# P-66 Amides, imides, hydrazides, nitriles, aldehydes, their chalcogen analogues and derivatives

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P-66.0 Introduction
P-66.1 Amides
P-66.2 Imides
P-66.3 Hydrazides
P-66.4 Amidines, amidrazones, hydrazidines
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# P-66.0 Introduction

The classes dealt with in this Section have in common the fact that their retained names are derived from those of acids by changing the 'ic acid' ending to a class name, for example 'amide', 'ohydrazide', 'nitrile' or 'aldehyde'. Their systematic names are formed substitutively by the suffix mode using one of two types of suffix, one that includes the carbon atom, for example, 'carbonitrile' for -CN, and one that does not, for example, '-nitrile' for -(C)N,. Amidines are named as amides, hydrazidines as hydrazides, and amidrazones as amides or hydrazides.

# P-66.1 Amides

P-66.1.0	Introduction
	Primary amides
P-66.1.2	Secondary and tertiary amides
P-66.1.3	Chalcogen analogues of amides
P-66.1.4	Lactams, lactims, sultams and sultims
P-66.1.5	Amides of carbonic, oxalic, cyanic, and polycarbonic acids
P-66.1.6	Polyfunctional amides

# P-66.1.0 Introduction

Amides are derivatives of oxoacids in which each hydroxy group has been replaced by an amino or substituted amino group. Chalcogen replacement analogues are called thio-, seleno- and telluroamides. Compounds having one, two or three acyl groups on a single nitrogen atom are generically included and may be designated as primary, secondary and tertiary amides, respectively.

**P-66.1.1** Primary amides

- P-66.1.1.1 Carboxamides
- P-66.1.1.2 Sulfonamides, sulfinamides, and related selenium and tellurium amides
- P-66.1.1.3 Substitution of primary amides
- P-66.1.1.4 Amides denoted as prefixes

# P-66.1.1.1 Carboxamides

Names of carboxamides are formed in two ways:

P-66.1.1.1.1 Substitutive nomenclatureP-66.1.1.1.2 Modification of retained names for acids

P-66.1.1.1.1 Amide names formed by substitutive nomenclature

**P-66-1.1.1.1.1** Aliphatic mono- and diamides are named substitutively by adding the suffix 'amide', to the appropriate parent hydride name, with elision of the final letter 'e' before 'a'. The multiplying prefix 'di' is used to name diamides.

Examples:

CH3-[CH2]4-CO-NH2H2N-OC-CH2-CH2-CH2-CH2-CO-NH2hexanamide (PIN)pentanediamide (PIN)

**P-66-1.1.1.1.2** If an unbranched chain is directly linked to more than two –CO-NH<sub>2</sub> groups, these groups are named from the parent hydride by substitutive use of the suffix 'carboxamide'.

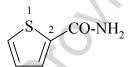
Example:

<sup>3</sup><sup>2</sup><sup>1</sup>H<sub>2</sub>N-CO-CH<sub>2</sub>-CH(CO-NH<sub>2</sub>)-CH<sub>2</sub>-CO-NH<sub>2</sub> propane-1,2,3-tricarboxamide (PIN)

**P-66-1.1.1.1.3** The suffix 'carboxamide' is always used to name amides having the  $-CO-NH_2$  group attached to a ring or ring system or to a heteroatom.

Examples:

H<sub>2</sub>P-CO-NH<sub>2</sub> phosphanecarboxamide (PIN)



thiophene-2-carboxamide (PIN)

 $H_2N$ -NH-CO- $NH_2$ 

hydrazinecarboxamide (PIN)

-CO-NH,

piperidine-1-carboxamide (PIN)

**P-66.1.1.1.2** Amide names formed by modifying retained names of acids

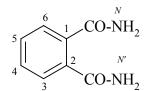
Names of amides derived from carboxylic acids listed in P-65.1.1 are formed by changing the 'ic acid' or '-oic acid' ending of the retained names of carboxylic acids into 'amide'. Names of amides formed by this method are either preferred IUPAC names or names only for use in general nomenclature according to the status of the corresponding acid; structures can be substituted in the same way as indicated for the corresponding acids (see P-65.1.1)

(a) Only the following two retained names are preferred IUPAC names and can be fully substituted. Systematic functional replacement names are used to generate acids modified by functional replacement.

CH <sub>3</sub> -CO-NH <sub>2</sub>	C <sub>6</sub> H <sub>5</sub> -CO-NH <sub>2</sub>
acetamide (PIN)	benzamide (PIN)

(b) For general nomenclature, only the names furamide, phthalamide, isophthalamide, and terephthalamide are retained with full substitution allowed (see P-34). Systematic names formed according to P-66.1.1.1.1 are the preferred IUPAC names.

Examples:



benzene-1,2-dicarboxamide (PIN) phthalamide

H<sub>2</sub>N-CO CO-NH<sub>2</sub>

benzene-1,4-dicarboxamide (PIN) terephthalamide

(c) Amides derived from retained acid names given in P-65.1.1.2 are only used in general nomenclature; no substitution is allowed, even on amide nitrogen atoms. Preferred IUPAC names are given systematic names as given by P-66.1.1.1.1.

Examples:

 $^{3}$   $^{2}$   $^{2}$   $^{1}$   $^{1}$   $^{2}$   $^{2}$   $^{1}$   $^{2}$ 

prop-2-enamide (PIN) acrylamide

> <sup>3</sup> <sup>2</sup> <sup>1</sup> CH<sub>3</sub>-CH(OH)-CO-NH<sub>2</sub>

2-hydroxypropanamide (PIN) (not lactamide)  $^{3}_{CH_2} = ^{2}_{CH-CO-NH-CH_3}$ 

*N*-methylprop-2-enamide (PIN) (not *N*-methylacrylamide; substitution not allowed on acrylamide)

<sup>3</sup> <sup>2</sup> <sup>1</sup> CH<sub>3</sub>-CH(OH)-CO-NH-CH<sub>3</sub>

2-hydroxy-*N*-methylpropanamide (PIN) (not *N*-methyllactamide)

(d) The traditional name 'formamide' is retained for  $HCO-NH_2$  and is the preferred IUPAC name. Substitution is permitted on the  $-NH_2$  group. Substitution of the aldehydic hydrogen is subject to limitations (see P-65.2.2.1).

Examples:

HCO-NH<sub>2</sub>

formamide (PIN)

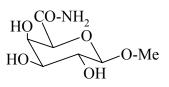
Cl-CO-NH<sub>2</sub>

carbono

carbonochloridic amide (PIN) (not 1-chloroformamide)

(e) Names for amides derived from carbohydrate acids and  $\alpha$ -amino acids are discussed in P-102.5.5.6.2.1 and P-103.2, respectively.

Examples:



$$R = -CO-NH_2$$

methyl β-D-galactopyranosiduronamide (PIN)

H<sub>2</sub>N-CH<sub>2</sub>-CO-NH<sub>2</sub> glycinamide (PIN)

P-66.1.1.2 Sulfonamides, sulfinamides, and related selenium and tellurium amides

Sulfonamides, sulfinamides, and the analogous selenium and tellurium amides are named substitutively using the following suffixes:

$-SO_2-NH_2$	sulfonamide	$-SO-NH_2$	sulfinamide
$-SeO_2-NH_2$	selenonamide	-SeO-NH <sub>2</sub>	seleninamide
-TeO <sub>2</sub> -NH <sub>2</sub>	telluronamide	-TeO-NH <sub>2</sub>	tellurinamide

These suffixes may be assigned to any position of a parent hydride. Examples:

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

 $SO-NH_2$ 1 4 3 CH<sub>3</sub>-CH<sub>2</sub>-CH-CH<sub>3</sub>

butane-2-sulfinamide (PIN)

methanesulfonamide (PIN)

eO-NH<sub>2</sub>

furan-2-seleninamide (PIN)

SO<sub>2</sub>-NH<sub>2</sub>

pyrrolidine-1-sulfonamide (PIN)

**P-66.1.1.3** Substitution of primary amides

**P-66.1.1.3.1** *N*-Substitution

**P-66.1.1.3.1.1** Substituted primary amides, with general structures such as R-CO-NHR' and R-CO-NR'R", and the corresponding amides derived from chalcogen acids are named by citing the substituents R' and R" as prefixes preceded by the locant N when one amide group is present; the locants N and N' are used to distinguish between two equivalent amide groups, and N locants preceded by the locant denoting of the position of the amide group on the parent hydride to distinguish nonequivalent groups (see also P-62.2.1.2.2)

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*N*-Substitution of primary amides is not allowed when amides having retained names designated as not substitutable.

Examples:

N HCO-N(CH<sub>3</sub>)<sub>2</sub> N,N-dimethylformamide (PIN) dimethylformamide H<sub>3</sub>C-CO-NH-CH(CH<sub>3</sub>)<sub>2</sub> N-(propan-2-yl)acetamide (PIN) CO-NH-CH<sub>2</sub> *N*-methylbenzamide (PIN) 1 2 3 NCH<sub>3</sub>-NH-CO-CH<sub>2</sub>-CH<sub>2</sub>-CO-NH<sub>2</sub> *N*-methylbutanediamide (PIN)

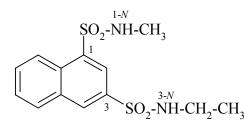
CH<sub>3</sub>-CH<sub>2</sub>-CO-N(CH<sub>3</sub>)<sub>2</sub>

*N,N*-dimethylpropanamide (PIN) (not *N,N*-dimethylpropionamide; substitution not allowed on propionamide)

 $CO-N(CH_2-CH_3)_2$ 

*N*,*N*-diethylfuran-2-carboxamide (PIN) *N*,*N*-diethyl-2-furanamide

> N' 5 4 3 2 1 N CH<sub>3</sub>-NH-CO-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CO-NH-CH<sub>3</sub> N,N' -dimethylpentanediamide (PIN)



3-N-ethyl-1-N-methylnaphthalene-1,3-disulfonamide (PIN)

**P-66.1.1.3.1.2** Locants for geminal carboxamide groups

When geminal carboxamide groups are present, the locants N, N', etc. are used in association with the numerical locant indicating the position of the groups on a chain or ring. Lowest locants are assigned to the most substituted group; when there is a choice, lowest locants are assigned to the first cited *N*-substituent. This system of *N*-locants in association with numerical locants is recommended for naming substituted amines (see P-62.2.1.2.2) and is extended to name geminal amidines (see P-66.4.1.3.3), amidrazones (see P-66.4.2.1), and hydrazidines (see P-66.4.3.1).

Examples:

1-N-ethyl-1-N',3-N-dimethylpropane-1,1,3-tricarboxamide (PIN)

# P-66.1.1.3.2 Anilides

*N*-Phenyl derivatives of primary amides are called 'anilides' and may be named using the term 'anilide' in place of 'amide' in systematic or retained names of amides. The locants for substituents in the *N*-phenyl ring are primed numbers. However, names expressing *N*-substitution by a phenyl group on an amide are preferred IUPAC names.

Examples:

HCO-NH-C<sub>6</sub>H<sub>5</sub>

*N*-phenylformamide (PIN) formanilide

CH<sub>3</sub>-CO-NH-C<sub>6</sub>H<sub>5</sub>

*N*-phenylacetamide (PIN) acetanilide

# $C_6H_5$ -CO-N(CH<sub>3</sub>)-C<sub>6</sub>H<sub>5</sub>

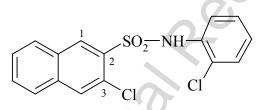
*N*-methyl-*N*-phenylbenzamide (PIN) *N*-methylbenzanilide

CH<sub>3</sub>-[CH<sub>2</sub>]<sub>4</sub>-CO-NH-C<sub>6</sub>H<sub>5</sub>

*N*-phenylhexanamide (PIN) hexananilide

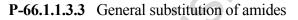
CH<sub>3</sub> H<sub>3</sub>

*N*,4-dimethyl-*N*-(3-methylphenyl)benzamide (PIN) *N*,3',4-trimethylbenzanilide



3-chloro-*N*-(2-chlorophenyl)naphthalene-2-sulfonamide (PIN) 2',3-dichloronaphthalene-2-sulfonanilide

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Substitution is expressed by prefixes; numerical and N and N' locants are used as required.

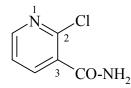
Examples:

Cl-CH<sub>2</sub>-CH<sub>2</sub>-CO-NH<sub>2</sub>

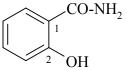
3-chloropropanamide (PIN) (not 3-chloropropionamide; no substitution on propionamide)

2 Cl-CH<sub>3</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CO-N(CH<sub>3</sub>)<sub>2</sub>

4-chloro-*N*,*N*-dimethylbutanamide (PIN) (not 4-chloro-*N*,*N*-dimethylbutyramide; no substitution on butyramide)



2-chloropyridine-3-carboxamide (PIN) 2-chloronicotinamide



2-hydroxybenzamide (PIN) (not salicylamide)

3,5-diamino-6-chloropyrazine-2-carboxamide (PIN)

CO-NH.

4-methylbenzene-1,2-dicarboxamide (PIN)

CO-NH,

CH<sub>3</sub>-CH<sub>2</sub>-CO-NH-OH

*N*-hydroxypropanamide (PIN) (not propanehydroxamic acid, see P-65.1.3.4)

P-66.1.1.4 Amides denoted as prefixes

Two different substituent groups can be derived from amides and expressed as prefixes in presence of a characteristic group having seniority for citation as suffix:

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H<sub>a</sub>(

H<sub>2</sub>N

Cl

4-methylphthalamide

P-66.1.1.4.1 Substituents of the types -CO-NH<sub>2</sub> and -SO<sub>2</sub>-NH<sub>2</sub>; P-66.1.1.4.2 Substituents of the types -NH-CO-R and -NH-SO<sub>2</sub>-R

**P-66.1.1.4.1** Substituent groups of the types  $-CO-NH_2$  and  $-SO_2-NH_2$  (and similar selenium and tellurium groups)

In presence of a characteristic group having priority for citation as suffix, the  $-CO-NH_2$  group is named in three different ways:

(1) by using the two prefixes 'amino' and 'oxo' to denote such groups on terminal atoms of carbon chains having more than one carbon atom;

(2) by using the acyl group name 'carbamoyl';

(3) by using the prefix 'aminocarbonyl'.

For generation of IUPAC preferred names, method (1) is preferred for chains and method (2) is preferred for rings and ring systems, heterogeneous chains, and on nonterminal atoms of carbon chains.

Derivatives of dicarboxylic acids having a retained name are called 'amic acids' when one carboxylic group has been changed to a carboxamide group. These acids may be named by replacing the 'ic acid' ending in the retained name by 'amic acid' (see P-65.1.6.1).

In presence of a characteristic group having priority for citation as suffix, the groups  $-SO_2-NH_2$ ,  $-SO-NH_2$  and related selenium and tellurium groups are named in two different ways corresponding to methods (2) and (3) for the  $-CO-NH_2$  group above:

- (2) by the acyl group 'sulfamoyl' (for sulfonamides only);
- (3) by the the prefixes 'amino-sulfonyl', '-sulfinyl', '-selenonyl', -seleninyl', -telluronyl', or 'tellurinyl'.

For generating preferred IUPAC names for  $-SO_2-NH_2$ , method (2) is preferred to method (3); method (3) is the sole method recommended for all other groups.

Substituted  $-CO-NH_2$ ,  $-SO_2-NH_2$ ,  $-SO-NH_2$  and related selenium and tellurium groups are named by substituting the groups 'carbamoyl' and 'sulfamoyl-', and by using substituted amino groups along with the prefix 'oxo' or the prefixes 'sulfonyl', sulfinyl, selenonyl, etc.

