hydride name. Preferred IUPAC names for cycloalkenes and cycloalkapolyenes are generated from cycloalkane names (see P-32.1.3.1).

Examples:



benzene (PIN)  
[6]annulene)

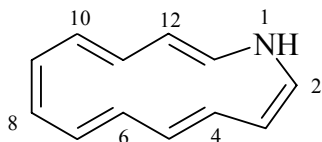


cyclohepta-1,3,5-triene (PIN)  
1*H*-[7]annulene (preferred IUPAC name for the  
parent component in fusion nomenclature,  
see P-25.3.2.1.1)

### P-52.2.2 Unsaturated heteromonocyclic compounds with more than ten ring members

Names derived from cycloalkanes modified by skeletal replacement ('a') nomenclature are preferred IUPAC names; [*n*]annulene names (see P-31.1.3.2) may be used in general nomenclature. A modified skeletal replacement ('a') name is used to designate these heterocyclic compounds as components in fusion names (see P-25.3.2.1.2) and is found in general nomenclature.

Example:



1-azacyclotrideca-2,4,6,8,10,12-hexaene (PIN)

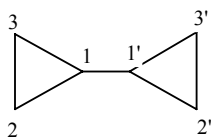
1-azacyclotridecine (preferred IUPAC name for the the principal component in a fusion name, see also P-25.2.2.1.2; 1-azacyclotridecino for an attached component, see P-25.3.2.2.2)

1*H*-1-aza[13]annulene

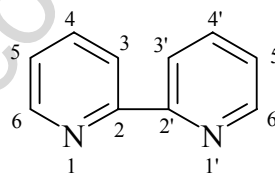
### P-52.2.3 Preferred names and numbering for ring assemblies

**P-52.2.3.1** Preferred IUPAC names for assemblies of two identical cyclic systems joined by a single bond are formed using the names of parent hydrides, except for benzene assemblies, biphenyl and the polyphenyls, rather than the names of substituent groups.

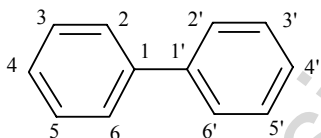
Examples:



1,1'-bi(cyclopropane) (PIN)  
1,1'-bi(cyclopropyl)



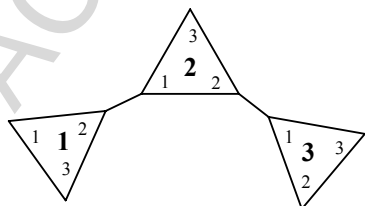
2,2'-bipyridine (PIN)  
2,2'-bipyridyl



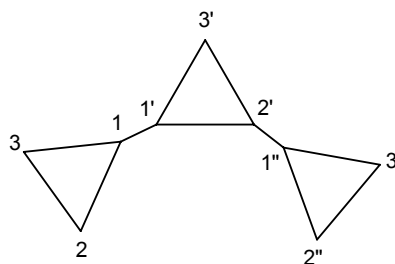
1,1'-biphenyl (PIN)  
biphenyl

**P-52.2.3.2** The preferred numbering for ring assemblies composed of three or more identical cyclic systems is by composite locants rather than primed locants.

Examples:



1<sup>1</sup>,2<sup>1</sup>:2<sup>2</sup>,3<sup>1</sup>-tercyclopropane (PIN)



1,1':2',1''-tercyclopropane

### **P-52.5** Selecting a preferred cyclic parent hydride

When two or more cyclic parent hydrides can be chosen to name a cyclic compound, one of them must be selected as the preferred parent hydride.

#### **P-52.5.1** General rule

The preferred parent hydride is one occurring first in the following list given in decreasing order of seniority:

- spiro system
- cyclic phane system
- fused system
- bridged fused system
- von Baeyer polycyclic system
- linear phane system
- ring assembly.

#### **P-52.5.2** Definitions

**P-52.5.2.1** Fused systems, bridged fused systems, spiro systems, bi- and polycyclic (von Baeyer) ring systems, and ring assemblies are described in Chapter 2.

It must be noted that for preferred IUPAC names fusion nomenclature is applicable only when two five membered rings are present. Thus, the name octahydropentalene (a fusion name) is preferred to bicyclo[3.3.0]octane. Systems without the required two five membered rings are given von Baeyer names, for example, bicyclo[2.2.0]hexane.

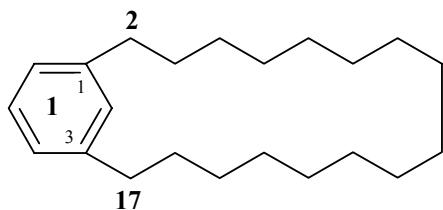
#### **P-52.5.2.2** Cyclic and linear phane systems

Cyclic and linear phane structures are defined in section P-26. For the purpose of selecting preferred IUPAC names for polycyclic systems and correctly applying P-52.5.1, cyclic and acyclic phane systems are defined more rigorously as follows:

- (1) cyclophanes are cyclic phane structures containing one or more rings or ring systems, at least one ring or ring system of which must be a monocyclic system attached to adjacent components at nonadjacent ring positions;
- (2) linearphanes consist of four or more rings or ring systems, two of which must be terminal, and together with acyclic atoms or chains must consist of at least seven nodes (components).

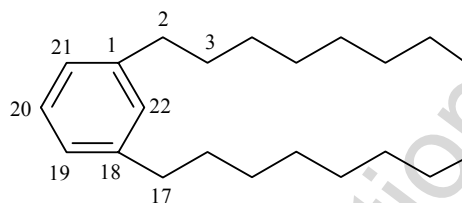
**P-52.5.3** Name selection. The following examples illustrate the application of P-52.5.1.

Examples:

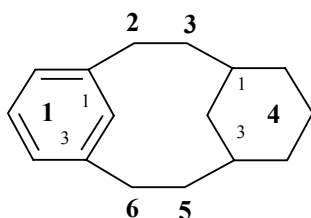


1(1,3)-benzenacycloheptadecane (PIN;  
phane name)

(a fusion name is not possible for this structure; a phane name is preferred to a von Baeyer name)

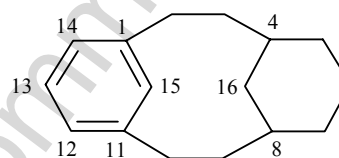


bicyclo[16.3.1]docosane-1(22),18,20-triene  
(von Baeyer name)

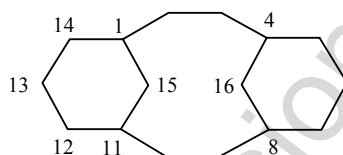


1(1,3)-benzena-4(1,3)-cyclohexanacyclohexaphane (PIN)

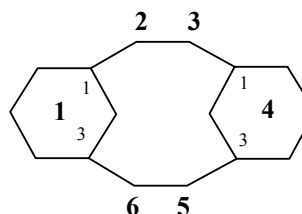
(a fusion name is not possible for this structure; a phane name is preferred to a von Baeyer name)



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

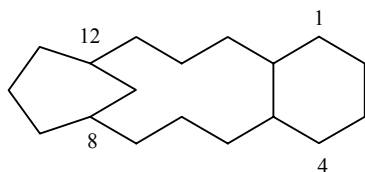


tricyclo[9.3.1.1<sup>4,8</sup>]hexadecane (PIN)

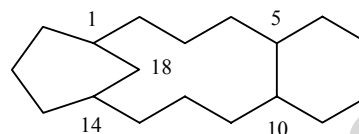


1,4(1,3)-dicyclohexanacyclohexaphane

(a fusion name is not possible; since there is no mancude ring present a phane name is not appropriate; therefore the von Baeyer name is the preferred IUPAC name)



(I)

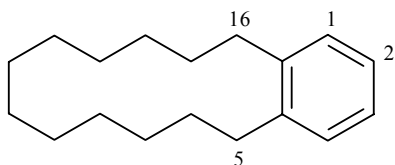


(II)

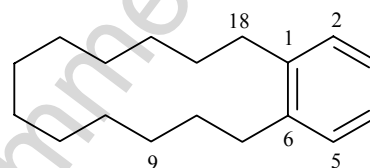
(I) hexadecahydro-1*H*-8,12-methanobenzo[13]annulene (PIN)

(II) tricyclo[12.3.1.0<sup>5,10</sup>]octadecane

[the bridged fused name (I) is preferred to von Baeyer name (II);  
since no mancude ring being present, a phane name is not allowed]

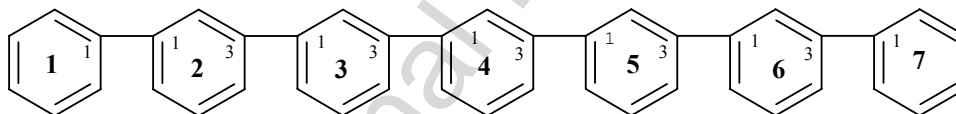


5,6,7,8,9,10,11,12,13,14,15,16-dodecahydro-  
benzo[14]annulene (PIN)



bicyclo[12.4.0]octadeca-1(14),17,19-triene

(a phane name is not allowed according to Rule P-52.5.3.2;  
a fusion name is preferred to a von Baeyer name)

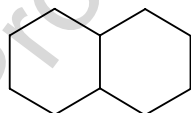


1,7(1),2,3,4,5,6(1,3)heptabenzenaheptaphane (PIN)

1<sup>1</sup>,2<sup>1</sup>,2<sup>3</sup>,3<sup>1</sup>,3<sup>3</sup>,4<sup>1</sup>,4<sup>4</sup>,5<sup>1</sup>,5<sup>3</sup>,6<sup>1</sup>,6<sup>3</sup>,7<sup>1</sup>-septiphenyl

1,1':3',1'':3'',1''':3''',1''':3''',1''''-septiphenyl

(a phane name, where permitted, is preferred to a ring assembly name)



decahydronaphthalene (PIN)

bicyclo[4.4.0]decane

(a fusion name is preferred to a von Baeyer name)



### P-53 Selecting a method for modifying the degree of hydrogenation

Three methods are used to modify the degree of hydrogenation of parent hydrides:

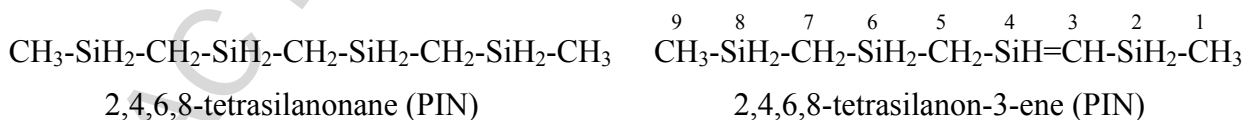
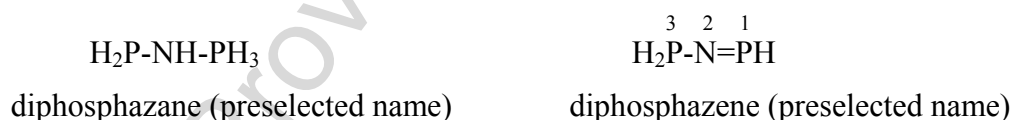
- (1) by changing the ending 'ane' in acyclic parent hydrides to 'ene' and 'yne';
- (2) by using 'hydro' prefixes to saturate one or more double bonds in mancude compounds;
- (3) by using 'dehydro' prefixes to introduce triple bonds in mancude compounds.

Systematic IUPAC names and retained names may be modified in the same way or in different ways.

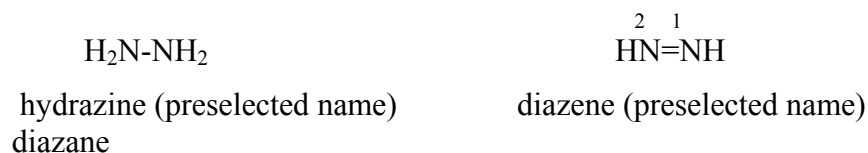
#### P-53.1 Changing the ending 'ane' into 'ene' and 'yne'

**P-53.1.1** Alkanes, homogenous chains, and heterogenous hetero chains composed in part or entirely of heteroatoms are modified by changing the ending 'ane' into 'ene' and 'yne' to generate preferred IUPAC names (see P-31.1.2.2.1).

Examples:

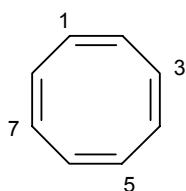


The retained name 'hydrazine' generates the systematic name 'diazene':

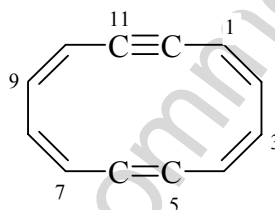


**P-53.1.2** Preferred IUPAC names for monocyclic mancude hydrocarbons (see P-31.1.3.1), von Baeyer polyalicyclic compounds (see P-31.1.4.1), and saturated spiro compounds (see P-31.1.5.1), are formed by modifying the ending 'ane' into 'ene'.

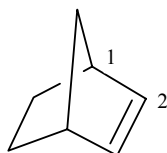
Example:



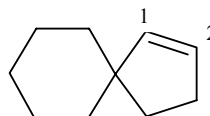
cycloocta-1,3,5,7-tetraene (PIN)  
[8]annulene



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



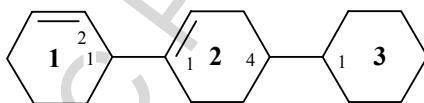
bicyclo[2.2.1]hept-2-ene (PIN)



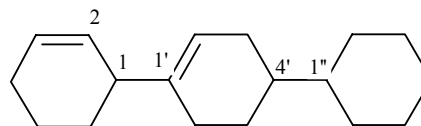
spiro[4.5]dec-1-ene (PIN)

**P-53.1.3** Assemblies of identical saturated rings and ring systems are modified by 'ene' and 'yne' endings (see P-31.1.6). Preferred IUPAC names are generated by the use of 'ene' and 'yne' endings using composite locants rather than primed locants (see P-28.3.1).

