

## CHAPTER 6 APPLICATIONS TO SPECIFIC CLASSES OF COMPOUNDS

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### P-60 Introduction

**P-60.1** The recommendations in this chapter illustrate how the general principles and specific rules set out in the preceding sections are applied to various types of compounds.

Section 61 describes compounds that are named substitutively only by the prefix mode. It includes and exemplifies binary compounds formed by substituting parent hydrides by substituents derived from other parent hydrides and by characteristic groups that are always used as prefixes.

Sections 62 to 66 include compounds that are named, in substitutive nomenclature, by suffixes and prefixes, and by means of other types of nomenclature. The traditional classes from acids to imines are described (see P-41).

Section 67 describes nomenclature of organic derivatives of noncarbon acids and their functional replacement analogs.

Section P-68 covers the nomenclature of organic compounds of the Groups 13, 14, 15, 16, and 17 elements not included in Sections 62-67.

Section 69 describes the nomenclature of organometallic compounds.

### P-60.2 Presentation of names.

Names described in this Chapter are presented in a systematic way. General methods recommended to generate IUPAC preferred names are all described in a simplified way with reference to the following full descriptions.

- (a) Names formed substitutively using suffixes follow the general method described in Section 15.1. Substitutive names are formed by adding a suffix such as 'al', 'ol', 'yl', 'carbaldehyde', 'carboxylic acid', etc., to the name of a parent hydride, with elision of the final letter 'e' of the parent hydride, if any, before 'a', 'i', 'o', 'u', and 'y'.
- (b) Names formed substitutively by using prefixes follow the general method. Substitutive names are formed by adding a prefix such as amino, hydroxy, etc., to the name of the parent hydride or parent compound; in order to preserve their formal identity, there is no elision of the last letter of these prefixes

- (c) Names formed by functional class nomenclature follow the general method described in Section 15.2. Functional class names are formed by citing the name of the class, such as alcohol, oxide, ketone, etc., preceded by the name of the substituent groups cited in alphabetical order and separated by a space, if required.
- (d) Names formed by skeletal replacement ('a') nomenclature follow the methodology described in Section 15.4.
- (e) Functional parents are discussed in terms of preferred names and names that can be used in general nomenclature.

The method to generate preferred IUPAC names is indicated by a phrase such as 'This method generates preferred IUPAC names' or 'Method (1) leads to preferred IUPAC names. The abbreviation 'PIN' is placed after preferred IUPAC names. Names that were recommended in the past but are not included in these recommendations are described parenthetically by the phrase 'no longer recommended'. For example, the prefix 'methylene' is 'no longer recommended' in IUPAC nomenclature to designate the  $=\text{CH}_2$  group.

Names preceded by 'not' are names that are not constructed in accordance with the rule described in this section. Thus, they are 'incorrect' names.' As they are not alternatives to preferred IUPAC names, they must not be used. For example, the name 'ethanolamine', which is still widely used, is badly constructed because of the presence of two suffixes; it is not an alternative to the preferred IUPAC name, '2-aminoethanol'.

### **P-61 Substitutive nomenclature: prefix mode**

- P-61.0 Introduction
- P-61.1 General methodology
- P-61.2 Hydrocarbyl groups and corresponding polyvalent groups
- P-61.3 Halogen compounds
- P-61.4 Diazo compounds
- P-61.5 Nitro and nitroso compounds
- P-61.6 Azides
- P-61.7 Isocyanates
- P-61.8 Isocyanides
- P-61.9 Fulminates/isofulminates
- P-61.10 Polyfunctional compounds

#### **P-61.0 Introduction**

This subsection describes the names of compounds formed by substitutive nomenclature that includes only prefixes denoting substituent groups and/or characteristic groups. These prefixes are detachable and cited in a name in alphabetical order.

Hydrocarbyl groups and their corresponding polyvalent groups (substituent groups derived from hydrocarbon parent hydrides) are included in this subsection because they occupy the penultimate rank in the seniority order of classes (see P-41) and thus are treated as prefixes in presence of a higher class. A similar situation prevails for halogen compounds in their standard bonding number, which are last in the order of seniority of classes.

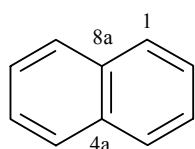
Nitro and nitroso compounds, azides, isocyanates, isocyanides, and fulminates/isofulminates are also included in this Section. Ethers, peroxides, and acetals are not considered in this Section, but are treated at length in association with hydroxy compounds and aldehydes (see P-63.2, P-63.5 and P-66.6.5, respectively).

The characteristic groups described here (see Table 4.6) are referred to as 'characteristic groups denoted, in substitutive nomenclature, only as prefixes' (see R-4.1, ref. 2). This statement must not be interpreted as a must for always using these characteristic groups as prefixes. Substitutive nomenclature is based on a seniority system based on classes. The senior class must be determined first (see for example, P-62.4).

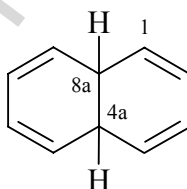
### P-61.1 General methodology

Substitutive nomenclature is based on the substitutive operation involving the exchange of one or more hydrogen atoms of a parent hydride or parent compound for another atom or group. This process is expressed by either a prefix or suffix denoting the atom or group being introduced. Substitution is not possible when no hydrogen atoms are present. However, if hydrogen atoms are added to a structure by an additive operation (to a double bond, for example), substitution then becomes possible. The formal addition of hydrogen atoms must precede the substitution operation when atoms or groups denoted by prefixes are involved; thus, they are cited after the alphabetized prefixes.

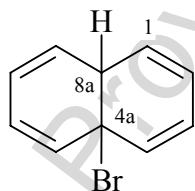
Examples:



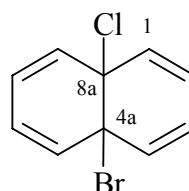
naphthalene (PIN)



4a,8a-dihydronaphthalene (PIN)



4a-bromo-4a,8a-dihydronaphthalene (PIN)



4a-bromo-8a-chloro-4a,8a-dihydronaphthalene (PIN)

The seniority order of parent structures, the principal chain, and the senior ring system are chosen in accordance with Rule P-44.

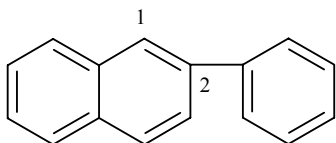
When there is a choice for numbering, the general rule described in P-14.4 is applied. The starting point and the direction of numbering of a compound are chosen so as to give lowest locants to the following structural features (if present) considered successively in the order given until a decision is reached.



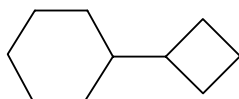
### P-61.2.2 Cyclic hydrocarbons

Names of rings or cyclic systems substituted by rings or ring systems are formed in accordance with the seniority order of rings and ring systems (see P-44.2).

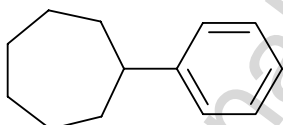
Examples:



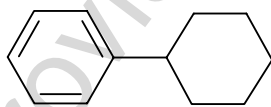
2-phenylnaphthalene (PIN)  
(naphthalene, having two rings, is senior to benzene, which has only one ring; see P-44.2.1)



cyclobutylcyclohexane (PIN)  
(cyclohexane has more ring atoms than cyclobutane; see P-44.2.1)



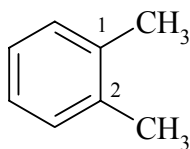
phenylcycloheptane (PIN)  
(cycloheptane has more ring atoms than benzene; see P-44.2.1)



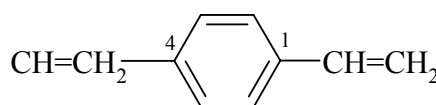
cyclohexylbenzene (PIN)  
(benzene has more multiple bonds; see P-44.2.3)

**P-61.2.3** Names of cyclic hydrocarbons substituted by chains are formed by substituting chains, saturated or unsaturated, into rings (see P-44.1.2.2). This rule must be strictly applied in the context of preferred IUPAC names. The name 'toluene' is retained with no substitution allowed for preferred IUPAC names, but substitution is allowed on both the ring and side chain with certain restrictions (see P-46.3.1) for general nomenclature; the names 'xylene', 'mesitylene' and 'styrene' are retained, but no substitution is allowed even for general nomenclature (see P-22.1.3).

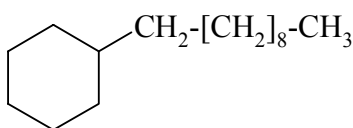
Examples:



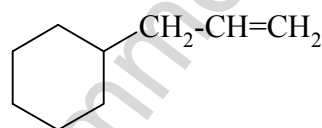
*o*-xylene (PIN)  
1,2-dimethylbenzene  
(not *o*-methyltoluene, substitution of toluene by additional methyl groups not allowed; see P-46.3.1.2)



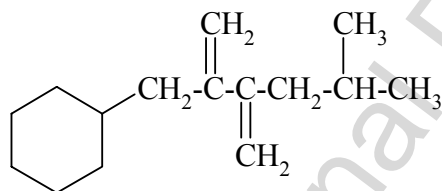
1,4-diethenylbenzene (PIN)  
*p*-divinylbenzene  
(not *p*-vinylstyrene; substitution of styrene not allowed: see P-22.1.3)



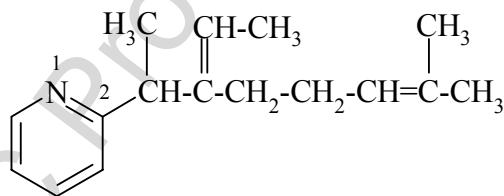
decylcyclohexane (PIN)  
(ring preferred to chain, see P-58.3.1.6)  
1-cyclohexyldecane



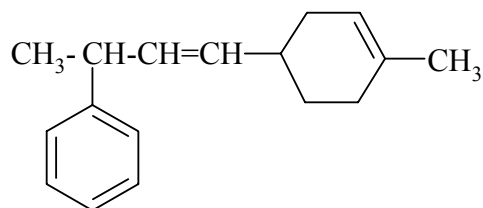
prop-2-en-1-ylcyclohexane (PIN)  
(ring preferred to chain, see P-58.3.1.6)  
allylcyclohexane



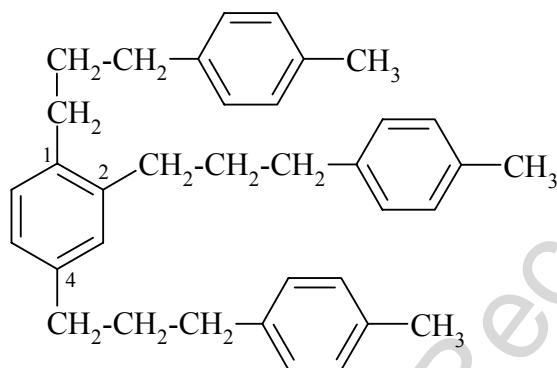
(5-methyl-2,3-dimethylidenehexyl)cyclohexane (PIN);  
(the longest chain is preferred to the shorter unsaturated chain, see P-44.3)  
[2-methylidene-3-(2-methylpropyl)but-3-en-1-yl]cyclohexane



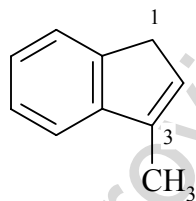
2-(3-ethylidene-7-methyloct-6-en-2-yl)pyridine (PIN)  
(preferred parent substituent prefix, see P-45.1)  
2-(2-ethylidene-1,6-dimethylhept-5-en-1-yl)pyridine



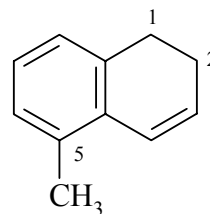
[4-(4-methylcyclohex-3-en-1-yl)but-3-en-2-yl]benzene (PIN; see P-56.1.1)  
[1-methyl-3-(4-methylcyclohex-3-en-1-yl)allyl]benzene



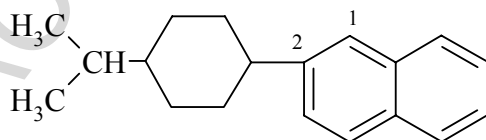
1,1',1''-(benzene-1,2,4-triyl)tripropyltris(4-methylbenzene) (PIN)  
(multiplicative name, see P-51.2)  
1,2,4-tris[3-(4-methylphenyl)propyl]benzene  
1,2,4-tris(3-*p*-tolylpropyl)benzene



3-methyl-1*H*-indene (PIN)



5-methyl-1,2-dihydronaphthalene (PIN)



2-[4-(propan-2-yl)cyclohexyl]naphthalene (PIN)  
2-(4-isopropylcyclohexyl)naphthalene

### P-61.3 Halogen compounds

Halogen compounds are always expressed by prefixes in substitutive nomenclature or, as the principal characteristic group, expressed as a separate word in functional class nomenclature.

**P-61.3.1** Halogen compounds are named in two ways:

- (1) by substitutive nomenclature, using the prefixes 'bromo', 'chloro', 'fluoro', and 'iodo' and appropriate multiplicative prefixes, as required; or
- (2) by functional class nomenclature, in which names are formed by citing the name of the organic 'groups' followed by the class name 'fluoride', 'chloride', 'bromide', and 'iodide', as a separate word, preceded, if necessary, by a multiplicative prefix. Functional class names usually are used to denote simple structures, having one kind of halogen, and are not used to name more complex structures. Additive names, such as stilbene dibromide, are not recommended.

Method (1) leads to preferred IUPAC names.

Examples:

$\text{CH}_3\text{-I}$   
iodomethane (PIN)  
methyl iodide

$\text{C}_6\text{H}_5\text{-CH}_2\text{-Br}$   
(bromomethyl)benzene (PIN)  
(no substitution on toluene)  
 $\alpha$ -bromotoluene ( see P-46.3 for toluene  
substitution rules)  
benzyl bromide

$\begin{array}{c} \text{Cl} \\ | \\ \text{CH}_3\text{-C-CH}_3 \\ | \\ \text{CH}_3 \end{array}$   
2-chloro-2-methylpropane (PIN)  
*tert*-butyl chloride

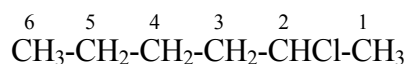
$\begin{array}{c} 1 \quad 2 \\ \text{Br-CH}_2\text{-CH}_2\text{-Br} \end{array}$

1,2-dibromoethane (PIN)  
ethylene dibromide

$\begin{array}{c} 1 \quad 2 \\ \text{C}_6\text{H}_5\text{-CHBr-CHBr-C}_6\text{H}_5 \end{array}$   
1,1'-(1,2-dibromoethane-1,2-diyl)dibenzene ((PIN)  
(multiplicative name, see P-51.2)  
1,2-dibromo-1,2-diphenylethane (substitutive name)  
stilbene dibromide (additive name, not recommended)



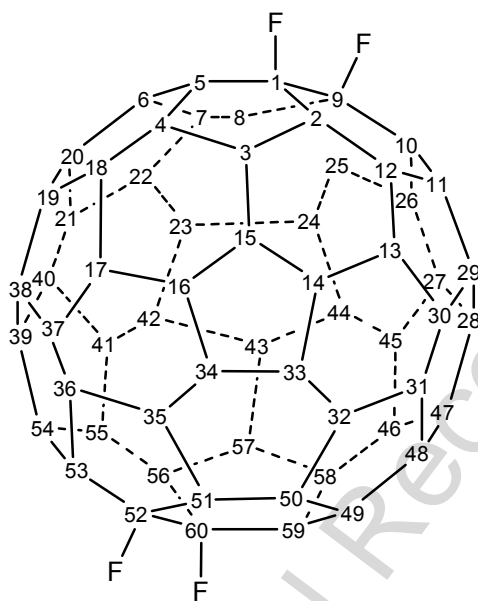




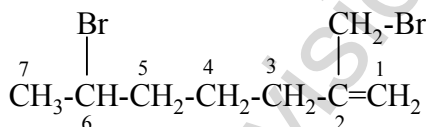
2-chlorohexane (PIN)  
 hexan-2-yl chloride  
 1-methylpentyl chloride



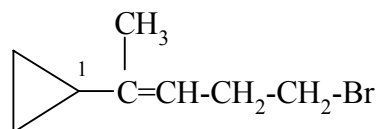
tetrafluorourea (PIN)  
 tetrafluorocarbonic diamide



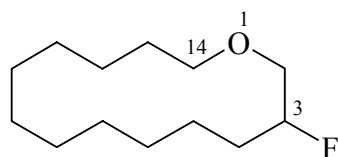
1,9,52,60-tetrafluoro-1,9,52,60-tetrahydro( $\text{C}_{60}\text{I}_h$ )[5,6]fullerene (PIN)  
 ( $\text{C}_{60}\text{I}_h$ )[5,6]fullerene-1,9,52,60-tetrayl tetrafluoride



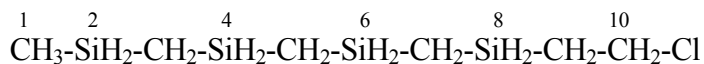
6-bromo-2-(bromomethyl)hept-1-ene (PIN)  
 2-methyleneheptan-1,6-diyl dibromide



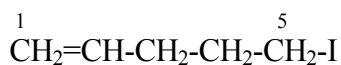
1-(5-bromopent-2-en-2-yl)cyclopropane (PIN)  
 (ring preferred to chain, see P-58.3.1.6;  
 preferred substituent prefix, see P-45.1)  
 1-(4-bromo-1-methylbut-1-en-1-yl)cyclopropane  
 5-bromo-2-cyclopropylpent-2-ene



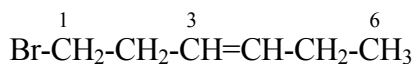
3-fluoro-1-oxacyclotetradecane (PIN)  
 1-oxacyclotetradecan-3-yl fluoride



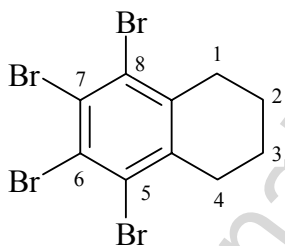
10-chloro-2,4,6,8-tetrasiladecane (PIN)  
2,4,6,8-tetrasiladecan-1-yl chloride



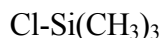
5-iodopent-1-ene (PIN)  
pent-4-en-1-yl iodide



1-bromohex-3-ene (PIN)  
hex-3-en-1-yl bromide



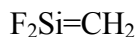
5,6,7,8-tetrabromo-1,2,3,4-tetrahydronaphthalene (PIN)  
5,6,7,8-tetrahydronaphthalene-1,2,3,4-tetrayl tetrabromide



chlorotrimethylsilane (PIN; silane is a preselected name; see P-12)  
trimethylsilyl chloride



trichloro(iodomethyl)silane (PIN; silane is a preselected name; see P-12)



difluoro(methylidene)silane (PIN; silane is a preselected name; see P-12)

**P-61.3.2** Compounds containing the groups  $-XO$ ,  $-XO_2$  or  $XO_3$  ( $X = \text{halogen}$ ) are expressed by the following prefixes in substitutive nomenclature:

$-XO$	chlorosyl (no longer chloroso), bromosyl, ioderyl, fluorosyl
$-XO_2$	chloryl (no longer chloroxy), bromyl, iodyl, fluoryl
$-XO_3$	perchloryl, perbromyl, periodyl, perfluoryl

Examples:

$C_6H_5-ClO_3$	$C_6H_5-IO$
perchlorylbenzene (PIN)	iodosylbenzene (PIN)

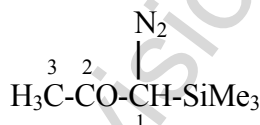
**P-61.3.3** Compounds containing the group  $-I(OH)_2$  or similar groups are named substitutively by using prefixes based on the preselected parent hydride name  $\lambda^3$ -iodane, as indicated in P-21.1.2.

#### P-61.4 Diazo compounds

Compounds containing a group  $=N_2$  attached to a single carbon atom are named by adding the prefix 'diazo-' to the name of the parent hydride or functional parent hydride.