Examples:

<sup>10</sup>H<sub>2</sub>N-CO-[CH<sub>2</sub>-]<sub>8</sub>-COOH

- (1) 10-amino-10-oxodecanoic acid (PIN)
- (2) 9-carbamoylnonanoic acid

(3) 9-(aminocarbonyl)nonanoic acid

(1) 3-amino-3-oxopropanoic acid (PIN)

H<sub>2</sub>N-CO-CH<sub>2</sub>-COOH

- (2) carbamoylacetic acid
- (3) (aminocarbonyl)acetic acid malonamic acid (see P-65.1.6.1)

 $\begin{array}{c|c} & \text{CO-N(CH_3)_2} \\ & 5 & 4 & 2 & 1 \\ \text{HOOC-CH_2-CH-CH_2-COOH} \end{array}$ 

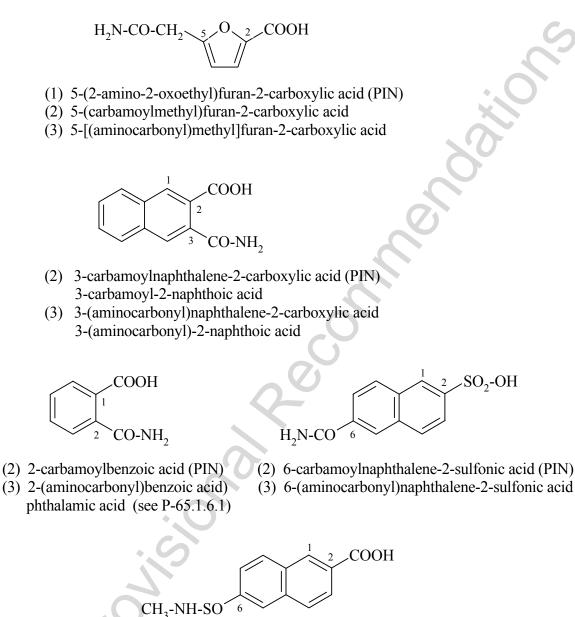
(2) 3-(dimethylcarbamoyl)pentanedioic acid (PIN)

(3) 3-[(dimethylamino)carbonyl]pentanedioic acid

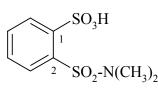
 $C_6H_5$ -NH-SO<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CO-O-CH<sub>3</sub>

(2) methyl 3-(phenylsulfamoyl)propanoate (PIN)

(3) methyl 3-[(phenylamino)sulfonyl]propanoate

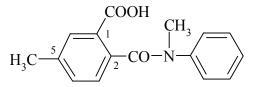


(3) 6-[(methylamino)sulfinyl]naphthalene-2-carboxylic acid (PIN)(3) 6-[(methylamino)sulfinyl]-2-naphthoic acid



(2) 2-(dimethylsulfamoyl)benzene-1-sulfonic acid (PIN)

(3) 2-[(dimethylamino)sulfonyl]benzene-1-sulfonic acid



(2) 5-methyl-2-[(methyl(phenyl)carbamoyl]benzoic acid (PIN)

(3) 5-methyl-2-[(N-methylanilino)carbonyl]benzoic acid

**P-66.1.1.4.2** When a group having preference for citation as a principal characteristic group is present, the group R-CO-NH<sup>-</sup>, or R-SO<sub>2</sub>-NH<sup>-</sup> (and selenium and tellurium analogues) of an *N*-substituted amide is named in two ways:

- (1) substitutively, by using a prefix named formed by changing the final letter 'e' in the complete name of the amide to 'o', thus changing the suffixes 'amide' and 'carboxamide' into 'amido' and 'carboxamido', respectively, 'diamide' to 'diamido' or 'sulfonamide' to 'sulfonamido', etc.;
- (2) substitutively, by using 'acylamino' prefixes formed by combining the name of the acyl group with that of the substituent group 'amino'

Method (1) generates preferred IUPAC names.

Examples:

HCO-NH COOH

4-formamidobenzoic acid (PIN) 4-(formylamino)benzoic acid

 $As(O)(OH)_2$ CH<sub>3</sub>-CO-NH

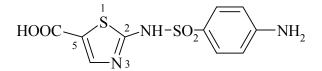
(4-acetamido-3-methylphenyl)arsonic acid (PIN) [4-(acetylamino)-3-methylphenyl]arsonic acid

CH<sub>3</sub>-SO<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-COOH

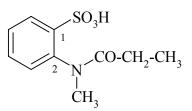
3-(methanesulfonamido)propanoic acid (PIN)3-(methanesulfonylamino)propanoic acid

C<sub>6</sub>H<sub>5</sub>-CO-NH SO<sub>2</sub>-OH

4-benzamidobenzesulfonic acid (PIN) 4-(benzoylamino)benzenesulfonic acid



2-(4-aminobenzenesulfonamido)-1,3-thiazole-5-carboxylic acid (PIN) (not 2-sulfanilamidothiazole-5-carboxylic acid; sulfanilic acid is not a retained name)



2-(*N*-methylpropanamido)benzene-1-sulfonic acid (PIN) 2-[methyl(propanoyl)amino]benzene-1-sulfonic acid

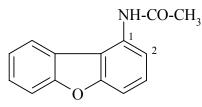
4,4'-butanediamidodibenzoic acid (PIN) 4,4'-succinamidodibenzoic acid

When an amide is the principal function, it must be named as such. The traditional method of considering amides as substituents on polycyclic ring systems, described in the 1993 Recommendations, should be avoided, even in general nomenclature.

Examples:



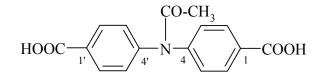
*N*-methyl-*N*-(quinolin-4-yl)acetamide (PIN) (not 4-(*N*-methylacetamido)quinoline) (not 4-[acetyl(methyl)amino]quinoline)



*N*-(dibenzofuran-1-yl)acetamide (PIN) (not 1-acetamidodibenzofuran) (not 1-(acetylamino)dibenzofuran)

**P-66.1.1.4.3** When a group having preference for citation as a principal characteristic group is present, the groups R-CO-N $\leq$  and R-CO-N=, or R-SO<sub>2</sub>-N $\leq$  and R-SO<sub>2</sub>-N= (and selenium and tellurium analogues) of an *N*-substituted amide are named by combining acyl group names with those of the appropriate nitrogen substituent groups, azanediyl and imino, respectively.

Examples:



4,4'-(acetylazanediyl)dibenzoic acid (PIN)

$$CH_3-SO_2-N_4$$
 CO-OCH<sub>3</sub>

methyl 4-(methanesulfonylimino)cyclohexane-1-carboxylate (PIN)

P-66.1.2 Secondary and tertiary amides

**P-66.1.2.1** Amides having general formulas,  $(R-CO)_2NH$ ,  $(R-SO_2)_2NH$ , etc., and  $(R-CO)_3N$ ,  $(R-SO_2)_3N$ , etc., respectively, are named as *N*-acyl derivatives of the senior primary amide. Names based on the substitution of the parent hydride 'azane' or the pseudo parent hydride 'amine' by acyl groups, for example, diacetylazane or diacetylamine, as recommended in the 1993 Recommendations (ref 2) are not included in these recommendations, nor are trivial names such as diacetamide, triacetamide, dibenzamide and tribenzamide.

Examples:

HCO-NH-O-CH

*N*-formylformamide (PIN) (not diformylazane) (not diformylamine) (not diformamide) CH<sub>3</sub>-CO-NH-CO-CH<sub>3</sub>

*N*-acetylacetamide (PIN) (not diacetylazane) (not diacetylamine) (not diacetamide)

*N*-(furan-2-carbonyl)furan-2-carboxamide (PIN) [not di(furan-2-carbonyl)azane] [not di(furan-2-carbonyl)amine]

*N,N*-di(cyclohexanecarbonyl)cyclohexanecarboxamide (PIN) [not tri(cyclohexanecarbonyl)azane] [not tri(cyclohexanecarbonyl)amine]

C<sub>6</sub>H<sub>5</sub>-CO-NH-CO-CH<sub>3</sub>

*N*-acetylbenzamide (PIN) [not acetyl(benzoyl)azane] [not acetyl(benzoyl)amine]

#### CO-CH<sub>3</sub> | C<sub>6</sub>H<sub>5</sub>-CO-N-CO-CH<sub>2</sub>-CH<sub>2</sub>-Cl

*N*-acetyl-*N*-(3-chloropropanoyl)benzamide (PIN) [not acetyl(benzoyl)(3-chloropropanoyl)azane] [not acetyl(benzoyl)(3-chloropropanoyl)amine]

 $N(CO-CH_3)_2$ 

CO-CH<sub>3</sub> -CO-C<sub>c</sub>H<sub>5</sub>

*N*-acetyl-*N*-cyclopentylacetamide (PIN) [not diacetyl(cyclopentyl)azane] [not diacetyl(cyclopentyl)amine] N-acetyl-N-(naphthalen-2-yl)benzamide (PIN) [not acetyl(benzoyl)(naphthalen-2-yl)azane] [not acetyl(benzoyl)(naphthalen-2-yl)amine]

**P-66.1.2.2** In the presence of a characteristic group higher than amide, a secondary amide group is expressed as an *N*-acylamido prefix or as a diacylamino prefix. The *N*-acylamido prefix method leads to preferred IUPAC names.

Example:

(CH<sub>3</sub>-CO)<sub>2</sub>N-CH<sub>3</sub>-CH<sub>2</sub>-COOH

3-(*N*-acetylacetamido)propanoic acid (PIN) 3-(diacetylamino)propanoic acid

P-66.1.2.3 Hidden amides

An *N*-acyl group attached to a nitrogen atom of a heterocyclic system has been called a 'hidden amide', i.e., an amide that cannot be named as such. The traditional way to name such compounds by using acyl groups as substituents on the nitrogen atom of the heterocyclic system is discontinued. Such compounds are treated as pseudoketones (see P-64.3).

Examples:

CO-CH<sub>3</sub>

1-(piperidin-1-yl)ethan-1-one (PIN) (not 1-acetylpiperidine)

CO-CH<sub>2</sub>-CH<sub>3</sub>

1-(1,2,3,4-tetrahydroquinolin-1-yl)propan-1-one (PIN) (not 1-propanoyl-1,2,3,4-tetrahydroquinoline) (not 1-propionyl-1,2,3,4-tetrahydroquinoline)

P-66.1.3 Chalcogen analogues of amides

Chalcogen analogues of amides are named systematically. Prefixes are no longer used with retained names.

P-66.1.3.1 Chalcogen amide suffixes

**P-66.1.3.1.1** Names are formed by using suffixes modified by functional replacement nomenclature using prefixes and infixes.

Examples:

$-(C)S-NH_2$	thioamide
-CS-NH <sub>2</sub>	carbothioamide
$-S(O)(S)-NH_2$	sulfonothioamide
$-S(S)(S)-NH_2$	sulfonodithioamide
$-S(S)-NH_2$	sulfinothioamide

For a more extended list, see Table 4.4.

Examples:

HCS-NH<sub>2</sub>

methanethioamide (PIN) thioformamide

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

ethanethioamide (PIN) thioacetamide C<sub>6</sub>H<sub>5</sub>-CS-NH<sub>2</sub>

benzenecarbothioamide (PIN) thiobenzamide

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pyridine-2-carbothioamide (PIN)

CS-NH,

pyridine-4-carbothioamide (PIN) thioisonicotinamide

**P-66.1.3.1.2** In presence of a function having priority for citation as suffix, the amide function is expressed by the appropriate prefixes, such as amino in conjunction with sulfanylidene or thioxo, as well as carbonothioyl (not thiocarbonyl) for -CS- or carbamothioyl (not thiocarbamoyl) for -CS- NH<sub>2</sub>.

Examples:

 $H_2N$ -CS- $CH_2$ -COOH

3-amino-3-sulfanylidenepropanoic acid (PIN)3-amino-3-thioxopropanoic acid carbamothioylacetic acid (aminocarbonothioyl)acetic acid

CH<sub>3</sub>-CS-NH CO-NH,

4-ethanethioamidobenzamide (PIN)4-(ethanethioylamino)benzamide [not 4-(thioacetamido)benzamide] naphthalene-2-sulfonodithioamide (PIN)

P-66.1.4 Lactams, lactims, sultams, sultims

P-66.1.4.1 Lactams and lactims

Intramolecular amides of amino carboxylic acids, -CO-NH-, are called 'lactams' and their tautomers, -C(OH)=N-, are 'lactims'. Lactams are named:

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- (1) as heterocyclic pseudoketones;
- (2) by substituting 'lactam' for the 'ic acid' ending of a systematic 'oic acid' name for the parent acid without the amino substituent, and inserting a locant designating the position of the amino group between the 'o' and 'lactam'. Lactims are named in the same way, using 'lactim' in place of 'lactam'.

Method (1) generates preferred IUPAC names.

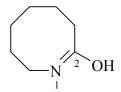
Examples:

pyrrolidin-2-one (PIN) butano-4-lactam 2-pyrrolidone tetrahydropyrrol-2-one

OH

2,3,4,5-tetrahydropyridin-2-ol (PIN) pentano-5-lactim

1-azacyclotridecan-2-one (PIN) dodecano-12-lactam



hexahydro-2,3,4,5,6,7-azocin-2-ol (PIN) 1,2-didehydroazocan-2-ol heptano-7-lactim

P-66.1.4.2 Sultams, sultims, and intramolecular amides of sulfinic acids.

**P-66.1.4.2.1** Intramolecular amides of amino sulfonic acids are called 'sultams' and may be named in three ways.

- (1) as heterocyclic heterones;
- (2) by citing the term 'sultam' denoting the cyclic –NH-SO<sub>2</sub>– group after the name of the appropriate parent hydride preceded by a pair of locants describing the points of

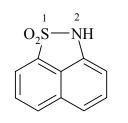
attachment of the sulfonyl group and the nitrogen atom, respectively; the locant of the sulfonyl group is cited first, and, if there is a choice, is the lower locant. Multiplying prefixes and pairs of locants separated by a colon are used to indicate two or more sultam rings.

(3) as heterocycles according to functional class names using the class term 'oxide'.

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Method (1) leads to preferred IUPAC names.

Examples:



1

 $1\lambda^{6}$ -2*H*-naphtho[1,8-*cd*][1,2]thiazole-1,1-dione (PIN) 2*H*-naphtho[1,8-*cd*][1,2]thiazole 1,1-dioxide naphthalene-1,8-sultam

HO

HC

 $1\lambda^{6}$ ,2-thiazinane-1,1-dione (PIN) 1,2-thiazinane 1,1-dioxide butane-1,4-sultam

**P-66.1.4.2.2** Sultims are tautomers of sultams and are named as described above for sultams, using the term 'sultim' in place of 'sultam'.

Examples:

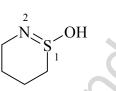
1-hydroxy-4,5-dihydro-3*H*-1 $\lambda^6$ ,2-thiazol-1-one (PIN) 1-hydroxy-4,5-dihydro-3*H*-1 $\lambda^4$ ,2-thiazole 1-oxide propane-4-sultim

1-hydroxy- $1\lambda^6$ -thia-2-azacyclododec-1-en-1-one (PIN) 1-hydroxy- $1\lambda^4$ -thia-2-azacyclododec-1-ene 1-oxide decane-11-sultim P-66.1.4.2.3 Intramolecular amides of amino sulfinic acids.