Example:



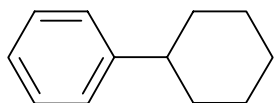
[1<sup>1</sup>,2<sup>1</sup>:2<sup>4</sup>,3<sup>1</sup>-tercyclohexane]-1<sup>2</sup>,2<sup>1</sup>-diene (PIN)  
(see also P-28.3.1)



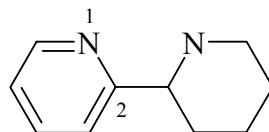
[1,1':4',1''-tercyclohexane]-1',2-diene  
(see also P-28.3.1)

When assemblies of otherwise identical rings contain both mancude and saturated rings, substitutive names lead to preferred IUPAC names and when the requirements for the formation of phane names are met, phane names are the preferred IUPAC names.

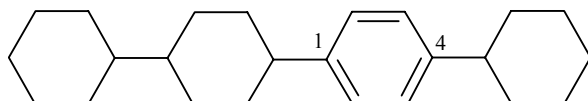
Examples:



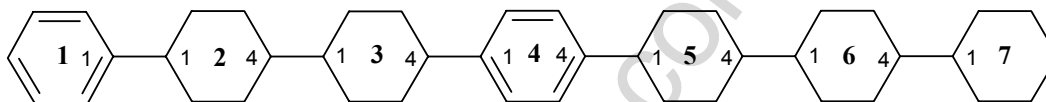
cyclohexylbenzene (PIN)



2-(piperidin-2-yl)pyridine (PIN)



4-(cyclohexylphenyl)-1,1'-bicyclohexane (PIN)



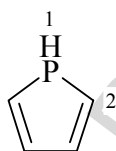
1(1), 4(1,4)-dibenzena-2,3,5,6(1,4),7(1)-pentacyclohexanaheptaphane (PIN)  
1-[4-(4'-phenyl-[1,1'-bicyclohexan]-1-yl)phenyl]-1<sup>1</sup>,2<sup>1</sup>:2<sup>4</sup>,3<sup>1</sup>-tercyclohexane

## P-53.2 Names modified by 'hydro' prefixes

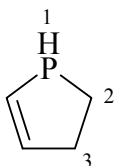
### P-53.2.1 Monoheterocycles having Hantzsch-Widman names

Preferred IUPAC names for Hantzsch-Widman rings correspond to either fully unsaturated or fully saturated compounds (see P-22.2.2.1.1). 'Hydro' prefixes added to names of fully unsaturated Hantzsch-Widman rings lead to preferred IUPAC names for partially unsaturated rings.

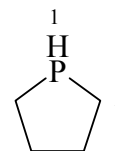
Examples:



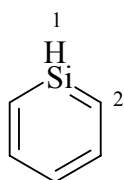
1*H*-phosphole (PIN)



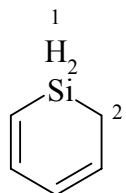
2,3-dihydro-1*H*-phosphole (PIN)



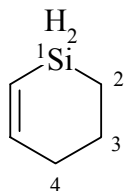
phospholane (PIN)



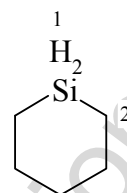
silinine (PIN)



1,2-dihydrosilinine (PIN)



1,2,3,4-tetrahydrosilinine (PIN)



silinane (PIN)

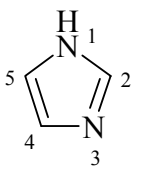
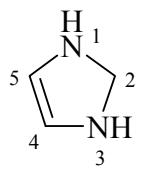
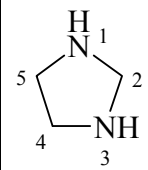
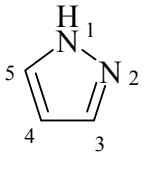
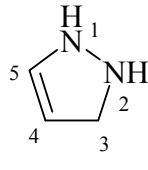
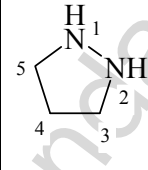
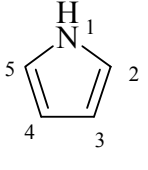
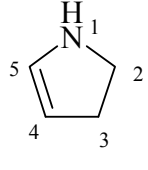
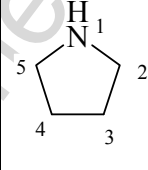
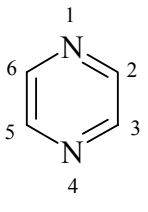
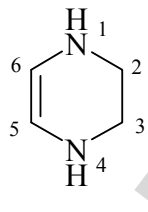
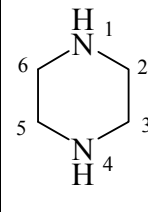
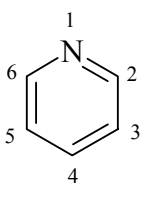
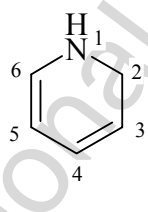
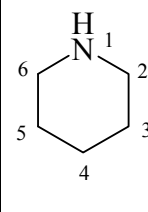
### P-53.2.2 Heteromonocyclic compounds with retained names

Retained names are used for unsaturated and saturated heteromonocyclic compounds before modification with 'hydro' prefixes and for saturated compounds after modification by 'hydro' prefixes, in accordance with Table 5.1. Hantzsch-Widman names are described in P-22.2.2; retained names are listed in P-22.2.1 and in Tables 2.2 and 2.3.

Names of fully saturated compounds can also be formed by adding the maximum number of 'hydro' prefixes, for example 'hexahydropyridine'; these names are not preferred IUPAC names but are acceptable in general nomenclature.

**Table 5.1 Retained heteromonocyclic names modified by 'hydro' prefixes**

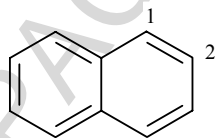
Structure	Name before modification by 'hydro' prefixes	Structure	Name after partial modification by 'hydro' prefixes	Structure	Name after full modification by 'hydro' prefixes
	furan (PIN)		2,3-dihydrofuran (PIN)		oxolane (PIN) tetrahydrofuran
	2 <i>H</i> -pyran (PIN)		2,3-dihydro-2 <i>H</i> -pyran (PIN)		oxane (PIN)
	4 <i>H</i> -oxazine (PIN)		2 <i>H</i> -3,4-dihydro-oxazine (PIN)		morpholine (PIN) tetrahydro-2 <i>H</i> -oxazine

	1 <i>H</i> -imidazole (PIN)		2,3-dihydro-1 <i>H</i> -imidazole (PIN)		imidazolidine (PIN)
	1 <i>H</i> -pyrazole (PIN)		2,3-dihydro-1 <i>H</i> -pyrazole (PIN)		pyrazolidine (PIN)
	1 <i>H</i> -pyrrole (PIN)		2,3-dihydro-1 <i>H</i> -pyrrole (PIN)		pyrrolidine (PIN)
	pyrazine (PIN)		1,2,3,4-tetrahydro pyrazine (PIN)		piperazine (PIN)
	pyridine (PIN)		1,2-dihydro pyridine (PIN)		piperidine (PIN)

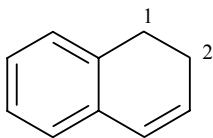
### P-53.2.3 Fused ring systems and mancude ring assemblies

**P-53.2.3.1** Retained fusion names are used for the fully unsaturated compounds (see P-25); they are the preferred IUPAC names. Preferred IUPAC names for the partially saturated and fully saturated compounds are formed by using 'hydro' prefixes. Preferred IUPAC names for partially saturated and mancude ring assemblies are formed in the same way.

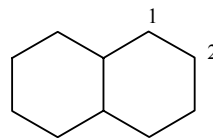
Examples:



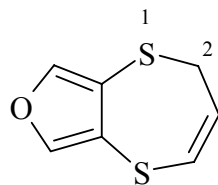
naphthalene (PIN)



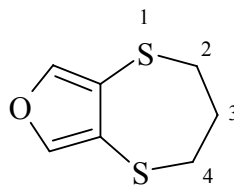
1,2-dihydronaphthalene (PIN)



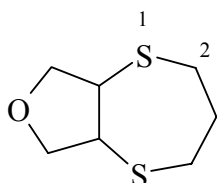
decahydronaphthalene (PIN)  
bicyclo[4,4,0]decane



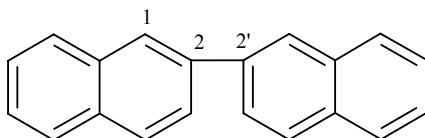
2*H*-thiepine[1,3-*c*]furan (PIN)



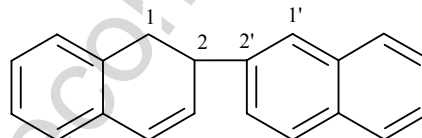
3,4-dihydro-2*H*-thiepine[1,3-*c*]furan (PIN)



hexahydro-2*H*-thiepine[1,3-*c*]furan (PIN)



2,2'-binaphthalene (PIN)  
2,2'-binaphthyl



1,2-dihydro-2,2'-binaphthalene (PIN)  
1,2-dihydro-2,2'-binaphthyl

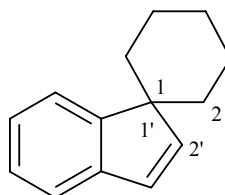
**P-53.2.3.2** The retained names for the partially saturated heterocycles, 'indane', 'indoline', 'isoindoline', 'chromane', and 'isochromane' are not used as preferred IUPAC names, but are acceptable for use in general nomenclature (see P-31.2.3.3.1).

### P-53.3 Names modified by 'ene' and 'yne' endings and 'hydro' prefixes

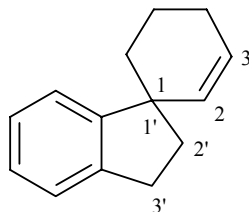
#### P-53.3.1 Spiro compounds

Saturated and mancude components, when present in a spiro compound, are modified individually in accordance with the rule applicable to the component.

Example:



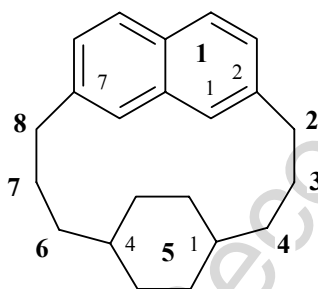
spiro[cyclohexane-1,1'-indene] (PIN)



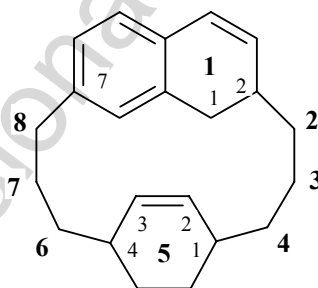
2',3'-dihydrospiro[cyclohexane-1,1'-indene]-2-ene (PIN)

**P-53.3.2** Mancude and saturated amplifcants, when present in a phane system, are each modified in accordance with the rules applicable to each individual amplifcant.

Example:



1(2,7)-naphthalena-5(1,4)-cyclohexanacyclooctaphane (PIN)

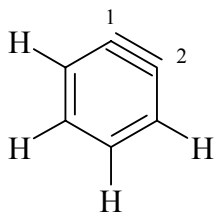


1<sup>1</sup>,1<sup>2</sup>-dihydro-1(2,7)-naphthalena-5(1,4)-cyclohexanacyclooctaphan-5<sup>2</sup>-ene (PIN)

#### **P-53.4 Names modified by 'dehydro' prefixes**

'Dehydro' prefixes are used to generate preferred IUPAC names of dehydrogenated mancude compounds. They may be used in general nomenclature to introduce double and triple bonds in saturated parent hydrides.

Example:



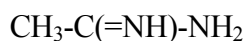
1,2-dehydrobenzene (PIN)  
cyclohexa-1,3-dien-5-yne  
(not benzyne)

#### P-54 Selecting suffixes

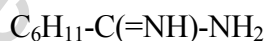
Suffixes have always been described as unique elements of the formation of names. In the past, some suffixes have been discarded and replaced by new ones.

**P-54.1** The suffixes ‘amidine’ and ‘carboxamidine’ for  $-\text{C}(=\text{NH})-\text{NH}_2$ , are no longer recommended; the new suffixes ‘imidamide’ and ‘carboximidamide’ (see P-66.4.1) are used in preferred IUPAC names.

Examples:



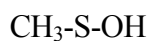
ethanimidamide (PIN)  
(no longer acetamidine)



cyclohexanecarboximidamide (PIN)  
(no longer cyclohexanecarboxamidine)

**P-54.2** The suffix ‘sulfenic acid’ for  $-\text{S}-\text{OH}$  was discarded in the 1993 recommendations (ref 2); in these recommendations, it is replaced by the new suffix, ‘*SO*-thioperoxol’ (see P-63.3.2).