Examples:

$CH_2N_2$	$N_2CH-CO-O-C_2H_5$
diazomethane (PIN)	ethyl diazoacetate (PIN)



1-diazo-1-(trimethylsilyl)propan-2-one (PIN)  
1-diazo-1-(trimethylsilyl)acetone

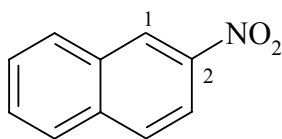
#### P-61.5 Nitro, nitroso and related compounds

##### P-61.5.1 Nitro and nitroso compounds

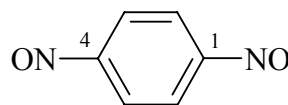
Compounds containing the  $-NO_2$  or the  $-NO$  group are named by means of the prefixes 'nitro' and 'nitroso', respectively, unless these groups are to be named on the basis of the parent structures nitric and nitrous acids,  $NO_2-OH$  and  $NO-OH$ , respectively, or their corresponding esters, anhydrides, amides and hydrazides.

Examples:

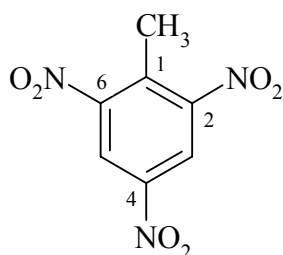
CH<sub>3</sub>-NO<sub>2</sub>  
 nitromethane (PIN)



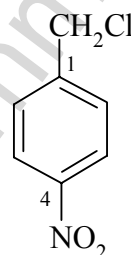
2-nitronaphthalene (PIN)



1,4-dinitrosobenzene (PIN)  
*p*-dinitrosobenzene



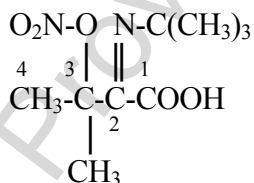
1-methyl-2,4,6-trinitrobenzene (PIN)  
 2,4,6-trinitrotoluene (see P-46.3 for  
 toluene substitution rules)



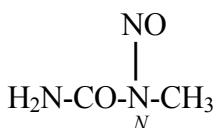
1-(chloromethyl)-4-nitrobenzene (PIN)  
 α-chloro-4-nitrotoluene (see P-46.3 for  
 toluene substitution rules)  
 4-nitrobenzyl chloride

**P-61.5.2** In the presence of a characteristic group having seniority to be named as suffix or parent structure, nitro and nitroso groups can be attached to any atom. When linked to another nitrogen atom they are not considered to lengthen the nitrogen chain.

Examples:



2-(*tert*-butylimino)-3-methyl-3-(nitrooxy)butanoic acid (PIN)



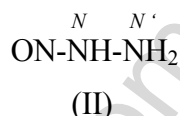
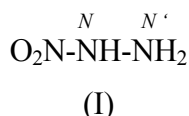
*N*-methyl-*N*-nitrosourea (PIN)

**P-61.5.3** Amides and hydrazides of nitric and nitrous acids

Nitramines are amides of nitric acid (see ref. 17). The class is composed of ‘nitramide’ (a shortened form of nitric amide),  $\text{NO}_2\text{-NH}_2$ , and its derivatives formed by substitution and named as such. Nitrosamines are amides of nitrous acid (see ref. 17); they are named as derivatives of this amide. Nitric acid and nitrous acid are preferred preselected names, see P-12.

Formerly, nitramines and nitrosamines were named as nitro and nitroso amines. This former method can be used in general nomenclature, but preferred IUPAC names are those of substituted amides, in accordance with the seniority order of classes.

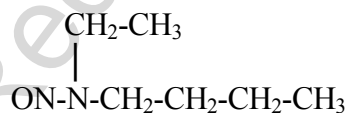
Similarly, nitric hydrazide (I) and nitrous hydrazide (II) are preferred preselected names used as parent structures for generation of preferred IUPAC names.



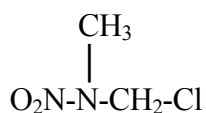
Examples:



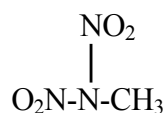
*N,N*-dipropylnitrous amide (PIN)  
*N*-nitroso-*N*-propylpropan-1-amine



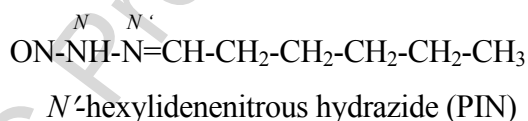
*N*-butyl-*N*-ethylnitrous amide (PIN)  
*N*-ethyl-*N*-nitrosobutan-1-amine



*N*-(chloromethyl)-*N*-methylnitramide (PIN)  
 1-chloro-*N*-methyl-*N*-nitromethanamine



*N*-methyl-*N*-nitronitramide (PIN)  
*N,N*-dinitromethanamine



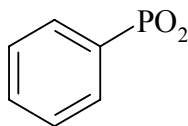
**P-61.5.4** *aci*-Nitro compounds

Compounds containing the group  $\text{=N(O)OH}$  are named as derivatives of azinic acid,  $\text{H}_2\text{N(O)-OH}$ , a preferred preselected name, and by using the prefix name hydroxy(oxo)- $\lambda^5$ -azanylidene, when a characteristic group having priority for citation as a suffix is present. The use of the prefix ‘*aci*-nitro’ is no longer recommended (see P-67.1.6).

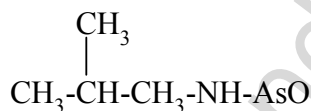
**P-61.5.5** Compounds containing the  $\text{-PO}_2$ ,  $\text{-PO}$ ,  $\text{-AsO}_2$ , or  $\text{-AsO}$  groups are described by the compulsory prefix names phospho, phosphoso, arso, and arsoroso.

Note: The term 'phospho' is widely used in biochemical nomenclature in place of phosphono for designating the  $-P(O)(OH)_2$  group linked to a heteroatom, as in phosphocholine and 6-phospho-D-glucose; and as an infix to describe phosphoric diesters, as in glycerophosphocholine.

Examples:



phosphobenzene (PIN)  
dioxo(phenyl)- $\lambda^5$ -phosphane

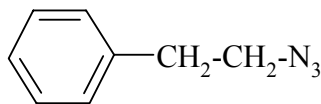


*N*-arsoroso-2-methylpropanamine (PIN)  
*N*-(2-methylpropyl)oxoarsanamine

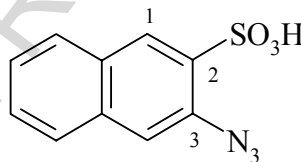
### P-61.6 Azides

Compounds containing a  $-N_3$  ( $-N=N^+=N^-$ ) group attached to a parent hydride, are named using substitutive nomenclature and the prefix 'azido'. This method gives preferred IUPAC names rather than names based on the class name 'azide' in functional class nomenclature.

Examples:



(2-azidoethyl)benzene (PIN)  
phenethyl azide



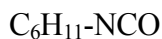
3-azidonaphthalene-2-sulfonic acid (PIN)

### P-61.7 Isocyanates

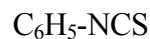
In these Recommendations, preferred IUPAC names are generated by using the prefix 'isocyanato' as a compulsory prefix, i.e., it is attached directly to a parent hydride in substitutive nomenclature. Previously, functional class names were recommended for this class.

Compounds containing the  $-N=C=O$  group attached to a parent hydride structure, are named by using substitutive nomenclature and the prefix 'isocyanato'. This method leads to preferred IUPAC names rather than names based on functional class nomenclature and the functional class name 'isocyanate'. Chalcogen analogues are named by inserting the appropriate functional replacement prefix 'thio', 'seleno', or 'telluro' into the names 'isocyanate' or 'isocyanato' just after 'iso'.

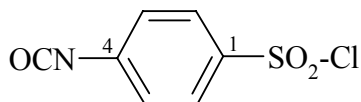
Examples:



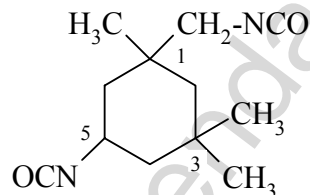
isocyanatocyclohexane (PIN)  
cyclohexyl isocyanate



isothiocyanatobenzene (PIN)  
phenyl isothiocyanate



4-isocyanatobenzenesulfonyl chloride (PIN)



5-isocyanato-1-(isocyanatomethyl)-1,3,3-trimethylcyclohexane (PIN)  
3-(isocyanatomethyl)-3,5,5-trimethylcyclohexyl isocyanate



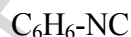
isothiocyanatosilane (PIN; silane is a preselected name; see P-12)

### P-61.8 Isocyanides

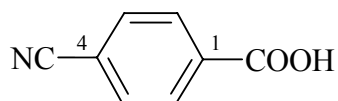
In these Recommendations, preferred IUPAC names are formed by using the prefix 'isocyano' as a compulsory prefix, i.e., it is attached directly to a parent hydride in substitutive nomenclature. Previously, functional class names were recommended for this class.

Compounds containing the  $\text{-NC}$  group attached to a parent hydride structure, are named by substitutive nomenclature and the prefix 'isocyano'. This method leads to preferred IUPAC names rather than names based on functional class nomenclature and the functional class name 'isocyanide'.

Examples:



isocyanobenzene (PIN)  
phenyl isocyanide



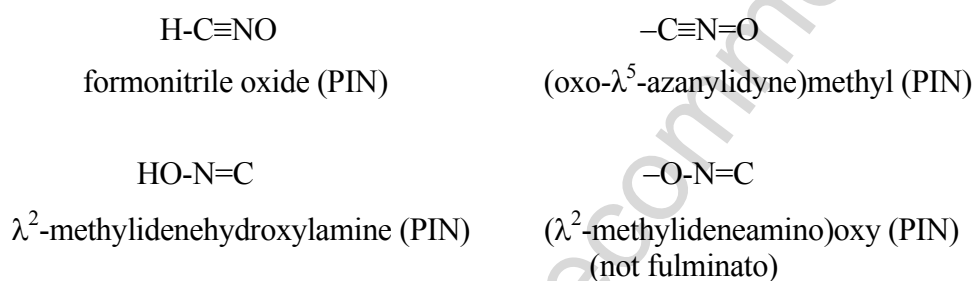
4-isocyanobenzoic acid (PIN)



### P-61.9 Fulminates and isofulminates

The structure of fulminic acid was indicated in the 1979 Recommendations (Rule C-833.1, ref. 1) and in the 1993 Recommendations (Rule R-5.7.9.2, ref. 2) as HO-N≡C by the class name fulminate and the compulsory prefix fulminato. Although consistent with the pseudohalogen cyanate, the structure of this acid in the literature is claimed to be HCNO. Accordingly, the name fulminic acid and of its substituent group fulminato must be deprecated; and the names isofulminic acid and isofulminate must also be deprecated. The IUPAC preferred name for the structure HCNO is formonitrile oxide (see P-66.5.3) and the IUPAC preferred name for its isomer, HO-N=C, is based on hydroxylamine (see P-68.3.1.1).

Examples:



### P-61.10 Polyfunctional compounds

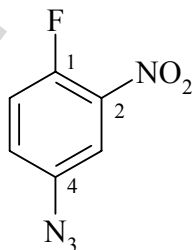
In substitutive names, detachable prefixes in names are cited in alphanumerical order. Low locants are assigned to:

- (1) the prefixes as a set, and if there is a choice,
- (2) to the prefix that is cited first in a name.

In functional class nomenclature, names are formed by using the order of classes (see P-41) and the order of seniority of halides and pseudohalides (see P-41 and P-65.5.2.1) to choose the principal function. Names formed substitutively rather than functional class names are preferred IUPAC names.

**P-61.10.1** Low locants are assigned as a set, without regard to kind.

Examples:



4-azido-1-fluoro-2-nitrobenzene (PIN)  
4-azido-2-nitrophenyl fluoride



## P-62.1 General methodology

The general methodology is based on the following principles:

- (a) Definitions, as given in the Glossary of Class Names Based on Structure (ref. 17), classify amines and imines unambiguously as follows:
  - (1) amines are compounds formally derived from ammonia by replacing one, two, or three of its hydrogen atoms by hydrocarbyl groups, and having the general structures  $R-NH_2$  (primary amines),  $R_2NH$  (secondary amines),  $R_3N$  (tertiary amines).
  - (2) imines are compounds having the structure  $R-N=CR_2$  ( $R = H$ , hydrocarbyl), corresponding either to ketimines,  $RR'C=NR''$  or to aldimines,  $RCH=NR'$ .
- (b) amines are senior to imines in the seniority order of classes.
- (c) methods for naming amines and imines will be restricted to a minimum, preference being given to the substitutive method using the suffix 'amine'.
- (d) a minimum of traditional names will be retained.

## P-62.2 Amines

P-62.2.1 Amines derived from parent hydrides

P-62.2.2 Modification of the degree of saturation/unsaturation of amines

### P-62.2.1 Amines derived from parent hydrides

P-62.2.1.1 Primary amines

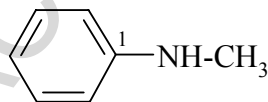
P-62.2.1.2 Secondary and tertiary amines

P-62.2.1.3 Polyamines

#### P-62.2.1.1 Primary amines

**P-62.2.1.1.1** One trivial name only for a primary amine is retained as a preferred name, i.e., aniline, for  $C_6H_5-NH_2$ , with full substitution permitted on the ring and on the nitrogen atom. Rules for substituting aniline are described in P-46.2.

Examples:



*N*-methylaniline (PIN)  
*N*-methylbenzenamine



4-chloroaniline (PIN)  
4-chlorobenzenamine

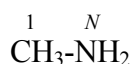
**P-62.2.1.1.2** Primary amines, R-NH<sub>2</sub>, are systematically named in two ways:

- (1) by adding the suffix 'amine' to the name of the parent hydride;
- (2) by adding the name of the substituent group R- to the term 'amine' used as a parent hydride name.

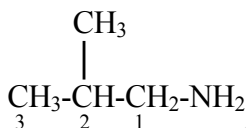
Two or more 'amine' suffixes are indicated by an appropriate multiplying numerical prefix 'di', 'tri', 'tetra', etc. The terminal letter 'a' of a numerical prefix is elided before the suffix amine, i. e., 'tetramine', not 'tetraamine', but not before the parent name amine. Numerical locants, including '1' in the case of amines derived from mononuclear parent hydrides, are used to denote substitution on atoms of the parent hydride and '*N*' locants for substitution on the nitrogen atom for amines named by method (1).

Method (1) leads to preferred IUPAC names.

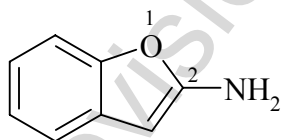
Examples:



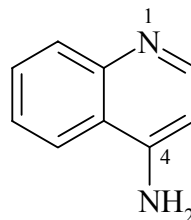
- (1) methanamine (PIN)
- (2) methylamine



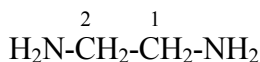
- (1) 2-methylpropan-1-amine (PIN)
- (2) (2-methylpropyl)amine



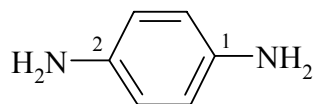
- (1) 1-benzofuran-2-amine (PIN)
- (2) 1-benzofuran-2-ylamine



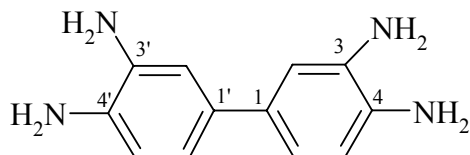
- (1) quinolin-4-amine (PIN)
- (2) (quinolin-4-yl)amine
- (3) 4-quinolylamine



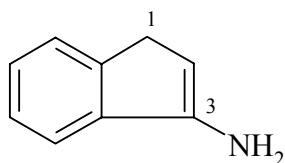
- (1) ethane-1,2-diamine (PIN)
- (2) ethylenediamine



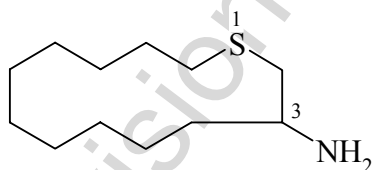
benzene-1,4-diamine (PIN)  
1,4-phenylenediamine  
*p*-phenylenediamine



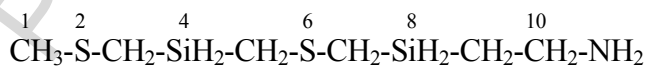
[1,1'-biphenyl]-3,3',4,4'-tetramine (PIN; note elision of 'a' from 'tetra' in 'tetramine')  
[1,1'-biphenyl-3,3',4,4'-tetrayl]tetraamine (note no elision of 'a' from 'tetra' in 'tetraamine')



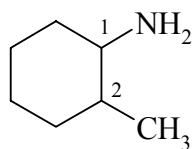
1*H*-inden-3-amine (PIN)  
1*H*-inden-3-ylamine



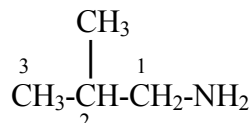
1-thiacyclotridecan-3-amine (PIN)  
(1-thiacyclotridecan-3-yl)amine



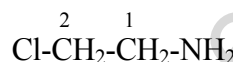
2,6-dithia-4,8-disiladecan-10-amine (PIN)  
(2,6-dithia-4,8-disiladecan-10-yl)amine



2-methylcyclohexan-1-amine (PIN)  
 (2-methylcyclohexyl)amine



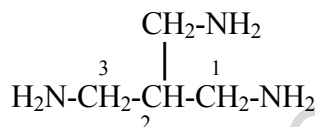
2-methylpropan-1-amine (PIN)  
 isobutylamine  
 (2-methylpropyl)amine



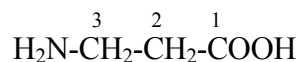
2-chloroethanamine (PIN)  
 (2-chloroethyl)amine

**P-62.2.1.1.3** When all amino groups cannot be expressed as suffixes, or when the  $-NH_2$  group is not the principal characteristic group, the prefix 'amino', not azanyl, is used in preferred IUPAC names. Azanyl may be used in general nomenclature. The substituent prefix name anilino is no longer recommended.

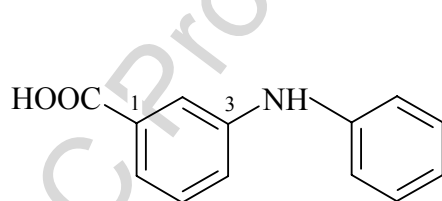
Examples:



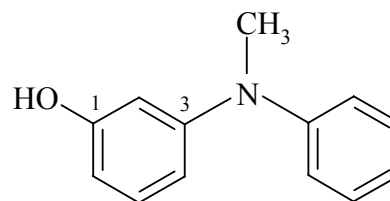
2-(aminomethyl)propane-1,3-diamine (PIN)  
 2-(azanylmethyl)propane-1,3-diamine  
 [2-(aminomethyl)propane-1,3-diyl]diamine



3-aminopropanoic acid (PIN)  
 3-azanylpropanoic acid



3-anilinobenzoic acid (PIN)  
 3-(phenylamino)benzoic acid

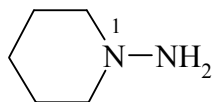


3-(*N*-methylanilino)phenol (PIN)  
 3-[methyl(phenyl)amino]phenol

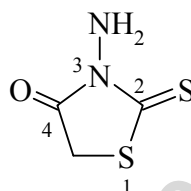
#### P-62.2.1.1.4 Amino groups attached to heteroatoms

When attached to heteroatoms, amino groups are expressed as suffixes when representing the principal characteristic group and by the amino prefix in presence of a characteristic group having seniority over amines.

Examples:



piperidin-1-amine (PIN)  
1-aminopiperidine



3-amino-2-sulfanylidene-1,3-thiazolidin-4-one (PIN)  
(not 3-amino-2-thioxo-1,3-thiazolidin-4-one)

#### P-62.2.1.2 Secondary and tertiary amines

**P-62.2.1.2.1** Symmetrical and unsymmetrical secondary and tertiary amines are named by the same two methods.

- (1) substitutively using the retained name aniline or the suffix 'amine' with further *N*-substitution;
- (2) substitutively, by prefixing, in alphabetical order when required, the name(s) of the substituent group(s) R, R' or R'' to the parent hydride name 'amine'. In order to avoid ambiguity, the second prefix in secondary amines, and the second and the third prefixes in tertiary amines must be enclosed in parentheses when these prefixes denote simple substituents.