Cyclic amides of amino sulfinic acids and their tautomers are named as heterocyclic compounds. Examples:

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 $1\lambda^4$ ,2-thiazinan-1-one (PIN)

3,4,5,6-tetrahydro- $1\lambda^4$ ,2-thiazin-1-ol (PIN)

P-66.1.5 Amides derived from carbonic, oxalic, cyanic, and the polycarbonic acids

- P-66.1.5.1 Amides derived from carbonic acid
- P-66.1.5.2 Amides derived from cyanic acid
- P-66.1.5.3 Amides derived from oxalic acid
- P-66.1.5.4 Amides derived from polycarbonic acids

P-66.1.5.1 Amides derived from carbonic acid and related compounds

- P-66.1.5.1.1 Urea, H<sub>2</sub>N-CO-NH<sub>2</sub>, and its derivatives
- P-66.1.5.1.2 Isourea, H<sub>2</sub>N-C(=NH)-OH, and its derivatives
- P-66.1.5.1.3 Chalcogen analogues of urea and isourea
- P-66.1.5.1.4 Condensed ureas

P-66.1.5.1.1 Urea and its substitutive derivatives

**P-66.1.5.1.1.1** The compound  $H_2N$ -CO- $NH_2$  has the retained named 'urea', which is the preferred IUPAC name with locants 1,2, and 3 as shown below. The systematic name is 'carbonic diamide' with locants N and N', as shown below.

$$H_{2N}^{1} - CO - NH_{2N}^{3}$$

**P-66.1.5.1.1.2** Derivatives of urea formed by substitution on the nitrogen atom(s) are named as substitution products in accordance with the seniority order of urea that is ranked as an amide of carbonic acid. Amides of the cyanic, oxalic, and the polycarboxylic acids follow the same seniority as the corresponding acid (see P-42.2)

Examples:

$$CH_3-\underset{N}{\overset{3}{\underset{N}{\text{H-CO-NH-CH}}}}^2_{N'}$$

1,3-dimethylurea (PIN) *N,N'*-dimethylcarbonic diamide

$$H_2N-CO-N=C(CH_3)_2$$

propan-2-ylideneurea (PIN) isopropylideneurea *N*-(propan-2-ylidene)carbonic diamide

$$CN$$

$$3 \qquad 1 \qquad | \\CH_3-NH-CO-NH-CH-CH_2-CH_2-S-CH_2$$

1-[1-cyano-3-(methylsulfanyl)propyl]-3-methylurea (PIN) *N*-[1-cyano-3-(methylsulfanyl)propyl]-*N*'-methylcarbonic diamide

**P-66.1.5.1.1.3** The prefixes for appropriate substituent groups derived from urea are systematically derived. The prefix names "ureido" and "ureylene" are not recommended.

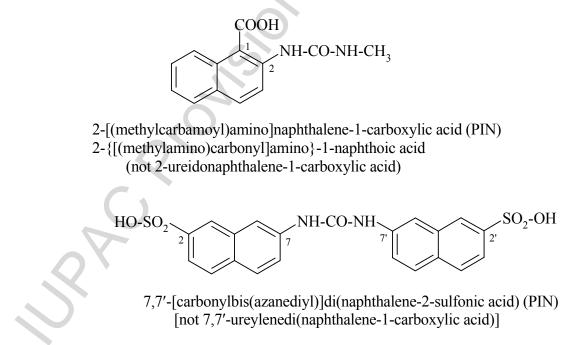
H<sub>2</sub>N-CO-NH-

-HN-CO-NH-

carbamoylamino (PIN) (not ureido)

carbonylbis(azanediyl) (PIN) (for use in multiplicative nomenclature) (not ureylene)

Examples:



 $C_6H_5$ -CO-NH-CO-NH<sub>2</sub>

*N*-carbamoylbenzamide (PIN) *N*-(aminocarbonyl)benzamide

# C<sub>6</sub>H<sub>5</sub>-SO<sub>2</sub>-NH-CO-NH<sub>2</sub>

*N*-carbamoylbenzene-1-sulfonamide (PIN) *N*-(aminocarbonyl)benzene-1-sulfonamide

$$H_2N-CO-NH-CO-CH_2-C_6H_5$$

*N*-carbamoyl-2-phenylacetamide (PIN) *N*-(aminocarbonyl)-2-phenylacetamide

P-66.1.5.1.1 4 Carboxylic acid derivatives of urea

Two carboxylic acids are related to urea; they have been known as 'allophanic acid' and 'hydantoic acid'. These names are no longer recommended. Preferred IUPAC names for these two acids and their derivatives are formed systematically.

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Examples:

<sup>3</sup> <sup>2</sup> <sup>1</sup> H<sub>2</sub>N-CO-NH-COOH

carbamoylcarbamic acid (PIN) (aminocarbonyl)carbamic acid

H<sub>2</sub>N-CO-NH-CO-

carbamoylcarbamoyl (PIN) [(aminocarbonyl)amino]carbonyl

H<sub>2</sub>N-CO-NH-CH<sub>2</sub>-COOH

*N*-carbamoylglycine (PIN) (carbamoylamino)acetic acid

P-66.1.5.1.1.5 Seniority order of urea among amides

Amides are ranked in the same way than corresponding acids (see P-42). Thus, in substitutive nomenclature amides from carboxylic acids, which includes formamide, are senior to urea.

Examples:

# H<sub>2</sub>N-CO-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CO-CH<sub>3</sub>

*N*-[2-(carbamoylamino)ethyl]acetamide (PIN) *N*-{2-[(aminocarbonyl)amino]ethyl}acetamide <sup>3</sup> <sup>1</sup> H<sub>2</sub>N-CO-NH-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-HN-CHO [3-(carbamoylamino)propyl]formamide (PIN) (not 1-(3-formamidopropyl)urea) (not 1-[3-(formylamino)propyl]urea) (formamide preferred to urea, see P-41)

# P-66.1.5.1.2 Isourea

**P-66.1.5.1.2.1** The imidic acid tautomer of urea,  $H_2N$ -C(OH)=NH, is named 'carbamimidic acid', a shortened form of the systematic functional replacement name 'carbonamidimidic acid'. The name 'isourea' is no longer recommended. Numerical locants are used in preferred IUPAC names when the positions of substituent groups are known; the locant N is used when the position of the double bond is unknown.

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$$H_2 N-C(OH) = NH$$

carbamimidic acid (PIN)

Examples:

$$(C_6H_5)_{2N}^{1} - C(=_{N'}^{3} - CH_3) - O - CH_2 - CH_3$$

ethyl 3-methyl-1,1-diphenylcarbamimidate (PIN) (not *O*-ethyl-*N*/-methyl-*N*,*N*-diphenylisourea)

$$(C_6H_5)_2$$
<sup>1</sup>N-C(=NH)-O-CH<sub>2</sub>-CH<sub>3</sub>  
<sub>N'</sub>O-CH<sub>2</sub>-CH<sub>3</sub>

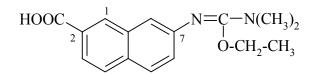
ethyl 1,1-diphenylcarbamimidate (PIN) (not *O*-ethyl-*N*,*N*-diphenylisourea)

 $C_{6}H_{5}-\underset{N}{\overset{1}{\underset{N}}}H-C(=\underset{N'}{\overset{3}{\underset{N}}}H)-\underset{O}{\overset{2}{\underset{O}}}-CH_{2}-CH_{3} \qquad \leftrightarrows \qquad \underset{N}{\overset{1}{\underset{N}}}MH_{2}-C(=\underset{N'}{\overset{3}{\underset{N}}}-C_{6}H_{5})-\underset{O}{\overset{2}{\underset{O}}}-CH_{2}-CH_{3}$ ethyl N-phenylcarbamimidate (PIN)

(not *O*-ethyl-*N*-phenylisourea)

**P-66.1.5.1.2.2** The groups HN=C(OH)-NH- and  $-N=C(OH)-NH_2$  are named '(*C*-hydroxy-carbonimidoyl)amino' and '[amino(hydroxy)methylidene]amino', respectively. The letter locant '*C*' is used in the former to prevent possible ambiguity with *N*-substitution and parentheses are used around 'hydroxy' to emphasize that 'amino' is not substituted by 'hydroxy'.

The prefixes 1-isoureido and 3-isoureido are no longer recommended. Example:



7-{[(dimethylamino)(ethoxy)methylidene]amino}naphthalene-2-carboxylic acid (PIN) (not 7-(2-ethyl-1,1-dimethyl-3-isoureido)naphthalene-2-carboxylic acid)

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P-66.1.5.1.3 Chalcogen analogues of urea and isourea

**P-66.1.5.1.3.1** Chalcogen analogues of urea are named by functional replacement nomenclature using the prefixes 'thio', 'seleno' and 'telluro'. Preferred IUPAC names use numerical locants. Examples:

 $\begin{array}{cccc} & & & 3 & 2 & 1 \\ H_2 \underset{N}{N}-CS-\underset{N'}{NH_2} & & & H_2 \underset{N'}{N}-CS-\underset{N}{NH-C(CH_3)-CH_2-CH_3} \\ \text{thiourea (PIN)} & & & 1-(butan-2-yl) \text{selenourea (PIN)} \\ \text{carbonothioic diamide} & & N-(butan-2-yl) \text{carbonoselenoic diamide} \end{array}$ 

**P-66.1.5.1.3.2** Chalcogen analogues of isourea are named by functional replacement nomenclature using the appropriate chalcogen infixes. Preferred IUPAC names use the locants N and N'. When the position of the double bond is not known, locants *S*, *Se*, *Te* and *N* are used to assign substituents to the appropriate atoms.

Examples:

$$S-CH_2CH_3$$

$$3 \mid 1$$

$$HN=C-N(CH_3)_2$$

ethyl *N'*-methylcarbamimidothioate (PIN)

S-CH<sub>2</sub>CH<sub>3</sub>

ethyl *N*,*N*-dimethylcarbamimidothioate (PIN) (not 2-ethyl-1,1-dimethylisothiourea)

(not 2-ethyl-3-methylisothiourea)

For the second example, when the position of the double bond is not known the names are ethyl *N*-methylcarbamimidothioate (PIN) and *S*-ethyl *N*-methylisothiourea.

**P-66.1.5.1.3.3** Prefix names for the groups  $H_2N$ -CS-NH– , HN=C(SH)-NH–, and -N=C(SH)-NH<sub>2</sub>, are 'carbamothioylamino', '(*C*-sulfanylcarbonimidoyl)amino', and '(*C*-sulfanylcarbonimidoyl)amino', and

Example:

# <sup>3</sup><sup>2</sup><sup>1</sup> H<sub>2</sub>N-CS-NH-CH<sub>2</sub>-CH<sub>2</sub>-COOH

3-(carbamothioylamino)propanoic acid

# P-66.1.5.1.4 Condensed ureas

Condensed ureas,  $H_2N$ -[CO-NH]<sub>n</sub>-H, where n = 2, 3, or 4 are named systematically as diamides of triimidodicarbonic acid, pentaimidotricarbonic acid, and heptatriimidotetracarbonic acid. The names biuret, triuret, etc., are no longer recommended as preferred IUPAC names. Chalcogen analogues are described by functional replacement prefixes. Locants, as shown, are used to indicate the positions of substituents and functional replacement prefixes, where needed. Preferred IUPAC names use the locants prescribed for the amides of imidopolycarbonic acids (see P-66.1.5.4).

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2-imidodicarbonic diamide (PIN) (numbering above structure) biuret (numbering below structure)

2,4-diimidotricarbonic diamide (PIN) (numbering above structure) triuret (numbering below structure)

Examples:

<sup>N</sup>CH<sub>3</sub>-NH-CO-NH-CO-NH<sub>2</sub>

N-methyl-2-imidodicarbonic diamide (PIN)

CH<sub>3</sub>-NH-CS-NH-CO-NH<sub>2</sub>

*N*-methyl-2-imido-1-thiodicarbonic diamide (PIN)

N 1 2 3 4 5 N' CH<sub>3</sub>-NH-CO-NH-CS-NH-CO-NH<sub>2</sub>

*N*-methyl-2,4-diimido-3-thiotricarbonic diamide (PIN)

For polyurets, where n = 5 and higher, skeletal replacement ('a') nomenclature leads to preferred IUPAC names.

Example:

#### <sup>1</sup> <sup>2</sup> <sup>3</sup> <sup>4</sup> <sup>5</sup> <sup>6</sup> <sup>7</sup> <sup>8</sup> <sup>9</sup> H<sub>2</sub>N-CO-NH-CO-NH-CO-NH-CO-NH-CO-NH<sub>2</sub>

3,5,7-trioxo-2,4,6,8-tetraazanonanediamide (PIN) pentauret

P-66.1.5.2 Amides derived from cyanic acid.

The traditional name 'cyanamide' is retained for  $NC-NH_2$  and is the preferred IUPAC name. Substitution is allowed on the  $-NH_2$  group.

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Examples:

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

(propan-2-yl)cyanamide (PIN) (not propan-2-ylcarbononitridic amide) NC-N(CH<sub>2</sub>-CH<sub>3</sub>)<sub>2</sub>

diethylcyanamide (PIN) (not diethylcarbononitridic amide)

P-66.1.5.3 Amides of oxalic acid

The name 'oxamide' is retained for  $H_2N$ -CO-CO- $NH_2$  and is the preferred IUPAC name. Substitution is allowed. The structure is numbered as shown below.

$$H_2^{N-1}$$
  $H_2^{2}$   $H_2^{N'}$   $H_2^{N'}$ 

Example:

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

*N*-ethyl-*N*'-methyloxamide (PIN) *N*-ethyl-*N*'-methyloxalic diamide

Chalcogen analogues are described by functional replacement prefixes.

Example:

 $(CH_3)_3C-NH-CS-CO-NH_2$ 

*N-tert*-butyl-1-thiooxamide (PIN) *N-tert*-butyl-1-thiooxalic diamide

The prefixes used to indicate appropriate substituent groups derived from oxamide are:

H<sub>2</sub>N-CO-CO-NH-

oxamoylamino (PIN) carbamoylformamido aminooxoacetamido

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H <sub>2</sub> N-CO-CO-N=	oxamoylimino (PIN)
H <sub>2</sub> N-CO-CO-N<	oxamoylazanediyl (PIN)
-HN-CO-CO-NH-	oxalylbis(azanediyl) (PIN) (used in multiplicative nomenclature)
>N-CO-CO-N<	oxalyldinitrilo (PIN) (used in multiplicative nomenclature)
=N-CO-CO-N=	oxalylbis(azanylylidene) (PIN) (used in multiplicative nomenclature)

#### P-66.1 5.4 Amides of the polycarbonic acids.

Systematic names are formed by adding the functional class name 'amide' to that of the corresponding acid, preceded by the numerical prefix 'di' to indicate the presence of two  $-NH_2$  groups. Chalcogen analogues are described by functional replacement prefixes. Numerical and letter locants are used to number the structures.

 $\begin{matrix} N & 1 & 2 & 3 & N' \\ H_2 N\text{-}CO\text{-}O\text{-}CO\text{-}NH_2 \end{matrix}$ 

dicarbonic diamide (PIN)

H<sub>2</sub>N-CO-O-CO-OH<sub>2</sub>

N 1 2 3 4 5 N'

tricarbonic diamide (PIN)

Examples:

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

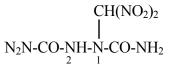
*N*-(propan-2-yl)dicarbonic diamide (PIN) *N*-isopropyldicarbonic diamide  $\begin{array}{c} N & 1 & 2 \\ \text{CH}_3\text{-}\text{NH-CO-S-CO-O-CO-NH}_2 \end{array}$ 

*N*-methyl-2-thiotricarbonic diamide (PIN)

#### **P-66.1.6** Polyfunctional amides

Amides follow acids, anhydrides, esters, and acid halides in the seniority order of compound classes expressed by suffixes (see P-41) and within the amide class, amides rank in the same order as the corresponding acid. Seniority for numbering polyfunctional amides follows that described for acids for which see P-65.1.2.3 and P-65.3.4.