Example:



methane-*SO*-thioperoxol (PIN)  
(no longer methanesulfenic acid)

**P-54.3** The suffix ‘ylene’ was used to describe divalent substituent groups in which the free valences do not form a double bond, i.e.,  $-\text{E}-$  or  $\text{E}<$ , in contrast to substituent groups in which the free valences form a double bond, i.e.,  $\text{E}=\text{}$ . The suffix ‘ylene’ has been replaced by the suffixes ‘diyl’ to express the  $-\text{E}-$  or  $\text{E}<$  type, and ‘ylidene’ for  $\text{E}=\text{}$ , for example, methanediyl for  $\text{H}_2\text{C}<$  and methylydene for  $\text{H}_2\text{C}=\text{}$ , respectively. However, the name ‘methylene’ is retained to describe the substituent group  $\text{H}_2\text{C}<$ ; it is used in preferred IUPAC names rather than methanediyl. In these recommendations, preferred names are expressed as follows:



methylene (PIN, retained name)  
methanediyl



methylydene (PIN)  
(formerly methylene)



$-\text{CH}_2-\text{CH}_2-$ ethane-1,2-diyl (PIN) ethylene	$\text{CH}_3-\text{CH}=\text{}$ ethylidene (PIN)
$-\text{SiH}_2-$ silanediyl (preselected name) (not silylene, a name still used by CAS)	$\text{H}_2\text{Ge}=\text{}$ germylidene (preselected name) (not germylene, a name still used by CAS)
$-\text{BH}-$ boranediyl (preselected name) (not borylene, a name still used by CAS)	$\text{HB}=\text{}$ boranylidene (preselected name) (not borylene, a name still used by CAS)
$-\text{SbH}-$ stibanediyl (preselected name) stibinediyl (not stibylene, a name still used by CAS)	$\text{HSb}=\text{}$ stibanylidene (preselected name) stibinylidene (not stibylene, a name still used by CAS)
$-\text{NH}-\text{CO}-\text{NH}-$ carbonylbis(azanediyl) (PIN, a name used in multiplicative nomenclature) (carbonyldiimino, a name still used by CAS) (not ureylene)	

### P-55 Preferred retained names

Trivial names (names having no part used in a systematic sense) and semisystematic names retained for use in naming organic compounds are given in this Section. Some of them are used as preferred IUPAC names; all of them may be used in general nomenclature. References to rules established in Chapters 2 and 3 are given.

Trivial or semisystematic names retained for naming organic compounds are known as 'retained names'. Their number was sharply reduced in the 1979 Rules, and reduced still further in the 1993 Recommendations. The following list gives the recommendations for 2005 and is to be considered limiting, unless specified otherwise; see, for example, fusion nomenclature in P-25, and phane nomenclature in P-26. Substituent groups names not derived from a systematic transformation are given in Section P-56. All the names in the list can be used in general nomenclature.

Retained names are classified into three types based on their substitutability (see also P-29.6, P-35, P-35, and P-46).

**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.

**P-55.1** Acyclic, alicyclic, monocyclic, and partially saturated hydrocarbons

The preferred IUPAC names for acyclic, alicyclic and monocyclic hydrocarbons, with the exception of toluene and xylene, have no restriction as to their ability to be substituted by substituent groups and by characteristic groups cited as suffixes and/or prefixes.

IUPAC preferred retained names			Retained names only for general nomenclature		
acetylene	Type 3	P-34.3.1	allene	Type 2b	P-34.3.1
adamantane	Type 1	P-23.7	[ <i>n</i> ]annulene	Type 1	P-22.1.2
benzene	Type 1	P-22.1.2	cubane	Type 1	P-23.7
butane	Type 1	P-21.1.1	indane	Type 1	P-31.3.2.1
ethane	Type 1	P-21.1.1	isoprene	Type 3	P-34.3.1
methane	Type 1	P-21.1.1	mesitylene	Type 3	P-22.1.3
propane	Type 1	P-21.1.1	styrene	Type 3	P-34.3.1
toluene	Type 2c	P-22.1.3			
xylene	Type 3	P-22.1.3			

**P-55.1.2** Polycyclic fully unsaturated (mancude) hydrocarbons

The retained names for fully unsaturated (mancude) hydrocarbons given below are all IUPAC preferred names, fully substitutable, and are listed in Table 2.5, P-25.1.1.

anthracene	azulene	chrysene	coronene
fluoranthene	fluorene	<i>as</i> -indacene	<i>s</i> -indacene
indene	naphthalene	ovalene	perylene
phenalene	phenanthrene	picene	pleiadene
pyrene	pyranthrene	rubicene	

## P-55.2 Heterocycles

### P-55.2.1 Fully unsaturated (aromatic) heteromonocycles

**P-55.2.1.1** The retained names for fully unsaturated (aromatic) heteromonocycles given below are all IUPAC preferred names, fully substitutable, and are listed in Table 2.2, P-22.2.1.

furan	imidazole	pyran	pyrazine
pyrazole	pyridazine	pyridine	pyrimidine
pyrrole	selenophene	tellurophene	thiophene

### P-55.2.1.2.

The retained names for fully unsaturated (aromatic) heteromonocycles given below are not preferred IUPAC preferred names, but are acceptable in general nomenclature. They are fully substitutable, and are listed in Table 2.2, P-22.2.1.

isothiazole	isoxazole	oxazole	thiazole
1,2-thiazole (PIN)	1,2-oxazole (PIN)	1,3-oxazole (PIN)	1,3-thiazole (PIN)

### P-55.2.2 Saturated heterocycles

**P-55.2.1.1** The retained names for the saturated heteromonocycles given below are all IUPAC preferred names, fully substitutable, and are listed in Table 2.3, P-22.2.1.

imidazolidine	morpholine	piperazine	piperidine
pyrazolidine	pyrrolidine		

**P-55.2.1.2** The retained names for the saturated or partially saturated heteropolycycles given below are not preferred IUPAC names, but are acceptable for general nomenclature, are fully substitutable, and, except for quinuclidine, are listed in P-31.3.2.

quinuclidine (see P-23.7)  
1-azabicyclo[2.2.2]octane (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  
3,4-dihydro-2*H*-1-benzothiopyran (PIN)

selenochromane  
3,4-dihydro-2*H*-1-benzoselenopyran (PIN)

tellurochromane  
3,4-dihydro-2*H*-1-benzotelluopyran (PIN)

isochromane 3,4-dihydro-1 <i>H</i> -2-benzopyran (PIN)	isothiochromane 3,4-dihydro-1 <i>H</i> -2-benzothiopyran (PIN)
isoselenochromane 3,4-dihydro-1 <i>H</i> -2-benzoselenopyran (PIN)	isotellurochromane 3,4-dihydro-1 <i>H</i> -2-benzotelluropyran (PIN)

**P-55.2.3** Fully unsaturated (mancude) heteropolycycles

**P-55.2.3.1** The retained names for the fully unsaturated (mancude) heteropolycycles given below are all IUPAC preferred names, fully substitutable, and are listed in Tables 2.6 and 2.7, P-25.1.

acridarsine	acridine	acridophosphine	arsanthridine
arsindole	arsinoline	carbazole	chromene
cinnoline	imidazole	indazole	indole
indolizine	isoarsindole	isoarsinoline	isochromene
isoindole	isophosphindole	isophosphinoline	isoquinoline
naphthyridine	perimidine	phenanthridine	phenanthroline
phenazine	phosphindole	phosphinoline	phthalazine
pteridine	purine	pyrazine	pyrrolizine
quinazoline	quinoline	quinolizine	quinoxaline
xanthene			

**P-55.2.3.2** The retained names for the fully unsaturated (mancude) heteropolycycles given below are not preferred IUPAC names, but are acceptable in general nomenclature. They are fully substitutable and are included in Tables 2.6 and 2.7, P-25.1.

$\beta$ -carboline 9 <i>H</i> -pyrido[3,4- <i>b</i> ]indole (PIN)	isobenzofuran 1 <i>H</i> -2-benzofuran (PIN)
isobenzothiopyran 1 <i>H</i> -2-benzothiofuran (PIN)	isobenzoselenopyran 1 <i>H</i> -2-benzoselenofuran (PIN)
isobenzotelluropyran 1 <i>H</i> -2-benzotellurofuran (PIN)	

**P-55.3** Retained names for nitrogen parent hydrides. The following are the preferred IUPAC names for the fully substitutable structures given in P-34.3.8.

hydrazine (preselected name, see P-12)	formazan (PIN)
--	----------------

**P-55.4** Retained functional parent names

The following retained names for functional parent compounds are used as preferred names and are used in general nomenclature. Substitution of the corresponding structures follows the general types as given in P-55.0, except that substitution by groups corresponding to the same or higher functional class is not allowed.

**P-55.4.1** Hydroxy compounds and ethers

IUPAC preferred retained names			Retained names only for general nomenclature		
anisole	Type 3	P-34.3.2	anisole	Type 2c	P-34.3.3
phenol	Type 1	P-34.3.2	ethylene glycol	Type 3	P-34.3.3
			glycerol	Type 3	P-34.3.3
			<i>p</i> -cresol (also <i>o</i> - and <i>m</i> - isomers)	Type 3	P-34.3.3
			picric acid	Type 3	P-34.3.3

**P-55.4.2** Carbonyl compounds. The following retained names are not preferred IUPAC names but are acceptable in general nomenclature (all compounds are given in P-34.3.2)

acetone	Type 2a
ketene	Type 2b
acetophenone	Type 3
benzophenone	Type 3
1,4-benzoquinone (also 1,2- isomer)	Type 2a
9,10-anthraquinone (also 1,2-, 1,4-and 2,3- isomers)	Type 2a
1,4-naphthoquinone (also 1,2- and 2,3- isomers)	Type 2a

**P-55.4.3** Carboxylic acids

**P-55.4.3.1** The retained names for the carboxylic acids given below are IUPAC preferred names, fully substitutable (Type 2a), except for formic acid which is Type 2c, and are listed in Tables 2.6 and 2.7, P-34.3.4.

acetic acid	benzoic acid	formic acid (Type 2c)
phthalic acid	terephthalic acid	

**P-55.4.3.2** The retained names for the carboxylic acids given below are not preferred IUPAC names but are acceptable in general use; they are not substitutable (Type 3), and are listed in P-34.3.4.

acrylic acid	glutaric acid	methacrylic acid	propionic acid
adipic acid	isonicotinic acid	naphthoic acid	pyruvic acid
butyric acid	isophthalic acid	nicotinic acid	stearic acid
cinnamic acid	lactic acid	oleic acid	succinic acid
citric acid	malonic acid	palmitic acid	tartaric acid
furoic acid			

**P-55.4.4** Retained names for other 'carbon acids' (carbonic acid and oxalic acid) and related acids given below are IUPAC preferred names, and are fully substitutable where the possibility of substitution exists. They are listed in P-34.3.5.

carbonic acid	carbamic acid
cyanic acid	
oxalic acid	oxamic acid
oxaldehydic acid	

**P-55.4.5** Nitrogen functional parent structures

Preferred IUPAC retained names			Retained names only for general nomenclature		
aniline	Type 2a	P-34.3.6	benzidine	Type 3	P-34.3.4
formazan	Type 2b	P-34.3.4	semicarbazide	Type 2b	P-34.3.4
urea	Type 2b	P-34.3.4	biuret	Type 2b	P-34.3.4
guanidine	Type 2b	P-34.3.4	biguanide	Type 2b	P-34.3.4
hydroxylamine	Type 2c	P-34.3.4			

**P-55.4.6 Preferred IUPAC names for natural products**

**P-55.4.6.1** Names of alkaloids, steroids, terpenes and other natural product parent hydrides are retained because they carry implied stereochemical configuration, have widespread usage, and may have a complex structure. Preferred IUPAC names and names for use only in general nomenclature are listed in Table 10.1 in Chapter 10. The list is nonlimiting. Some structures are also given in Chapter 10; all are listed in the Appendix in ref 9.

**P-55.4.6.2** Preferred IUPAC names for functional parent structures, such as carbohydrates and  $\alpha$ -amino acids, follow the nomenclature procedures for these compound classes as given in P-102 through P-107.

**P-56 Names of substituent groups derived from parent structures**

**P-56.1** Substituent groups derived from parent structures with retained names.

This Section describes preferred IUPAC names that are retained names of substituent groups derived from parent structures described in P-55 as well as names for use in general nomenclature. Names of substituent groups derived from the parent structures in P-33 that are formed by a systematic procedure given in P-29 and P-32 are NOT included. References to rules established in Chapters 2 and 3 are given. The substitutability of each structure is indicated in the same manner as for the parent structures in P-55.