Method (1) generates preferred IUPAC names. Names like diethylamine and triethylamine are deprecated.

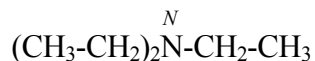
Preferred IUPAC names for prefixes corresponding to  $-NHR$  or  $-NRR'$  or  $-NR_2$  are formed by prefixing the names of the groups R and R' to the prefix 'amino', for example 'methylamino', for  $-NH-CH_3$ . Prefixes such as azanyl and azanylidene may be used in general nomenclature.

Examples:



*N*-phenylaniline (PIN)  
diphenylamine

(not azanediylidibenzene; the retained name 'aniline' must be used for all *N* derivatives)



*N,N*-diethylethanamine (PIN)  
triethylamine



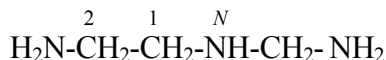




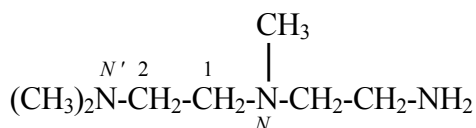
**P-62.2.1.3 Polyamine systems**

Polyamine systems are composed of two or more amines, identical or different. They are named by *N*-substitution of the senior amine. The senior amine is chosen in accordance with the choice of a principal chain or a senior ring or ring system. Alphanumerical order is applied when a choice is to be made. Multiplicative nomenclature, skeletal replacement ('a') nomenclature, or phane names are used when the conditions required by these types of nomenclature are fulfilled.

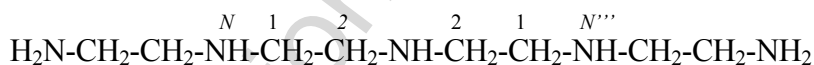
Examples:



*N*-(aminomethyl)ethane-1,2-diamine (PIN)  
 (regular substitutive nomenclature; the diamine having the longest carbon chain is chosen as parent structure)



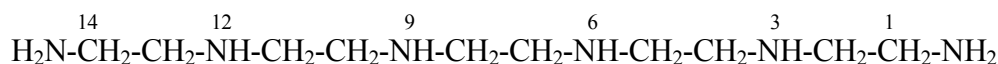
*N*-(2-aminoethyl)-*N,N,N'*-trimethylethane-1,2-diamine (PIN; numbering shown)  
 (the most substituted diamine is chosen as parent structure)  
 (not *N,N*-dimethyl-2,2'-(methylazanediyl)diethanamine; the preferred IUPAC name must be a diamine)



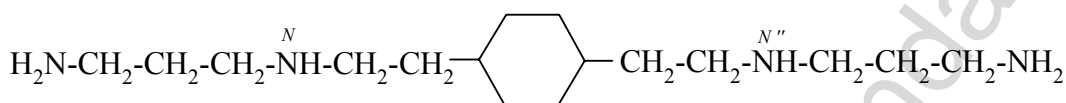
*N,N''*-(azanediyl)diethane-2,1-diylbis(ethane-1,2-diamine) (PIN; numbering shown)  
*N*-(2-aminoethyl)-*N'*-{2-[(2-aminoethyl)amino]ethyl}ethane-1,2-diamine  
 (not 2,2'-azanediylbis[*N*-(2-aminoethyl)ethanamine]; the preferred IUPAC name must be a diamine)



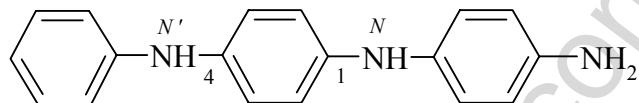
*N*-{2-[(2-aminoethyl)amino]ethyl}-*N'*-(2-aminomethyl)ethane-1,2-diamine (PIN)  
 (not *N*-(2-aminomethyl)-*N'*-{2-[(2-aminoethyl)amino]ethyl}ethane-1,2-diamine;  
 'aminoethyl' precedes 'aminomethyl' in alphanumerical order)  
 (not *N*-(aminoethyl)-*N'*-(aminomethyl)-2,2'-azanediyl)diethanamine;  
 the preferred IUPAC name must be a diamine)



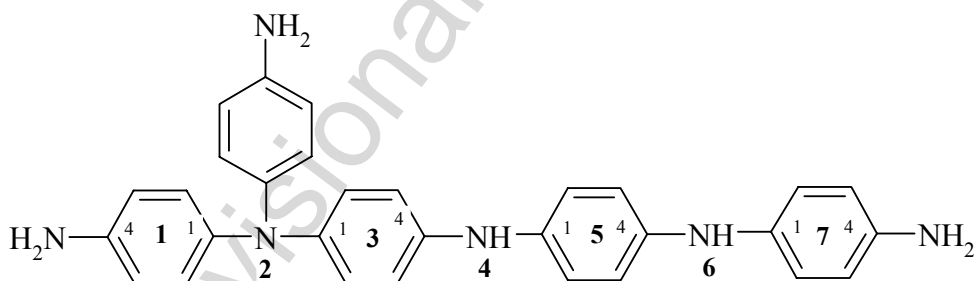
3,6,9,12-tetraazatetradecane-1,14-diamine (PIN)  
 (skeletal replacement ('a') name; see P-51.3.2)



*N,N''*-(cyclohexane-1,4-diyl)bis(propane-1,3-diamine) (PIN)  
 (multiplicative nomenclature allows four amine characteristic groups to be included in the parent structure)



*N*-(4-aminophenyl)-*N'*-phenylbenzene-1,4-diamine (PIN)  
 [maximum number of substituents cited as prefixes; see P-44.2.3(g) and P-44.3(k)]



2-(4-aminophenyl)-2,4,6-triaza-1,7(1),3,5(1,4)-tetrabenzenaheptaphane-1<sup>4</sup>,7<sup>4</sup>-diamine (PIN)  
 (four benzene rings and a total of seven phane nodes justify a phane name; see P-51.4)

#### P-62.2.2.2 Modification of the degree of saturation/unsaturation of amines

##### P-62.2.2.2.1 General methodology

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

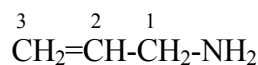
- fixed numbering (naphthalene, bicyclo[2.2.2]octane, etc.)
- heteroatoms in heterocycles and in acyclic parent structures

- (c) indicated hydrogen [for unsubstituted compounds; a higher locant may be needed at another position to provide for a substituent suffix in accordance with the 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)

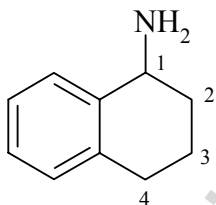
**P-62.2.2.2.2** Modification of the degree of saturation/unsaturation of primary amines

Criteria (d), (e) and (f) described in the general methodology (P-62.2.2.2.1) are used.

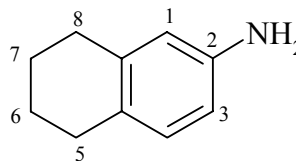
Examples:



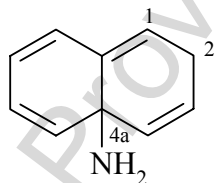
prop-2-en-1-amine (PIN)  
allylamine



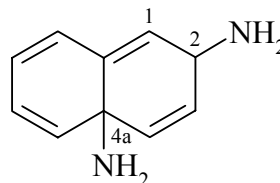
1,2,3,4-tetrahydronaphthalen-1-amine (PIN)



5,6,7,8-tetrahydronaphthalen-2-amine (PIN)



naphthalen-4a(2H)-amine (PIN)  
2,4a-dihydronaphthalen-4a-amine  
(see P-53.1)

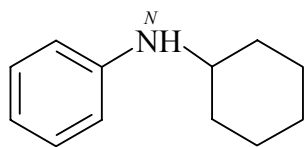


naphthalene-2,4a(2H)-diamine (PIN)  
2,4a-dihydronaphthalene-2,4a-diamine  
(see P-53.1)

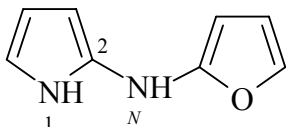
**P-62.2.2.3** Selection of the principal chain or senior ring system in secondary and tertiary amines

Names of amines formed substitutively by using the retained name aniline or the suffix 'amine' are based on a principal chain and a senior ring system (see P-44.1). When a choice for parent

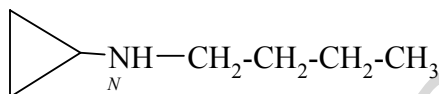




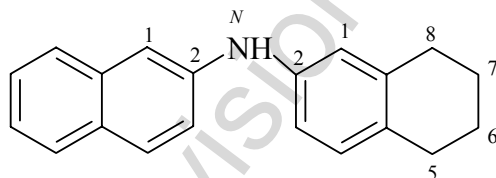
*N*-cyclohexylaniline (PIN)  
cyclohexyl(phenyl)amine



*N*-(furan-2-yl)pyrrol-2-amine (PIN)  
(furan-2-yl)(pyrrol-2-yl)amine  
2-furyl(1*H*-pyrrol-2-yl)amine



*N*-butylcyclopropanamine (PIN)  
*N*-cyclopropylbutan-1-amine  
cyclopropyl(butyl)amine



*N*-(5,6,7,8-tetrahydronaphthalen-2-yl)naphthalen-2-amine (PIN)  
2-naphthyl(5,6,7,8-tetrahydro-2-naphthyl)amine  
(not 5,6,7,8-tetrahydrodi-2-naphthylamine)

### P-62.3 Imines

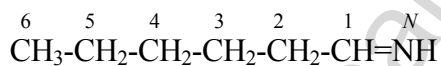
Compounds having the general structure  $R-CH=NR'$  or  $R(R')C=NR''$  are called generically 'aldimines' and 'ketimines', respectively. Imines are characterized by a double bond between a carbon atom and a nitrogen atom. Thus, *N*-substituted imines,  $R-CH=N-R'$  or  $R(R')C=N-R''$ , must be classified as imines and not as amines in spite of the fact that there is a single bond between a carbon atom and the nitrogen atom; amines must have three single bonds linked to carbon atoms (see P-62.0).

### P-62.3.1 Substitutive names of imines

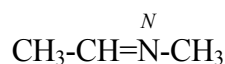
**P-62.3.1.1** All imines are named substitutively using the suffix ‘imine’; the presence of several ‘imine’ characteristic groups is denoted by the numerical multiplying prefixes ‘di’, ‘tri’, etc. When there is a choice for numbering, the starting point and the direction of numbering of a compound are chosen so as to give lowest locants to the following structural features (if present) considered successively in the order given until a decision is reached.

- fixed numbering (naphthalene, bicyclo[2.2.2]octane, etc.)
- heteroatoms in heterocycles and in acyclic parent structures
- indicated hydrogen [for unsubstituted compounds; a higher locant may be needed at another position to provide for a substituent suffix in accordance with the structural feature (d)]
- principal group named as suffix
- added hydrogen (consistent with the structure of the compound and in accordance with further substitution)
- saturation (‘hydro’/‘dehydro’ prefixes) or unsaturation (‘ene’, ‘yne’ endings)
- substituents named as prefixes (low locants are allocated for substituents regardless of kind; then, if necessary, in the order of citation)

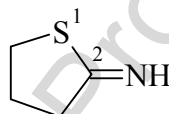
Examples:



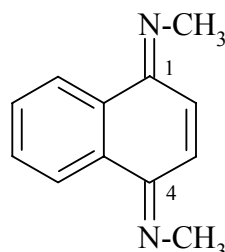
hexan-1-imine (PIN)



*N*-methylethanimine (PIN)  
(not *N*-ethylidenemethanamine)  
[not *N*-ethylidene(methyl)amine]

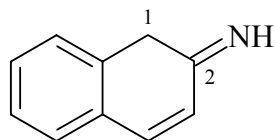


thiolan-2-imine (PIN)

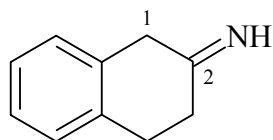


*N,N'*-dimethylnaphthalene-1,4-diimine (PIN;  
see also P-53.1)

*N,N'*-dimethyl-1,4-dihydronaphthalene-1,4-diimine  
(not *N,N'*-dimethyl-1,4-naphthoquinone diimine;  
two suffixes of different kinds are incompatible)  
[not *N,N'*-naphthalene-1,4-ylidenebis(methanamine)]  
[not *N,N'*-naphthalene-1,4-diylidenebis(methylamine)]  
[not dimethyl(naphthalene-1,4-diylidene)bis(amine)]



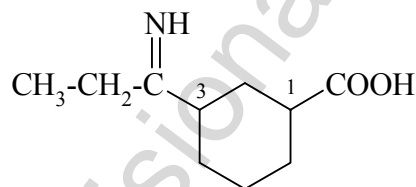
naphthalen-2(1*H*)-imine (PIN; see also P-53.1)  
1,2-dihydronaphthalen-2-imine



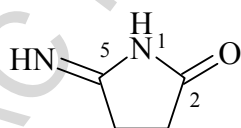
3,4-dihydronaphthalen-2(1*H*)-imine (PIN; see also P-53.1)  
1,2,3,4-tetrahydronaphthalen-2-imine

**P-62.3.1.2** The prefix 'imino' for =NH is used in presence of characteristic groups having seniority over imines. In multiplicative nomenclature, the prefix 'azanylylidene' for -N= is used. Substituent groups attached to rings, ring systems or heteroatoms of the type R-(C=NH)-, where R- is a ring or a chain, are named as acyl groups (see imidic acids, P-65.1.3.1 and acyl groups P-65.2).

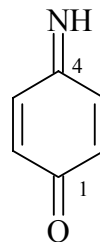
Examples:



3-propanimidoylcyclohexane-1-carboxylic acid (PIN)

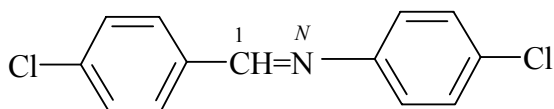


5-iminopyrrolidin-2-one (PIN)  
5-imino-2-pyrrolidone

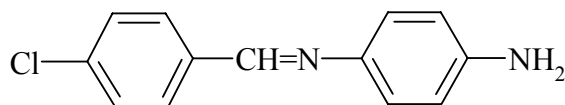


4-iminocyclohexa-2,5-dien-1-one (PIN)  
(not *p*-benzoquinone monoimine)

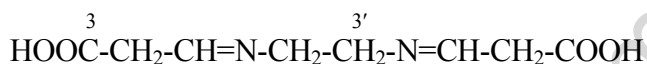




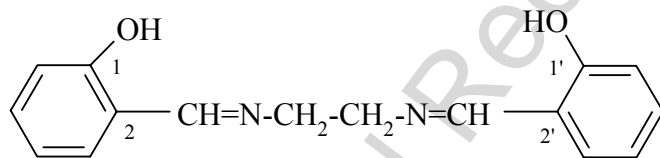
*N*,1-bis(4-chlorophenyl)methanimine (PIN) (see following example)



4-[[4-chlorophenyl)methylidene]amino}aniline (PIN)



3,3'-[ethane-1,2-diylbis(azanylylidene)]dipropanoic acid (PIN)

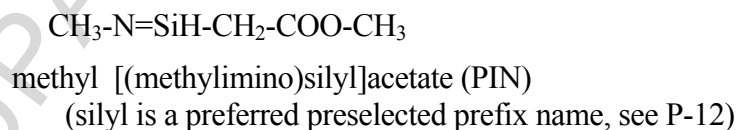
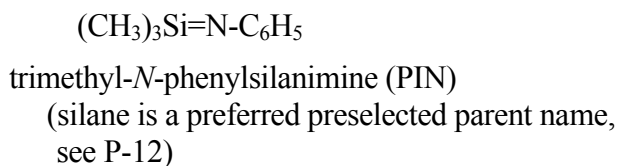
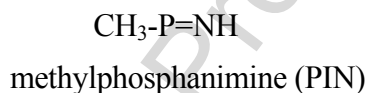


2,2'-[ethane-1,2-diylbis(azanylylidenemethanylylidene)]diphenol (PIN)

### P-62.3.1.3 Imino groups attached to heteroatoms (pseudoinimines)

Compounds containing the group X=NH, where X is a heteroatom and =NH the principal characteristic group, are named as imines; the prefix 'imino' is used to express the =NH group when another characteristic groups has seniority over imines.

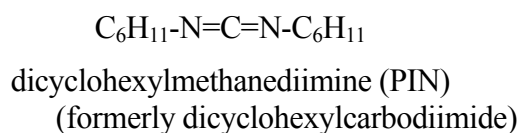
Examples:



#### P-62.3.1.4 Carbodiimides

The hypothetical compound  $\text{HN}=\text{C}=\text{NH}$  is named systematically 'methanediimine'. Its derivatives are named as substitution products thereof. These names are preferred to those based on the retained name 'carbodiimide', which now should be used only as a class name.

Example:



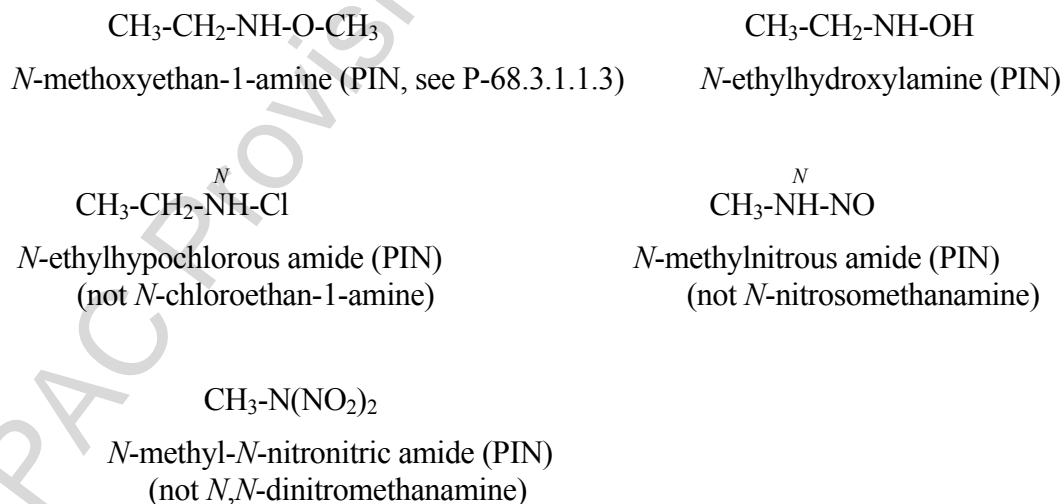
#### P-62.4 N-Substitution of amines and imines

Traditionally, substitution on the nitrogen atom of amines and imines was allowed for substituents always cited as prefixes (see P-46.1), such as  $-\text{Cl}$  and other halogen atoms,  $-\text{NO}$ ,  $-\text{NO}_2$ ,  $-\text{O-R}$  and even  $-\text{OH}$  groups, and chalcogen analogues.

In accordance with the seniority of classes (see P-41), compounds such as  $\text{R-NH-Cl}$ ,  $\text{R-NH-NO}$ , and  $\text{R-NH-NO}_2$  are named as derivatives of amides (see P-67.1.2.3). Compounds such as  $\text{R-NH-OH}$  are named as *N*-derivatives of hydroxylamine,  $\text{NH}_2\text{-OH}$  (see P-68.3.1.1.1). Names based on *N*-substitution of amines are not recommended in these cases.

Substitution of amines is permitted by  $-\text{OR}$ ,  $-\text{SR}$ ,  $-\text{SeR}$ , and  $-\text{TeR}$  groups, where R is an alkyl or aryl substituent group.

Examples:



### P-62.5 Amine oxides and imine oxides

Amine oxides and imine oxides are named:

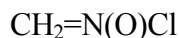
- (1) by functional class nomenclature using the class name 'oxide';
- (2) by use of prefixes derived from the parent name  $\lambda^5$ -azane;
- (3) as zwitterions (see P-74.2.1.2)

Method (1) is used when the oxide is located on a nitrogen atom of the parent structure so that, if a locant is necessary, it can be used to unambiguously locate the oxide. Because of the zwitterionic nature of a nitrogen oxide, amine and imine oxides are placed with zwitterions in the order of compound classes (see P-41). Method (2) is used when the oxide is on a nitrogen atom of a substituent to the parent structure. Methods (1) and (2) lead to preferred IUPAC names. When method (3) is used, the zwitterion is the parent structure.