Examples:



1-(dinitromethyl)hydrazine-1,2-dicarboxamide (PIN)

$$NO_2 NO_2$$

$$| | |$$

$$CH_2=CH-CO-NH-CH_2-N-CH_2-N-CH_2-NH-CO-CH_3$$

*N*-[({[(acetamidomethyl)nitroamino]methyl}nitroamino)methyl]prop-2-enamide (PIN) *N*- {[({[(acetylamino)methyl]nitroamino}methyl)nitroamino]methyl}prop-2-enamide

 $\begin{array}{c} CH_3 \\ \mid _{2 \quad 1} \\ H_2N-CH_2-C=N-NH-CO-NH_2 \end{array}$ 

2-(1-aminopropan-2-ylidene)hydrazine-1-carboxamide (PIN)

HO-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CO-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-OH

4-[(2-hydroxyethyl)amino]-N-{2-[(2-hydroxyethyl)amino]ethyl}butanamide (PIN)

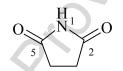
 $^{2}$   $^{1}$   $H_{2}N-CH_{2}-CO-N(CH_{3})-CH_{2}-CHOH-CH_{2}OH$ 

2-amino-N-(2,3-dihydroxypropyl)-N-methylacetamide (PIN)

# P-66.2 Imides

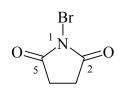
Imides are compounds containing the structural grouping –CO-NH-CO–. Acyclic imides are named according to P-66.1.2. Cyclic imides are preferably named as heterocyclic pseudoketones. They may also be named by replacing the suffixes 'dioic acid', or 'dicarboxylic acid' of the corresponding dibasic acid, or 'ic acid' in retained names of diacids, by 'imide' or 'dicarboximide'.

Examples:



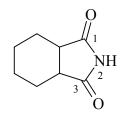
pyrrolidine-2,5-dione (PIN) succinimide

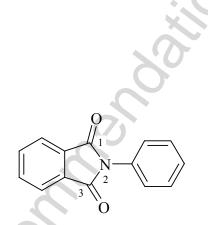
1*H*-pyrrole-2,5-dione (PIN) pyrrole-2,5-dione



1-bromopyrrolidine-2,5-dione (PIN) (not *N*-bromosuccinimide; substitution not allowed on succinimide)

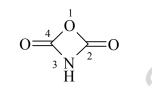
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hexahydroisoindole-1,3-dione (PIN) cyclohexane-1,2-dicarboximide

2-phenylisoindole-1,3-dione (PIN) *N*-phenylphthalimide



2H-1,3-oxazete-2,4(3H)-dione (PIN)

# P-66.3 Hydrazides

- P-66.3.0 Definition
- P-66.3.1 Systematic names
- P-66.3.2 Substituent groups derived from hydrazides
- P-66.3.3 Substituted hydrazides
- P-66.3.4 Functional replacement by chalcogen atoms
- P-66.3.5 Hydrazides of carbonic, cyanic, oxalic, and the polycarbonic acids
- P-66.3.6 Semioxamazones

# P-66.3.0 Definition

Hydrazides are compounds derived from oxoacids by replacing –OH groups by –NR-NR'R" groups (R groups are commonly H).

P-66.3.1 Systematic names

Hydrazides of the type R-CO-NH-NH<sub>2</sub> are named in two ways:

P-66.3.1.1 substitutive nomenclature:

P-66.3.1.2 modification of retained names of carboxylic acids.

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# P-66.3.1.1 Substitutive names

Hydrazides may be named substitutively in two ways:

(1) by the following suffixes:

–(C)O-NH-NH <sub>2</sub>	hydrazide
-CO-NH-NH <sub>2</sub>	carbohydrazide
$-SO_2$ -NH-NH <sub>2</sub>	sulfonohydrazide (and corresponding Se and Te suffixes)
-SO-NH-NH <sub>2</sub>	sulfinohydrazide (and corresponding Se and Te suffixes)

The suffix 'hydrazide' is recommended in place of 'ohydrazide' in accordance with the general use of suffixes that are added to names of parent hydrides, for example pentanehydrazide for CH<sub>3</sub>-CH<sub>3</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CO-NH-NH<sub>2</sub>, not pentanohydrazide.

The suffix 'hydrazide' is used to name acyclic compounds. The suffix 'carbohydrazide' is used to denote the -CO-NH-NH<sub>2</sub> characteristic group attached to cyclic compounds and in chains having more than two -CO-NH-NH<sub>2</sub> characteristic groups, or when the group is attached to a heteroatom of a heterocycle. Multiplicative nomenclature may be used when the symmetry conditions for its use are met.

(2) as acyl derivatives of hydrazine; multiplicative nomenclature is used when conditions allow this type of nomenclature.

Method (1) leads to preferred IUPAC names.

N = N'The nitrogen atoms in hydrazides are identified by N and N' locants as  $-CO-NH-NH_2$ , even though hydrazine, itself, is numbered using the numerical locants 1 and 2, as NH<sub>2</sub>-NH<sub>2</sub>. Examples:

(1) pentanehydrazide (PIN) (2) pentanoylhydrazine

CH<sub>3</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CO-NH-NH<sub>2</sub> H<sub>2</sub>N-NH-CO-CH<sub>2</sub>-CH<sub>2</sub>-CO-NH-NH<sub>2</sub>

- (1) butanedihydrazide (PIN) succinohydrazide (see P-66.2.1.3)
- (2) (ethane-1,2-diyldicarbonyl)dihydrazine succinyldihydrazine

CO-NH-NH<sub>2</sub>

cyclohexanecarbohydrazide (PIN) (cyclohexanecarbonyl)hydrazine

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

methanesulfonohydrazide (PIN)

**P-66.3.1.2** Names formed by modifying retained names of carboxylic acids

Names of hydrazides are formed by changing the 'ic acid' or '-oic acid' ending of the retained names of carboxylic acids into 'ohydrazide', as described in P-34.4.3.

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(a) Only the following two retained names are preferred IUPAC names and can be fully substituted. Systematic substitutive names are used to generate acids modified by functional replacement.

HCO-NH-NH<sub>2</sub>

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

formohydrazide (PIN) hydrazinecarbaldehyde (see P-66.6.1.4) acetohydrazide (PIN)

CO-NH-NH,

piperidine-1-carbohydrazide (PIN)

[(piperidin-1-yl)carbonyl]hydrazine

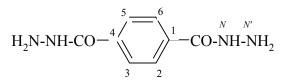
C<sub>6</sub>H<sub>5</sub>-CO-NH-NH<sub>2</sub> benzohydrazide (PIN)

(b) For general nomenclature, only the names furohydrazide, phthalohydrazide, isophthalohydrazide, and terephthalohydrazide are retained with full substitution allowed (see P-34). Systematic names are preferred IUPAC names (see P-66-3.1.1).

Examples:

$$\begin{array}{c} & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & &$$

benzene-1,2-dicarboxamide (PIN) phthalohydrazide



benzene-1,4-dicarboxamide (PIN) terephthalohydrazide

(c) Retained names for carboxylic acids (see P-65.1.1.2) are used only in general nomenclature and hydrazide formation is governed by the above rule; but substitution is not allowed, including substitution on the nitrogen atom(s) of the hydrazides.

Example:

# CH<sub>3</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CO-NH-NH<sub>2</sub>

butanehydrazide (PIN) butyrohydrazide (substitution not allowed)

(d) Hydrazides derived from carbohydrate acids and  $\alpha$ -amino acids are discussed in P-102.5.5.6.2.1 and P-103.2, respectively.

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Examples:

NH<sub>2</sub>-CH<sub>2</sub>-CO-NH-NH<sub>2</sub> glycinohydrazide (PIN)

```
<sup>1</sup>CO-NH-NH<sub>2</sub>
H-C-OH
HO-C-H
H-C-OH
H-C-OH
H-C-OH
CH<sub>2</sub>-OH
```

gluconohydrazide (PIN)

P-66.3.2. Substituent groups derived from hydrazides

Substituent groups corresponding to hydrazides are of two types;

P-66.3.2.2.1 Substituent groups of the type -CO-NH-NH<sub>2</sub>, -SO<sub>2</sub>-NH-NH<sub>2</sub>, etc.; P-66.3.2.2.2 Substituent groups of the type -NH-NH-CO-R, -NH-NH-SO<sub>2</sub>-R, etc.

**P-66.3.2.1** Substituent groups of the type  $-CO-NH-NH_2$ ,  $-SO_2-NH-NH_2$ , etc., may be named in two ways:

(1) as acyl groups derived from the corresponding acids or the appropriate carbonohydrazidoyl acyl prefix; the former are preferred IUPAC names:

H<sub>2</sub>N-NH-COOH

hydrazinecarboxylic acid (PIN) carbonohydrazidic acid

H<sub>2</sub>N-NH-CO-

hydrazinecarbonyl (PIN; (see P-68.3.1.2.1.2) carbonohydrazidoyl

H<sub>2</sub>N-NH-SO<sub>2</sub>OH

hydrazinesulfonic acid (PIN)

H<sub>2</sub>N-NH-SO<sub>2</sub>– hydrazinesulfonyl (PIN; see P-68.3.1.2.1.2)

(2) by the prefixes 'hydrazinyl' and 'oxo' when the -CO-NHNH<sub>2</sub> group is located at the end of a chain.

Examples:

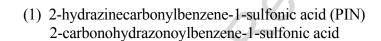
$$^{3}$$
  $^{2}$   $^{1}$   $^{1}$   $H_2$ N-NH-CO-CH<sub>2</sub>-COOH

- (1) 3-hydrazinyl-3-oxopropanoic acid (PIN)
- (2) 2-hydrazinecarbonylacetic acid 2-carbonohydrazidoylacetic acid

H<sub>2</sub>N-NH-SO<sub>2</sub>-CH<sub>2</sub>-COOH

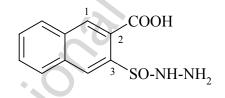
(1) hydrazinesulfonylacetic acid (PIN)

2-carbonohydrazidoylacetic acid



SO<sub>3</sub>H

CO-NH-NH<sub>2</sub>



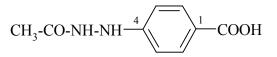
(1) 3-(hydrazinesulfinyl)naphthalene-2-carboxylic acid (PIN)

**P-66.3.2.2** When a group having priority for citation as a principal characteristic group is present, a hydrazide group of the type R-CO-NH-NH–, or R-SO<sub>2</sub>-NH-NH– (or related selenium and tellurium group) is named:

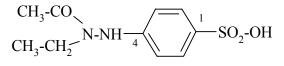
- (1) as an acylhydrazinyl compound; the hydrazinyl group is numbered by using numerical locants 1 and 2; the locant '1' is the nitrogen atom adjacent to the free valence;
- (2) by expressing the corresponding hydrazide as a prefix by replacing the final letter 'e' in the name of the hydrazide by the letter 'o', for example, 'acetohydrazido', 'propanehydrazido', and 'benzenecarbohydrazido'. The locant *N* designates the nitrogen atom adjacent to the -CO- group.

Method (1) generates preferred IUPAC names.

Example:

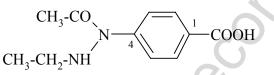


4-(2-acetylhydrazin-1-yl)benzoic acid (PIN) 4-(acetohydrazido)benzoic acid



4-(2-acetyl-2-ethylhydrazin-1-yl)benzene-1-sulfonic acid (PIN) 4-(*N*-ethylacetohydrazido)benzene-1-sulfonic acid

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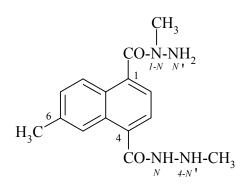
4-(1-acetyl-2-ethylhydrazin-1-yl)benzoic acid (PIN) 4-(*N*'-ethylacetohydrazido)benzoic acid

# **P-66.3.3** Substituted hydrazides

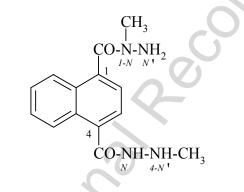
**P-66.3.3.1** Alkyl, aryl, cycloalkyl, etc substituents on the nitrogen atoms of hydrazides are described by the appropriate prefix names and the locants N or 1' for the imido nitrogen atom and N' or 2' for the amino nitrogen atom as illustrated below. Preferred IUPAC names use the locants N and N' rather than the locants 1' and 2'.

When two hydrazide groups are present, each is identified by the locants N and N'. To distinguish the four nitrogen atoms, the symbols are preceded by the locant of the skeletal atom of the parent structure to which the hydrazide group is attached, followed by a hyphen.

Examples:



1-*N*,4-*N*',6-trimethylnaphthalene-1,4-dicarbohydrazide (PIN) (the numbering for this compound is based on the lowest set of locants for the three substituent groups)



1-N,4-N'-dimethylnaphthalene-1,4-dicarbohydrazide (PIN) (numbering is based on the lower set of locants: since N is lower than N', the set 1-N, 4-N' is lower than 1-N',4-N)

P-66.3.3.2 Acyl, diacyl, and triacyl derivatives of hydrazides are named:

- (1) by substituting the senior hydrazide by the appropriate acyl groups (the senior hydrazide is the one derived from the senior acid), or
- (2) by substituting the parent hydride, hydrazine (hydrazine, a retained name, is preferred to diazane for preferred IUPAC names).

Method (1) leads to preferred IUPAC names.

Examples:

$$C_6H_5$$
-CO-NH-NH-CO-C<sub>6</sub>H<sub>5</sub>

H<sub>3</sub>C CH<sub>2</sub>CH<sub>3</sub> | |CH<sub>3</sub>-CH<sub>2</sub>-CO-N-N-CO-CH<sub>3</sub>  $^{2}$   $^{2}$   $^{1}$ 

*N*'-benzoylbenzohydrazide (PIN) *N* 1,2-dibenzoylhydrazine 1

*N*'-acetyl-*N*'-ethyl-*N*-methylpropanehydrazide (PIN) 1-acetyl-1-ethyl-2-methyl-2-propanoylhydrazine

**P-66.3.4** Functional replacement by chalcogen atoms

Thiohydrazides may be named in three ways; seleno and tellurohydrazides may be named in a similar manner.

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- (1) substitutively using suffixes formed by functional replacement, i.e., 'thiohydrazide', '-carbothiohydrazide', 'sulfonothiohydrazide', etc.;
- (2) by substituting hydrazine with appropriately modified acyl groups;
- (3) retained names modified by the prefixes 'thio', 'seleno', telluro'.

Examples:

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

- (1) propanethiohydrazide (PIN)
- (2) (propanethioyl)hydrazine (thiopropionyl)hydrazine

- $C_6H_5$ -CS-NH-NH<sub>2</sub>
- (1) benzenecarbothiohydrazide (PIN)
- (2) benzenecarbothioylhydrazine (thiobenzoyl)hydrazine

P-66.3.5 Hydrazides from carbonic, cyanic, oxalic, and the polycarbonic acids

**P-66.3.5.1** Preferred IUPAC names of hydrazides derived from carbonic and cyanic acids are as follows:

H <sub>2</sub> N-NH-CN	cyanohydrazide (PIN) hydrazinecarbonitrile carbononitridic hydrazide
H <sub>2</sub> N-NH-CO-OH	hydrazinecarboxylic acid (PIN) carbonohydrazidic acid
H <sub>2</sub> N-NH-CO-NH-NH <sub>2</sub>	hydrazinecarbohydrazide (PIN) carbonic dihydrazide

**P-66.3.5.2** Names of hydrazides derived from oxalic and the polycarbonic acids are formed by adding the functional class name 'hydrazide' to that of the corresponding acid, preceded by the numerical locant 'di' to express multiplicity of hydrazide groups, when necessary. Chalcogen and other replacement analogues are described by the appropriate functional replacement prefix.