**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

To facilitate the choice of a preferred prefix, all usual prefixes, including those described below, are listed in Appendix 2, with clear indications as to their preferred status in the nomenclature of organic compounds

**P-56.1.1** Substituent groups derived from parent hydrides.

Preferred IUPAC retained names			Retained names only for general nomenclature		
adamantyl 1- and 2- isomers	Type 2a	P-29.6	allyl	Type 2b	P-32.3

benzyl	Type 2c	P-29.6	allylidene	Type 2b	P-32.3
benzylidene	Type 2c	P-29.6	anthryl 1-, 2-, and 9- isomers	Type 2a	P-29.6.1
benzylidyne	Type 2a	P-29.6	ethylene	Type 2a	P-29.6.1
<i>tert</i> -butyl	Type 3	P-29.6	furyl 2- and 3- isomers	Type 2a	P-29.6.1
hydrazinyl	Type 2a	P-29.6	isopropyl	Type 3	P-29.6.3
hydrazinylidene	Type 2a	P-29.6	isopropylidene	Type 3	P-29.6.3
methylene	Type 2a	P-29.6	isoquinolyl 1-, 2-, 3-, 4-, 5-, 6-, 7-, and 8- isomers	Type 2a	P-29.6.1
phenyl	Type 2a	P-29.6	naphthyl 1-, and 2- isomers	Type 2a	P-29.6.1
phenylene 1,2-, 1,3-, and 1,4- isomers	Type 2a	P-29.6.1	phenanthryl 1-, 2-, 3-, 4-, and 9- isomers	Type 2a	P-29.6.1
trityl	Type 3	P-29.6.3	piperidyl 1-, 2-, 3-, and 4- isomers	Type 2a	P-29.6.1
			pyridyl 2-, 3-, and 4- isomers	Type 2a	P-29.6.1
			quinolyl 2-, 3-, 4-, 5-, 6-, 7-, and 8- isomers	Type 2a	P-29.6.1
			styryl	Type 3	P-29.6.3
			thienyl		



			1-, 2- and 3- isomers	Type 2a	P-29.6.1
			tolyl <i>o</i> -, <i>m</i> -, and <i>p</i> - isomers)	Type 2a	P-29.6.3
			vinyl	Type 2a	P-32.3
			vinylidene	Type 2a	P-32.3

**P-56.1.2** Substituent groups derived from functional parents

IUPAC preferred retained names			Retained names only for general nomenclature		
acetyl	Type 2a	P-34.4.1	acetonyl	Type 3	P-34.3.3
butoxy	Type 2a	P-34.4.2	<i>sec</i> -butoxy	Type 3	P-34.4.2
<i>tert</i> -butoxy	Type 3	P-34.4.2	<i>tert</i> -butoxy	Type 3	P-34.4.2
carbonyl	NA	P-35.2.3	butyryl	Type 3	P-34.4.1
ethoxy	Type 2a	P-34.4.2	cyano	NA	P-35.2.1
formyl	Type 2c	P-34.4.1	glutaryl	Type 3	P-34.4.1
methoxy	Type 2a	P-34.4.2	isopropoxy	Type 3	P-34.3.1
oxalo	NA	P-65.2.3	malonyl	Type 3	P-34.4.1
oxalyl	NA	P-34.4.1	propionyl	Type 3	P-34.4.1
oxamoyl	Type 2a	P-34.4.1	succinyl	Type 3	P-34.4.1
oxaldehydoyl	Type 2c	P-65.2.3			
phenoxy	Type 2a	P-34.4.2			
propoxy	Type 2a	P-34.4.2			
seleninyl	NA	P-35.2.3			

selenonyl	NA	P-35.2.3
sulfinyl	NA	P-35.2.3
sulfonyl	NA	P-35.2.3
tellurinyl	NA	P-35.2.3
telluronyl	NA	P-35.2.3

**P-56.1.3** 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 rules for selection of preferred IUPAC names and the same substitution rules as the corresponding acid given above.

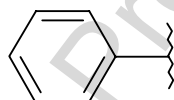
The retained names anilino, formazan-1-yl, formazan-3-yl, and formazan-5-yl are preferred IUPAC names, are used in general nomenclature, and are classified as Type 2 for the purposes of substitution.

**P-56.2** Selection of preferred substituent group names between retained names and systematic names for which two methods of formation are recommended according to P-29 and P-32. The following rules are recommended for the selection of preferred IUPAC names. Names of substituent groups are listed in Appendix 2, with indications concerning their use as preferred names or for general nomenclature only.

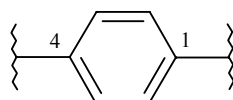
**P-56.2.1** Methylene and phenylene



methylene (PIN; not used to indicate a double bond)  
methanediyl



phenyl (PIN)

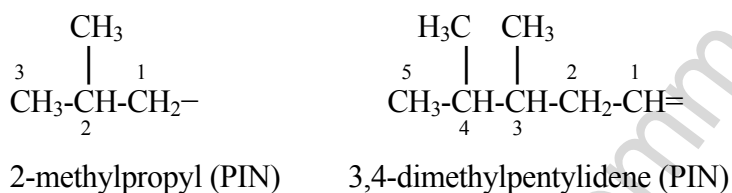
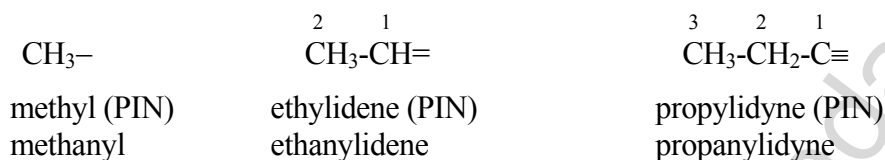


1,4-phenylene (PIN)  
(also, the 1,2- and 1,3-isomers are preferred IUPAC names)  
*p*-phenylene

**P-56.2.2** Selecting preferred IUPAC names for acyclic hydrocarbon substituent groups

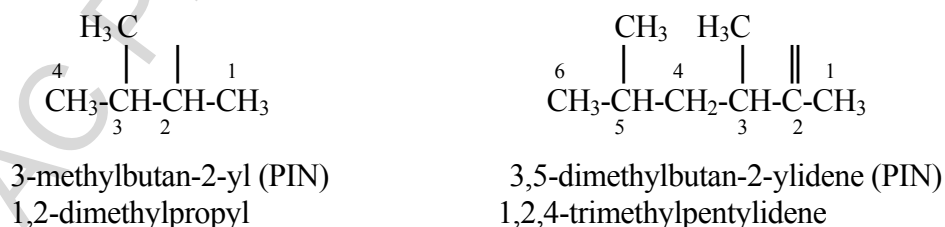
**P-56.2.2.1** When the free valence(s) are at the end of the longest chain of an alkane, alkyl substituent prefixes are preferred IUPAC names, not alkanyl substituent prefixes.

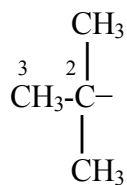
Examples:



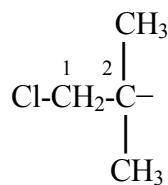
**P-56.2.2.2** Alkanyl substituent prefixes are preferred IUPAC names when the free valence(s) is (are) located on a nonterminal atom of the longest continuous chain. These names are preferred to those formed by substituting alkyl groups.

Examples:

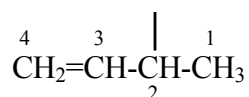




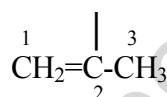
*tert*-butyl (PIN)  
2-methylpropan-2-yl  
1,1-dimethylethyl



1-chloro-2-methylpropan-2-yl (PIN)  
2-chloro-1,2-dimethylethyl



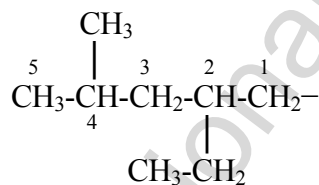
but-3-en-2-yl (PIN)  
1-methylprop-2-en-1-yl



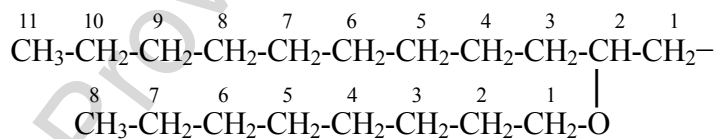
prop-1-en-2-yl (PIN)  
1-methylethenyl

**P-56.2.2.3** For compound substituent groups (substituted substituent groups), P-56.1.2.1 or P-56.1.2.2 is applied according to the requirements for each chain. When the longest chain of the parent substituent or of each substituent chain terminates at the free valence, it is named as an alkyl substituent. When the free valence is not at the end of the longest chain of the parent substituent or of each substituent chain, it is named as an alkanyl group.

Examples:

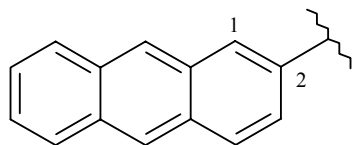


2-ethyl-4-methylpentyl (PIN)

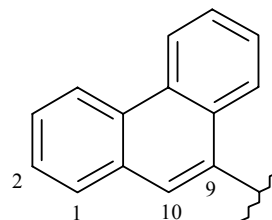


2-(octyloxy)undecyl (PIN)

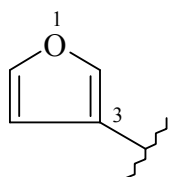




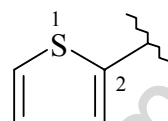
anthracen-2-yl (PIN)  
2-anthryl



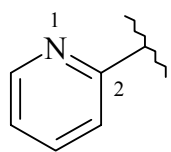
phenanthren-9-yl (PIN)  
9-phenanthryl



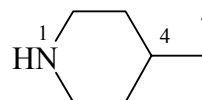
furan-3-yl (PIN)  
3-furyl



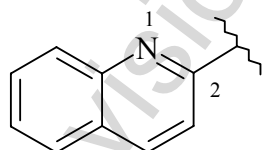
thiophen-2-yl (PIN)  
2-thienyl



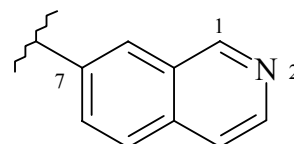
pyridin-2-yl (PIN)  
2-pyridyl



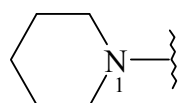
piperidin-4-yl (PIN)  
4-piperidyl



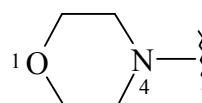
quinolin-2-yl (PIN)  
2-quinolyl



isoquinolin-7-yl (PIN)  
7-isoquinolyl



piperidin-1-yl (PIN)  
1-piperidyl  
(not piperidino)



morpholin-4-yl (PIN)  
(not morpholino)

**P-56.3** Retained names for characteristic groups expressed as prefixes

Prefixes denoting characteristic groups that are derived from parent structures are classified into four categories.

- P-56.3.1 Retained names for simple characteristic groups
- P-56.3.2 Names derived from retained names rather than systematic names of parent structures.
- P-56.3.3 Systematic names preferred to traditional retained names
- P-56.3.4 Systematic names used to replace traditional prefixes

Prefixes denoting characteristic groups are listed in Appendix 2; preferred prefixes are indicated when one or two alternative prefixes are recommended. In this section, retained and systematically formed prefixes are listed. They are simple prefixes; their multiplicity is denoted by the basic multiplying prefixes 'di', 'tri', etc.

**P-56.3.1** Retained names for simple characteristic groups

The following names are retained as preselected IUPAC names. The corresponding systematic names, with the exception of azanylidyne, are not recommended as preselected IUPAC names, but may be used in general nomenclature, for example 'amino' is a preselected IUPAC name but 'azanyl' is not.

$\text{H}_2\text{N}-$	$\text{HN}=\text{}$	$\begin{array}{c}   \\ -\text{N}- \end{array}$
amino (preselected name) azanyl	imino (preselected name) azanylidene	nitriolo (preselected name) azanetriyl
$\text{HO}-$	$-\text{O}-$	$\text{O}=\text{}$
hydroxy (preselected name) (not oxidanyl)	oxy (preselected name) (not (oxidanediyl))	oxo (preselected name) (not oxidanylidene)
$\text{HOO}-$	$-\text{OO}-$	
hydroperoxy (preselected name) (not dioxidanyl)	peroxy (preselected name) (not dioxanediyl) (not dioxy)	
$\text{F}-$	$\text{Cl}-$	
fluoro (preselected name) (not fluoranyl)	chloro (preselected name) (not chloranyl)	

Br-	I-
bromo (preselected name) (not bromanyl)	iodo (preselected name) (not iodanyl)

**P-56.3.2** Names derived from retained names rather than systematic names of parent structures.

Names derived from hydrazine and formazan are preferred to those derived from diazane and (hydrazinylidenemethyl)diazene, respectively. In turn, the traditional prefixes ending with the letter 'o' are no longer recommended.