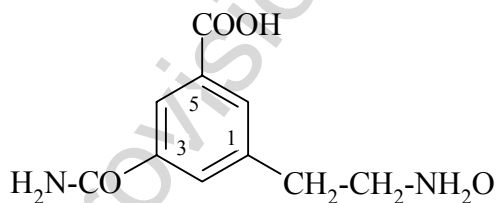
Examples:



- (1) *N,N*-dimethylmethanamine oxide (PIN)  
trimethylamine oxide
- (3) (trimethylazaniumyl)oxidanide



- (1) *N*-chloromethanimine oxide (PIN)
- (3) [chloro(methylidene)azaniumyl]oxidanide (see also P-74.2.1.2)



- (1) 2-(3-carbamoyl-5-carboxyphenyl)ethanamine oxide (PIN)
- (3) {[2-(3-carbamoyl-5-carboxyphenyl)ethyl]azaniumyl} oxidanide (see also P-74.2.1.2)



2-(oxo- $\lambda^5$ -azanyl)ethyl (PIN)

## P-63 Hydroxy compounds, ethers, peroxols, peroxides and chalcogen analogues

- P-63.0 Introduction
- P-63.1 Hydroxy compounds and chalcogen analogues
- P-63.2 Ethers and chalcogen analogues
- P-63.3 Peroxides and chalcogen analogues
- P-63.4 Hydroperoxides (peroxols) and chalcogen analogues
- P-63.5 Cyclic ethers and peroxides and chalcogen analogues
- P-63.6 Sulfoxides and sulfones
- P-63.7 Polyfunctional compounds

### P-63.0 Introduction

Traditionally, hydroxy compounds are compounds having one or more hydroxy groups attached to carbon atoms. Alcohols, phenols, enols and ynols are recognized as hydroxy compounds. The category is extended so as to include compounds having one or more hydroxy groups attached to atoms other than carbon without being classified as acids as defined in the seniority of classes. For instance,  $\text{H}_2\text{Si-OH}$  is classified and named as a hydroxy compound, silanol, but  $\text{Si(OH)}_4$  is classified and named as an acid, orthosilicic acid.

Several changes are recommended in naming of characteristic groups having two contiguous chalcogen atoms. The suffix 'peroxol' is now introduced to name the group  $-\text{OOH}$ , formerly named by functional class nomenclature as 'hydroperoxide'. □

### P-63.1 Hydroxy compounds and chalcogen analogues

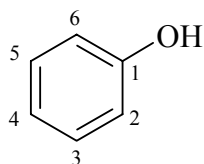
Names generated substitutively are preferred IUPAC names rather than functional class names or retained names, with the exception of the retained name 'phenol' that can be fully substituted. Functional class names are traditional names that are restricted today to alcohols,  $\text{R-OH}$ , where the  $\text{R-}$  group is a simple aliphatic or alicyclic group.

- P-63.1.1 Retained names
- P-63.1.2 Systematic names of alcohols, phenols, enols, and ynols
- P-63.1.3 Heterols
- P-63.1.4 Substitutive nomenclature, prefix mode
- P-63.1.5 Sulfur, selenium and tellurium analogues of hydroxy compounds
- P-63.1.6 Polyfunctional hydroxy compounds

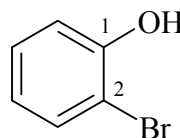
#### P-63.1.1 Retained names

Only one name is retained, phenol, for  $\text{C}_6\text{H}_5\text{-OH}$ , both as a preferred name and for general nomenclature. The structure is substitutable at any position. Locants 2, 3, and 4 are preferred to the prefixes *o*, *m*, and *p*. Naphthol (both isomers) and anthrol (all isomers) are retained names for general nomenclature only; they are substitutable at any position.

Examples:



phenol (PIN; retained name)



2-bromophenol (PIN)  
*o*-bromophenol

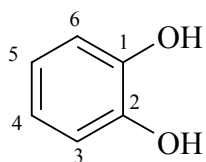
### P-63.1.2 Systematic names of alcohols, phenols, enols, and ynols

Hydroxy compounds are named in four ways.

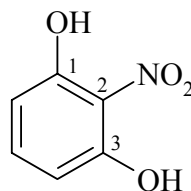
- (1) substitutively, using the suffix 'ol' and the prefix 'hydroxy'. The presence of several 'ol' characteristic groups is denoted by the numerical multiplying prefixes 'di', 'tri', etc.; the final letter 'a' in a multiplying prefix is elided before the suffix 'ol'. Rule P-44 is applied when a principal chain or a senior ring system must be chosen. When there is a choice for numbering, the starting point and the direction of numbering of a compound are chosen so as to give lowest locants to the following structural features (if present) considered successively in the order given until a decision is reached.
  - (a) fixed numbering (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 the 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')
  - (g) substituents named as prefixes (low locants are allocated for substituents regardless of kind; then, if necessary, in the order of citation)
- (2) by using functional nomenclature and the functional class term 'alcohol'
- (3) as assemblies of identical units when the conditions of symmetry are fulfilled
- (4) retained names for general nomenclature only

Method (1) generates preferred IUPAC names rather than functional class names and names of assemblies of identical units are preferred to those that are formed by normal substitution.

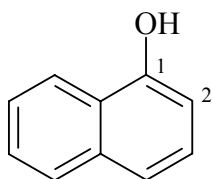
Examples:



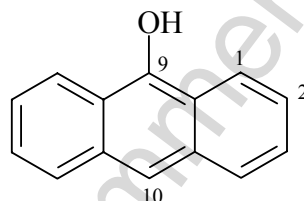
(1) benzene-1,2-diol (PIN)  
(not pyrocatechol)



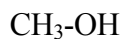
(1) 2-nitrobenzene-1,3-diol (PIN)



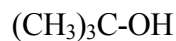
(1) naphthalen-1-ol (PIN)  
(4) 1-naphthol



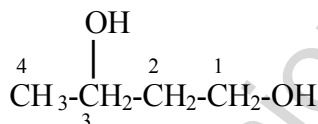
(1) anthracen-9-ol (PIN)  
(4) 9-anthrol



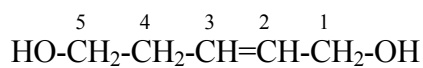
(1) methanol (PIN)  
(2) methyl alcohol



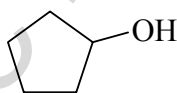
(1) 2-methylpropan-2-ol (PIN)  
(2) *tert*-butyl alcohol



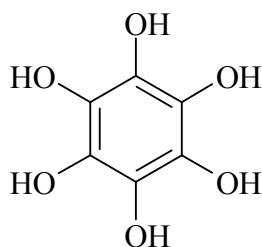
(1) butane-1,3-diol (PIN)



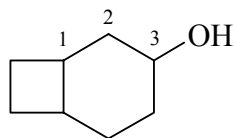
(1) pent-2-ene-1,5-diol (PIN)



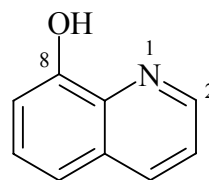
(1) cyclopentanol (PIN)



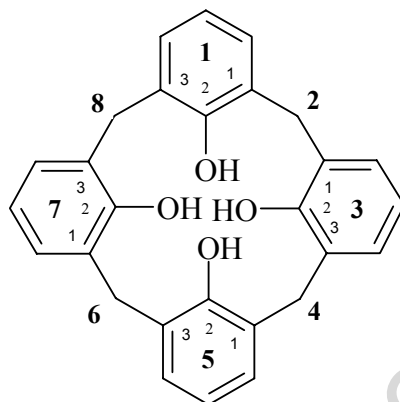
(1) benzenehexol (PIN)



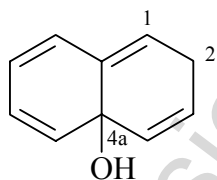
(1) bicyclo[4.2.0]octan-3-ol (PIN)



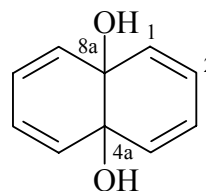
(1) quinolin-8-ol (PIN)



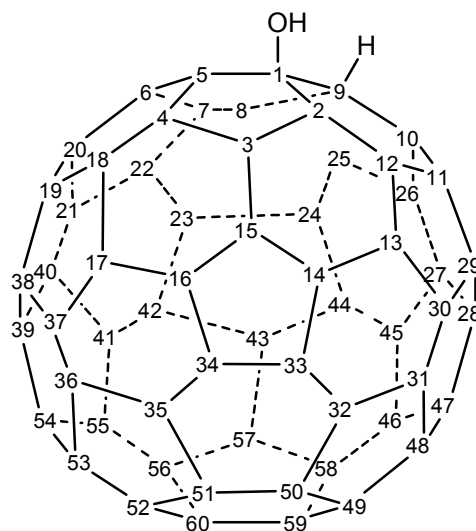
1,3,5,7(1,3)-tetrabenzenacyclooctaphane-1<sup>2</sup>,3<sup>2</sup>,5<sup>2</sup>,7<sup>2</sup>-tetrol (PIN)



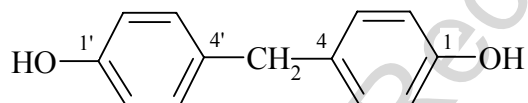
(1) naphthalen-4a(2*H*)-ol (PIN)  
2,4a-dihydronaphthalen-4a-ol  
(see P-53.1)



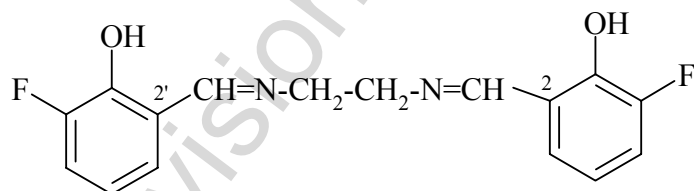
(1) naphthalene-4a,8a-diol (PIN)  
4a,8a-dihydronaphthalene-4a,8a-diol  
(see P-53.1)



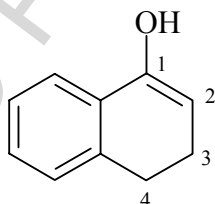
- (1) (C<sub>60</sub>-I<sub>h</sub>)[5,6]fulleren-1(9H)-ol (see P-53.1) (PIN)  
 1,9-dihydro(C<sub>60</sub>-I<sub>h</sub>)[5,6]fulleren-1-ol (see P-53.1)



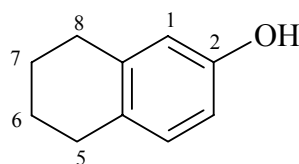
- (3) 4,4'-methylenediphenol (PIN)  
 (1) 4-[(4-hydroxyphenyl)methyl]phenol



- (3) 2,2'-[ethane-1,2-diylbis(azanylylidene)methanylylidene]bis(6-fluorophenol) (PIN)

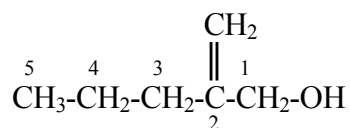


- (1) 3,4-dihydronaphthalen-1-ol (PIN)

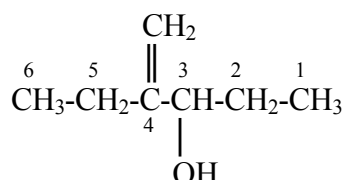


- (1) 5,6,7,8-tetrahydronaphthalen-2-ol (PIN)

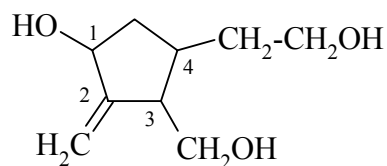




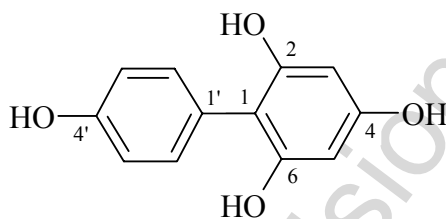
(1) 2-methylidenepentan-1-ol (PIN)



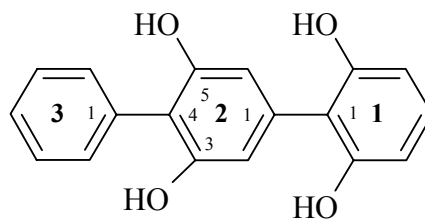
(1) 4-methylidenehexan-3-ol (PIN)



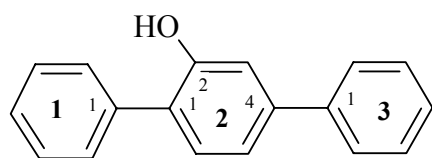
(1) 4-(2-hydroxyethyl)-3-(hydroxymethyl)-2-methylidenecyclopentan-1-ol (PIN)



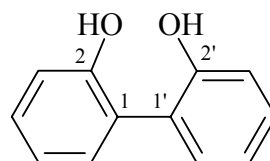
(1) [1,1'-biphenyl]-2,4,4',6-tetrol (PIN)  
 biphenyl-2,4,4',6-tetrol



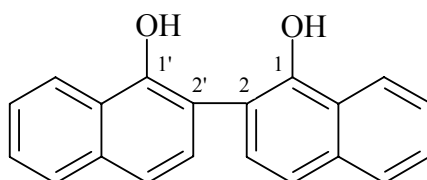
(1) [1<sup>1</sup>,2<sup>1</sup>:2<sup>4</sup>,3<sup>1</sup>-terphenyl]-1<sup>2</sup>,1<sup>6</sup>,2<sup>3</sup>,2<sup>5</sup>-tetrol (PIN)  
 [in the preferred name brackets enclose the name of an assembly requiring locants when suffixes are present; for numbering, see P-28.3.1(a)]  
 1,1':4',1''-terphenyl-2,3',5',6-tetrol  
 [see P-28.3.1(b)]



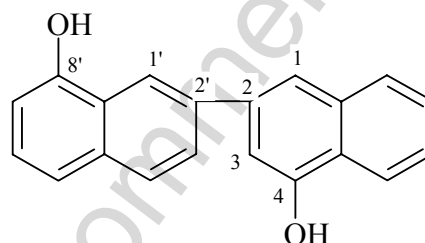
[1<sup>1</sup>,2<sup>1</sup>:2<sup>4</sup>,3<sup>1</sup>-terphenyl]-2<sup>2</sup>-ol (PIN;  
 see P-28.3.1(a))  
 1,1':4',1''-terphenyl-2'-ol [P-28.3.1(b)]



[1,1'-biphenyl]-2,2'-diol (PIN)  
 (not 2,2'-biphenol)



[2,2'-binaphthalene]-1,1'-diol (PIN)  
 (not 2,2'-bi-1-naphthol)

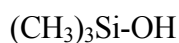


[2,2'-binaphthalene]-4,8'-diol (PIN)  
 (not 3,7'-bi-1-naphthol)

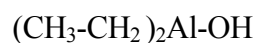
### P-63.1.3 Heterols

When the hydroxy group is attached to an atom other than carbon, hydroxy compounds belong to a class called heterols. They are classified as hydroxy compounds and named using the suffix 'ol', unless they are classified as acids and denoted by a retained name. Names formed using a suffix are preferred to those formed by means of the prefix 'hydroxy'.

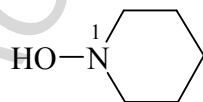
Examples:



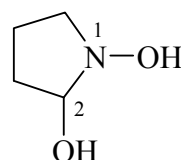
trimethylsilanol (PIN)  
 hydroxy(trimethyl)silane  
 (silane is a preferred preselected  
 name; see P-12)



diethylalumanol (PIN)  
 diethyl(hydroxy)alumane  
 (alumane is a preferred  
 preselected name; see P-12)



piperidin-1-ol (PIN)  
 1-hydroxypiperidine  
*N*-hydroxypiperidine



pyrrolidine-1,2-diol (PIN)  
 1-hydroxypyrrolidin-2-ol  
*N*-hydroxypyrrolidin-2-ol

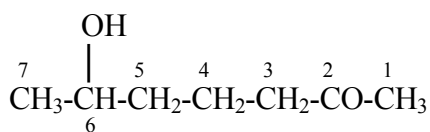
$\text{P(OH)}_3$	$\text{H}_2\text{As-OH}$
phosphorous acid (retained preselected name) (not phosphanetriol)	arsinous acid (retained preselected name) (not arsanol)

**P-63.1.4** Substitutive nomenclature, prefix mode

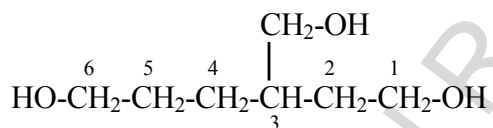
Hydroxy groups are indicated by the prefix 'hydroxy' when:

- (1) a group having priority for citation as the principal characteristic group is present; or
- (2) a hydroxy group cannot be denoted by a suffix.

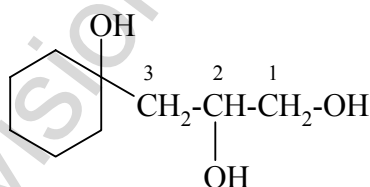
Examples:



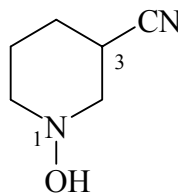
(1) 6-hydroxyheptan-2-one (PIN)



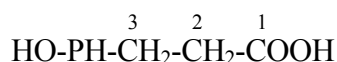
(2) 3-(hydroxymethyl)hexane-1,6-diol (PIN)



(2) 3-(1-hydroxycyclohexyl)propane-1,2-diol (PIN)



(1) 1-hydroxypiperidine-3-carbonitrile (PIN)



- (1) 3-(hydroxyphosphanyl)propanoic acid (PIN)  
3-(hydroxyphosphanyl)propionic acid

**P-63.1.5** Sulfur, selenium, and tellurium analogues of hydroxy compounds

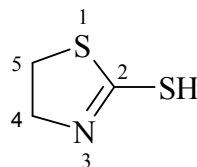
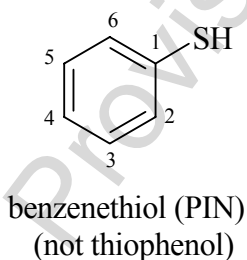
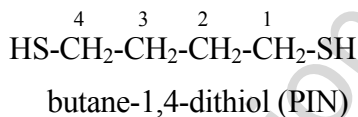
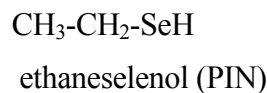
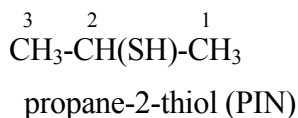
Sulfur, selenium, and tellurium analogues of hydroxy compounds are named substitutively using the suffixes 'thiol', 'selenol', and 'tellurol', and the prefixes 'sulfanyl', 'selanyl', and 'tellanyl', respectively; the presence of several of the same kind of 'ol' characteristic groups is denoted by the numerical multiplying prefixes 'di', 'tri', etc. The prefixes 'mercapto' (–SH), and 'hydroseleno' (–SeH) are no longer recommended.

Functional class nomenclature is not used.

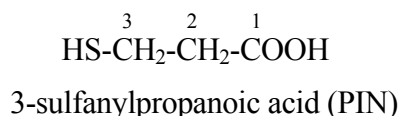
Names of assemblies of identical units are formed by the general method described in P-15.3 and are preferred to those formed substitutively.

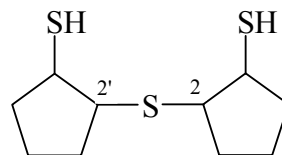
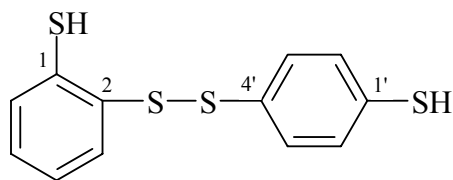
The seniority order of sulfur, selenium, and tellurium analogues of hydroxy compounds is:  
O > S > Se > Te.