Examples:

#### P-66.3.5.3 Corresponding substituent groups

When a group having priority for citation as a principal characteristic group is present, the hydrazide group is named:

- (1) as an acylhydrazinyl compound; the hydrazinyl group is numbered by using numerical locants 1 and 2;
- (2) by expressing the corresponding hydrazide as a prefix by replacing the final letter 'e' in the name of the hydrazide by the letter 'o', for example, 'formohydrazido'. The locant N designates the nitrogen atom adjacent to the -CO- group

Method (1) generates preferred IUPAC names.

Examples:

OHC-NH-NH-CH<sub>2</sub>-CH<sub>2</sub>-COOH

3-(2-formylhydrazin-1-yl)propanoic acid (PIN) 3-formohydrazidopropanoic acid

H<sub>2</sub>N-NH-CO-NH-NH-CH<sub>2</sub>-COOH

2-(2-hydrazinecarbonylhydrazin-1-yl)acetic acid (PIN) 2-hydrazinecarbohydrazidoacetic acid

H<sub>2</sub>N-NH-CO-O-CO-NH-NH-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-COOH

4-{2-[(hydrazinecarbonyloxy)carbonyl]hydrazin-1-yl}butanoic acid (PIN)

### P-66.3.6 Semioxamazones

Semioxamazones have the general structure R=N-NH-COCO-NH<sub>2</sub> and are named as substituted hydrazido oxamides.

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Example:

C<sub>6</sub>H<sub>5</sub>-CH=N-NH-COCO-NH<sub>2</sub>

N'-benzylidene-2-hydrazidooxamide (PIN) 2-(2-benzylidenehydrazin-1-yl)-2-oxoacetamide

## P-66.4 Amidines, amidrazones, and hydrazidines, and amide oximes (amidoximes)

P-66.4.1 Amidines P-66.4.2 Amidrazones P-66.4.3 Hydrazidines P-66.4.4 Amide oximes (amidoximes)

### P-66.4.1 Amidines

Compounds having the general structure R-C(=NH)-NH<sub>2</sub> are generically known as '(carbox)amidines'; those having the general structure R-S(=NH)-NH<sub>2</sub> are 'sulfinamidines'.

Compounds with the structure 
$$\begin{array}{ccc} O & NH \\ \parallel & \parallel \\ R-S-NH_2 \text{ or } R-S-NH_2 \text{ are generically called 'sulfonimidamides} \\ \parallel & \parallel \\ NH & NH \end{array}$$
 and not amidines.

P-66.4.1.1	Suffixes for amidines
P-66.4.1.2	Amidines of carbonic, oxalic, and the polycarbonic acids
P-66.4.1.3	Prefixes for the amidine characteristic group
P-66.4.1.4	Substituted amidines
P-66.4.1.5	Formamidine disulfides
P-66.4.1.6	Diamidides
P-66.4.1.7	Amide oximes

## **P-66.4.1.1** Suffixes for amidines

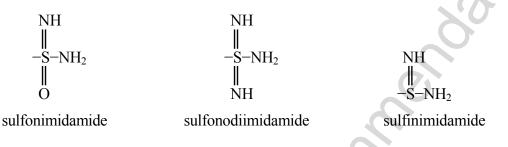
Amidines are named as amides in which the =O atom has been replaced by the =NH group by functional replacement nomenclature. As a principal characteristic group they are designated by the following suffixes, formed by functional replacement by using the prefix or the infix 'imido'.

-(C)(=NH)-NH <sub>2</sub>	$-C(=NH)-NH_2$
imidamide	carboximidamide

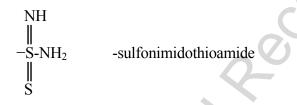
The suffixes 'amidine' and 'carboxamidine' are no longer recommended.

Suffixes for sulfonic acid, sulfinic acid and selenium and tellurium analogues are named similarly.

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The suffixes for groups containing S, Se and Te in place of O in a sulfonimidamide suffix are named by functional replacement, for example:



The suffix 'imidamide' is used to denote an acyclic amidine with one terminal amidine characteristic group; two terminal amidine characteristic groups on an acyclic parent hydride are denoted by the suffix 'bis(imidamide)' (the multiplicative prefix 'bis' is used to avoid the possibility of ambiguity). All the other suffixes are used to name acyclic polyamidines and all amidines having the suffix attached to a cyclic parent hydride or a heteroatom of a heteroacyclic parent hydride.

Retained names of amidines are formed by replacing the 'amide' ending in names of amides by 'imidamide', but are not preferred IUPAC names; preferred IUPAC names are derived systematically. Other than that, the nomenclatural properties of amides are transferred to amidines; thus, names of amidines correspond to preferred names of amides; and amides that are not substitutable generate nonsubstitutable amidines.

Examples:

<sup>6</sup> CH<sub>3</sub>-[CH<sub>2</sub>]<sub>4</sub>-C(=NH)-NH<sub>2</sub> hexanimidamide (PIN) (no longer hexanamidine)

 $C_6H_{11}$ -C(=NH)-NH<sub>2</sub>

cyclohexanecarboximidamide (PIN) (no longer cyclohexanecarboxamidine)

 $CH_3-C(=NH)-NH_2$ 

ethanimidamide (PIN) acetimidamide (no longer acetamidine)

 $HC(=NH)-NH_2$ 

methanimidamide (PIN) formimidamide (no longer formamidine)

 $H_2N-C(=NH)-CH_2-CH_2-CH_2-C(=NH)-NH_2$ 

pentanebis(imidamide)(PIN) (no longer pentanediamidine)

H<sub>2</sub>N-C(=NH)-CH<sub>2</sub>-CH<sub>2</sub>-C(=NH)-NH<sub>2</sub>

butanebis(imidamide) (PIN) succinimidamide

$$\begin{array}{c} 5 \\ 4 \\ 2 \\ 2 \\ C(=NH)-NH_{2} \end{array}$$

benzene-1,2-dicarboximidamide (PIN) phthalimidamide (no longer benzene-1,2-dicarboxamidine)  $H_2N-C(=NH)-SiH_2-SiH_2-C(=NH)-NH_2$ 

disilanedicarboximidamide (PIN) (no longer disilanedicarboxamidine)

H<sub>2</sub>N-(HN=)C
$$\xrightarrow{4}$$
 $\xrightarrow{5}$  $\xrightarrow{6}$ 1  
3 2 C(=NH)-NH<sub>2</sub>

benzene-1,4-dicarboximidamide (PIN) terephthalimidamide (no longer benzene-1,4-dicarboxamidine)

P-66.4.1.2 Amidines of carbonic, oxalic, and the polycarbonic acids

P-66.4.1.2.1 Guanidine, H<sub>2</sub>N-C(=NH)-NH<sub>2</sub>, and its derivatives

**P-66.4.1.2.1.1** The preferred IUPAC name for the 'amidine' related to carbonic acid,  $H_2N-C(=NH)-NH_2$ , is the retained name 'guanidine'; the locants 1, 2, and 3 are used, not N, N' and N''.

$$H_{2N} - C(=NH) - NH_{2}$$

The systematic functional replacement name 'carbonimidic diamide' may be used in general nomenclature and uses the locants N, N' and N''.

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

methanesulfinimidamide (PIN)

(no longer methanesulfinamidine)

**P-66.4.1.2.1.2** Hydrocarbyl derivatives are named as substituted guanidines. The locants N and N' are used when the position of the double bond is unknown; when there is a choice, a minimum number of primes is used. Examples:

1,1,3,3-tetramethyl-2-phenylguanidine (PIN)1,1,3-trimethylguanidine (PIN)N,N,N',N'-tetramethyl-N"-phenylguanidineN,N,N'-trimethylguanidineN,N,N',N'-tetramethyl-N"-phenylguanidic diamideN,N,N'-trimethylguanidic diamide

 $CH_3-NH-C(=NH)-N(CH_3)_2$ 

**P-66.4.1.2.1.3** In presence of a characteristic group having seniority over guanidine (see P-42.2), the following prefixes are used. The prefix guanidino is no longer recommended.

<sup>N</sup>, <sup>N</sup>, <sup>N</sup>, <sup>N</sup>, <sup>N</sup> H<sub>2</sub>N-C(=NH)-NH–

carbamimidamido (PIN) carbamimidoylamino (not guanidino)

 $(H_2N)_2C=N-$ 

(diaminomethylidene)amino (PIN)

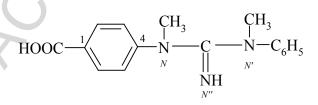
Examples:

(H<sub>2</sub>N)<sub>2</sub>C=N-CH<sub>2</sub>-COOH

*N*-(diaminomethylidene)glycine (PIN) [(diaminomethylidene)amino]acetic acid

 $(H_2N)_2C=N-CH_2-CH_2-CH_2-COOH$ 

4-[(diaminomethylidene)amino]butanoic acid (PIN)



4-(*N*,*N*′-dimethyl-*N*′-phenylcarbamimidamido)benzoic acid (PIN) 4-[methyl(*N*-methyl-*N*-phenylcarbamimidoyl)amino]benzoic acid  $H_2N-C(=NH)-NH-CHO$ 

*N*-carbamimidoylformamide (PIN) (not *N*-formylguanidine)  $H_2N-C(=NH)-NH-CO-NH_2$ 

carbamimidoylurea (PIN) (not *N*-carbamoylguanidine)

$$H_2N-C(=NH)-NH-CO-CH_3$$

*N*-(*C*-aminocarbonimidoyl)acetamide (PIN) (not *N*-acetylguanidine)

P-66.4.1.2.2 Condensed guanidines.

The names biguanide, triguanide, etc., are no longer recommended. Condensed guanidines,  $H_2N$ -[C(=NH)-NH]<sub>n</sub>-H, where n = 2, 3, or 4 are named systematically as the diamides of triimidodicarbonic acid, pentaimidotricarbonic acid, and heptatriimidotetracarbonic acid. Locants, as shown, are used to indicate the positions of substituents.

N 1	N''	2	3	N'''	N '
$H_2N-C$	(=NH)	-NE	I-C(=	=NH)	-NH <sub>2</sub>

1,2,3-triimidodicarbonic diamide (PIN)

N = 1 N'' = 2 N''' = 4 5 N''' = N''H<sub>2</sub>N-C(=NH)-NH-C(=NH)-NH-C(=NH)-NH<sub>2</sub> 1,2,3,4,5-pentadiimidotricarbonic diamide (PIN)

Example:

 $H_2N-C_3(=NH)-NH-C(=N-CH_2-CH_3)-N(C_6H_5)_2$ 

*N*,*N*-diphenyl-*N*"-ethylimidodicarbonodiimidic diamide (PIN)

For polyguanides, where n = 5 and higher skeletal replacement ('a') nomenclature leads to preferred IUPAC names

Example:

 $H_2N-C(=NH)-NH-C(=NH)-NH-C(=NH)-NH-C(=NH)-NH-C(=NH)-NH-C(=NH)-NH_2$ 3,5,7-triimino-2,4,6,8-tetraazanonanebis(imidamide) (PIN)

**P-66.4.1.2.3** Preferred names for amidines related to oxalic acid and the polycarbonic acids are diamides of imido acids in which the imido groups are indicated by the functional replacement prefix imido (see also P-66-1.5.6.1.2).

Examples:

> N 1 N" 2 N"' N' H<sub>2</sub>N-C(=NH)-C(=NH)-NH<sub>2</sub> 1,2-diimidooxalic diamide (PIN) (not oxalimidamide; see P-65.2.5)

 $H_2N-C(=NH)-NH-C(=NH)-NH_2$ 

1,2,3-triimidodicarbonic diamide (PIN)

P-66.4.1.3 Prefixes for the amidine characteristic group

**P-66.4.1.3.1** The systematic name for the group  $-C(=NH)-NH_2$  is 'carbamimidoyl'; it is the name of the acyl group derived from the name carbamimidic acid, HO-C(=NH)-NH<sub>2</sub>. The prefix 'amidino' is no longer recommended. In the acyl group, the  $-NH_2$  group is denoted by the locant *N* and the =NH group by *N*'.

Examples:

$$H_2N-C(=NH)$$
  $4$   $1$  COOH

4-carbamimidoylbenzoic acid (PIN) (no longer 4-amidinobenzoic acid)

$$(CH_3)_2^N - C(=N-CH_2-CH_3) \xrightarrow{4} 1$$
 COOH

4-(*N*'-ethyl-*N*,*N*-dimethylcarbamimidoyl)benzoic acid (PIN) [no longer 4-(*N*'-ethyl-*N*,*N*-dimethylamidino)benzoic acid]

**P-66.4.1.3.2** When the carbon atom of the  $H_2N-C(=NH)$ – group terminates a chain, the groups  $-NH_2$  and =NH are designated by the prefixes 'amino' and 'imino', respectively.

Example:

$$(CH_3)_2N-C(=N-CH_2-CH_3)-CH_2-CH_2-CO-O-CH_3$$

methyl 4-(dimethylamino)-4-(ethylimino)butanoate (PIN) (not methyl 3-[C-(dimethylamino)-N-ethylcarbonimidoyl]propanoate) (not methyl 3-( $N^2$ -ethyl- $N^1$ , $N^1$ -dimethylamidino)propionate)

**P-66.4.1.3.3** The substituent group HN=CH-NH– is named 'methaneimidamido'; it can also be named as a compound substituent 'formimidoylamino' or '(iminomethyl)amino'. The name 'methanimidamido' leads to preferred IUPAC names. The substituent group  $H_2N$ -CH=N– can only be named as a compound substituent group, '(aminomethylidene)amino'.

Example:

HN=CH-NH COOH

4-methanimidamidobenzoic acid (PIN) 4-[(iminomethyl)amino]benzoic acid 4-(formimidoylamino)benzoic acid

**P-66.4.1.3.4** Substituent prefixes corresponding to the suffixes sulfonimidamide, sulfinimidamide, and related selenium and tellurium suffixes are formed systematically by concatenation using the prefix 'amino-' and the the name of the appropriate acyl group:

$-S(O)(=NH)-NH_2$	$-S(=NH)_2-NH_2$	$-S(=NH)-NH_2$
S-aminosulfonimidoyl	S-aminosulfonodiimidoyl	S-aminosulfinimidoyl

The italic letter locant 'S' is used to avoid potential ambiguity regarding substitution on the imido nitrogen atom

Example:

H<sub>2</sub>N-S(=NH)-CH<sub>2</sub>-CH<sub>2</sub>-COOH

3-(S-aminosulfinimidoyl)propanoic acid (PIN)

**P-66.4.1.3.5** In the presence of a characteristic group cited as a suffix, the group R-C(=NH)NH-, or R-S(O)(=NH)NH- (and selenium and tellurium analogues) is named in two ways.

- (1) substitutively, by using a prefix named formed by changing the final letter 'e' in the complete name of the amide to 'o', thus changing the suffixes 'imidamide' and 'carboximidamide' into 'imidamido' and 'carboximidamido', respectively, or 'sulfonimidamide' to 'sulfonimidamido', etc..
- (2) substitutively, by using 'acylamino' prefixes formed by substituting the name of the acyl group to the substituent 'amino'

Method (1) generates preferred IUPAC names.

Examples:

4-ethanimidamidobenzoic acid (PIN) 4-(acetimidoylamino)benzoic acid 4-acetimidamidobenzoic acid

2-ethanesulfonodiimidamidobenzoic acid (PIN) 2-(ethanesulfonodiimidoylamino)benzoic acid

P-66.4.1.4 Substituted amidines

**P-66.4.1.4.1** *N*-Substituted amidines are named by prefixing the name of the appropriate substituent to the name of the unsubstituted amidine, with N or  $N^1$  and N' or  $N^2$  locants; N or  $N^1$  refers to the amino group and N' or  $N^2$  refers to the imino group. Because of tautomerism, the plain locant N is used when only one substituent is present. The locants N and N' are used in preferred IUPAC names.