Examples:

-NHNH <sub>2</sub>	=NNH <sub>2</sub>
hydrazinyl (preselected name) diazanyl (not hydrazino)	hydrazinylidene (preselected name) diazanylidene (not hydrazono)

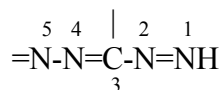
=N-N=	-NH-NH-
hydrazinediylidene (preselected name) diazanediylidene (not azino)	hydrazine-1,2-diyl (preselected name) diazane-1,2-diyl (not hydrazo nor hydrazi)

$\begin{array}{cccccc} & 5 & 4 & 3 & 2 & 1 \\ & \text{H}_2\text{N} & \text{N} & =\text{CH} & \text{N} & =\text{N}- \end{array}$	$\begin{array}{cccccc} & 1 & 2 & 3 & 4 & 5 \\ & \text{HN} & =\text{N} & \text{CH} & =\text{N} & \text{NH}- \end{array}$
formazan-1-yl (PIN) (hydrazinylidenemethyl)diazenyl	formazan-5-yl (PIN) (diazenylmethylidene)hydrazinyl

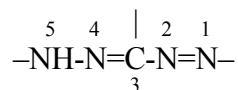
$\begin{array}{cccccc} & 5 & 4 & & 2 & 1 \\ & \text{H}_2\text{N} & \text{N} & =\text{C} & \text{N} & =\text{NH} \\ & & & & 3 & \end{array}$	$\begin{array}{cccccc} & 5 & 4 & 3 & 2 & 1 \\ & \text{NH} & \text{N} & =\text{CH} & \text{N} & =\text{N}- \end{array}$
formazan-3-yl (PIN) (hydrazinylhydrazinylidene)methyl	formazan-1,5-diyl (PIN)

$\begin{array}{cccccc} & 1 & 2 & & 4 & 5 \\ & \text{HN} & =\text{N} & \text{C} & =\text{N} & \text{NH}- \\ & & & 3 & & \end{array}$	$\begin{array}{cccccc} & 5 & 4 & 3 & 2 & 1 \\ & =\text{N} & \text{N} & =\text{CH} & \text{N} & =\text{N}- \end{array}$
formazan-3,5-diyl (PIN)	formazan-1-yl-5-ylidene (PIN)





formazan-3-yl-5-ylidene (PIN)



formazan-1,3,5-triyl (PIN)

**P-56.3.3** Systematic names that are preselected IUPAC names; traditional retained names may be used in general nomenclature

S=	sulfanylidene (preselected name)	Se=	selanylidene (preselected name)
	thioxo		selenoxo
Te=	tellanylidene (preselected name)		
	telluroxo		

**P-56.3.4** Systematic names that are preselected IUPAC names rather than traditional prefix names.

-S-  
sulfanediyl (preselected name)  
thio

-SS-  
disulfanediyl (preselected name)  
dithio

-Se-  
selanediyl (preselected name)  
(not seleno)

-SeSe-  
diselanediyl (preselected name)  
(not diseleno)

-Te-  
tellanediyl (preselected name)  
(not telluro)

-TeTe-  
ditellanediyl (preselected name)  
(not ditelluro)

-NH-  
azanediyl (preselected name)  
(not imino)

-N=  
azanylylidene (preselected name)  
(not nitrilo)

N≡  
azanylidyne (PIN)  
(not nitrilo)

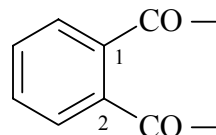
**P-56.3.5** Acyl groups

**P-56.3.5.1** The following names are retained as preferred names for acyl groups derived from the carboxylic acids listed in Section P-34.4.5, and the sulfur acids in P-34.7.

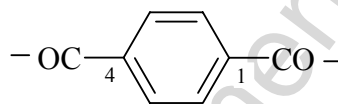
HCO–  
formyl (PIN)

CH<sub>3</sub>-CO–  
acetyl (PIN)

C<sub>6</sub>H<sub>5</sub>-CO–  
benzoyl (PIN)



phthaloyl (PIN)



terephthaloyl (PIN)

H<sub>2</sub>N-CO–  
carbamoyl (PIN)  
aminocarbonyl

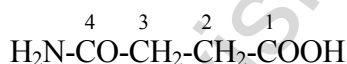
H<sub>2</sub>N-C(=NH)–  
carbamimidoyl (PIN)  
aminoiminomethyl

H<sub>2</sub>N-SO<sub>2</sub>–  
sulfamoyl (preselected name)  
aminosulfonyl

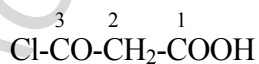
**P-56.3.5.2** Preferred IUPAC names for acyl group prefixes

When acyl groups derived from carboxylic acids described in P-56.2.3 are attached to a carbon chain, preferred IUPAC names are formed by making the carbon atom of the acyl group part of the principal chain and appropriate prefixes are used. Note, however, that the –COOH group is never fragmented.

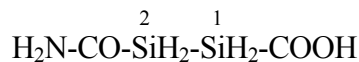
Examples:



4-amino-4-oxobutanoic acid (PIN)  
3-carbamoylpropanoic acid  
3-(aminocarbonyl)propanoic acid  
[not (aminoformyl)propanoic acid]  
succinamic acid



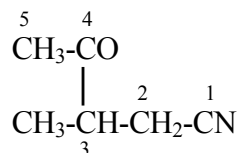
3-chloro-3-oxopropanoic acid (PIN)  
2-(carbonochloridoyl)acetic acid  
2-(chlorocarbonyl)acetic acid  
[not (chloroformyl)acetic acid]



2-carbamoyldisilane-1-carboxylic acid (PIN)

2-(aminocarbonyl)disilane-1-carboxylic acid

[not 2-(aminoformyl)disilane-1-carboxylic acid]



3-methyl-4-oxopentanenitrile (PIN)

(not 3-acetylbutanenitrile)

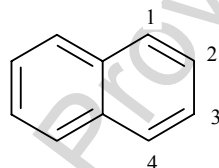
**P-56.4** Substitution in compounds having the maximum number of noncumulative double bonds (mancude compounds) at positions where there is an insufficient number of hydrogen atoms for the substitutive operation.

**P-56.4.1.** Compounds without indicated hydrogen atoms

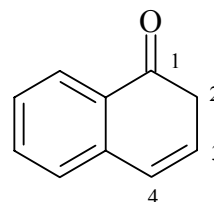
After introduction of free valences, radical or ionic centers, or principal characteristic groups, the maximum number of noncumulative double bonds is inserted and any hydrogen atoms needed to achieve tetravalency are denoted as ‘added hydrogen’ (see P-14.6). Lowest permissible locants are assigned first to suffixes and then to any ‘added hydrogen atoms’.

In names, each ‘added hydrogen’ is expressed by the letter *H* preceded by the appropriate locant. The ‘added hydrogen’ expression is enclosed in parentheses and inserted into the name after the locant or locants denoting the free valence(s), radical or ionic center(s), or principal characteristic group(s).

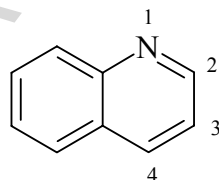
Examples:



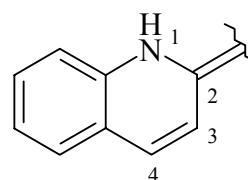
naphthalene (PIN, parent hydride)



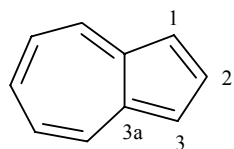
naphthalene-1(2*H*)-one (PIN)



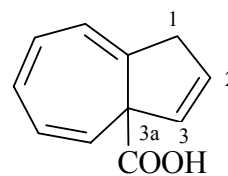
quinoline (PIN, parent hydride)



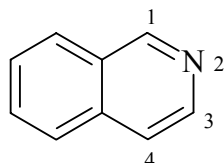
quinolin-2(1*H*)-ylidene (PIN)



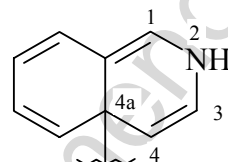
azulene (PIN, parent hydride)



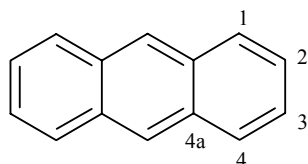
azulene-3a(1*H*)-carboxylic acid (PIN)



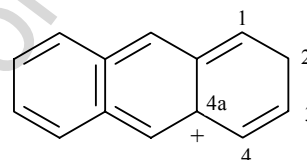
isoquinoline (PIN, parent hydride)



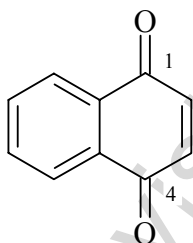
isoquinolin-4a(2*H*)-yl (PIN)



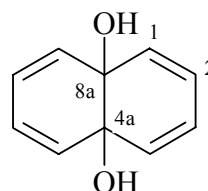
anthracene (PIN, parent hydride)



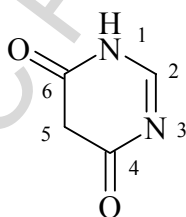
anthracen-4a(2*H*)-ylium (PIN)



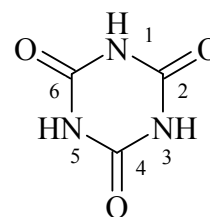
naphthalene-1,4-dione (PIN)



naphthalene-4a,8a-diol (PIN)



pyrimidine-4,6(1*H*,5*H*)-dione (PIN)

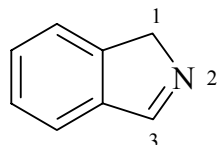


1,3,5-triazine-2,4,6(1*H*,3*H*,5*H*)-trione (PIN)

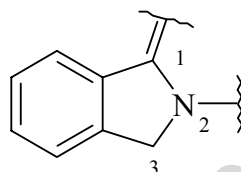
**P-56.4.2** Substitution in compounds with indicated hydrogen atoms

Indicated hydrogen atoms are assigned the lowest locants permitted by the structure unless they can accommodate structural features elsewhere in the structure. Then, lowest possible locants are assigned to the nomenclatural feature cited as suffix and finally to added hydrogen atom(s), as noted in P-56.4.1.

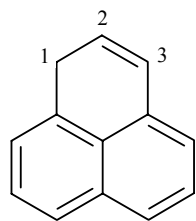
Examples:



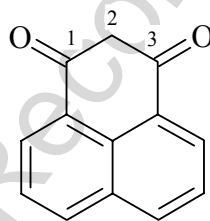
1*H*-indole (PIN)



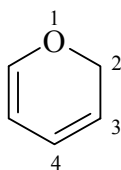
1*H*-indol-2(3*H*)-yl-1-ylidene (PIN)  
(not 2*H*-indol-2-yl-1(3*H*)-ylidene)



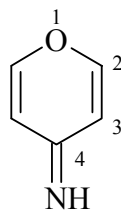
1*H*-phenalene (PIN)



1*H*-phenalen-1,3(2*H*)-dione (PIN)



2*H*-pyran (PIN)



4*H*-pyran-4-imine (PIN)

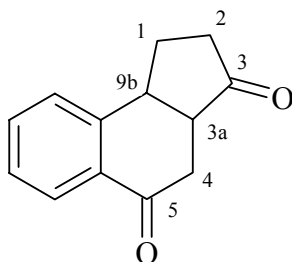
**P-56.4.3** Compounds with indicated and/or added hydrogen atoms and additional saturation

Hydro prefixes are used to indicate additional saturation of double bonds in compounds already containing indicated and/or added hydrogen atoms. Lowest locants are assigned in the following order:

- indicated hydrogen atoms
- suffixes and associated added hydrogen atoms
- hydro prefixes

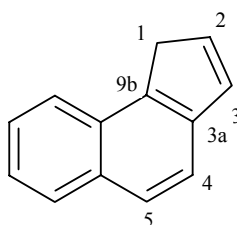
In names, hydro prefixes, indicated hydrogen, parent hydride, and suffixes appear in that order.

Examples:

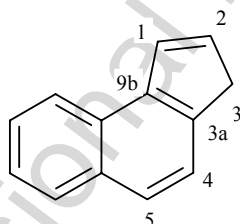


1,3a,4,9b-tetrahydro-3*H*-cyclopenta[*a*]naphthalene-3,5(2*H*)-dione (PIN)

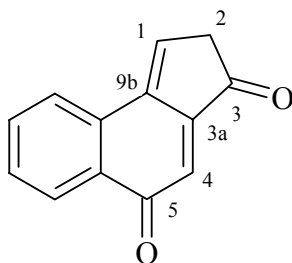
Guide to name construction.



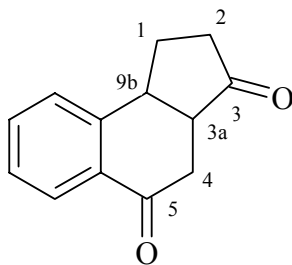
Step 1: Parent structure: 1*H*-cyclopenta[*a*]naphthalene (PIN, parent hydride)  
(indicated hydrogen atom at the lowest possible position)



Step 2: 3*H*-cyclopenta[*a*]naphthalene (PIN, parent hydride; indicated hydrogen atom moved from position 1 to position 3 to accommodate further substitution by the ketone suffix 'one')



Step 3: 3*H*-cyclopenta[*a*]naphthalene-3,5(2*H*)-dione (PIN, at position 3, the ketone suffix 'one' introduced by direct substitution; at position 5, the introduction of the one suffix requires an added hydrogen atom at position 2, the position with the lowest locant possible)

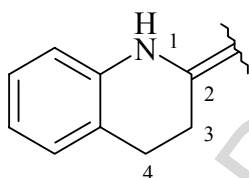


Step 4: 1,3a,4,9a-tetrahydro-3*H*-cyclopenta[*a*]naphthalene-3,5(2*H*)-dione (PIN)  
(the prefix tetrahydro is added to saturate double bonds  
at 1-9a and 3a-4)

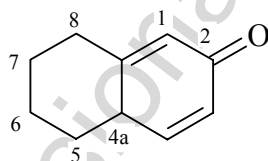
These four steps lead to the preferred IUPAC name:

1,3a,4,9b-tetrahydro-3*H*-cyclopenta[*a*]naphthalene-3,5(2*H*)-dione (PIN)

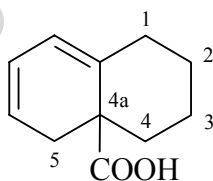
Further examples:



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



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



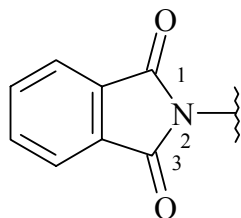
1,3,4,5-tetrahydronaphthalene-4a(2*H*)-carboxylic acid (PIN)

#### P-56.4.4 Compounds with detachable prefixes

Substituent groups denoted by detachable (alphabetized) prefixes are introduced, as required, as the last step in the name construction. The addition of the necessary amount of hydrogen atoms to saturate double bonds is a prerequisite to the introduction of detachable substituents. In names,

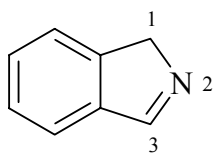
detachable prefixes denoting substituent groups are placed at the front of the name, before hydro prefixes.