Examples:

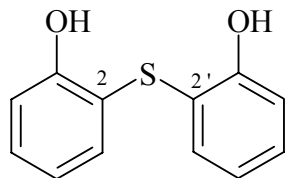


4,5-dihydrothiazole-2-thiol (PIN)

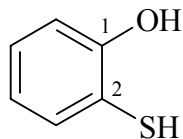




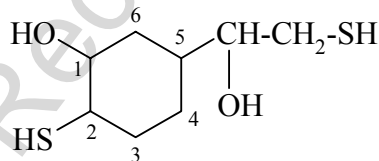
2,4'-disulfaneyldi(benzene-1-thiol) (PIN) 2,2'-sulfaneyldi(cyclopentane-1-thiol) (PIN)



2,2'-sulfaneyldiphenol (PIN)  
2-[(2-hydroxyphenyl)sulfanyl]phenol



2-sulfanylphenol (PIN)



5-(1-hydroxy-2-sulfanylethyl)-2-sulfanylcyclohexan-1-ol (PIN)  
(ring preferred to chain, see P-58.3.1.6)  
1-(3-hydroxy-4-sulfanylcyclohexyl)-2-sulfanylethan-1-ol

## P-63.2 Ethers and chalcogen analogs

P-63.2.1 Definitions and general methodology

P-63.2.2 Names of substituent groups R'-O-, R'-S-, R'-Se-, and R'-Te-

P-63.2.3 Retained names

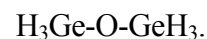
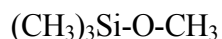
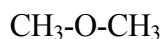
P-63.2.4 Systematic names of ethers

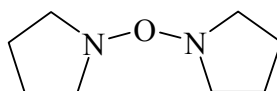
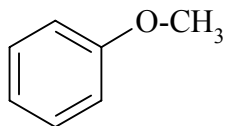
P-63.2.5 Chalcogen analogs of ethers: sulfides, selenides and tellurides

### P-63.2.1 Definitions and general methodology

Ethers have the general formula R-O-R', in which R = R' or R ≠ R'; R and R' can be any substituent group, aliphatic or cyclic, organyl (the free valence attached to a carbon atom) or organoheteryl (the free valence attached to an atom other than carbon), derived from the parent hydrides described in P-28.

Examples:





Chalcogen analogues are generically called sulfides, R-S-R', selenides, R-Se-R', and tellurides, R-Te-R'.

Names for ethers and their chalcogen analogues are formed by different methods in accordance with the principles of substitutive nomenclature, multiplicative nomenclature, skeletal replacement ('a') nomenclature, phane nomenclature, and functional class nomenclature. However, some ethers and chalcogen analogues are classified as parent hydrides and named as such, for example H<sub>3</sub>Ge-O-GeH<sub>3</sub>, digermoxane, and similar compounds described in Section P-21.2.3.1. These compounds are thus not named by the methods described in this Section, because their names are subject to selection rules with regard to heteroatom content.

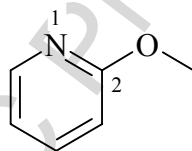
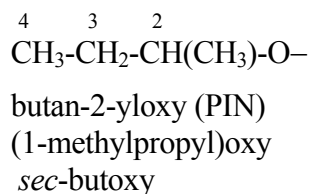
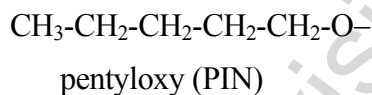
In substitutive nomenclature, when R is different from R', R is chosen as parent hydride and R'-O- is cited as a substituent to it. Names of these substituent groups are described in Section P-63.4.2. In functional class nomenclature, R and R' are used as substituent groups.

**P-63.2.2** Names of substituent groups R'-O-, R'-S-, R'-Se-, and R'-Te-

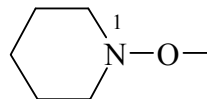
**P-63.2.2.1** Systematic names

**P-63.2.2.1.1** Substituent prefix names for R'-O- groups are formed by concatenation, i.e., by adding the prefix 'oxy' to the substituent prefix name for the group R'. These compound prefixes require the numerical multiplying prefixes 'bis', 'tris', etc.

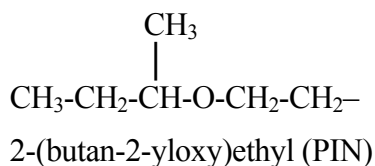
Examples:



pyridin-2-yloxy (PIN)  
2-pyridyloxy

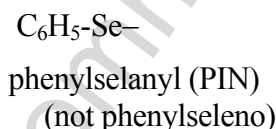
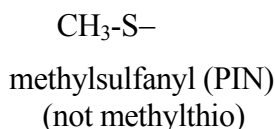


piperidin-1-yloxy (PIN)  
piperidinoxy



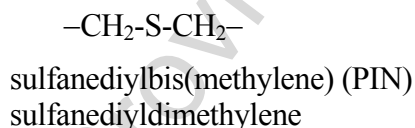
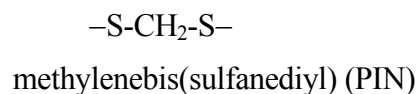
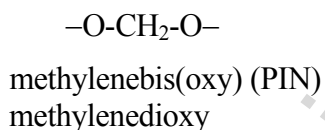
**P-63.2.2.1.2** Substituent prefixes for R'S-, R'Se-, and R'Te-, are substituents whose names are formed by substitution of the groups HS-, sulfanyl; HSe-, selanyl; and HTe-, tellanyl. The prefixes thus formed are preferred to compound prefixes formed by adding the name of the appropriate substituent to the prefix names thio, -S-; seleno, -Se-; or telluro, -Te-. The latter require the multiplicative prefixes 'bis', 'tris', etc.

Examples:



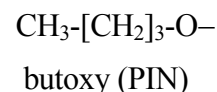
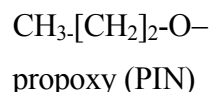
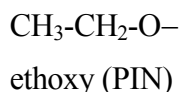
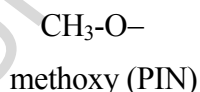
**P-63.2.2.1.3** Divalent groups, such as -O-Y-O- or -S-Y-S-, are named by adding the prefixes oxy, sulfanediyl, etc. to the name of the divalent group Y. The multiplying prefix 'bis' is used in preferred names instead of 'di' to avoid ambiguity. Parentheses are used after the multiplying prefix 'bis', 'tris' etc., even around simple prefixes.

Examples:



#### **P-63.2.2.2** Retained names

Some contracted names are retained for R-O- substituent groups. They are used both as preferred IUPAC names and in general nomenclature; they are fully substitutable (with the exception of *tert*-butoxy), are compulsory prefixes, and are considered as simple prefixes requiring the numerical prefixes 'di', 'tri', etc. They are:





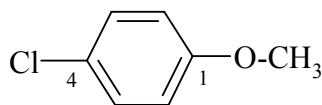
The following names are retained for use in general nomenclature only; no substitution is allowed:



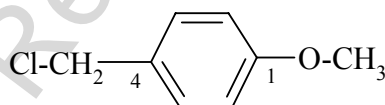
### P-63.2.3 Retained names of ethers

Anisole,  $C_6H_5-O-CH_3$ , is the only name in the class of ethers which is retained both as a preferred IUPAC name and for use in general nomenclature. For preferred IUPAC names, no substitution is allowed; for general nomenclature substitution is allowed on the ring and on the side chain under certain conditions (see P-34.3.2, and P-46.3).

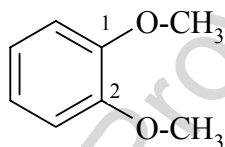
Examples:



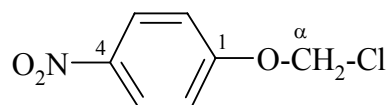
1-chloro-4-methoxybenzene (PIN)  
(no substitution on anisole)  
4-chloroanisole



1-(chloromethyl)-4-methoxybenzene (PIN)  
(no substitution on anisole)  
4-(chloromethyl)anisole  
(not 4-methoxybenzyl chloride; no  
substitution on benzyl)

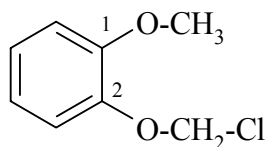


1,2-dimethoxybenzene (PIN)  
(no substitution on anisole)  
(not 2-methoxyanisole; see  
P-46.3 for substitution rules  
for anisole)

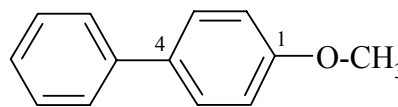


1-(chloromethoxy)-4-nitrobenzene (PIN)  
(no substitution on anisole)  
 $\alpha$ -chloro-4-nitroanisole (see P-46.3 for  
substitution rules for anisole)

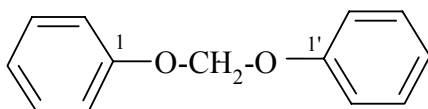




1-(chloromethoxy)-2-methoxybenzene (PIN)  
(no substitution on anisole)  
 $\alpha$ -chloro-2-methoxyanisole  
(not 2-(chloromethoxy)anisole)



4-methoxy-1,1'-biphenyl (PIN)  
(not 4-phenylanisole nor 1-methoxy-4-phenylbenzene; the biphenyl ring system is senior to a single benzene ring)



1,1'-[methylenebis(oxy)]dibenzene (PIN)  
 $\alpha$ -phenoxyanisole

#### P-63.2.4 Systematic names of ethers

Ethers having the general structure R-O-R' (R=R', or R $\neq$ R') have the class names 'ethers' and are named by one of the five following methods:

- (1) substitutively by prefixing the name of the R'-O - group to that of the parent hydride;
- (2) by functional class nomenclature, using the term 'ether' and, when the groups are different, citing the two substituent groups in alphanumerical order;
- (3) by multiplicative nomenclature, when R and R' are cyclic components;
- (4) by skeletal replacement ('a') nomenclature;
- (5) by phane nomenclature.

**P-63.2.4.1** Names of ethers, when R and R' are both aliphatic groups or when one is cyclic, are formed by methods (1), (2), or (4). Methods (1) and (5) lead to preferred IUPAC names.

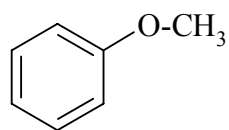
Examples:



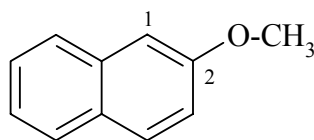
- (1) methoxymethane (PIN)
- (2) dimethyl ether



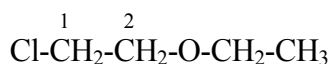
- (1) methoxyethane (PIN)
- (2) ethyl methyl ether



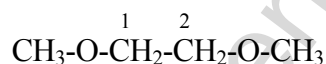
- (1) anisole (PIN; retained name)  
methoxybenzene
- (2) methyl phenyl ether



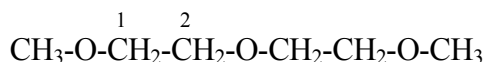
- (1) 2-methoxynaphthalene (PIN)
- (2) methyl naphthalen-2-yl ether  
methyl 2-naphthyl ether



- (1) 1-chloro-2-ethoxyethane (PIN)
- (2) 2-chloroethyl ethyl ether  
(not 2-chloroethyl ethyl oxide)



- (1) 1,2-dimethoxyethane (PIN)
- (2) ethane-1,2-diyl dimethyl ether



- (1) 1-methoxy-2-(2-methoxyethoxy)ethane (PIN)

Skeletal replacement ('a') nomenclature [method (4)] generates preferred IUPAC names, when the conditions for using this type of nomenclature are met; otherwise substitutive nomenclature must be used.

Examples:

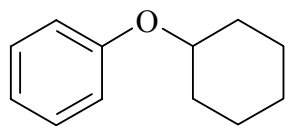


- (4) 2,5,8,11-tetraoxadodecane (PIN)
- (1) 1-methoxy-2-[2-(2-methoxyethoxy)ethoxy]ethane

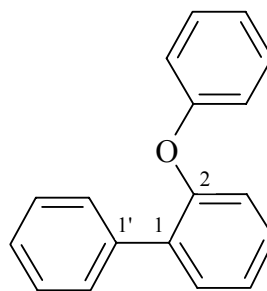
**P-63.2.4.2** The names of ethers when both R and R' groups are cyclic are formed by methods (1), (2), (3), and (5). Methods (1), (2), and (5) lead to preferred IUPAC names.

When method (1), substitutive nomenclature, is used, the senior ring or ring system must be chosen as the parent hydride (see P-44).

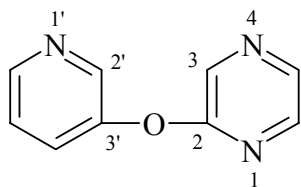
Examples:



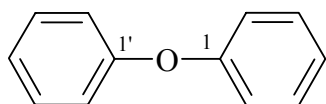
- (1) (cyclohexyloxy)benzene (PIN)  
(2) cyclohexyl phenyl ether



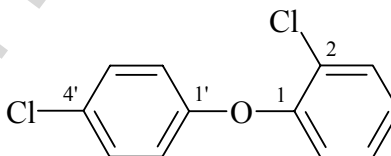
- (1) 2-phenoxybiphenyl (PIN)  
(2) biphenyl-2-yl phenyl ether



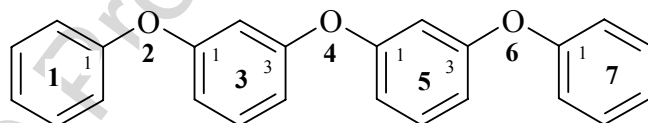
- (1) 2-(pyridin-3-yloxy)pyrazine (PIN)  
(2) pyrazin-2-yl 3-pyridyl ether



- (2) 1,1'-oxydibenzene (PIN)  
(1) phenoxybenzene  
(3) diphenyl ether



- (2) 2,4'-dichloro-1,1'-oxydibenzene (PIN)  
(1) 1-chloro-2-(4-chlorophenoxy)benzene  
(3) 2-chlorophenyl 4-chlorophenyl ether



- (5) 2,4,6-trioxa-1,7(1),3,5(1,3)-tetrabenzenaheptaphane (PIN)

### P-63.2.5 Names of chalcogen analogs of ethers: sulfides, selenides and tellurides

#### P-63.2.5.1 General methodology

Sulfides, R-S-R', selenides R-Se-R', and tellurides R-Te-R', are named by the following methods:

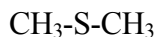
- (1) by prefixing the names of the substituent groups R'-S -, R'-Se -, or R'-Te -, i.e., R'-sulfanyl, R'-selanyl, and R'-tellanyl, respectively, to that of the appropriate parent hydride; the names R'-thio, R'-seleno, and R'-telluro are no longer recommended. The prefixes R'-sulfanyl, R'-selanyl, and R'-tellanyl are compulsory prefixes and can be attached to any atom of any parent hydride;
- (2) by functional class nomenclature using the terms sulfides, selenides and tellurides for -S-, -Se-, and -Te-, respectively;
- (3) by multiplicative nomenclature in the case of cyclic parent hydrides, using the prefixes sulfanediyl, -S- (not thio); selanediyl -Se- (not seleno); and tellanediyl -Te- (not telluro), respectively;
- (4) by skeletal replacement ('a') nomenclature;
- (5) by phane nomenclature;

Names formed by substituting the parent hydrides oxidane, sulfane, selane, and tellane for H<sub>2</sub>O, H<sub>2</sub>S, H<sub>2</sub>Se, and H<sub>2</sub>Te, respectively, by the appropriate substituent groups are not recommended.

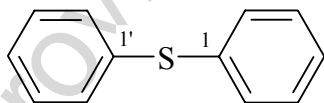
Names formed by functional replacement nomenclature of the retained name anisole are no longer recommended. Class names such as thiooxide are not recommended.

Method (1), substitutive nomenclature, is preferred to method (2), functional class nomenclature, for the formation of preferred IUPAC names; methods (3), (4), and (5) are applied in place of method (1) when the conditions for their use are satisfied.

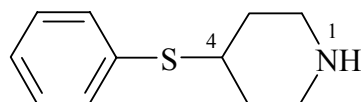
Examples:



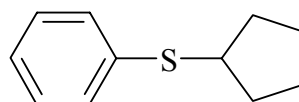
- (1) (methylsulfanyl)methane (PIN)
- (2) dimethyl sulfide



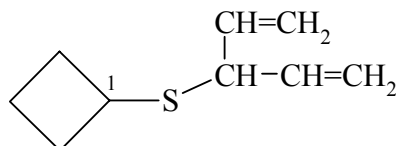
- (3) 1,1'-sulfanediylbenzene (PIN)  
(not 1,1'-thiodibenzene)
- (1) (phenylsulfanyl)benzene
- (2) diphenyl sulfide



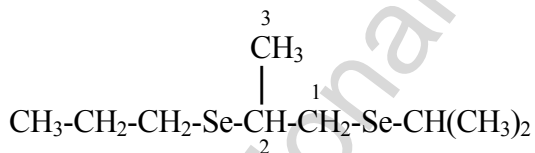
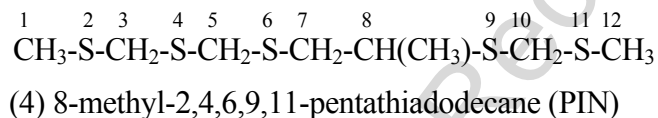
- (a) 4-(phenylsulfanyl)piperidine (PIN)  
 [not 4-(phenylthio)piperidine]  
 (b) phenyl piperidin-2-yl sulfide



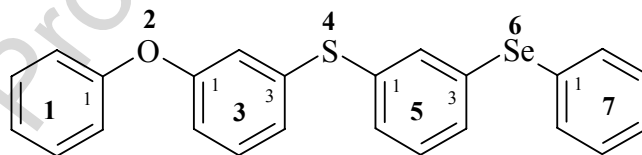
- (a) (cyclopentylselanyl)benzene (PIN)  
 [not (cyclopentylseleno)benzene]  
 (b) cyclopentyl phenyl selenide



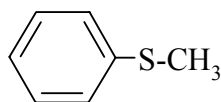
- (1) 1-[(penta-1,4-dien-3-yl)sulfanyl]cyclobutane (PIN)  
 (ring preferred to chain, see P-58.3.1.6)  
 (2) cyclobutyl penta-1,4-dien-3-yl sulfide



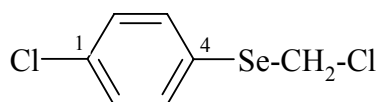
- (1) 1-(propan-2-ylselanyl)-2-(propylselanyl)propane (PIN)  
 (not 2,5-dimethyl-3,6-diselenanonane; skeletal replacement ('a')  
 nomenclature requires four heterounits)



- (5) 2-oxa-4-thia-6-selena-1,7(1),3,5(1,3)-tetrabenzenaheptaphane (PIN)



- (1) (methylsulfanyl)benzene (PIN)  
 (not thioanisole)



- (1) 1-chloro-4-(chloromethyl)selenanyl]benzene (PIN)  
 (not  $\alpha$ ,4-dichloroselenoanisole)

### P-63.3 Peroxides and chalcogen analogues

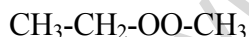
#### P-63.3.1 Peroxides, disulfides, diselenides, and ditellurides

Compounds with the general structures R-OO-R', R-SS-R', R-SeSe-R', and R-TeTe-R' are named in the following ways:

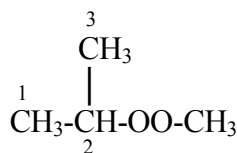
- (1) substitutively by combining the prefix name for R' additively with 'peroxy' giving the names 'R'-peroxy', 'R'-disulfanyl', 'R'-diselanyl' or 'R'-ditellanyl' prefixed to the name of the parent hydride corresponding to R;
- (2) by functional class nomenclature by citing the names of the groups R and R', in alphanumerical order if two different groups are present, and the class name, peroxide, disulfide, diselenide, and ditelluride, respectively, as a separate word (class names such as dithioperoxide are not recommended);
- (3) by ring assembly nomenclature, multiplicative nomenclature, skeletal replacement ('a') nomenclature, or phane nomenclature, when the conditions for their application are fulfilled.