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Examples:

$$C_{6}H_{5}-C(=N-CH_{3})-N(C_{6}H_{5})_{2}$$

*N'*-methyl-*N*,*N*-diphenylbenzenecarboximidamide (PIN)

N<sup>2</sup>-methyl-N<sup>1</sup>,N<sup>1</sup>-diphenylbenzamidine (no longer N'-methyl-N,N-diphenylbenzamidine)

$$C_{6}H_{5}-C(=NH)-NH-C_{6}H_{5}$$

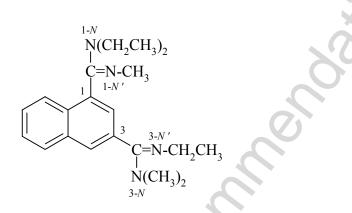
*N*-phenylbenzenecarboximidamide (PIN) (no longer *N*-phenylbenzamidine) (not benzimidanilide)

$$C_{6}H_{5}-C(=N-CH_{2}-CH_{3})-NH-CH_{3}$$

N'-ethyl-N-methylbenzenecarboximidamide (PIN) N<sup>2</sup>-ethyl-N<sup>1</sup>-methylbenzamidine (no longer N'-ethyl- N-methylbenzamidine)

**P-66.4.1.4.2** When it is necessary to identify the position of substituents in a polyamidine system, the *N* locants described above are preceded by the locant of the position occupied by each amidine characteristic group.

Example:

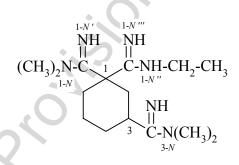


1-N,1-N,3-N'-triethyl-1-N',3-N,3-N-trimethylnapthalene-1,3-dicarboximidamide (PIN)

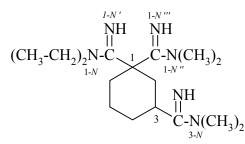
#### P-66.4.1.4.3 Geminal carboxamidine groups

When geminal carboximidamide groups are present, the locants N, N', etc. are used in association with the numerical locant indicating the position of the groups on a chain or cycle. Lowest locants are assigned to the most substituted group; when there is a choice, lowest locants are assigned to the first cited *N*-substituent. This system of *N*-locants in association with numerical locants is recommended for naming substituted amines (see P-62.2.1.2.2) and substituted amides (see P-66.1.1.3.1.2).

Examples:



1-*N*,1-*N*,3-*N*,3-*N*-tetramethyl-1-*N*"-ethylcyclohexane-1,1,3-tricarboximidamide (PIN)



1-*N*,1-*N*-diethyl-1-*N*",1-*N*",3-*N*-,3-*N*-tetramethylcyclohexane-1,1,3-tricarboximidamide (PIN)

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P-66.4.1.5 Formamidine disulfides.

The compound  $H_2N-C(=NH)-S-S-C(=NH)-NH_2$  and its derivatives have been named previously on the basis of the parent structure 'formamidine disulfides'. They are now named on the basis of:

(1) the parent hydride 'disulfane'; or

(2) the parent compound 'dicarbonic acid'.

Method (1) generates preferred IUPAC names.

Example:

 $CH_3-CH_2-NH-C(=NH)-S-S-C(=NH)-NH-CH_3$ 

*N*-ethyl-*N*'-methyldisulfanedicarboximidamide (PIN) *N*-ethyl-*N*'-methyl(dithioperoxy)dicarbonimidic diamide (traditionally  $N^1$ -ethyl- $N^2$ -methyl- $\alpha, \alpha'$ -dithiobisformamidine)

P-66.4.1.6 Diamidides

Diamidides are analogues of acyclic carboxylic anhydrides in which the =O atoms have been replaced by =NR groups and the anhydride oxygen atom by -NR- giving the general formula RC(=NR')-NR''-(=NR''')CR''''. They are named systematically as *N*-imidoylimidamides.

Example:

N<sup>N</sup> CH<sub>3</sub>-C(=NH)-NH-C(=NH)-CH<sub>3</sub> N-ethanimidovlethanimidamide (PIN)

*N*-acetimidoylacetimidamide (PIN)

P-66.4.1.7 Amide oximes

Amide oximes are formally oximes of carboxamides, i.e., compounds having the general structure  $R-C(=N-OH)-NH_2$  and derivatives formed by substitution. Preferred IUPAC names are

*N'*-hydroxy- or *N'*-alkyloxy- derivatives of carboximidamides (amidines). Suffixes such as 'amide oxime' or 'carboxamide oxime' are no longer recommended.

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Example:

$$CH_3-C(=N-OH)-NH-CH_3$$

*N'*-hydroxy-*N*-methylacetimidamide (PIN) (no longer *N*-methylacetamide oxime)

$$\begin{array}{c}
H \\
N \\
M \\
M \\
M
\end{array}$$

$$\begin{array}{c}
N \\
C = N-O-CH_2CH_3
\end{array}$$

*N'* -ethoxyimidazole-2-carboximidamide (PIN) (no longer imidazole-2-carboxamide *O*-ethyloxime)

P-66.4.2 Amidrazones

P-66.4.2.1 Amidrazone suffixes

Compounds having the general structure  $R-C(-NH_2)=N-NH_2$  or the tautomeric  $R-C(=NH)-NH-NH_2$  have the class name 'amidrazones' and are named substitutively using the suffixes 'hydrazonamide' or 'imidohydrazide', respectively, or 'carbohydrazonamide' or 'carboximidohydrazide', respectively. *N*-Substitution, when the position of the double bond is known, is designated according to the following numbering:

for carbohydrazonamides	$R-C(=N-NH_2)-NH_2$
for carboximidohydrazides	$R-C(=NH)-NH-NH_2$

Locants N, N' and N'' as shown are recommended. The previous methods of naming amidrazones as 'amide hydrazones' or 'hydrazide imides', or amidrazones when the structure is not known are no longer recommended.

When the position of the double bond is unknown, the senior characteristic group, carbohydrazonamide, is chosen to denote the tautomers, with appropriate locants N and N'' to denote substitution. When the position of the substituted suffixes must be indicated in a name, locants designating the positions of the suffixes are added in front of the appropriate N locants, separated by a hyphen.

Retained names of amidrazones are formed by replacing the 'amide' ending in names of amides by 'ohydrazonamide' and are only used in general nomenclature. Preferred IUPAC names of amidrazones are formed systematically. Otherwise, the nomenclatural properties of amides are transferred to amidrazones; thus, preferred names of amidrazones correspond to preferred names of amides and amides that are not substitutable generate nonsubstitutable amidrazones.

Examples:

N '' $N-N=C(CH_3)_2$ N HC-N(CH<sub>3</sub>)<sub>2</sub>

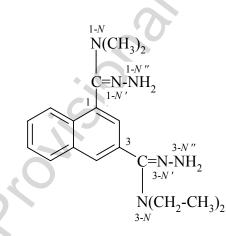
*N*,*N*-dimethyl-*N*"-propan-2-ylidenemethanehydrazonic amide (PIN) *N*,*N*-dimethyl-*N*"-isopropylideneformohydrazonic amide (not *N*,*N*-dimethylformamide isopropylidenehydrazone)

 $\begin{array}{c} C_{6}H_{5} \\ N'' \mid N N' \\ CH_{3}\text{-}CH_{2}\text{-}N=C\text{-}N(CH_{3})\text{-}NH\text{-}C_{6}H_{5} \end{array}$ 

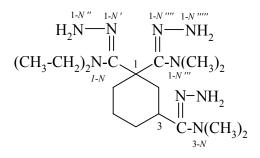
N''-ethyl-N-methyl-N'-phenylbenzenecarboximidohydrazide (PIN) (not  $N^{1}$ -methyl- $N^{2}$ -phenylbenzohydrazide ethylimide)

1 2 3 4 1 2 H<sub>2</sub>N-C(=NH)-NH-NH-N=N-C(=NH)-NH-NH-NO

4-[*C*-(2-nitrosohydrazinecarbonimidoyl)tetraaz-3-ene-1-carboximidamide (PIN) [an imidamide is senior to an imidohydrazide (an amidrazone)]



3-N,3-N-diethyl-1-N,1-N-dimethylnaphthalene-1,3-dicarbohydrazonamide (PIN)



1-*N*,1-*N*-diethyl-1-*N*<sup>'''</sup>,3-*N*,3-*N*-tetramethylcyclohexane-1,1,3-tricarbohydrazonamide (PIN) (for locants *N*,*N* ', etc. in association with numerical locants, see P-62.2.1.2.2 and P-66.4.1.3.3)

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Amidrazones derived from sulfonic acid, and similar acids, are named in accordance with the same principles.

Example:

$$C_6H_5$$
-S(=NNH<sub>2</sub>)-NH<sub>2</sub>

benzenesulfinohydrazonamide (PIN)

P-66.4.2.2 Amidrazones of carbonic, oxalic, and the polycarbonic acids

The general methodology discussed in P-65.2 is applied to generate the names for amidrazones derived from carbonic, oxalic, and the polycarbonic acids.

Examples:

 $\begin{array}{c} 2 \quad 1 \\ H_2N-NH-C(=NH)-NH-NH_2 \end{array}$ 

hydrazinecarboximidohydrazide (PIN) carbonimidic dihydrazide

 $H_2N-C(=N-NH_2)-NH_2$ 

carbonohydrazonic diamide (PIN)

 $H_2N-NH-C(=NH)-O-C(=NH)-NH-NH_2$ 

1,3-diimidodicarbonic dihydrazide (PIN)

$$H_2N-C(=N-NH_2)-O-C(=N-NH_2)-NH_2$$
  
1,3-dihydrazonodicarbonic diamide (PIN)

#### $H_2N-NH-C(=NH)-O-C(=NNH_2)-NH_2$

(hydrazinecarboximidoyloxy)formohydrazonic amide (PIN) (carbamohydrazonoyloxy)methanimidohydrazide

 $H_2N-NH-C(=NH)-C(=NH)-NH-NH_2$ 

1,2-diimidooxalic dihydrazide (PIN)

 $H_2N-C(=N-NH_2)-C(=N-NH_2)-NH_2$ 

1,2-dihydrazonooxalic diamide (PIN)

H<sub>2</sub>N-NH-C(=NH)-C(=N-NH<sub>2</sub>)-NH<sub>2</sub>

hydrazinecarboximidoylmethanehydrazonic amide (PIN) carbamohydrazonoylmethanimidohydrazide

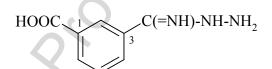
## P-66.4.2.3 Amidrazone prefixes

**P-66.4.2.3.1** The prefix name for the group  $-C(=NH)-NHNH_2$  is 'hydrazinecarboximidoyl'. When this group is located at the end of a carbon chain, the prefixes 'imino' and 'hydrazinyl' are preferred in order to avoid fragmenting the chain.

Examples:

 $H_2N-NH-(HN=)C-CH_2-COOH$ 

3-imino-3-hydrazinylpropanoic acid (PIN) hydrazinecarboximidoylacetic acid

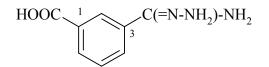


3-hydrazinecarboximidoylbenzoic acid (PIN)

**P-66.4.2.3.2** The prefix name for the group  $-C(=N-NH_2)-NH_2$  is 'carbamohydrazonoyl'. When this group is located at the end of a carbon chain, the prefixes 'amino' and 'hydrazinylidene' are preferred in order to avoid fragmenting the chain.

Examples:

3-amino-3-hydrazinylidenepropanoic acid (PIN) carbamohydrazonoylacetic acid



3-carbamohydrazonoylbenzoic acid (PIN)

**P-66.4.2.3.3** The prefix names for the groups  $-NH-CH=N-NH_2$  and  $-N=CH-NH-NH_2$  are compound prefixes and are '(hydrazinylidenemethyl)amino' and '(hydrazinylmethylidene)amino', respectively.

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Example:

H<sub>2</sub>N-NH-CH=N COOH

4-[(hydrazinylmethylidene)amino]benzoic acid (PIN)

**P-66.4.2.3.4** Prefix names for the H<sub>2</sub>N-CH=N-NH–, HN=CH-NH-NH–, and HC(=NNH<sub>2</sub>)-NH– groups are compound prefixes, which are: 2-(aminomethylidene)hydrazinyl (PIN)', '2-methanimidoylhydrazinyl (PIN)' or 'methanimidohydrazido' or '2-(iminomethyl)hydrazinyl', and 'methanehydrazonoylamino (PIN)' or methanehydrazonamido, respectively.

Example:

$$H_2N-CH=NH-NH-CH_2-CH_2-COOH$$

3-[2-(aminomethylidene)hydrazin-1-yl]propanoic acid (PIN)

**P-66.4.2.3.5** When a group having preference for citation as a principal characteristic group is present, the group  $R-C(=N-NH_2)-NH^-$ , or  $R-S(O)(=N-NH_2)-NH^-$  (and selenium and tellurium analogues) of an *N*-substituted amide is named in two ways.

- (1) substitutively, by using a prefix named formed by changing the final letter 'e' in the complete name of the amide to 'o';
- (2) substitutively, by using 'acylamino' prefixes formed by substituting the name of the acyl group to the substituent 'amino'

Method (1) generates preferred IUPAC names.

Example:

$$C_6H_5$$
-S(=N-NH<sub>2</sub>)-NH<sup>4</sup>/\_COOH

4-benzenesulfinohydrazonamidobenzoic acid (PIN))4-(benzenesulfinohydrazonoylamino)benzoic acid

**P-66.4.2.3.6** When a group having priority for citation as a principal characteristic group is present, a hydrazide group of the type R-C(=NH)-NHNH–, or R-S(=NH)<sub>2</sub>-NHNH– (or analogous selenium and tellurium group) is named:

- (1) as an acylhydrazinyl prefix; the hydrazinyl group is numbered by using the numerical locants 1 and 2;
- (2) by expressing the corresponding hydrazide as a prefix by replacing the final letter 'e' in the name of the hydrazide by the letter 'o'.

Method (1) generates preferred IUPAC names.

Example:

4-(2-benzenecarboximidoylhydrazin-1-yl)benzoic acid (PIN) 4-(2-benzenecarboximidohydrazido)benzoic acid

P-66.4.3 Hydrazidines

**P-66.4.3.1** Hydrazidine suffixes

Compounds with the general structure R-C(NH-NH<sub>2</sub>)=N-NH<sub>2</sub> have the class name 'hydrazidines' and are named substitutively by using the suffixes 'hydrazonohydrazide' and 'carbohydrazonohydrazide' as prescribed for hydrazides. The former method of naming hydrazidines as hydrazones of the corresponding hydrazides is no longer recommended.

Locants are assigned to nitrogen atoms as follows:

$$R-C(=N-NH_{2})-NH-NH_{2}$$

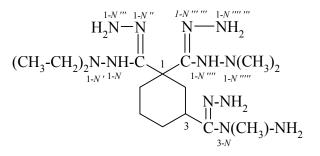
When necessary, the appropriate N locants are preceded by the locant indicating the position of the hydrazidine characteristic group on the parent structure.

Names of hydrazidines formally derived from carboxylic acids having retained names, formed by replacing the 'ohydrazide' ending in names of hydrazides by 'hydrazonohydrazide' may be used in general nomenclature. Preferred IUPAC names are formed systematically. Otherwise, the nomenclatural properties of hydrazides are transferred to hydrazidines; thus, preferred names of

hydrazidines correspond to preferred names of hydrazides, and hydrazides that are not substitutable generate nonsubstitutable hydrazidines.