Examples:

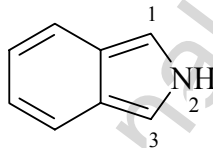


1,3-dioxo-1,3-dihydro-2*H*-isoindol-2-yl (PIN)

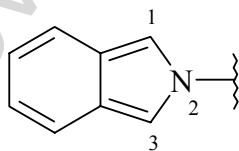
Guidelines for name construction:



Step 1.: 1*H*-isoindole (PIN, parent hydride)  
(‘indicated hydrogen’ atom at the lowest possible position)

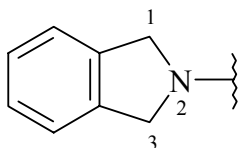


Step 2. 2*H*-isoindole (PIN, parent hydride)  
(‘indicated hydrogen’ atom moved to position 2 to accommodate the introduction of the free valence)

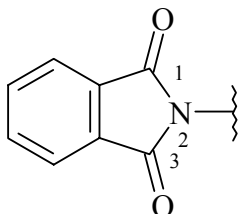


Step 3. 2*H*-isoindol-2-yl (PIN)  
(the suffix ‘yl’ indicates the presence of a free valence in position 2; no ‘added hydrogen’ is necessary)





Step 4. 1,3-dihydro-2*H*-isoindol-2-yl (PIN)  
(hydro prefixes are necessary to introduce the number of hydrogen atoms required for the introduction of the divalent 'ylidene' suffix)



Step 5. 1,3-dioxo-1,3-dihydro-2*H*-isoindol-2-yl (PIN)  
(two ketonic substituent groups introduced denoted by the detachable prefix 'oxo')

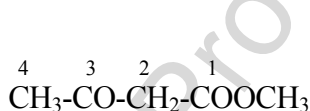
These five steps lead to the preferred IUPAC name:

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

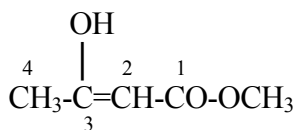
### P-57 Selecting names for tautomeric structures

Naming tautomers is not a major problem for preferred IUPAC nomenclature, because each tautomer can be named individually. It is traditional to denote a mixture of tautomers by naming the component belonging to the highest class. A preferred IUPAC name for a tautomeric structure is given in accordance with the indicated structure chosen by the authors that selected a preferred structure.

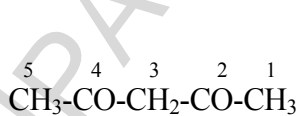
Examples:



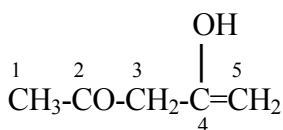
methyl 3-oxobutanoate (PIN)



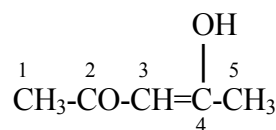
methyl 3-hydroxybut-2-enoate (PIN)



pentane-2,4-dione (PIN)



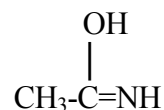
4-hydroxypent-4-en-2-one (PIN)



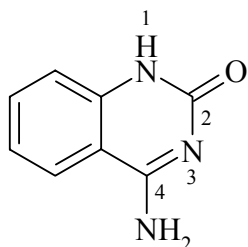
4-hydroxypent-3-en-2-one (PIN)



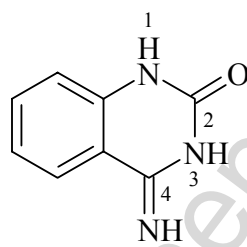
acetamide (PIN)



acetimidic acid (PIN)



4-aminoquinazolin-2(1*H*)-one (PIN)



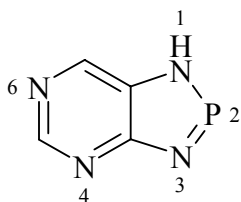
4-imino-3,4-dihydroquinazolin-2(1*H*)-one (PIN)



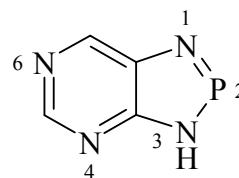
acetohydrazoneamide (PIN)



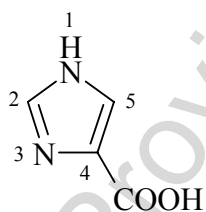
acetimidohydrazide (PIN)



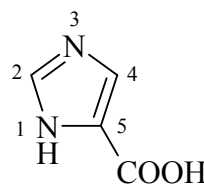
1*H*-1,3,2-diazaphospholo[4,5-*d*]pyrimidine (PIN)



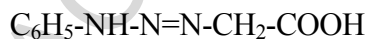
3*H*-1,3,2-diazaphospholo[4,5-*d*]pyrimidine (PIN)



1*H*-imidazole-4-carboxylic acid (PIN)



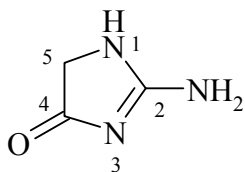
1*H*-imidazole-5-carboxylic acid (PIN)



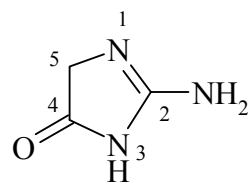
(3-phenyltriaz-1-en-1-yl)acetic acid (PIN)



(3-phenyltriaz-2-en-1-yl)acetic acid (PIN)

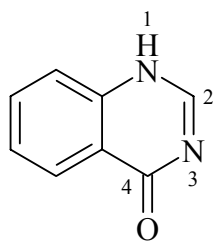


2-amino-1,5-dihydro-4*H*-imidazol-4-one (PIN)

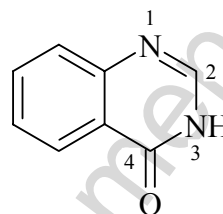


2-amino-3,5-dihydro-4*H*-imidazol-4-one (PIN)

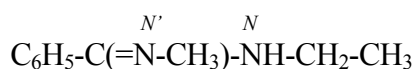
:



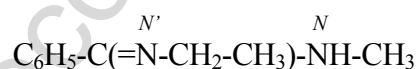
quinazolin-4(1*H*)-one (PIN)



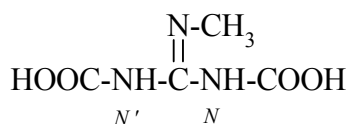
quinazolin-4(3*H*)-one (PIN)



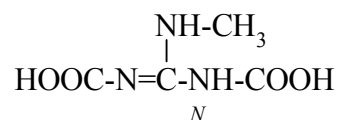
*N*-ethyl-*N'*-methylbenzenecarboximidamide (PIN)



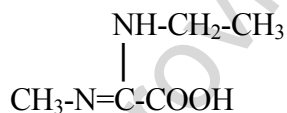
*N'*-ethyl-*N*-methylbenzenecarboximidamide (PIN)



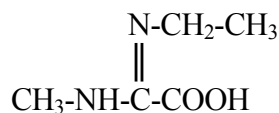
*N,N'*-(methylcarbonimidoyl)di-carbamic acid (PIN)



[*N'*-carboxy-*N*-methylcarbamimidoyl]-carbamic acid (PIN)



(ethylamino)(methylimino)acetic acid (PIN)



(ethylimino)(methylamino)acetic acid (PIN)

## P-58 Name construction

P-58.0 Introduction

P-58.1 General methodology

P-58.2 Suffixes and prefixes

P-58.3 Examples illustrating the methodology

## P-58.0 Introduction

This Section describes the procedure for the systematic formation of a preferred IUPAC name for an organic compound. This procedure can also be followed for generation of names for general nomenclature.

### P-58.1 General methodology

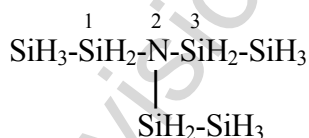
The procedure for formation of a preferred systematic name for an organic compound involves a number of steps outlined in this and in the following subsections, to be taken as far as they are applicable in the following order.

**P-58.1.1** From the nature of the compound, determine the type(s) of nomenclature (see P-15) and operations (see P-13) to be used. Although the so-called 'substitutive nomenclature' is the preferred type of nomenclature, other nomenclature types must be used when specified by strict rules, for instance 'skeletal replacement ('a') nomenclature, and 'functional class nomenclature' for compounds such as esters, and acid halides.

**P-58.1.2** Determine the class to which the compound belongs and the characteristic group to be cited as the suffix (if any) in accord with the seniority order of classes as indicated in P-41 or as a functional class name (see P-15.2). Only one kind of characteristic group (known as the principal group) can be cited as suffix or functional class name. All atoms or groups not so cited must be specified as substituent prefixes. Radicals and ions are named using suffixes that have the unique property of being cumulative, both among themselves and in conjunction with certain suffixes that express characteristic groups.

**P-58.1.3** Determine the senior parent hydride, including any appropriate nondetachable prefixes as described in Chapter 2 and in P-52 for preferred names, or functional parent compound as described in P-34 and P-55 for preferred names.

Example:



2-disilanyl-1,3-bis(silyl)disilazane (preselected name)

[disilazane is a parent hydride, not a functional parent compound (see P-21.2.3.1) and since N containing parent hydrides > Si containing parent hydrides, disilazane must be chosen over disilane]

**P-58.1.4** Name the parent hydride and the principal characteristic group, if any, or the functional parent compound, using rules indicated in P-58 in order to take functional modifications into consideration.

**P-58.1.5** Determine affixes and/or prefixes, in accordance with P-15.5 and Appendix 2, and appropriate multiplying prefixes (see P-14.2) and number the parent structure as far as possible using the general rule P-14.4.

**P-58.1.6** Name the detachable substitutive prefixes in accordance with P-56 and P-57 for preferred prefixes and complete the numbering of the structure, if necessary.

**P-58.1.7** Assemble the components into a complete name, using alphanumerical order described in P-14.4 and P-14.5 for all substitutive detachable prefixes.

**P-58.1.8** Complete the name with all required descriptors for indicating changes from standard valences, isotopic modifications, and stereochemical features.

**P-58.2** Suffixes and prefixes

In substitutive nomenclature, some characteristic groups can be denoted either as suffixes or prefixes (see P-33 and P-36), but others only as prefixes (see Table 5.2). Functional class names differ in that a separate word (or a suffix in some languages) designating the name of a functional class is associated with a substituent group name describing the remainder of the structure.

Characteristic groups that can be cited as suffixes in substitutive nomenclature are not necessarily identical with groups designated by the name of a corresponding functional class when functional class names are formed (e.g., butanone and ethyl methyl ketone, where 'one' denotes =O and 'ketone' denotes -CO-).

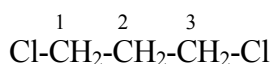
The characteristic groups listed in Table 5.2 are always cited as prefixes to the name of the parent structure described in Chapter 2. Multiplying prefixes (see P-14.2) and locants are added as necessary (see P-14.3)

**Table 5.2 Characteristic groups always cited as prefixes in substitutive nomenclature**

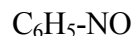
Characteristic group	Prefix	Characteristic group	Prefix
-Br	bromo	=N <sub>2</sub>	diazo
-Cl	chloro	-N <sub>3</sub>	azido
-ClO	chlorosyl	-NO	nitroso
-ClO <sub>2</sub>	chloryl	-NO <sub>2</sub>	nitro
-ClO <sub>3</sub>	perchloryl-	-PO	phosphoroso
-F	fluoro	-PO <sub>2</sub>	phospho
-I	iodo	-NCO	isocyanato
-IO	iodosyl	-NC	isocyano
-IO <sub>2</sub>	iodyl	-OR	(R)-oxy

\* R designates an 'organic' substituent group.

Examples:



1,3-dichloropropane (PIN)



nitrosobenzene (PIN)

Characteristic groups other than those listed in Table 5.2 may be cited as either suffixes or prefixes to the name of the parent hydride.

If characteristic groups other than those given in Table 5.2 are present, one (and only one) kind must be cited as suffix (the principal characteristic group) for classes other than radicals and ions.

When a compound contains more than one kind of characteristic group not given in Table 5.2, the principal characteristic group is the one that characterizes the class occurring earliest (i.e., nearest to the top) in the seniority order of classes (see P-41.2, and P-42 and P-43, if necessary). All other characteristic groups are cited as prefixes.

If, and only if, the complete suffix (that is, the suffix plus its multiplying prefixes, if any, as described in Appendix 1) begins with a vowel, a terminal letter 'e' (if any) of the preceding parent hydride name is elided. Elision or retention of the terminal letter 'e' is independent of the presence of numerals between it and the following letter.

When a substituent is itself substituted (compound substituent, see P-35, P-36, and P-46), all the subsidiary substituents are named as prefixes. The substituent bearing the subsidiary substituent is regarded as a parent substituent (analogous to a parent hydride). The nomenclature of the whole substituent is subject to all the procedures adopted for compounds, with two exceptions, which are:

- (a) that no characteristic group is expressed as a suffix (instead, a suffix such as 'yl', 'ylidene', etc., is used); and
- (b) that the point of attachment of the substituent has the lowest permissible locant.

When the parent hydride (principal chain, ring system), principal group and substituents have been selected and named, the numbering of the complete compound is allocated using the rule of lowest locants. General rules for locants and numbering are described in P-14.4. They do apply each and every time a name is constructed, not only for substitutive and functional class nomenclature, but for all types of nomenclature.