Method (1) leads to preferred IUPAC names.

Examples:



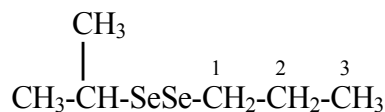
- (1) (methylperoxy)ethane (PIN)  
 (2) ethyl methyl peroxide



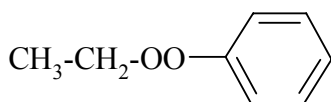
- (1) 2-(methylperoxy)propane (PIN)  
 (2) isopropyl methyl peroxide



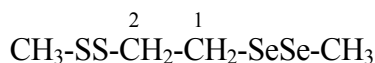
- (1) (methyldisulfanyl)methane (PIN)  
 (2) dimethyl disulfide



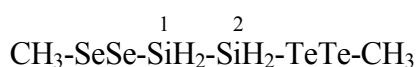
- (1) 1-(propan-2-yl)diselanyl]propane (PIN)  
 (2) isopropyl propyl diselenide



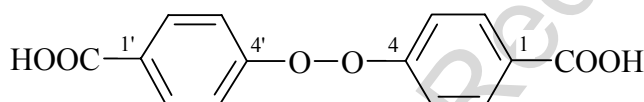
- (1) (ethylperoxy)benzene (PIN)  
 (2) ethyl phenyl peroxide



- (1) 1-(methyldiselanyl)-2-(methyldisulfanyl)ethane (PIN)



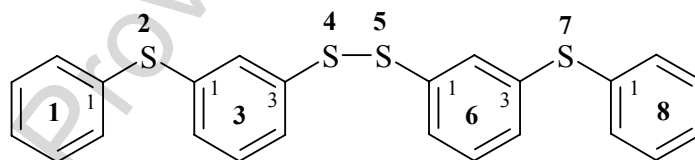
- (1) 1-(methyldiselanyl)-2-(methyltellanyl)disilane (PIN)  
 (disilane is a preferred preselected name, see P-12)



- (3) 4,4'-peroxydibenzoic acid (PIN)  
 [4-(4-carboxyphenyl)peroxy]benzoic acid



- (3) 2,4,5,8,11-pentathiadodecane (PIN)



- (3) 2,4,5,7-tetrathia-1,8(1),3,6(1,3)-tetrabenzenaoctaphane (PIN)

### P-63.3.2 Mixed chalcogen analogs of peroxides

Mixed chalcogen structures such as R-XY-R' in which X and Y are O, S, Se, or Te atoms are named by two methods:

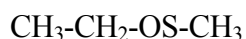
- (1) by prefixing the names of the substituent groups R'-S -, R'-Se -, or R'-Te -, i.e., R'-sulfanyl, R'-selanyl, and R'-tellanyl, respectively, to that of the appropriate parent

hydride. The prefixes R'-sulfanyl, R'-selanyl, and R'-tellanyl are compulsory prefixes and can be attached to any atom of any parent hydride; multiplicative nomenclature is used when the conditions for its use are fulfilled;

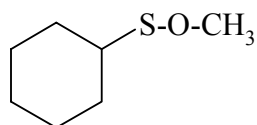
- (2) by citing the prefix names of the groups R and R', in alphanumerical order, followed by an appropriate class name 'thioperoxide', 'diselenoperoxide', 'selenothioperoxide', etc. Each prefix R and R' is preceded by a capital italicized letter locant, as appropriate;
- (3) by skeletal replacement ('a') nomenclature or phane nomenclature, when the conditions for its use are fulfilled.

Method (1) leads to preferred IUPAC names.

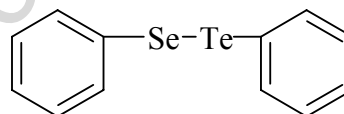
Examples:



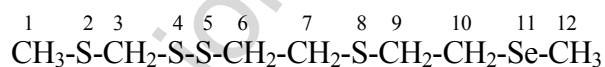
- (1) [(methylsulfanyl)oxy]ethane (PIN)
- (2) *O*-ethyl *S*-methyl thioperoxide



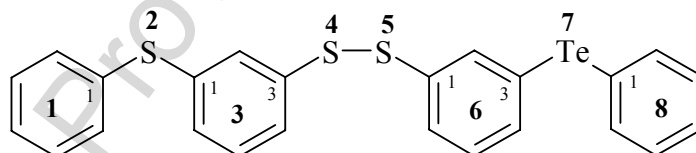
- (1) (methoxysulfanyl)cyclohexane (PIN)
- (2) *S*-cyclohexyl *O*-methyl thioperoxide



- (1) (selanediyltellanediyl)dibenzene (PIN)
- (2) diphenyl selenothioperoxide



- (3) 2,4,5,8-tetrathia-11-selenadodecane (PIN)



- (3) 2,4,5-trithia-7-tellura-1,8(1),3,6(1,3)-tetrabenzenaoctaphane (PIN)

## P-63.4 Hydroperoxides (peroxols) and chalcogen analogues

### P-63.4.1 Hydroperoxides

The suffix 'peroxol' is recommended for the characteristic group -OOH.



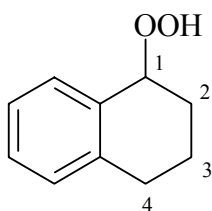
Compounds with the general structure R-OOH are called generically 'hydroperoxides'. The class name 'peroxols' could be more appropriate. They are named in two ways when the -OOH group is the principal function.

- (1) substitutively using the suffix 'peroxol';
- (2) by functional class nomenclature using the class name 'hydroperoxide'.

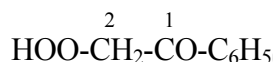
The prefix 'peroxy, not 'dioxy', is retained for the group -OO- (see P-63.4). The prefix 'hydroperoxy' is formed by concatenation to describe the group -OOH as a substituent in the presence of a characteristic group having priority for citation as a suffix.

Method (1) leads to preferred IUPAC names.

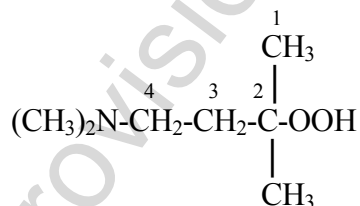
Examples:



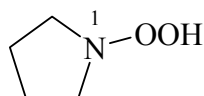
- (1) 1,2,3,4-tetrahydronaphthalene-1-peroxol (PIN)
- (2) 1,2,3,4-tetrahydronaphthalen-1-yl hydroperoxide



2-hydroperoxy-1-phenylethan-1-one (PIN)



- (1) 4-(dimethylamino)-2-methylbutane-2-peroxol (PIN)
- (2) [3-(dimethylamino)-1,1-dimethylpropyl] hydroperoxide  
[3-(dimethylamino)-2-methylbutan-2-yl] hydroperoxide



- (1) pyrrolidine-1-peroxol (PIN)
- (2) pyrrolidin-1-yl hydroperoxide

**P-63.4.2** Chalcogen analogues of hydroperoxides.

**P-63.4.2.1** Compounds having the general structure R-SOH or R-OSH are called generically 'thiohydroperoxides' or 'thioperoxols'. Similarly, compounds R-SeOH or R-OSeH and R-TeOH or R-OTeH, are called 'selenohydroperoxides' or 'selenoperoxols' and tellurohydroperoxides' or 'telluroperoxols', respectively. When representing the principal function, they are named by two methods.

- (1) by substitutive nomenclature and the appropriate suffix listed in Table 6.1, formed by functional replacement, to denote a principal function;
- (2) by functional class nomenclature using the name of the class 'thiohydroperoxide', 'selenohydroperoxide' and 'tellurohydroperoxide'; when required, the prefixes, 'thio', 'seleno' and 'telluro' are placed in alphabetical order, for example, 'selenothiohydroperoxide', etc.; the locants *O*, *S*, *Se*, or *Te* designate the bonding of the R- group; when the same element is present the class names 'disulfide', 'diselenide', or 'ditelluride' are used.

Compounds of the type R-SOH, R-SeOH and R-TeOH and their chalcogen analogues were previously named sulfenic, selenenic and tellurenic acids, using the suffixes 'sulfenic acid', 'selenenic acid', and 'tellurenic acid', respectively; this method is no longer recommended.

Method (1) generates preferred IUPAC names.

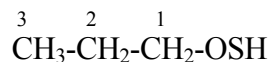
**Table 6.1 Suffixes to denote peroxols (hydroperoxides) modified by functional replacement nomenclature (in decreasing order of seniority as principal group)**

-S-OH	-SO-thioperoxol	-Se-SH	-SeS-selenothioperoxol
-Se-OH	-SeO-selenoperoxol	-Te-SH	-TeS-tellurothioperoxol
-Te-OH	-TeO-telluroperoxol	-S-SeH	-SSe-selenothioperoxol
-O-SH	-OS-thioperoxol	-S-TeH	-STe-tellurothioperoxol
-O-SeH	-OSe-selenoperoxol	-Se-SeH	-diselenoperoxol
-O-TeH	-OTe-telluroperoxol	-Te-SeH	-TeSe-selenotelluroperoxol
-S-SH	-dithioperoxol	-Se-TeH	-SeTe-selenotelluroperoxol
		-Te-TeH	-ditelluroperoxol

Examples:



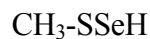
- (1) methane-SO-thioperoxol (PIN)
- (2) *S*-methyl thiohydroperoxide  
(no longer methanesulfenic acid)



- (1) propane-1-OS-thioperoxol (PIN)
- (2) *O*-propyl thiohydroperoxide



- (1) ethanedithioperoxol (PIN)
- (2) ethyl hydrodisulfide  
ethyl dithiohydroperoxide



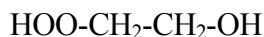
- (1) methane-SSe-selenothioperoxol (PIN)
- (2) *S*-methyl selenothiohydroperoxide

**P-63.4.2.2** Prefixes corresponding to the suffixes described in P-63.4.2.1 are formed:

- (1) by using prefixes such as ‘hydroperoxy’, –OOH; ‘disulfanyl’, –SSH, or by combining simple prefixes, ‘hydroxy’ –OH; ‘oxy-’, –O–; ‘sulfanyl’, –SH; etc.; or
- (2) by using prefixes such as dithiohydroperoxy, –SSH; *SO*-thiohydroperoxy, –OSH; *SeS*-selenothiohydroperoxy, –SSeH; etc.

Method (1) leads to preferred IUPAC names.

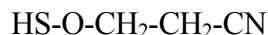
Examples:



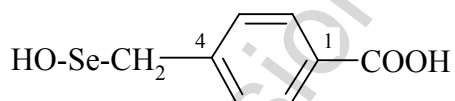
2-hydroperoxyethanol (PIN)



- (1) 2-disulfanylacetic acid (PIN)
- (2) (dithiohydroperoxy)acetic acid



3-(sulfanyloxy)propanenitrile (PIN)  
3-(*SO*-thiohydroperoxy)propanenitrile



4-[(hydroxyselanyl)methyl]benzoic acid (PIN)  
4-(*OSe*-selenohydroperoxymethyl)benzoic acid

### **P-63.5** Cyclic ethers, sulfides, selenides, and tellurides

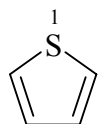
Cyclic ethers, sulfides, selenides and tellurides are heterocycles named by the following methods:

- (1) preferred retained names described in P-55 are chosen first;
- (2) for monocycles, by the extended Hantzsch-Widman system or by replacement nomenclature when the Hantzsch-Widman system is not applicable;
- (3) by bridged fused nomenclature;
- (4) by detachable prefixes ‘epoxy’, ‘epithio’, ‘episeleno’, or ‘epitelluro’ in substitutive nomenclature;

- (5) by additive names formed by the addition of the terms 'oxide', 'sulfide', selenide', or 'telluride' to the name of an unsaturated compound to the term.

As a general rule, names of heterocyclic compounds are preferred IUPAC names.

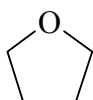
Examples:



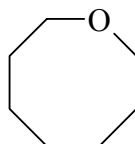
(1) thiophene (PIN)



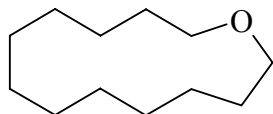
(1) tellurophene (PIN)



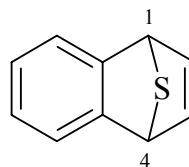
(1) oxolane (PIN)  
tetrahydrofuran



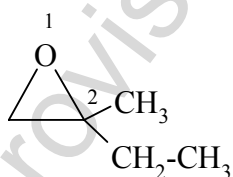
(1) thioctane (PIN)



(2) oxacyclotridecane (PIN)



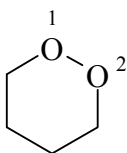
(3) 1,4-dihydro-1,4-sulfanonaphthalene (PIN)



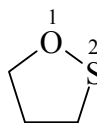
(2) 2-ethyl-2-methyloxirane (PIN)  
(4) 1,2-epoxy-2-methylbutane



(2) oxirane (PIN)  
(3) ethylene oxide



1,2-dioxane (PIN)



1,2-oxathiolane (PIN)

### P-63.6 Sulfoxides and sulfones

Compounds with the general structures R-SO-R' and R-SO<sub>2</sub>-R' are called generically 'sulfoxides' and 'sulfones', respectively, when R and R' are hydrocarbyl groups. They are named in three ways as follows;

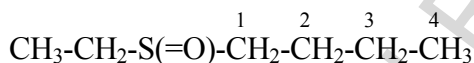
- (1) substitutively, by prefixing the name of the acyl group R'-SO- or R'-SO<sub>2</sub>- to the name of the parent hydride corresponding to R as described in P-65.3.2.2.2;
- (2) by functional class nomenclature, using the class names 'sulfoxide' and 'sulfone', respectively;
- (3) by multiplicative nomenclature, except where R and R' are alkyl groups.

Method (1) generates preferred names.

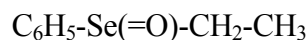
Selenium and tellurium analogues are named in the same way using acyl groups derived from the appropriate seleninic, selenonic, tellurenic, and telluronic acids, and the class names 'selenoxide', 'selenone', 'telluroxide', 'tellurone'.

Prefix names such as 'alkylsulfinyl' or 'arylsulfonyl' are no longer recommended.

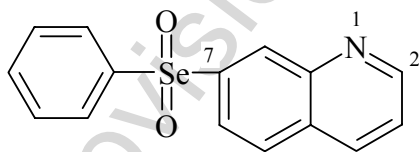
Examples:



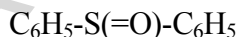
- (1) 1-(ethanesulfinyl)butane (PIN)  
[not 1-(ethylsulfinyl)butane]
- (2) butyl ethyl sulfoxide



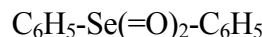
- (1) (ethaneseleninyl)benzene (PIN)  
[not (ethylseleninyl)benzene]
- (2) ethyl phenyl selenoxide



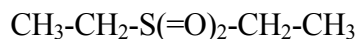
- (1) 7-(benzeneselenonyl)quinoline (PIN)  
[not 7-(phenylselenonyl)quinoline]
- (2) phenyl quinolin-7-yl selenone  
phenyl 7-quinolyl selenone



- (3) sulfinyldibenzene (PIN)
- (2) diphenyl sulfoxide
- (1) benzenesulfinylbenzene  
[not (phenylsulfinyl)benzene]



- (3) selenonyldibenzene (PIN)
- (2) diphenyl selenone
- (1) (ethaneselenonyl)ethane  
[not (phenylselenonyl)benzene]



- (1) (ethanesulfonyl)ethane (PIN)  
[not (ethylsulfonyl)ethane]
- (2) diethyl sulfone
- (3) multiplication of acyclic hydrocarbons is not permitted)

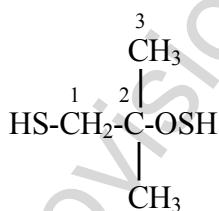
### P-63.7 Polyfunctional compounds

In the order of seniority of classes, hydroxy compounds and hydroperoxides are ranked in descending order after aldehydes and ketones, but before amines and imines. Chalcogen analogues are ranked after each class, according to the maximum number of O, S, Se, and Te atoms. In descending order, they are as follows.

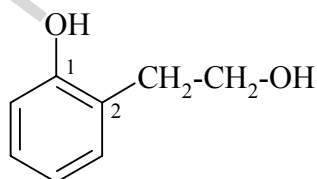
- (1) hydroxy compounds  $\text{-OH}$ , then their chalcogen analogues  $\text{-SH} > \text{-SeH} > \text{-TeH}$
- (2) hydroperoxides  $\text{-OOH}$ , then their chalcogen analogues  $\text{-SOH} > \text{-SeOH} > \text{-TeOH}$ , etc. (see Table 63.1)
- (3) amines  $>$  imines
- (4) ethers  $\text{-O-}$ , then their chalcogen analogues  $\text{-S-} > \text{-Se-} > \text{-Te-}$
- (5) peroxides  $\text{-OO-}$ , then their chalcogen analogues  $\text{-OS-} > \text{-OSe-} > \text{-OTe-}$ , etc.

There is no seniority order between phenols and hydroxy compounds. The choice for parent hydride is decided by the maximum number of hydroxy groups cited as suffixes; and a ring is preferred to a chain when there is a choice (see P-58.3.1.6).

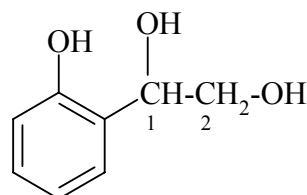
Examples:



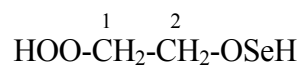
2-methyl-2-(sulfanyloxy)propane-1-thiol (PIN)



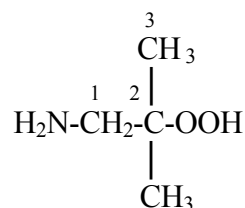
2-(2-hydroxyethyl)phenol (PIN)  
2-(2-hydroxyphenyl)ethan-1-ol  
(the ring is senior to the chain in the preferred name, see P-58.3.1.6)



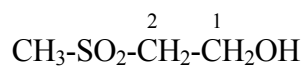
1-(2-hydroxyphenyl)ethane-1,2-diol (PIN)  
[not 2-(1,2-dihydroxyethyl)phenol; two principal groups are senior to one]



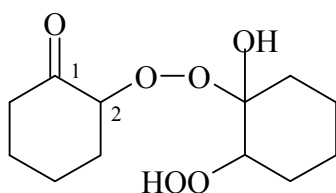
2-(selanyloxy)ethaneperoxol (PIN)



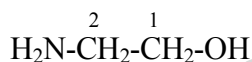
1-amino-2-methylpropane-2-peroxol (PIN)



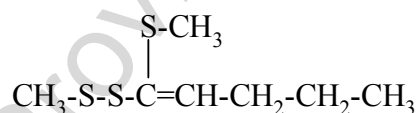
2-methanesulfonylethanol (PIN)



2-[(2-hydroperoxy-1-hydroxycyclohexyl)peroxy]cyclohexan-1-one (PIN)  
 (a ketone is senior to alcohols and peroxols)



2-aminoethan-1-ol (PIN)  
 (not ethanolamine)



1-(methyldisulfanyl)-1-(methylsulfanyl)pent-1-ene (PIN)  
 1-methyl-2-[1-(methylsulfanyl)pent-1-en-1-yl]disulfane  
 methyl 1-(methylsulfanyl)pent-1-en-1-yl disulfide  
 (not 1-methyl-2-[1-(methylthio)pent-1-en-1-yl]disulfane;  
 nor methyl 1-(methylthio)pent-1-en-1-yl disulfide)





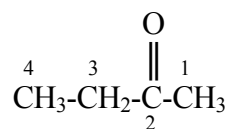
classes compounds other than ketones. Full systematization based on the strict application of the suffix 'one' for denoting the principal characteristic group =O is recommended in this Section.

Traditionally, the nomenclature of ketones was described with that of aldehydes. In these recommendations, the two classes are discussed separately (for aldehydes, see P-66.6), to emphasize the similarities between carboxylic acids and aldehydes with respect to nomenclature. Finally, to avoid fragmentation, the nomenclature of acetals and ketals is discussed with that of aldehydes in Section P-66.6.