Examples:

 $HC(=NNH_2)-NH-NH_2$ methanehydrazonohydrazide (PIN) (not methanehydrazide hydrazone) CH<sub>3</sub>-CH<sub>2</sub>-CH<sub>2</sub>-C(=NNH<sub>2</sub>)-NHNH<sub>2</sub> butanehydrazonohydrazide (PIN) (not butanehydrazide hydrazone) -NH-CH<sub>3</sub> NH-NH-CH N',N"'-dimethylthiophene-2-carbohydrazonohydrazide (PIN) (not  $N^2$ ,  $N^4$ -dimethyl-2-thenohydrazide hydrazone) =CH-C<sub>6</sub>H<sub>5</sub>  $H-N=CH-C_6H_5$ N', N''-dibenzylidene-1,3-thiazole-4-carbohydrazonohydrazide (PIN) (not  $N^2$ ,  $N^4$ -dibenzylidenethiazole-4-carbohydrazide hydrazone)  $-NH_2$  $\text{C-NH-N(CH}_{3})_2$ 2 CH, H<sub>2</sub>N-N N-NH, 1,2-N',2-N',6-N -tetramethylnaphthalene-2,6-dicarbohydrazonohydrazide (PIN)



1-*N*',1-*N*'-diethyl-1-*N*''' ",1-*N*''' ",3-*N*-trimethylcyclohexane-1-1-3-tricarbohydrazonohydrazide (PIN) (for locants *N*,*N*', etc. in association with numerical locants, see P-62.2.1.2.2, P-66.4.1.3.3 and P-66.4.2.1).

**P-66.4.3.2** Hydrazidines derived from sulfonic acid, and similar selenium and tellurium acids, are named in accordance with the same principles.

Example:

 $C_6H_5-S(=NNH_2)-NH-NH_2$ 

benzenesulfinohydrazonohydrazide (PIN)

**P-66.4.3.3** Hydrazidines derived from carbonic acid, oxalic acid, and the polycarbonic acid follow the procedure for the corresponding hydrazides given above (see P-66.3.5).

Example:

H<sub>2</sub>N-NH-C(=N-NH<sub>2</sub>)-NH-NH<sub>2</sub>

hydrazinecarbohydrazonohydrazide (PIN) carbonohydrazonic dihydrazide

<sup>1</sup> <sup>2</sup> <sup>3</sup> H<sub>2</sub>N-NH-C(=N-NH<sub>2</sub>)-O-C(=N-NH<sub>2</sub>)-NH-NH<sub>2</sub> dihydrazonodicarbonic dihydrazide (PIN)

 $H_2N-NH-C(=N-NH_2)-C(=N-NH_2)-NH-NH_2$ 

dihydrazonooxalic dihydrazide (PIN)

 $N' N N'' 1 2 N''' N'' N'' N'' N'' N'' N'' H_2N-NH-(H_2NN=)C-C(=NNH_2)-NH-NH_2$ 

dihydrazonooxalic dihydrazide (PIN)

**P-66.4.3.4** Hydrazidine prefixes

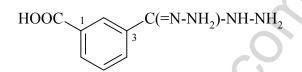
**P-66.4.3.4.1** Prefix names for the group  $-C(=NNH_2)-NH-NH_2$  are 'hydrazinecarbohydrazonoyl' or '*C*-hydrazinylcarbonohydrazonoyl'; preferred IUPAC names use the former prefix. When this group is located at the end of a carbon chain, the prefixes 'hydrazinyl' and 'hydrazinylidene' are preferred in order to avoid fragmenting the chain.

Examples:

 $H_2N-NH-(H_2N-N=)C-CH_2-COOH$ 

3-hydrazinyl-3-hydrazinylidenepropanoic acid (PIN) 2-hydrazinecarbohydrazonoyl)acetic acid

2-(C-hydrazinylcarbonohydrazonoyl)acetic acid



3-(hydrazinecarbohydrazonoylbenzoic acid (PIN) 3-(*C*-hydrazinylcarbonohydrazonoyl)benzoic acid

4-{2-[(carbamimidoyloxy)methanimidoyl]hydrazin-1-yl}benzoic acid (PIN)

**P-66.4.3.4.2** The prefix names for the groups -NH-NH-CH=N-NH<sub>2</sub> and -NH-N=CH-NH-NH<sub>2</sub> are compound prefixes and are: '2-(hydrazinylidenemethyl)hydrazinyl' or '(2-methanehydrazonoyl-hydrazin-1-yl) (PIN)' and '2-(hydrazinylmethylidene)hydrazinyl (PIN)', respectively.

Example:

H<sub>2</sub>N-NH-CH=N-NH-CH<sub>2</sub>-COOH

2-(2-methanehydrazonoylhydrazin-1-yl)acetic acid (PIN) [2-(hydrazinylmethylidene)hydrazin-1-yl]acetic acid

DRAFT 7 October 2004

# P-66.5 Nitriles

- P-66.5.0 Introduction
- P-66.5.1 Nitriles and cyanides
- P-66.5.2 Substituted nitriles and cyanides
- P-66.5.3 Nitriles/cyanides corresponding to carbonic, oxalic, and the polycarbonic acids
- P-66.5.4 Nitrile oxides

# P-66.5.0 Introduction

Compounds with the general structure R-C=N are called 'nitriles' or 'cyanides'. Nitriles and cyanides are derived from hydrocyanic acid, HC=N. When the point of attachment of the -C=N group to R is a carbon atom or a heteroatom, these compounds form the class of nitriles and are named substitutively as nitriles. They may also be named as cyanides according to the principles of functional class nomenclature. These two types of nomenclature are fully discussed in this Section.

P-66.5.1 Nomenclature for generating preferred names of nitriles

Compounds of the general structure R-C≡N have the class names 'nitriles' and are named in three ways:

- (a) substitutively, using the suffixes 'nitrile' for -(C)N and carbonitrile' for -CN
- (b) by changing the 'ic acid' or 'oic acid' endings in retained names of carboxylic acids into 'onitrile'; the nomenclatural properties of acids are transferred to nitriles; thus, preferred names of nitriles correspond to preferred names of carboxylic acids (see P-55) and carboxylic acids that are not substitutable generate nonsubstitutable nitriles (see P-65.1.1.1.2)
- (c) by functional class nomenclature, using the class name 'cyanide'

P-66.5.1.1 Substitutive and functional class names for nitriles

P-66.5.1.1.1 Acyclic mono- and dinitriles are named in the following two ways:

(1) substitutively by using the suffix 'nitrile', and

(2) by functional class nomenclature using the class name 'cyanide'.

Method (1) leads to preferred IUPAC names.

Examples:

 $CH_3$ -[CH<sub>2</sub>]<sub>4</sub>-CN

hexanenitrile (PIN)) pentyl cyanide 5 4 3 2 1 NC-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CN

pentanedinitrile (PIN)) propane-1,3-diyl dicyanide

**P-66.5.1.1.2** If an unbranched alkane is linked to more than two terminal cyano groups, all cyano groups are named from the parent hydride by the substitutive suffix 'carbonitrile', preceded by appropriate multiplying prefix and locants.

Example:

<sup>4</sup> <sup>1</sup> CH<sub>3</sub>-[CH<sub>2</sub>]<sub>2</sub>-C(CN)<sub>3</sub> butane-1,1,1-tricarbonitrile (PIN)

**P-66.5.1.1.3** The suffix 'carbonitrile' is always used to name nitriles having the –CN group attached to a ring or ring system or to an acyclic heteroatom.

Examples:

H<sub>3</sub>Si-CN

silanecarbonitrile (PIN) silyl cyanide

H<sub>2</sub>N-NH-CN

hydrazinecarbonitrile (PIN) hydrazinyl cyanide

cyclohexanecarbonitrile (PIN) cyclohexyl cyanide piperidine-1-carbonitrile (PIN)

-CN

**P-66.5.1.1.4** When a group is present that has priority for citation as the principal characteristic group or when all –CN groups cannot be expressed as the principal characteristic group, the –CN group is designated by the prefix 'cyano'. The prefix 'cyano' **must** also be used when the –CN group is located at the end of a chain.

Examples:

COOH 5-cyanofuran-2-carboxylic acid (PIN) 5-cyano-2-furoic acid NC-CH<sub>2</sub>-CH<sub>2</sub>-COOH 3-cyanopropanoic acid (PIN)

$$\begin{array}{c} \text{CH}_2\text{-CN} \\ 7 & 6 & 5 & 3 & 2 & 1 \\ \text{NC-CH}_2\text{-CH}_2\text{-CH}_2\text{-CH}_2\text{-CH}_2\text{-CH}_2\text{-CN} \end{array}$$

4-(cyanomethyl)heptanedinitrile (PIN)

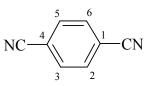
P-66.5.1.2 Names of nitriles derived from retained names of carboxylic acids

(a) The following names are retained as preferred names, with unlimited substitution, except for formonitrile whose substitution rules are the same as formic acid (see P-65.1.8)

HCN	CH <sub>3</sub> -CN	C <sub>6</sub> H <sub>5</sub> -CN
formonitrile (PIN) methanenitrile hydrogen cyanide	acetonitrile (PIN) ethanenitrile	benzonitrile (PIN) benzenecarbonitrile

(a) For general nomenclature, only the names furocarbonitrile, phthalonitrile, isophthalonitrile, and terephthalonitrile are retained with full substitution allowed (see P-34). Systematic names (P-66.1.1.1.1) are the preferred IUPAC names.

Examples:



benzene-1,2-dicarbonitrile (PIN) phthalonitrile

benzene-1,4-dicarbonitrile (PIN) terephthalonitrile

(c) Nitriles derived from retained acid names given in P-65.1.1.2 are only used in general nomenclature; no substitution is allowed. Preferred IUPAC names are given systematic names (P-66.5.1.1).

Examples:

CH<sub>3</sub>-CH<sub>2</sub>-CN

propiononitrile propanenitrile (PIN) NC-CH<sub>2</sub>-CH<sub>2</sub>-CN succinonitrile butanedinitrile (PIN)

(d) Names of nitriles derived from carbohydrate acids and amino acids are discussed in P-102.5.5.6.2.1 and P-103.2, respectively.

Examples:

```
CN

|

HOCH

|

HCOH

|

HOCH

|

CH<sub>2</sub>OH

L-xylononitrile (PIN)

H<sub>2</sub>N-CH<sub>2</sub>-CN
```

glycinonitrile (PIN)

P-66.5.1.3 Functional class nomenclature for generating preferred IUPAC names of cyanides

Functional class nomenclature is used, when needed, to name compounds in accordance with the seniority of classes and to name compounds that cannot be named substitutively, for example, cyanides corresponding to sulfonic and sulfinic acids, selenium and tellurium analogues, carbonic acid, and inorganic acids.

**P-66.5.1.3.1** Nitriles with an  $\alpha$ -oxo group.

Compounds of the type R-CO-CN can be named as acyl cyanides in a way similar to that of acid halides. Since acyl cyanides are senior to nitriles, in the seniority of classes, functional class nomenclature must be used to correctly express the seniority order.

Examples:

HCO-CN	CH <sub>3</sub> -CO-CN	CH <sub>3</sub> -[CH <sub>2</sub> ] <sub>5</sub> -CO-CN
formyl cyanide (not oxoacetonitrile)	acetyl cyanide (PIN) (not pyruvonitrile)	heptanoyl cyanide (PIN) (not 2-oxooctanenitrile) (not 2-oxopropanenitrile)

P-66.5.1.3.2 Cyanides corresponding to the sulfur, selenium, and tellurium acid suffixes

Cyanides formally formed by replacing the –OH group in sulfonic acids, sulfinic acids, and similar Se and Te acids, are named by functional class nomenclature.

Examples:

CH<sub>3</sub>-SO<sub>2</sub>-CN

methanesulfonyl cyanide (PIN) benzenesel

C<sub>6</sub>H<sub>5</sub>-SeO-CN benzeneseleninyl cyanide (PIN)

ondation

P-66.5.2 Substituted nitriles

Substituents on the parent hydrides are denoted as prefixes. Nitriles, in the seniority order of classes, are senior to ketones, pseudoketones, heterones, hydroxy compounds, amines and imines; these classes must be cited as prefixes in the presence of a nitrile group. Seniority for numbering polyfunctional amides follows that described for acids, for which see P-65.1.2.3 and P-65.3.4.

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Examples:

<sup>6</sup> <sup>5</sup> <sup>1</sup> CH<sub>2</sub>-CO-[CH<sub>2</sub>]<sub>3</sub>-CN 5-oxohexanenitrile (PIN)

3 2 HO-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CN

4-hydroxybutanenitrile (PIN)4-hydroxybutyronitrile

NC-CH<sub>2</sub> <sup>3</sup> Br

3-amino-1H-pyrazole-4-carbonitrile (PIN)

(3-bromophenyl)acetonitrile (PIN) 3-bromobenzyl cyanide

NC-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-CN

3,3'-iminodipropanenitrile (PIN) 3,3'-iminodipropionitrile

CN <sup>1</sup> <sup>2</sup>O-CH<sub>3</sub>

2-chloro-6-nitrobenzonitrile (PIN)

2-methoxybenzonitrile (PIN)

<sup>3</sup><sup>2</sup><sup>1</sup> Cl-CH<sub>2</sub>-CH<sub>2</sub>-CO-CN

3-chloropropanoyl cyanide (PIN) (not 3-chloropropionyl cyanide) (not 4-chloro-2-oxopropanenitrile)

P-66.5.3 Nitriles/cyanides corresponding to carbonic, oxalic, and the polycarbonic acids

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**P-66.5.3.1** Nitriles corresponding to carbonic acid and related compounds, oxalic acid and the polycarbonic acids are named by functional class nomenclature

Eamples:

NC-CO-CN

carbonyl dicyanide (PIN) (not 2-oxopropanedinitrile) (not oxomalononitrile; no substitution allowed on malononitrile)

NC-C(=NH)-CN

carbonimidoyl dicyanide (PIN) (not 2-iminopropanedinitrile) NC-C(=NNH<sub>2</sub>)-CN

carbonohydrazonoyl dicyanide (PIN) (not 2-hydrazonopropanedinitrile)

H<sub>2</sub>N-CO-CN

carbamoyl cyanide (PIN)

NC-CO-CO-CN

oxalic dicyanide (PIN)

NC-CO-O-CO-CN dicarbonic dicyanide (PIN)

**P-66.5.4** Nitrile oxides

**P-66.5.4.1** Compounds with the general structure R-C=NO have the generic name 'nitrile oxides'. As zwitterions, they are classed with the zwitterion class in the order of compound classes. They are named by three methods.

- (1) by the term 'oxide' added to the name of the nitrile;
- (2) by applying the  $\lambda$ -convention and oxo substitution to the nitrogen atom (see P-14.1)
- (3) as zwitterions (see P-74.2.2.2)

Methods (1) and (2) lead to preferred IUPAC names.

Example:

 $C_6H_5-C\equiv N^+-O^-$ 

- (1) benzonitrile oxide (PIN)
- (2) benzylidyne( $\infty o$ )- $\lambda^5$ -azane
- (3)\_(benzylidyneammoniumyl)oxidanide

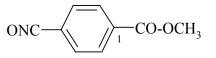
HC=N<sup>+</sup>-O<sup>-</sup> (1) formonitrile oxide (PIN) (2) methylidyne(oxo)- $\lambda^5$ -azane

(3) (methylidyneammoniumyl)oxidanide

**P-66.5.4.2** When necessary to cite the group  $-C \equiv NO$  group as a substituent prefix, method (2) is applied.

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Example:



methyl 4-[( $\infty - \lambda^5$ -azanylidene)methyl]benzoate (PIN) (no longer methyl 4-fulminatobenzoate)

# P-66.6 Aldehydes

- P-66.6.1 Systematic names of aldehydes
- P-66.6.2 Aldehydes from oxalic acid and the polycarbonic acids
- P-66.6.3 Chalcogen analogues of aldehydes
- P-66.6.4 Polyfunctional aldehydes
- P-66.6.5 Acetals and ketals, hemiacetals and hemiketals, and their chalcogen analogues

## P-66.6.0 Introduction.

The class name 'aldehyde' traditionally refers to compounds containing a –CH=O group attached to a carbon atom. However, when the attachment is to a heteroatom it is convenient to call the compound a pseudoaldehyde.