The list of seniority of structural features that receive lowest possible locants has been refined by reallocating the placement of 'a' prefixes for skeletal replacement in chains and by giving a special status of detachable prefix to hydro/dehydro prefixes.

Insofar as the preceding rules leave a choice, the starting point and direction of numbering of a compound are chosen so as to give lowest locants to the structural features (if present) considered successively in the order given until a decision is reached.

- (a) fixed numbering, as for naphthalene, bicyclo[2.2.2]octane, etc.
- (b) heteroatoms in heterocycles and in acyclic parent structures
- (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
- (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 in the name).

The various components having been selected, named and numbered, any necessary additive or subtractive modifications are made, and the complete name is assembled, prefixes being arranged in alphanumerical order. Notifications for changes in standard valences, isotopic modifiers and stereodescriptors are added, as required.

**P-58.3** Examples illustrating the methodology described above

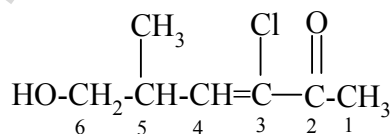
- P-58.3.1 Selection of parent compounds
- P-58.3.2 Seniority of heteroatoms over suffixes
- P-58.3.3 Seniority of suffixes over unsaturation
- P-58.3.4 Seniority of hydro/dehydro prefixes over detachable substituent prefixes
- P-58.3.5 Treatment of detachable prefixes

**P-58.3.1** Selection of parent compounds

After the principal group has been chosen and named, the parent compound is chosen by one of the following methods. For details of numbering, see Chapter 2 describing the numbering of the various parent hydrides and the general rule of lowest locants as formulated in P-14.3. For the arrangement of prefixes, see the general rule on alphanumerical order described in P-14.5.

**P-58.3.1.1** If the compound is purely acyclic, the principal chain is chosen as parent by the method described in P-44.

Example:



Analysis:

Principal group:	=CO	one
Principal chain:	CH <sub>3</sub> -CH <sub>2</sub> -CH <sub>2</sub> -CH <sub>2</sub> -CH <sub>2</sub> -CH <sub>3</sub>	hexane
Principal chain including principal group	CH <sub>3</sub> -CH <sub>2</sub> -CH <sub>2</sub> -CH <sub>2</sub> -CO-CH <sub>3</sub>	hexan-2-one
Subtractive modification	CH <sub>2</sub> -CH <sub>2</sub> -CH=CH-CO-CH <sub>3</sub>	hex-3-en-2-one
Prefixes:	Cl-	chloro
	HO-	hydroxy
	CH <sub>3</sub> -	methyl

Together with other rules, this analysis leads to the name:

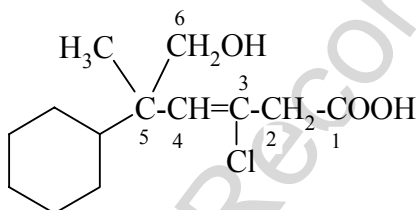
3-chloro-6-hydroxy-5-methylhex-3-en-2-one (PIN)

Guide to construction of this name.

The suffix 'one' receives the lowest possible locant, 2, thus determining the direction of numbering of the chain. Two hexane chains are possible; the principal chain, in accord with the criteria for selecting the principal chain, is the one that is most substituted (3 substituents compared to 2). Unsaturation is denoted by the ending 'ene'. The three prefixes are arranged in alphanumerical order to complete the name.

**P-58.3.1.2** If the principal group occurs only in a chain that carries a cyclic substituent, the compound is named as an acyclic compound into which the cyclic component is expressed by a substituent prefix.

Example:



Analysis:

Principal group:	-(C)OOH	oic acid
Principal chain:	CH <sub>3</sub> -CH <sub>2</sub> -CH <sub>2</sub> -CH <sub>2</sub> -CH <sub>2</sub> -CH <sub>3</sub>	hexane
Principal chain including principal group	CH <sub>3</sub> -CH <sub>2</sub> -CH <sub>2</sub> -CH <sub>2</sub> -CH <sub>2</sub> -COOH	hexanoic acid
Subtractive modification	CH <sub>3</sub> -CH <sub>2</sub> -CH=CH <sub>2</sub> -CH <sub>2</sub> -COOH	hex-3-enoic acid
Prefixes:	Cl-	chloro
	C <sub>6</sub> H <sub>11</sub> -	cyclohexyl
	HO-	hydroxy
	CH <sub>3</sub> -	methyl

Together with other rules, this analysis leads to the name:

3-chloro-5-cyclohexyl-6-hydroxy-5-methylhex-3-enoic acid (PIN)

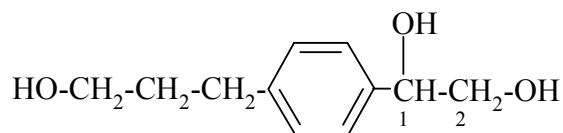
Guide to the construction of this name.

The presence of a carboxylic acid group at the end of the chain determines the direction of numbering of that chain. The 'ene' ending and the prefixes, in alphanumerical order, are located on the chain in accord with the determined numbering.



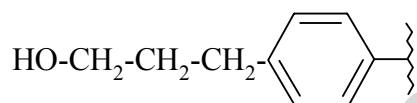
**P-58.3.1.3** If the principal group occurs in two or more carbon chains that are not attached to one another (that is, do not together form a continuous or branched chain but are separated by, for instance, a ring or a heteroatom), and when multiplicative nomenclature is not possible, then that chain carrying the largest number of the principal groups is chosen as parent for nomenclature; if the numbers of these groups in two or more chains are the same, choice is made by the principles for selection of the principal chain.

Example 1:



Analysis:

Principal group:	-OH	ol
Principal chain, carrying two OH groups:	HO-CH <sub>2</sub> -CH <sub>2</sub> -OH	ethanediol
Prefix:		



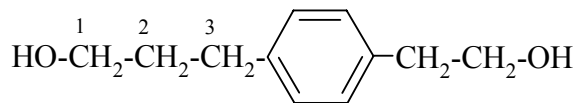
Prefix components:	-OH	hydroxy
	-CH <sub>2</sub> -CH <sub>2</sub> -CH <sub>3</sub>	propyl
	-C <sub>6</sub> H <sub>5</sub>	phenyl

Prefix name: 4-(3-hydroxypropyl)phenyl

Together with other rules, this analysis leads to the name:

1-[4-(3-hydroxypropyl)phenyl]ethane-1,2-diol (PIN)

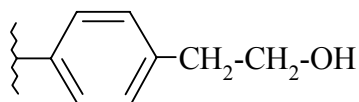
Example 2: In the following example, the longest chain is chosen as parent hydride, in accord with the criteria for selecting the principal chain. This compound can also be named by conjunctive nomenclature (see P-13.5)



Analysis:

Principal group:	-OH	ol
Parent hydride:	CH <sub>3</sub> -CH <sub>2</sub> -CH <sub>3</sub>	propane
Parent hydride + principal group	CH <sub>3</sub> -CH <sub>2</sub> -CH <sub>2</sub> -OH	propan-1-ol

Prefix:



Prefix components:	-OH	hydroxy
	-CH <sub>2</sub> -CH <sub>2</sub>	ethyl
	-C <sub>6</sub> H <sub>5</sub>	phenyl

Prefix name: 4-(2-hydroxyethyl)phenyl

Together with other rules, this analysis leads to the substitutive name:

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

Example 3: A multiplicative name is formed when identical parent structures are attached symmetrically to a central component (the parent structures may be unsymmetrically substituted). The numbering of the multiplied unit (including the characteristic group) is retained. This compound can also be named by conjunctive nomenclature; this procedure is illustrated in P-46.3.1.7.



Analysis:

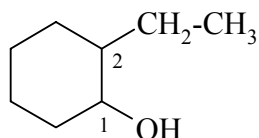
Principal group:	-OH	ol
Parent hydride:	CH <sub>3</sub> -CH <sub>2</sub> -CH <sub>3</sub>	propane
Parent hydride + principal group	<sup>3</sup> CH <sub>3</sub> - <sup>2</sup> CH <sub>2</sub> - <sup>1</sup> CH <sub>2</sub> -OH	propanol
Multiplicative connecting group:	-C <sub>6</sub> H <sub>4</sub> -	1,4-phenylene

This, together with other rules, leads to the name:

3,3'-(1,4-phenylene)di(propan-1-ol) (PIN)

**P-58.3.1.4** If the principal group occurs only in one cyclic system, that cyclic system forms the parent for nomenclature.

Example:



Analysis:

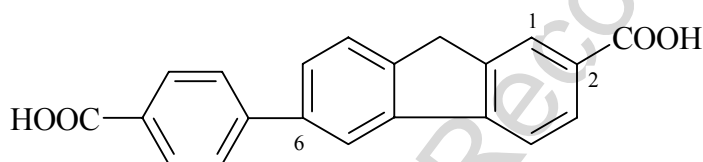
Principal group:	-OH	ol
Parent hydride:	C <sub>6</sub> H <sub>12</sub>	cyclohexane
Prefix:	-CH <sub>2</sub> -CH <sub>3</sub>	ethyl

Together with other rules, this analysis leads to the name:

2-ethylcyclohexan-1-ol (PIN)

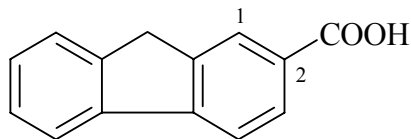
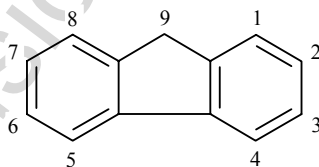
**P-58.3.1.5** If the principal group occurs in more than one cyclic system, the system chosen as parent for nomenclature is in accordance with the criteria for choosing a senior ring or ring system.

Example:



Analysis:

Principal group:	-COOH	carboxylic acid
Senior ring system for parent:	fluorene	



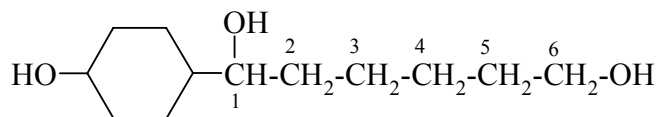
Name of parent including principal group:	fluorene-2-carboxylic acid
Prefixes	-C <sub>6</sub> H <sub>5</sub> -COOH
	phenyl carboxy

Together with other rules, this analysis leads to the name:

6-(4-carboxyphenyl)fluorene-2-carboxylic acid (PIN)

**P-58.3.1.6** If the principal group occurs both in a chain and in a cyclic system, the parent for nomenclature is that portion in which the principal group occurs in the greater number; if the number of occurrences of the principal group is the same in two or more portions, the ring or ring system is chosen as parent for nomenclature.

Example 1:



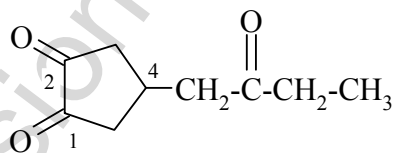
Analysis:

Principal group:		-OH	ol
Component with the greater number of the principal group:		HO-CH <sub>2</sub> -CH <sub>2</sub> -CH <sub>2</sub> -CH <sub>2</sub> -CH <sub>2</sub> -CH <sub>2</sub> -OH	
Name of parent including suffix:		hexane-1,6-diol	
Prefixes:	-C <sub>6</sub> H <sub>11</sub>	cyclohexyl	
	-OH	hydroxy	

Together with other rules this analysis leads to the name:

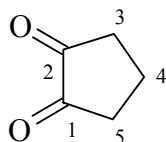
1-(4-hydroxycyclohexyl)hexane-1,6-diol (PIN)

Example 2:



Analysis:

Principal group:		=O	one
Component with the greater number of the principal group:			



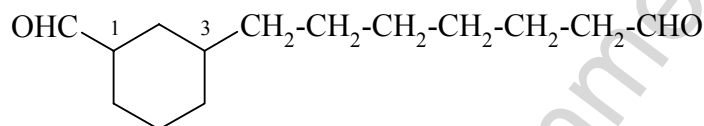
Name of parent including suffix:		cyclopentane-1,2-dione	
Prefixes:	=O	oxo	
	CH <sub>3</sub> -CH <sub>2</sub> -CH <sub>2</sub> -CH <sub>2</sub> -	butyl	

Together with other rules, this analysis leads to the name:

4-(2-oxobutyl)cyclopentane-1,2-dione (PIN)

**P-58.3.1.7** If the number of occurrences of the principal group is the same in two or more nomenclaturally significant parts of the compound, preferred IUPAC names are formed by choosing the ring or ring system as parent for nomenclature. In general nomenclature, a ring or ring system or a chain may be chosen as parent, depending on the importance given to a specific portion (Rule P-44.1.2.2). When the principal group identified by this suffix is not attached directly to a ring or ring system, a principal chain must be chosen.