### P-64.1 Definitions

**P-64.1.1** Ketones are defined classically as compounds in which a carbonyl group is bonded to two carbon atoms:  $R_2CO$  (neither R may be H) (see ref. 17).

Example:

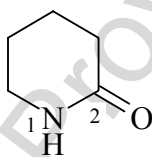


butan-2-one (PIN)

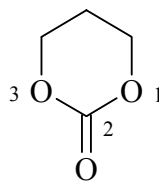
**P-64.1.2** Pseudoketones are

- cyclic compounds in which a carbonyl group in a ring is bonded to one or two skeletal heteroatoms; or
- compounds in which an acyclic carbonyl group is bonded to one or two acyclic skeletal heteroatoms, except nitrogen, halogen, or halogenoid atoms, or to a heteroatom of a ring or ring system. When the heteroatom of the ring is a nitrogen atom the compound has been called a 'hidden amide'.

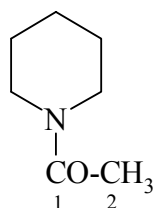
Examples:



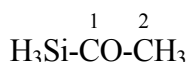
(a) piperidin-2-one (PIN)



(a) 1,3-dioxan-2-one (PIN)



- (b) 1-(piperidin-1-yl)ethan-1-one (PIN; a 'hidden amide')  
1-acetylpiperidine



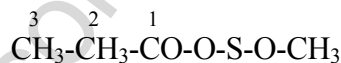
- (b) 1-silylethan-1-one (PIN)  
acetylsilane



- (b) 1-phosphanylpropan-1-one (PIN)  
propanoylphosphane



- (b) 1-(methoxydisulfanyl)ethan-1-one (PIN)  
(see also P-58.4.2)



- (b) 1-[(methoxysulfanyl)oxy]propan-1-one (PIN)  
(see also P-58.4.2)

### P-64.1.3 Heterones

Heterones are compounds having an oxygen atom formally doubly bonded to a heteroatom (see P-62.3.1.3 and P-63.1.3; see also P-68).

This systematization, the adjunction of two new subclasses to the general class of ketones, clarifies the general use of suffixes and prefixes in substitutive nomenclature by always giving precedence to suffixes that designate a principal characteristic group.

### P-64.2 Ketones

#### P-64.2.1 Retained names

For use in general nomenclature only, the names acetone, 1,4-benzoquinone, naphthoquinone, and anthraquinone are retained with full substitution on the corresponding structures. Also, the name ketene is retained for general nomenclature only, with substitution restricted to compulsory prefixes, and the names acetophenone and benzophenone are retained only for general nomenclature, but no substitution is allowed. (see P-34.3). Substitutive names, systematically constructed, are the preferred IUPAC names for ketones

**P-64.2.2** Systematic construction of names for ketones.

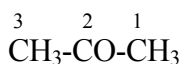
**P-64.2.2.1** Acyclic ketones

Unsubstituted acyclic ketones are systematically named in two ways:

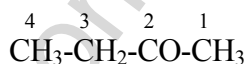
- (1) substitutively, using the suffix 'one' and the prefix 'oxo'; the presence of several 'one' characteristic groups is denoted by the numerical multiplying prefixes 'di', 'tri', etc.; the final letter 'a' of a numerical multiplying prefix is elided before the suffix '-one', for example, 'tetrone';
- (2) by functional class nomenclature using the class names 'ketone', 'diketone' etc.; substituent groups are placed, as separate words, in alphanumerical order before the class name.

Method (1) generates preferred IUPAC names.

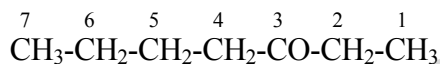
Examples:



propan-2-one (PIN)  
propanone  
acetone



butan-2-one (PIN)  
ethyl methyl ketone  
(not methyl ethyl ketone; groups must  
be cited in alphanumerical order)



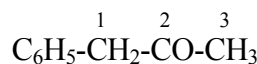
heptan-3-one (PIN)  
butyl ethyl ketone



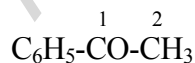
pentacosane-7,9,17,19-tetrone (PIN)



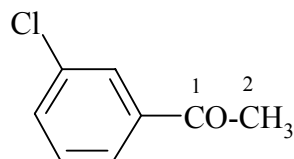
5-methylhexan-2-one (PIN)  
isopentyl methyl ketone



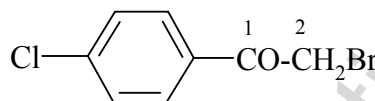
1-phenylpropan-2-one (PIN)  
benzyl methyl ketone



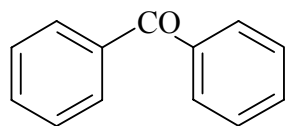
1-phenylethan-1-one (PIN)  
acetophenone (no substitution)



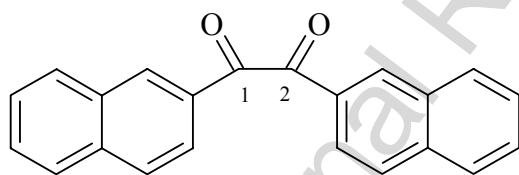
1-(3-chlorophenyl)ethan-1-one (PIN)  
(not 3'-chloroacetophenone;  
no substitution allowed for  
acetophenone)



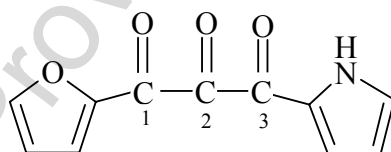
2-bromo-1-(4-chlorophenyl)ethan-1-one (PIN)  
(not 4-chlorophenacyl bromide)  
(not 2-bromo-4'-chloroacetophenone; no  
substitution allowed for acetophenone)



diphenylmethanone (PIN)  
benzophenone  
diphenyl ketone



1,2-di(naphthalen-2-yl)ethane-1,2-dione (PIN)  
di-2-naphthylethanedione  
di-2-naphthyl diketone



1-(furan-2-yl)-3-(1*H*-pyrrol-2-yl)propane-1,2,3-trione (PIN)  
1-(2-furyl)-3-(2-pyrrolyl)propanetrione  
2-furyl-2-pyrrolyl triketone

#### P-64.2.2.2 Cyclic ketones

Names of cyclic ketones are formed substitutively by using the suffix 'one'. As the formation of ketones is achieved by the conversion of a methylene,  $>CH_2$ , group into a  $>C=O$  group, the suffix 'one' with appropriate locants can be added to the name of parent hydrides having such groups.

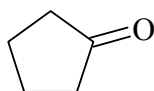
Methylene groups occur in saturated rings and ring systems and in mancude compounds having indicated hydrogen atoms.

Mancude compounds not having suitably located indicated hydrogen atoms or composed only of =CH- groups, must be hydrogenated in order to create >CH<sub>2</sub> groups; when the hydrogenation operation occurs simultaneously with substitution by the >C=O, it is called 'added hydrogen'. (see P-14.6). The added hydrogen method generates preferred IUPAC names.

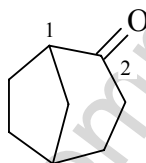
#### P-64.2.2.2.1 Alicyclic ketones

Ketones resulting from the substitution of >CH<sub>2</sub> groups are named substitutively using the suffix 'one' to designate the principal characteristic group.

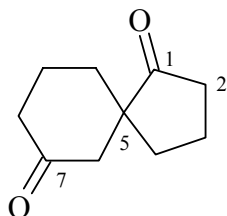
Examples:



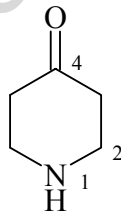
cyclopentanone (PIN)



bicyclo[3.2.1]octan-2-one (PIN)



spiro[5.6]decane-1,7-dione (PIN)

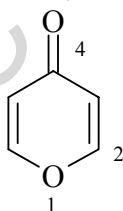


piperidin-4-one (PIN)

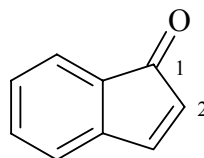
#### P-64.2.2.2.2 Ketones derived from mancude parent hydrides

Ketones derived from mancude parent hydrides having indicated hydrogen atoms are named by direct substitution of a >CH<sub>2</sub> group as indicated in P-64.2.2.2.1. When no indicated hydrogen is present, the methodology of 'added hydrogen' is applied (see P-14.6).

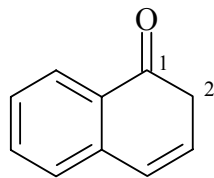
Examples:



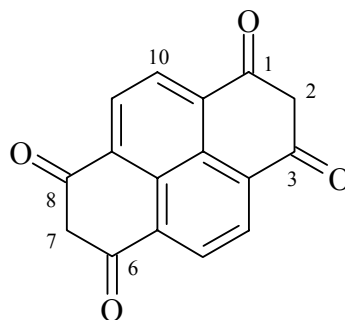
4*H*-pyran-4-one (PIN)  
pyran-4-one



1*H*-inden-1-one (PIN)  
inden-1-one



naphthalen-1(2*H*)-one (PIN)  
 1,2-dihydronaphthalen-1-one

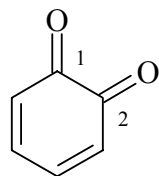


chrysene-1,3,6,8(2*H*,7*H*)-tetrone (PIN)  
 1,2,3,6,7,8-hexahydrochrysene-1,3,6,8-tetrone

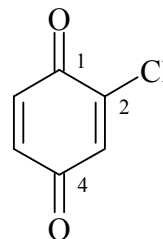
### P-64.2.2.2.3 Quinones

No retained quinone names are used as preferred IUPAC names. 1,4-benzoquinone, naphthoquinone, and anthraquinone are retained for use in general nomenclature with full substitution. All other quinones are named systematically. Diketones derived from mancade compounds without indicated hydrogen atoms by conversion of two or four =CH– groups into >C=O groups with any rearrangement of double bonds to a quinonoid structure are named systematically (see P-64.2.2.2.2).

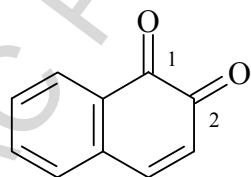
Examples:



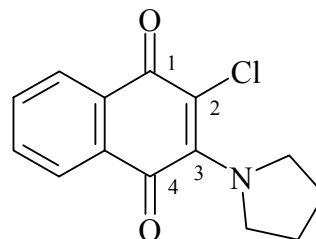
cyclohexa-3,5-diene-1,2-dione (PIN)  
 (not 1,2-benzoquinone)  
 (not *o*-benzoquinone)



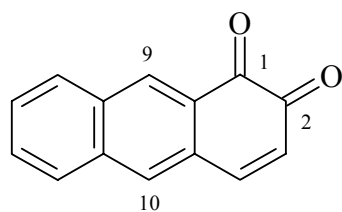
2-chlorocyclohexa-2,5-diene-1,4-dione (PIN)  
 2-chloro-1,4-benzoquinone  
 (not 2-chloro-*p*-benzoquinone)



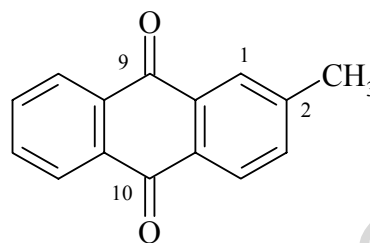
naphthalene-1,2-dione (PIN)  
 naphthalene-1,2-quinone



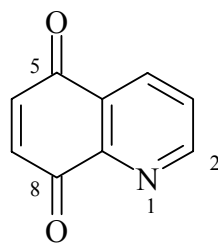
2-chloro-3-(pyrrolidin-1-yl)naphthalene-1,4-dione (PIN)  
 2-chloro-3-(pyrrolidin-1-yl)-1,4-naphthoquinone



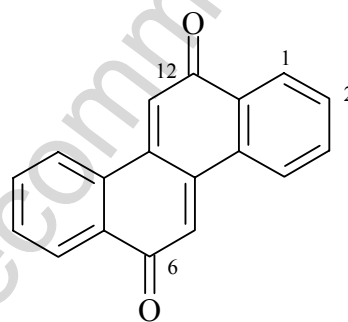
anthracene-1,2-dione (PIN)  
anthracene-1,2-quinone



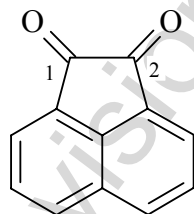
2-methylanthracene-9,10-dione (PIN)  
2-methylanthracene-9,10-dione  
2-methylanthracene-9,10-quinone



quinoline-5,8-dione (PIN)  
(not quinoline-5,8-quinone)



chrysene-6,12-dione (PIN)  
(not chrysene-6,12-quinone);



acenaphthylene-1,2-dione (PIN)  
acenaphthylene-1,2-quinone)

### P-64.2.2.3 Seniority order for numbering

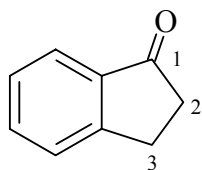
When there is a choice for numbering, the starting point and the direction of numbering of a compound are chosen so as to give lowest locants to the following structural features (if present) considered successively in the order given until a decision is reached.

- fixed numbering (naphthalene, bicyclo[2.2.2]octane, etc.)
- heteroatoms in heterocycles and in acyclic parent structures

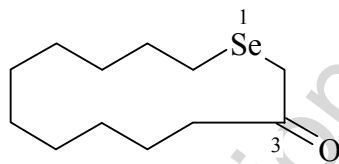
- (c) indicated hydrogen [for unsubstituted compounds; a higher locant may be needed at another position to provide for a substituent suffix in accordance with structural feature (d)]
- (d) principal group named as suffix
- (e) added hydrogen (consistent with the structure of the compound and in accordance 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).

Rule P-44 is applied when a choice for the principal chain or senior ring system is required.

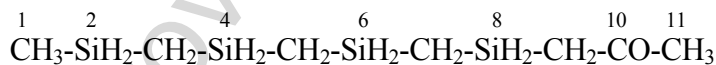
Examples:



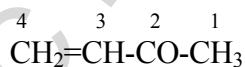
2,3-dihydro-1*H*-inden-1-one (PIN; see P-53.1)  
 indan-1-one



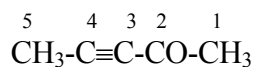
1-selenacyclotridecan-3-one (PIN)



2,4,6,8-tetrasilaundecan-10-one (PIN)



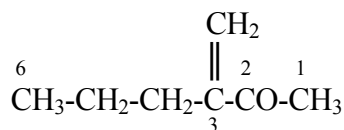
but-3-en-2-one (PIN)



pent-3-yn-2-one (PIN)

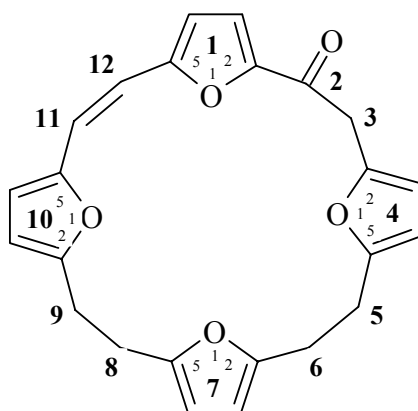


pent-1-en-4-yn-3-one (PIN)

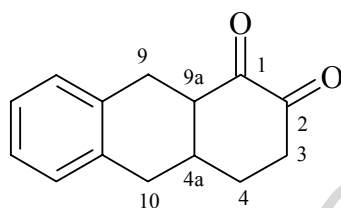


3-methylidenehexane-2-one (PIN)

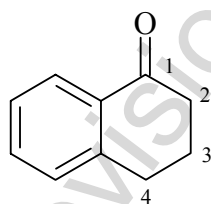




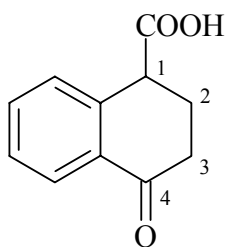
1,3,6,8(2,5)-tetrafuranylclodecaphane-11-en-2-one (PIN)



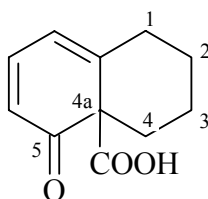
3,4,4a,9,9a,10-hexahydroanthracene-1,2-dione (PIN)  
(not 3,4,4a,9,9a,10-hexahydroanthraquinone)  
(not 1,2,3,4,4a,9,9a,10-octahydroanthracene-1,2-dione)



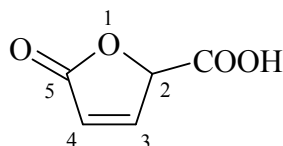
3,4-dihydronaphthalen-1(2H)-one (PIN; see P-53.1)  
1,2,3,4-tetrahydronaphthalen-1-one



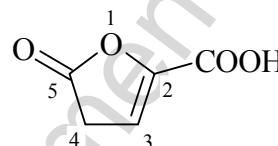
4-oxo-1,2,3,4-tetrahydronaphthalene-1-carboxylic acid (PIN)



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



5-oxo-2,5-dihydrofuran-2-carboxylic acid (PIN)

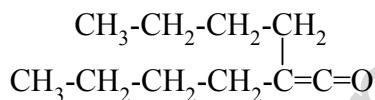


5-oxo-4,5-dihydrofuran-2-carboxylic acid (PIN)

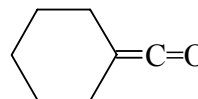
#### P-64.2.2.4 Ketenes

Ketene is the class name for  $\text{H}_2\text{C}=\text{C}=\text{O}$  and its derivatives; the name ketene can be used in general nomenclature to name the unsubstituted structure and derivatives named by compulsory prefixes. Other derivatives are named by using the principles for naming ketones.

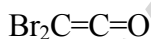
Examples:



2-butylhex-1-en-1-one (PIN)  
(not dibutylketene)



cyclohexylidenemethanone (PIN)



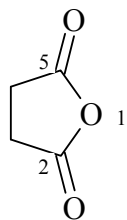
2,2-dibromoethen-1-one (PIN)  
dibromoketene

#### P-64.3 Pseudoketones.

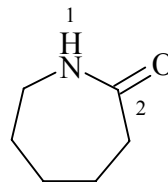
Pseudoketones are compounds having a carbonyl group joined to a carbon atom and a heteroatom,  $-\text{C}-\text{CO}-\text{X}-$ , or to two heteroatoms,  $-\text{X}-\text{CO}-\text{X}-$ , where  $\text{X} \neq \text{F}, \text{Cl}, \text{Br}, \text{I}$ , pseudohalogen, or acyclic N. These compounds are named substitutively using the suffix 'one', in accordance with rules expressed for ketones, when required.

**P-64.3.1** Cyclic anhydrides, esters and amides are named as pseudoketones; the resulting names are preferred IUPAC names.

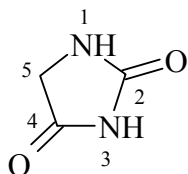
Examples:



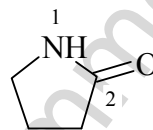
oxolane-2,5-dione (PIN)  
succinic anhydride (see P-65.7.3)



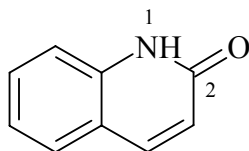
azepan-2-one ((PIN)  
hexano-6-lactam (see P-66.1.4.1)



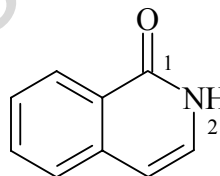
imidazolidine-2,4-dione (PIN)



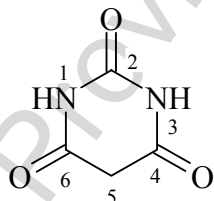
pyrrolidin-2-one (PIN)  
2-pyrrolidone



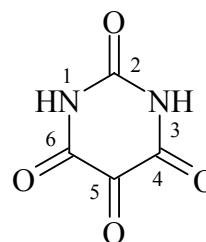
quinolin-2(1*H*)-one (PIN)  
1,2-dihydroquinolin-2-one



isoquinolin-1(2*H*)-one (PIN)  
1,2-dihydroisoquinolin-1-one



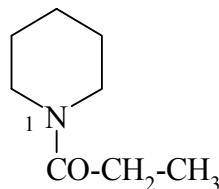
pyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (PIN)



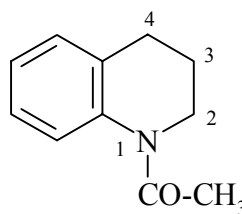
1,3,5-triazine-2,4,6(1*H*,3*H*,5*H*)-trione (PIN)

**P-64.3.2** Acyclic pseudoketones, including those in which the carbonyl group is linked to a heteroatom of a heterocycle (hidden amides, for instance), are named substitutively by using the suffix 'one' to indicate the principal function. This method is preferred to that using acyl groups, when present, to denote the  $-\text{CO-R}$  group.