**P-66.6.1** Systematic names of aldehydes

Aldehydes are systematically named in two ways:

(1) substitutively, using the suffixes 'al' for –(C)HO and 'carbaldehyde' for –CHO;

(2) by changing the 'ic acid' or 'oic acid' endings of retained names of carboxylic acids into 'aldehyde'; the nomenclatural properties of acids are transferred to aldehydes; thus, preferred names of aldehydes correspond to preferred names of acids and carboxylic acids that are not substitutable generate nonsubstitutable aldehydes.

P-66.6.1.1 Systematic substitutive names for aldehydes

Aldehydes are named substitutively using the suffixes 'al' or 'carbaldehyde', or the prefix 'oxo', denoting =O, or 'formyl-', denoting the substituent group -CHO.

**P-66.6.1.2** Mono- and dialdehydes derived from alkanes are named substitutively using the suffix 'al' added to the name of the parent hydride with elision of the final letter 'e' of the parent hydride before 'a'.

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Examples:

CH<sub>3</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CHO

pentanal (PIN)

OHC-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CHO pentanedial (PIN)

**P-66.6.1.3** The suffix 'carbaldehyde' is used when more than two –CHO groups are attached to an alkane.

Example:

CHO 1 OHC-CH2-CH-CH2-CH2-CHO

butane-1,2,4-tricarbaldehyde (PIN)

**P-66.6.1.4** The suffix 'carbaldehyde' is used when the –CHO group is attached to a carbon atom of a ring or ring system, or to a heteroatom.

Examples:

CHO

cyclohexanecarbaldehyde(PIN)

phosphanecarbaldehyde (PIN)

H<sub>2</sub>P-CHO

OHC 1 CHO

pyridine-2,6-dicarbaldehyde (PIN)

## H<sub>2</sub>NNH-CHO

hydrazinecarbaldehyde formohydrazide (PIN) (a hydrazide is senior to an aldehyde)

CH<sub>3</sub> (CH3)2N CHO

1,4,4-trimethyltetraaz-2-ene-1-carbaldehyde (PIN)

**P-66.5.1.2** Names of aldehydes derived from retained names of carboxylic acids

Names of aldehydes are formed by changing the 'ic acid' or 'oic acid' ending of the retained names of carboxylic acids to 'aldehyde'. Substitution of aldehydes parallels that of corresponding carboxylic acids.

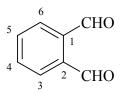
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(a) The following names are retained as preferred IUPAC names, with, except for formaldehyde, unlimited substitution. Substitution rules for formaldehyde are the same as for formic acid (see P-65.1.8)

НСНО	CH <sub>3</sub> -CHO	C <sub>6</sub> H <sub>5</sub> -CHO
formaldehyde (PIN)	acetaldehyde (PIN)	benzaldehyde (PIN)
methanal	ethanal	benzenecarboxaldehyde

(b) For general nomenclature, only the names furaldehyde, phthalaldehyde, isophthalaldehyde, and terephthalaldehyde are retained with full substitution allowed (see P-34). Systematic names (P-66.6.1.1) are the preferred IUPAC names.

Examples:



OHC  $-\frac{5}{4}$   $-\frac{6}{1}$  CHO

benzene-1,2-dicarbaldehyde (PIN) phthalaldehyde benzene-1,4-dicarbaldehyde (PIN) terephthalaldehyde

(c) Aldehydes derived from retained acid names given in P-65.1.1.2 are only used in general nomenclature; no substitution is allowed. Preferred IUPAC names are given systematic names (P-66.6.1.1).

Examples:

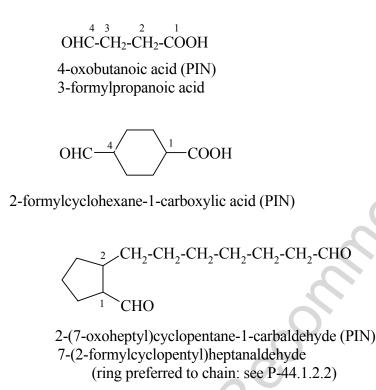
CH<sub>3</sub>-CH<sub>2</sub>-CHO propionaldehyde propanal (PIN))

OHC-CH<sub>2</sub>-CH<sub>2</sub>-CHO

succinaldehyde butanedial (PIN)

**P-66.6.1.3** In the presence of a characteristic group having priority to be cited as a suffix or when present on a side chain, a –CHO group is expressed by the prefix, 'oxo', if located at an end of a carbon chain, or, in other cases, by the prefix 'formyl'.

Examples:



P-66.6.2 Aldehydes from oxalic acid and the polycarbonic acids

**P-66.6.2.1** The retained name oxaldehyde is the preferred IUPAC name for the dialdehyde from oxalic acid. Substitution follows the rules for substituting formaldehyde or formic acid.

Example:

O=CH-CH=O

oxaldehyde (PIN) (a shortened form of oxalaldehyde) (not ethanedial)

**P-66.6.2.2** Aldehydes from di- and polycarbonic acids are named on the basis of the higher compound class. Multiplicative names based on formaldehyde can be used (see P-65.2.2.2)

Example

O=CH-O-CH=O

formic anhydride (PIN) (anhydride preferred to aldehyde) oxydiformaldehyde

# О=СН-О-СО-О-СН=О

carbonic diformic dianhydride (PIN) (anhydride preferred to ester) bis(oxomethyl) carbonate [carbonylbis(oxy)]diformaldehyde

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### P-66.6.3 Chalcogen analogues of aldehydes

Chalcogen analogues of aldehydes are named by using the following suffixes and prefixes modified by functional replacement. In the seniority order of classes, aldehydes are senior to ketones, hydroxy compounds, amines and imines. Names of chalcogen analogues corresponding to aldehydes with retained names are all systematically formed.

Group	Suffix	Prefix
-(C)HO	al	οχο
–(C)HS	thial	sulfanylidene (preferred to thioxo)
–(C)HSe	selenal	selanylidene (preferred to selenoxo)
–(C)HTe	tellural	tellanylidene (preferred to telluroxo)
-СНО	carbaldehyde	formyl
-CHS	carbothialdehyde	methanethioyl (preferred to thioformyl)
-CHSe	carboselenaldehyde	methaneselenoyl (preferred to selenoformyl)
-CHTe	carbotelluraldehyde	methanetelluroyl (preferred to telluroformyl)

Examples:

<sup>2</sup> <sup>1</sup> CH<sub>3</sub>-CHS ethanethial (PIN) thioacetaldehyde

6 CH<sub>3</sub>-[CH<sub>2</sub>]<sub>4</sub>-CHSe

hexaneselenal (PIN)

HOOC CHS

4-(methanethioyl)benzoic acid (PIN) 4-(thioformyl)benzoic acid C<sub>6</sub>H<sub>5</sub>-CHS benzenecarbothialdehyde (PIN) thiobenzaldehyde

<sup>5</sup> <sup>4</sup> <sup>3</sup> <sup>2</sup> <sup>1</sup> SHC-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>5</sub> pentanedithial (PIN)

CHSe HOOC

4-(methaneselenoyl)cyclohexane-1-carboxylic acid (PIN) 4-(selenoformyl)cyclohexane-1-carboxylic acid

CHSe

4-sulfanylidenecyclohexane-1-carboselenaldehyde (PIN) 4-thioxocyclohexane-1-carboselenaldehyde

P-66.6.4 Polyfunctional aldehydes

In presence of an aldehyde group, ketones, pseudoketones, heterones, hydroxy compounds, amines and imines are expressed by prefixes. Seniority for numbering polyfunctional aldehydes follows that described for acids, for which see P-65.1.2.3 and P-65.3.4.

Examples:

4 3 2 1 CH<sub>3</sub>-CO-CH<sub>2</sub>-CHO 3-oxobutanal (PIN) 3-oxobutyraldehyde

CHO OH

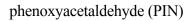
HO-CH CHO

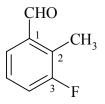
2-hydroxybenzaldehyde (PIN) (not salicylaldehyde) 5-(hydroxymethyl)furan-2-carbaldehyde (PIN)5-(hydroxymethyl)-2-furaldehyde (not 5-(hydroxymethyl)furfural)

 $CH_2$ 5 1 6 CH<sub>3</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-C-CHO

2-methylidenehexanal (PIN) [not 2-butylprop-2-enal, the longest chain is the principal chain (see P-44.3)]

О-СН,-СНО





3-fluoro-2-methylbenzaldehyde (PIN)

P-66.6.5 Acetals and ketals, hemiacetals and hemiketals, and chalcogen analogues

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P-66.6.5.1 Acetals and ketalsP-66.6.5.2 Hemiacetals and hemiketalsP-66.6.5.3 Chalcogen analogues

P-66.6.5.1 Acetals and ketals

**P-66.6.5.1.1** Compounds with the general structure RR'C(O-R'')(O-R''), where only R and R' may be, but need not be, hydrogen, have the class name 'acetals'. 'Ketals' constitute a subclass of acetals wherein neither R nor R' may be hydrogen. Acetals (ketals) are named in two ways:

- (1) substitutively as 'alkoxy', 'aryloxy', etc. derivatives of an appropriate parent hydride or functional parent compound;
- (2) by functional class nomenclature by citing the name of the aldehyde or ketone, the names of the *O*-substituents, in alphanumerical order if required, and finally the class terms 'acetal' or 'ketal'

Method (1), the substitutive method, leads to preferred IUPAC names.

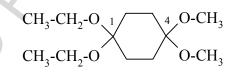
Examples:

<sup>3</sup> <sup>2</sup> <sup>1</sup> CH<sub>3</sub>-CH<sub>2</sub>-CH(OCH<sub>2</sub>-CH<sub>3</sub>)<sub>2</sub>

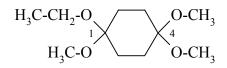
- (1) 1,1-diethoxypropane (PIN)
- (2) propanal diethyl acetal

- (1) 1-ethoxy-1-methoxycyclohexane (PIN)
- (2) cyclohexanone ethyl methyl ketal

(



(1) 1,1-diethoxy-4,4-dimethoxycyclohexane(2) cyclohexane-1,4-dione 1-(diethyl ketal) 4-(dimethyl ketal)



(1) 1-ethoxy-1,4,4-trimethoxycyclohexane (PIN)(2) cyclohexanedione 1-ethyl 1,4,4-trimethyl diketal

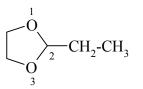
## P-66.6.5.1.2 Cyclic acetals and ketals

Cyclic acetals as the principal function are named as heterocyclic compounds and these names are preferred IUPAC names; cyclic ketals are spiro compounds that are named in accordance with the rules described in Section P-24 giving preferred IUPAC names.

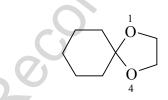
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Functional class nomenclature using the name of the appropriate divalent substituent groups may also be used.

Examples:



2-ethyl-1,3-dioxolane (PIN) propanal ethylene acetal



1,4-dioxaspiro[4.5]decane (PIN) cyclohexanone ethylene ketal

$$\underbrace{ \begin{array}{c} O \\ O \\ O \end{array} }^{O} \xrightarrow{2} CH_2 - CH_2 - Si(CH_3)_3$$

[2-(1,3-dioxolan-2-yl)ethyl]trimethylsilane (PIN) 3-(trimethylsilyl)propanal ethylene ketal

## P-66.6.5.2 Hemiacetals and hemiketals.

Compounds with the general structure RR'C(OH)(O-R") have the class name 'hemiacetals'. They are named substitutively as 'alkoxy', 'aryloxy', etc., derivatives of an appropriate hydroxy parent compound, such as an alcohol; these names are the preferred IUPAC names. Other names are formed by functional class nomenclature with the class name 'hemiacetal'; similarly derivatives of ketones are denoted by the class name 'hemiketal'.

Examples:

$$CH_{4}-CH_{2}-CH_{2}-CH_{2}-CH_{1}-OH_{1}$$

1-ethoxybutanol (PIN) butanal ethyl hemiacetal

1-methoxycyclohexan-1-ol (PIN) cyclohexanone methyl hemiketal

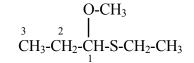
P-66.6.5.3 Chalcogen analogues of acetals and ketals

Sulfur analogues of acetals and ketals with the general structures RR'C(S-R")(S-R"') or RR'C(S-R")(O-R"'), have the class names 'dithioacetals' or 'monothioacetals', respectively. They are named substitutively as 'alkylsulfanyl', 'arylsulfanyl', 'alkoxy', or 'aryloxy' derivatives, as appropriate, of a parent hydride; these names are preferred IUPAC names. Other names can be generated by functional class nomenclature, using class names such as 'monothioacetal' and 'dithioketal'. Capital italic letter locants are used to provide structural specificity. Selenium, tellurium and mixed analogues are treated in the same way as their sulfur analogues.

Examples:

<sup>5</sup> <sup>4</sup> <sup>3</sup> <sup>2</sup> <sup>1</sup> <sup>1</sup> CH<sub>3</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>3</sub>)<sub>2</sub>

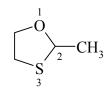
1,1-bis(methylsulfanyl)pentane (PIN) pentanal diethyl dithioacetal



1-(ethylsulfanyl)-1-methoxypropane (PIN) propanal S-ethyl O-methyl monothioacetal

O-CH<sub>2</sub>-CH<sub>3</sub>

1-ethoxy-1-(ethylsulfanyl)cyclopentane (PIN) cyclopentanone diethyl monothioketal

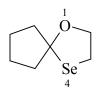


2-methyl-1,3-oxathiolane (PIN) ethan-1-one ethylene monothioketal

Se-CH<sub>2</sub>-CH<sub>3</sub>

1-(ethylselanyl)-1-(methylsulfanyl)cyclohexane (PIN) cyclohexanone *Se*-ethyl *S*-methyl selenothioketal

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1-oxa-4-selenaspiro[4.4]nonane (PIN) cyclopentanone ethylene monoselenoketal

P-66.6.5.4 Chalcogen analogues of hemiacetals and hemiketals

Sulfur analogues of hemiacetals and hemiketals with the general structures RR'C(SH)(S-R"), RR'C(OH)(S-R") or RR'C(SH)(O-R"), have the class names 'dithiohemiacetals' or 'monothiohemiacetals', respectively. They are named substitutively as 'alkylsulfanyl', 'arylsulfanyl', 'alkoxy', or 'aryloxy' derivatives, as appropriate, of a hydroxy parent compound; these are preferred IUPAC names. Other names can be generated by functional class nomenclature. Capital italic letter locants are used to provide structural specificity. Selenium, tellurium, and mixed analogues are treated in the same way as their sulfur analogues; generically, they are 'monoselenohemiacetals', 'ditellurohemiacetals, 'selenothiohemiacetals', etc.

Examples:

S-CH<sub>2</sub>-CH 3 2 CH<sub>3</sub>-CH<sub>2</sub>-CH-SH

O-CH<sub>2</sub>-CH<sub>3</sub> 3 2 | CH<sub>3</sub>-CH<sub>2</sub>-CH-SH

1-(ethylsulfanyl)propane-1-thiol (PIN) propanal ethyl dithiohemiacetal

1-ethoxypropane-1-thiol (PIN) propanal *O*-ethyl monothiohemiacetal

1-(ethylsulfanyl)cyclopentane-1-selenol (PIN) cyclopentanone S-ethyl selenothiohemiketal