Example:



Analysis:

Principal group:	-CHO	carbaldehyde or al
Parent:	ring	cyclohexane
	chain	heptane
Parent including suffix:	ring	cyclohexane-1-carbaldehyde
	chain	heptanal
Prefixes:	-CH <sub>2</sub> [CH <sub>2</sub> ] <sub>5</sub> -CHO	7-oxoheptyl
	-C <sub>6</sub> H <sub>4</sub> -CHO(3)	3-formylcyclohexyl

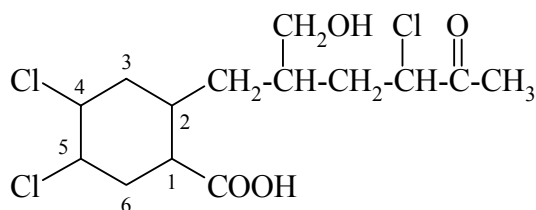
Together with other rules, this analysis leads to the names:

3-(7-oxoheptyl)cyclohexane-1-carbaldehyde (PIN)

7-(3-formylcyclohexyl)heptanal

**P-58.3.1.8** When a substituent is itself substituted, all the subsidiary substituents are named as prefixes. The substituent bearing the subsidiary substituents is regarded as a 'parent substituent' (analogous to a parent compound). The nomenclature of the whole substituent is subject to all the procedures adopted for compounds (for instance, choice of principal chain), with two exceptions, namely: (a) that no suffix is used, and (b) that the point of attachment of the substituent bears the lowest permissible locant number depending on the nomenclature of the substituent group, alkyl or alkanyl.

Example:



Analysis:

Principal group:	-COOH	carboxylic acid
Parent:		cyclohexane
Primary substituents to be named as prefixes:	-Cl	chloro
	-CH <sub>2</sub> -CH-CH <sub>2</sub> -CHCl-CO-CH <sub>3</sub>	
Parent substituent chain:	-CH <sub>2</sub> -CH <sub>2</sub> -CH <sub>2</sub> -CH <sub>2</sub> -CH <sub>2</sub> -CH <sub>3</sub>	hexyl

Secondary prefixes:	-Cl	chloro
	=O	oxo
	-CH <sub>2</sub> -OH	

Secondary compound prefix name composed of:

-CH <sub>3</sub>	methyl
-OH	hydroxy

Name of secondary compound prefix: hydroxymethyl

Name of substituted primary prefix: 4-chloro-2-(hydroxymethyl)-5-oxohexyl

Together with other rules, this analysis leads to the name:

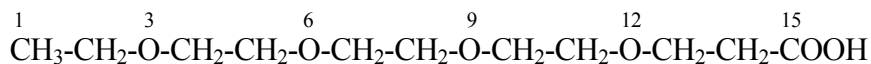
4,5-dichloro-2-[4-chloro-2-(hydroxymethyl)-5-oxohexyl]cyclohexane-1-carboxylic acid (PIN)

### P-58.3.2 Seniority of heteroatoms over suffixes

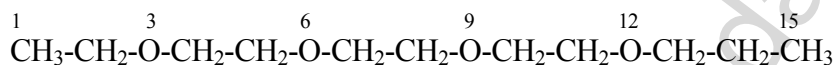
Heterocyclic compounds and chains modified by skeletal replacement ('a') nomenclature are treated similarly. They are considered as parent compounds with a fixed numbering. As a consequence, heteroatoms have seniority for low locants and suffixes are assigned the next lowest possible locants. For chains, this order is a major change from the 1979 organic nomenclature recommendations in which suffixes had seniority over heteroatoms.

**P-58.3.2.1** For chains the replacement operation is applied to the hydrocarbon parent to create a new parent hydride with a fixed numbering. Suffixes receive the lowest possible locants in accordance with the resulting numbering.

Example:



Principal group:	-(C)OOH	oic acid
Parent hydrocarbon	CH <sub>3</sub> -[CH <sub>2</sub> ] <sub>13</sub> -CH <sub>3</sub>	pentadecane
'a' Prefix	-O-	oxa
Heteroacyclic parent		



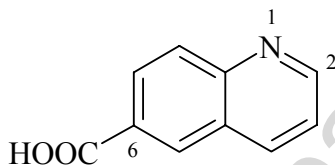
Name of heteroacyclic parent      3,6,9,12-tetraoxapentadecane

Together with other rules, this analysis leads to the name:

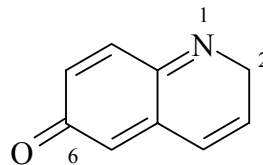
3,6,9,12-tetraoxapentadecan-15-oic acid (PIN)

**P-58.3.2.2** Heterocyclic compounds having retained and systematic names are considered as parent compounds. Thus, suffixes are added and assigned lowest possible locants in accordance with the fixed numbering of the heterocyclic ring or ring system. Added hydrogen atoms, if needed, are assigned next lowest possible locants.

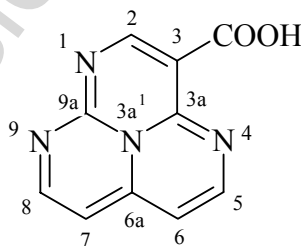
Examples:



quinoline-6-carboxylic acid (PIN)



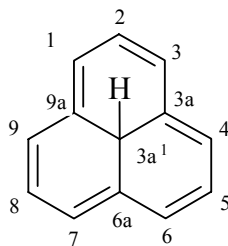
quinolin-6(2*H*)-one (PIN)



Analysis:

Principal group:	-COOH	carboxylic acid
Parent hydrocarbon:		3a <sup>1</sup> <i>H</i> -phenalene

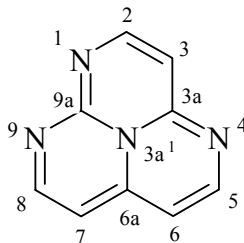
[Note the new system of numbering for internal atoms in fused systems, 3a<sup>1</sup> in place of 9b; see P-25.3.3.3.]



Skeletal replacement ('a') prefix:

-N<

aza



Name of parent heterocycle: 1,3a<sup>1</sup>,4,9-tetraazaphenalene

Together with other rules, this analysis leads to the name:

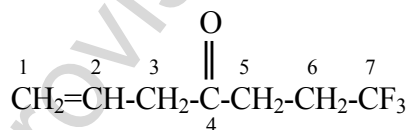
1,3a<sup>1</sup>,4,9-tetraazaphenalene-3-carboxylic acid (PIN)

[Note: The indicated hydrogen, 3a<sup>1</sup>H, of the parent hydrocarbon does not appear in the name of the heterocycle.]

### P-58.3.3. Seniority of suffixes over unsaturation

**P-58.3.3.1** After suffixes, if there is a choice, low locants are assigned to 'ene' and 'yne' endings, and then to detachable prefixes, if applicable.

Example:



Analysis:

Principal group:	=O	one
Parent hydride:	CH <sub>3</sub> -[CH <sub>2</sub> ] <sub>5</sub> -CH <sub>3</sub>	heptane
Parent hydride + principal group	CH <sub>3</sub> -[CH <sub>2</sub> ] <sub>2</sub> -CO-[CH <sub>2</sub> ] <sub>2</sub> -CH <sub>3</sub>	heptan-4-one
Subtractive modification	>C=C<	ene
Substituent prefix	-F	fluoro

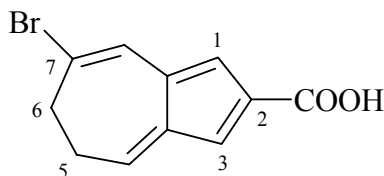
Together with other rules, this analysis leads to the name:

7,7,7-trifluorohept-1-en-4-one (PIN)



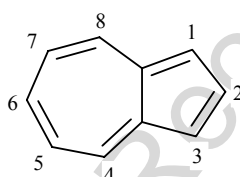
**P-58.3.3.2** Hydro and dehydro prefixes are used to express a change in the degree of hydrogenation of the parent hydride. In these recommendations, these prefixes are considered detachable but only in the context of numbering; they are not included among the detachable substituent prefixes. In names, they are cited immediately before the name of the parent compound, after those of detachable substituent prefixes arranged in alphanumerical order.

Example:

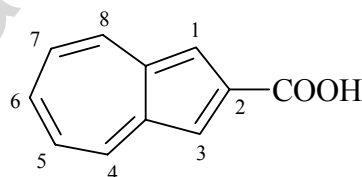


Analysis:

Principal group:  $-\text{COOH}$  carboxylic acid  
Parent hydride: azulene



Parent hydride + principal group:



azulene-2-carboxylic acid

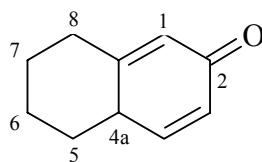
Saturation prefix	$-\text{H}$	hydro
Prefix	$-\text{Br}$	bromo

Together with other rules, this analysis leads to the name:

7-bromo-5,6-dihydroazulene-2-carboxylic acid (PIN)

**P-58.3.3.3** Mancude ketones, imines and 'ylidene' substituent groups are named by the 'added hydrogen' method. If there is a choice, 'indicated hydrogen' atoms have priority for low locants, then suffixes, 'added hydrogen' atoms and finally hydro prefixes, in that order.

Example 1:



Analysis:

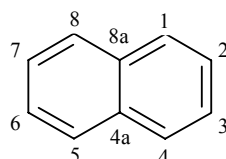
Principal group:

=O

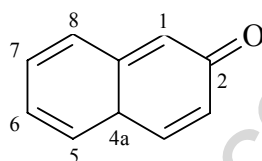
one

Parent hydride:

naphthalene



Parent hydride + principal group:



naphthalen-2(4aH)-one

Saturation Prefix

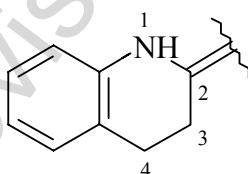
-H

hydro

Together with other rules, this analysis leads to the name:

5,6,7,8-tetrahydronaphthalen-2(4aH)-one (PIN)

Example 2:



Analysis:

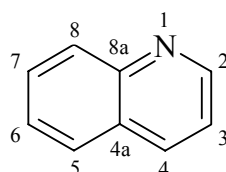
Free valences:

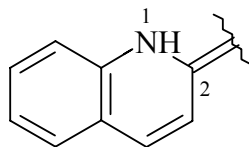
X=

ylidene

Parent hydride:

quinoline





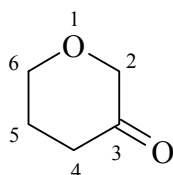
Parent hydride + free valences:      uinolin-2(1*H*)-ylidene

Saturation prefix:                      -H                      hydro

Together with other rules, this analysis leads to the name:

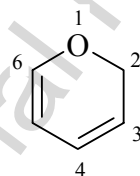
3,4-dihydroquinolin-2(1*H*)-ylidene (PIN)

Example 3:

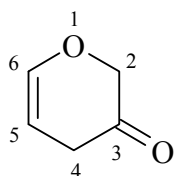


Analysis:

Principal group:                              =O                      one  
Parent hydride:                              2*H*-pyran



Parent hydride + principal group:



2*H*-pyran-3(4*H*)-one

Saturation prefix:                              -H                      hydro

Together with other rules, this analysis leads to the name:

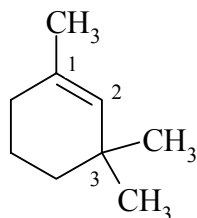
dihydro-2*H*-pyran-3(4*H*)-one (PIN)

(Note: no locants are required when the cyclic system becomes fully saturated using hydro prefixes; see P-14.3.3)

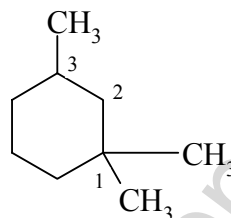
**P-58.3.4.** Seniority of hydro prefixes over detachable substituent prefixes

If there is a choice, low locants are assigned to 'ene' and 'yne' endings and 'hydro/dehydro' prefixes.

Examples:

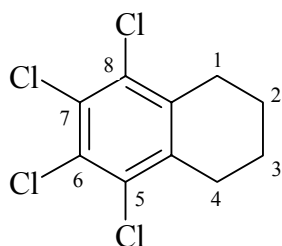


compare with

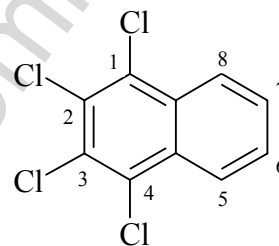


1,3,3-trimethylcyclohex-1-ene (PIN)

1,1,3-trimethylcyclohexane (PIN)



compare with



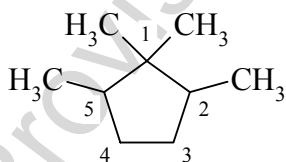
5,6,7,8-tetrachloro-1,2,3,4-tetrahydronaphthalene (PIN)

1,2,3,4-tetrachloronaphthalene (PIN)

**P-58.3.5** Treatment of detachable prefixes

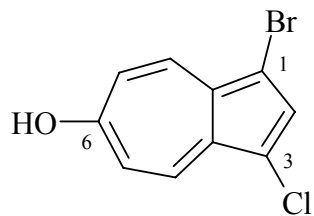
If there is a choice, low locants are assigned to detachable prefixes considered together, and, if there is a further choice, in alphanumerical order.

Examples:

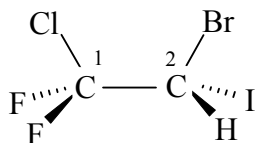


1,1,2,5-tetramethylcyclopentane (PIN)

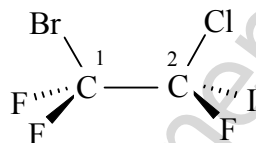
(not 1,2,2,3-tetramethylcyclopentane; the set of locants 1,1,2,5 is lower than 1,2,2,3)



1-bromo-3-chloroazulen-6-ol (PIN)



2-bromo-1-chloro-1,1-difluoro-  
2-iodoethane (PIN)



1-bromo-2-chloro-1,1,2-trifluoro-  
2-iodoethane (PIN)