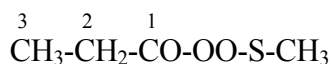
Examples:



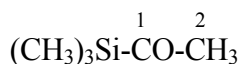
1-(piperidin-1-yl)propan-1-one (PIN)  
1-propanoylpiperidine



1-(1,2,3,4-tetrahydroquinolin-1-yl)ethan-1-one (PIN)  
1-acetyl-1,2,3,4-tetrahydroquinoline



1-[(methylsulfanyl)peroxy]propan-1-one (PIN)  
(see also P-68.4.2)



1-(trimethylsilyl)ethan-1-one (PIN)  
acetyl(trimethyl)silane

#### P-64.4 Heterones

Heterones are compounds having an oxygen atom formally doubly bonded to a heteroatom (see P-664,1,3, P-62.3.1.3, and P-63.1.3; see also P-68).

##### P-64.4.1 Acyclic heterones

##### P-64.4.2 Thioketone and thioaldehyde oxides

**P-64.4.1** Acyclic heterones are compounds having an oxygen atom doubly bonded to a heteroatom. They may be named in two ways.

- (1) by the suffix 'one';
- (2) by functional class names using the class name 'oxide' when the oxygen atom is bonded to a S, Se, Te, P, As, Sb, or Bi atom.

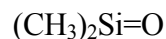
Method (1) leads to preferred IUPAC names.

The distinction between ketones, 'C-CO-C', and aldehydes, 'C-CHO', is not retained for naming compounds having the oxygen atom linked to a heteroatom. Sulfones, sulfoxides, and related chalcogen compounds are exceptions (see P-63.6)

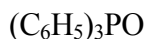
Examples:



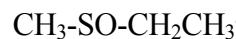
- (1) phosphanone (PIN)
- (2) phosphane oxide  
(not phosphine oxide)



dimethylsilanone (PIN)



- (1) triphenyl- $\lambda^5$ -phosphanone (PIN)
- (2) triphenylphosphane oxide  
(not triphenylphosphine oxide)



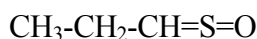
- methanesulfonyl ethane (PIN; see P-63.6)
- (2) ethyl methyl sulfoxide
  - (1) ethyl(methyl)- $\lambda^4$ -sulfanone

Thioketone oxides are named by two methods.

- (1) substitutively, as heterones, using the suffix 'one';
- (2) by functional class nomenclature, using the class name 'oxide', and 'dioxide', if required.

Method (1) leads to preferred IUPAC names.

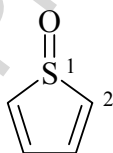
Example:



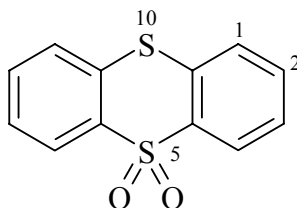
- (1) propylidene- $\lambda^4$ -sulfanone (PIN)
- (2) propanethial oxide

When a group  $-\text{SO}-$  or  $-\text{SO}_2-$  is part of a ring system, oxygen atom(s) are expressed substitutively by the suffix '-one' added to the name of the heterocycle in which the sulfur atoms are designated as  $\lambda^4$  or  $\lambda^6$  atoms (see P-14.10). This method generates preferred IUPAC names rather than those based on functional class nomenclature, in which the class name 'oxide' follows the name of the heterocycle.

Examples:



$1\lambda^4$ -thiophen-1-one (PIN)  
thiophene oxide



$5\lambda^6$ -thianthrene-5,5-dione (PIN)  
thianthrene 5,5-dioxide

### P-64.5 Expressing carbonyl groups as prefixes

When a carbonyl group is not the principal characteristic group expressed as a suffix, it is denoted by a prefix. Three types of prefixes are used:

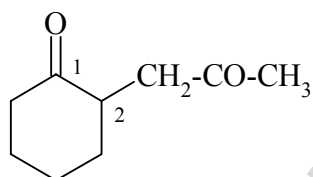
- (1) the prefix 'oxo' when the doubly bonded oxygen atom (ketone, pseudoketone, or heterone group) is not in position 1 of a side chain. Lowest possible locants are assigned to suffixes, and then to prefixes;
- (2) carbonyl groups in position 1 of a side chain, i.e.,  $-\text{CO}-\text{R}$ , are described by the appropriate acyl group name (see P-65.2 for names of acyl groups);
- (3) the group  $-\text{CO}-$  is named substitutively as the acyl group 'carbonyl'; the group  $=\text{C}=\text{O}$  is named substitutively as 'oxomethylidene'; the substituent group  $-\text{CHO}$  is named substitutively as the acyl group 'formyl', .

#### P-64.5.1 Ketones

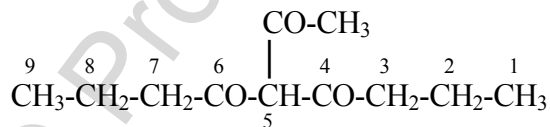
The prefix 'oxo' and/or acyl prefixes are used to denote carbonyl groups when:

- (a) all carbonyl or oxo groups cannot be cited as suffixes; or
- (b) in the presence of a characteristic group having priority to be cited as suffix.

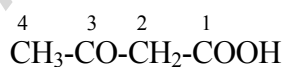
Examples:



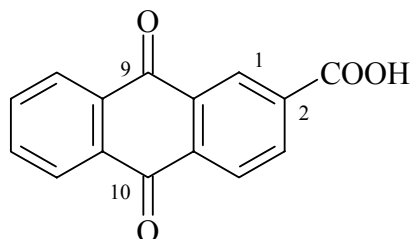
2-(2-oxopropyl)cyclohexan-1-one (PIN)  
(ring preferred to chain; see P-58.3.1.6)  
2-acetyl-cyclohexan-1-one  
2-(2-oxocyclohexyl)propan-2-one



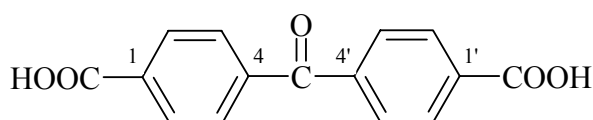
5-acetylnonane-4,6-dione (PIN)  
[not 5-(1-oxoethyl)nonane-4,6-dione]



3-oxopropanoic acid (PIN)  
(not 3-oxopropionic acid)



9,10-dioxo-9,10-dihydroanthracene-2-carboxylic acid (PIN)  
(not 9,10-anthraquinone-2-carboxylic acid)



4,4'-carbonyldibenzoic acid (PIN)  
4,4'-(oxomethylene)dibenzoic acid  
4-(4-carboxybenzoyl)benzoic acid (substitutive name)

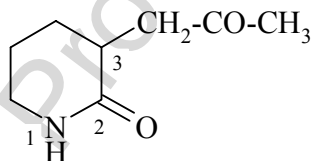
### P-64.5.2 Pseudoketones

**P-64.5.2.1** In cyclic pseudoketones, the prefix 'oxo' and/or acyl group prefixes are used to denote a carbonyl group:

- when all carbonyl groups cannot be cited as suffixes; or
- in the presence of a characteristic group having priority to be cited as suffix;

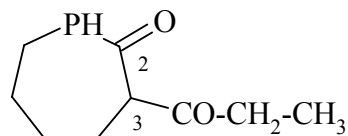
Formerly, acyl groups were used to name pseudoketones in so-called 'hidden amides' having the structure R-CO-N<, where the nitrogen atom is part of a ring or ring system.

Examples:

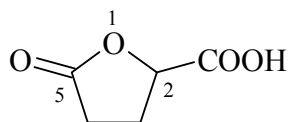


3-(2-oxopropyl)piperidin-2-one (PIN)  
(ring preferred to chain, see  
P-58.3.1.6)

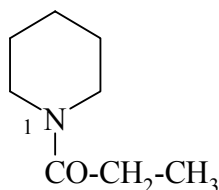
3-acetonylpiperidin-2-one  
3-(2-oxopiperidin-3-yl)propan-2-one



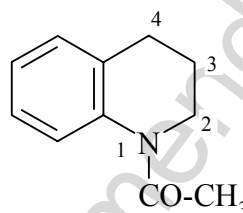
3-propanoylphospepan-2-one (PIN)  
3-propionylphospepan-2-one



5-oxoxolane-2-carboxylic acid (PIN)



1-(piperidin-1-yl)propan-1-one (PIN)  
1-propanoylpiperidine  
1-propionylpiperidine  
(a 'hidden amide')



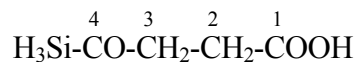
(1,2,3,4-tetrahydroquinolin-1-yl)ethan-1-one (PIN)  
1-acetyl-1,2,3,4-tetrahydroquinoline  
(a 'hidden amide')

**P-64.5.2.2** Acyclic pseudoketones are named in the same way; traditionally they have been named using acyl groups.

Examples:



1-phosphanylbutan-1-one (PIN)  
butanoylphosphane



4-oxo-4-silylbutanoic acid (PIN)  
3-silanecarbonylpropanoic acid

## P-64.6 Chalcogen analogs of ketones, pseudoketones and heterones

**P-64.6.1** Chalcogen analogs of ketones, pseudoketones and heterones are named by using the following suffixes and prefixes:

=S    '-thione' and 'sulfanylidene' (preferred to 'thioxo')

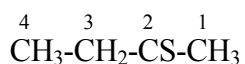
=Se   '-selone' and 'selanylidene' (preferred to 'selenoxo')

=Te   '-tellone' and 'tellanylidene' (preferred to 'telluroxo')

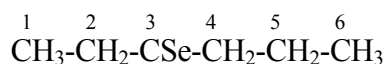
Acyl group prefixes are named by functional replacement of O by S, Se, and Te using infixes (see P-65.2). The use of functional replacement prefixes 'thio' or 'seleno' with retained names is no longer recommended; all preferred IUPAC names are systematically constructed.

Examples:

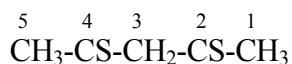




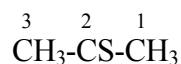
butane-2-thione (PIN)



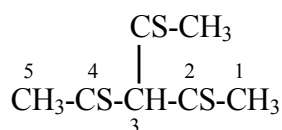
hexane-3-selone (PIN)



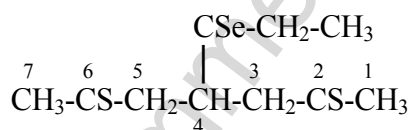
pentane-2,4-dithione (PIN)



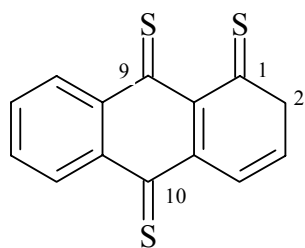
propane-2-thione (PIN)  
 (not thioacetone)



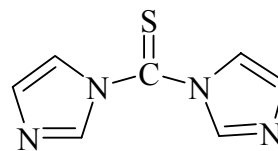
3-(thioacetyl)pentane-2,4-dithione (PIN)  
 3-(ethanethioyl)pentane-2,4-dithione



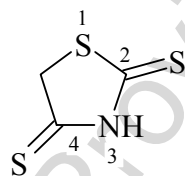
4-(propaneselenoyl)heptane-2,5-dithione (PIN)



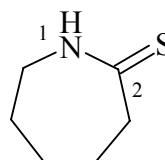
anthracene-1,9,10(2*H*)-trithione (PIN)



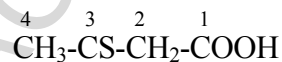
di(1*H*-imidazol-1-yl)methanethione (PIN)



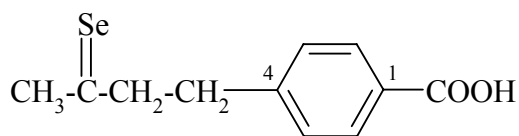
1,3-thiazolidine-2,4-dithione (PIN)



azepane-2-thione (PIN)



3-sulfanylidenebutanoic acid (PIN)  
 3-thioxobutanoic acid

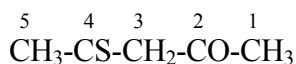


4-(3-selanylidenobutyl)benzoic acid (PIN)  
4-(3-selenoxobutyl)benzoic acid

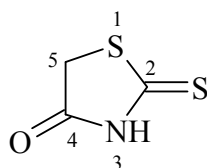
#### 64.6.2 Seniority order of suffixes

The order of seniority of suffixes is  $C=O > C=S > C=Se > C=Te$ . Lowest locants are assigned in accordance with that order.

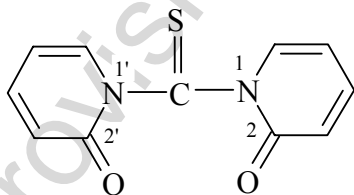
Examples:



4-sulfanylidene-2-pentanone (PIN)  
4-thioxopentan-2-one



2-sulfanylidene-1,3-thiazolidin-4-one (PIN)  
2-thio-1,3-thiazolidin-4-one

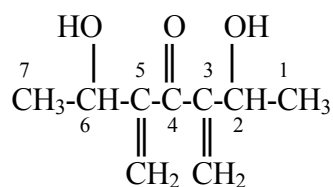


1,1'-carbonothioyl-di[pyridine-2(1H)-one] (PIN)  
1,1'-thiocarbonyl-di[pyridine-2(1H)-one]

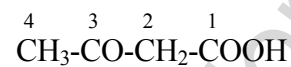
#### P-64.7 Polyfunctional ketones, pseudoketones, and heterones

**P-64.7.1** Ketones, pseudoketones and heterones, and their chalcogen analogs in the order  $=O > =S > =Se > =Te$ , are senior to hydroxy compounds and their chalcogen analogs, amines, and imines in the seniority order of classes. In the presence of a characteristic group having priority to be cited as suffix as described in P-64.4 and P-64, they are cited as prefixes (see P-41).

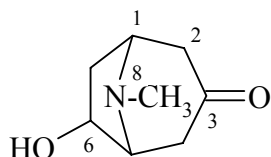
Examples:



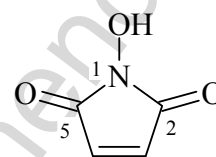
2,6-dihydroxy-3,5-dimethylideneheptan-3-one (PIN)



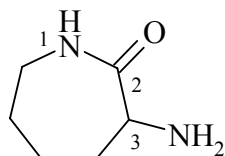
3-oxobutanoic acid (PIN)



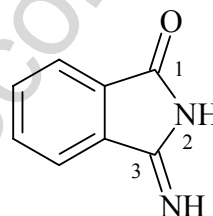
6-hydroxy-8-methyl-8-azabicyclo[3.2.1]octan-3-one (PIN)



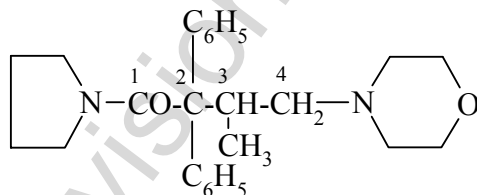
1-hydroxypyrrole-2,5-dione (PIN)



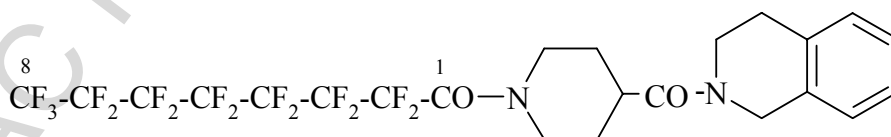
3-aminoazepan-2-one (PIN)



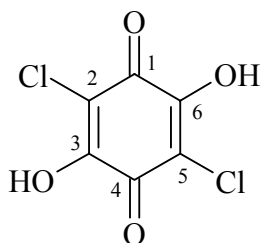
3-imino-2,3-dihydro-1*H*-isoindol-1-one (PIN)



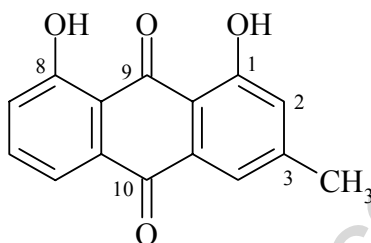
3-methyl-4-(morpholin-4-yl)-2,2-diphenyl-1-(pyrrolidin-1-yl)butan-1-one (PIN)



pentadecafluoro-1-[4-(1,2,3,4-tetrahydroisoquinolin-2-yl-carbonyl)piperidin-1-yl]octan-1-one (PIN)



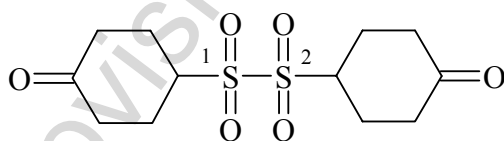
2,5-dichloro-3,6-dihydroxycyclohexadiene-1,4-dione (PIN)  
2,5-dichloro-3,6-dihydroxy-1,4-benzoquinone



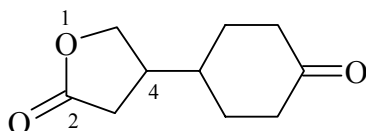
1,8-dihydroxy-3-methylantracene-9,10-dione (PIN)  
1,8-dihydroxy-3-methyl-9,10-anthraquinone

**P-64.7.2** There is no seniority order between ketones and pseudoketones. When necessary, the maximum number of carbonyl groups, the seniority order between chains and rings, and between rings and ring systems, are considered, as appropriate. Heterones follow the seniority order of the corresponding acyclic parent hydride.

Examples:



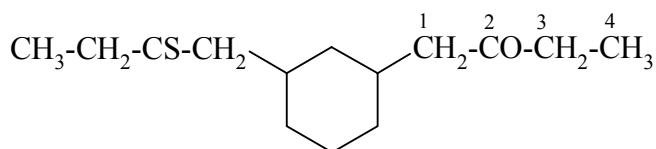
1,2-bis(4-oxocyclohexyl)-1 $\lambda^6$ ,2 $\lambda^6$ -disulfane-1,1,2,2-tetrone (PIN)  
(in the seniority order of classes, 1 $\lambda^6$ ,2 $\lambda^6$ -disulfanes  
are senior to carbon compounds, see P-41)



4-(4-oxocyclohexyl)oxolan-2-one (PIN)  
[not 4-(2-oxooxolan-4-yl)cyclohexanone; a heterocyclic  
ring is senior to a carbocyclic ring, see P-44.2.1)

**P-64.7.3** After functional replacement, the seniority order of ketones, pseudoketones, and heterones is O > S > Se > Te.

Example:



1-[3-(2-sulfanylidenebutyl)cyclohexyl]butan-2-one (PIN)  
(not 1-[3-(2-thioxobutyl)cyclohexyl]butan-2-one)

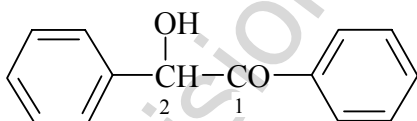
### P-64.8 Acyloins

$\alpha$ -Hydroxy ketones, RCH(OH)-CO-R, in which R is an alkyl, aryl, or a heterocyclic group, have the class name 'acyloins' and are named by substitutive nomenclature as substituted ketones, in accordance with the seniority order: ketones > hydroxy compounds (see P-41). Names ending in 'oin' are not recommended.

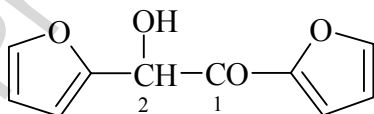
Examples:



3-hydroxybutan-2-one (PIN)  
(not acetoin)



2-hydroxy-1,2-diphenylethan-1-one (PIN)



1,2-di(furan-2-yl)-2-hydroxyethan-1-one (PIN)  
1,2-di(2-furyl)-2-hydroxyethan-1-one