P-65 Acids, acyl halides and pseudohalides, salts, esters, and anhydrides

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P-65.0 Introduction

This Chapter includes acids named substitutively by means of suffixes, that is, carboxylic acids, sulfonic, sulfinic, and analogous selenium and tellurium acids. Their derivatives, such as esters, acyl halides and anhydrides, are described. Salts are included in this Section although anions are formally treated in Chapter 7. Carbon acids not named substitutively, i.e., carbonic acid, formic acid, cyanic acid, oxalic acid, and the bi- and polynuclear carbon acids are also included here. Mononuclear and polynuclear noncarbon (inorganic) acids used as parent structures for organic derivatives are discussed in Section P-67.

The hydrogen atom of an acid group is not substitutable for the purposes of substitutive nomenclature; replacement of acid hydrogen atoms by specific atoms or groups is called 'functionalization', as other classes are generated, for example esters. Substitution takes place when other hydrogen atoms in the structure are exchanged with other atoms or groups, as illustrated by the name 'chloroacetic acid'.

P-65.1 Carboxylic acids and nitrogenous analogues

Carboxylic acids are 'oxoacids' having the structure R-C(=O)-OH, where R can be a hydrogen atom. Nitrogenous analogues are carboxylic acids in which =O has been replaced by =NH, =NNH₂, =N-OH, or in which –OH has been replaced by –NH-OH.

Names of α -amino acids, as well as carboxylic acids derived from carbohydrates, are not covered extensively in this Chapter. Traditional names are maintained, as recommended in specialized publications (ref. 23), and listed in Chapter 10 devoted to preferred IUPAC names for natural products.

P-65.1.1 Retained names

P-65.1.2 Systematic names

- P-65.1.3 Carboximidic, carbohydrazonic, carbohydroximic, and carbohydroxamic acids
- P-65.1.5 Chalcogen analogues of carboxylic acids
- P-65.1.6 Amic, anilic, and aldehydic acids.

P-65.1.7 Acyl groups derived from carboxylic and related acids

P-65.1.1 Retained names

Carboxylic acids derived from natural sources were often given trivial names reminiscent of their animal or vegetable origin. In both 1979 and 1993, the list of these trivial names was significantly reduced, systematic names being recommended.

P-65.1.1.1 Retained names as preferred IUPAC names

Only the following three retained names are preferred IUPAC names. All can be functionalized, but only acetic acid and benzoic acid can be fully substituted; for substitution rules regarding formic acid, see P-65.1.8. Systematic substitutive names are used to generate acids modified by functional replacement.

HCOOH formic acid (PIN) methanoic acid

acetic acid (PIN) ethanoic acid

CH₃-COOH

C₆H₅-COOH benzoic acid (PIN)

benzenecarboxylic acid

P-65.1.1.2 Retained names for general nomenclature

For general nomenclature, the following names are retained with full substitution allowed (see P-34).

furoic acid isophthalic acid phthalic acid terephthalic acid

The following names are retained for general nomenclature with functionalization but no substitution allowed. Functionalization leads to anhydrides, salts and esters, for example, the formation of esters leads to names such as methyl butyrate.

	acrylic acid	methacrylic acid
28	adipic acid	naphthoic acid
	butyric acid	nicotinic acid
	cinnamic acid	oleic acid
	fumaric acid	palmitic acid
	glutaric acid	propionic acid
	isonicotinic acid	stearic acid
	maleic acid	succinic acid
	malonic acid	

The names citric acid, lactic acid, glyceric acid, pyruvic acid, and tartaric acid, related to natural products, are also retained; no substitution is recommended, but the formation of salts and esters is allowed.

Names of α -amino acids related to peptides and proteins are also retained and used as preferred IUPAC names (see P-103). In particular, the name 'glycine' for H₂N-CH₂-COOH is used to form systematic substitutive preferred IUPAC names.

P-65.1.2 Systematic names

Carboxylic acids are named substitutively using the suffix 'oic acid' or 'carboxylic acid' and the prefix 'carboxy'.

P-65.1.2.1 Carboxylic acid groups, -COOH, that conceptually replace a $-CH_3$ group of methane or terminating an unbranched hydrocarbon chain are named by replacing the final 'e' of the name of the corresponding hydrocarbon by the suffix 'oic acid'. No locants are necessary to denote the positions of the carboxylic acid groups in a hydrocarbon chain; locants are used when hydrocarbon chains are modified by skeletal replacement, as shown in P-15.4.3.1.2. Except for formic acid (see P-65.1.8.1) and acetic acid (see P-65.1.1.1), systematically formed names are preferred IUPAC names; the names given in P-65.1.1.2 are retained names for use in general nomenclature.

Examples:

⁴ ³ ² ¹ CH₃-CH₂-CH₂-COOH butanoic acid (PIN)

butyric acid

¹⁰ ¹ CH₃-[CH₂]₈-COOH decanoic acid (PIN) ¹² 1 HOOC-[CH₂]₁₀-COOH dodecanedioic acid (PIN)

 $\overset{15}{\text{CH}_3\text{-}\text{CH}_2\text{-}\text{CH}_2\text{-}\text{O}\text{-}\text{O}\text{-}\text{CH}_2\text{-}\text{O}^2\text{-}\text{CH}_2\text{-}$

3,6,9,12-tetraoxapentadecan-1-oic acid (PIN)

P-65.1.2.2 The suffix 'carboxylic acid' is used for all carboxylic acids not covered by P-65.1.2.1, except for benzoic acid (see P-65.1.1.1). The carboxy group can be attached to any atom, carbon or heteroatom, of any parent hydride; the proper methodology must be applied in the case of mancude parent hydrides as exemplified in P-65.1.2.3.

P-65.1.2.2.1 If an unbranched chain is linked to more than two carboxy groups, all carboxy groups are named from the parent hydride by substitutive use of the suffix 'carboxylic acid', preceded by the appropriate numerical prefix 'tri', 'tetra' etc. and appropriate locants. Examples:

COOH

$$5 4 \begin{vmatrix} 2 & 1 \\ 2 & -1 \\ HOOC-CH_2-CH_2-CH-CH_2-CH_2-COOH \\ 3 \end{pmatrix}$$
pentane-1,3,5-tricarboxylic acid (PIN)

 $(\text{HOOC})_2^{1}\text{CH-CH}(\text{COOH})_2$

ethane-1,1,2,2-tetracarboxylic acid (PIN)

COOH

P-65.1.2.2.2 Carboxy groups attached to cyclic parent hydrides or heteroacyclic parent hydrides are always named by using the suffix 'carboxylic acid'.

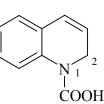
Examples:

COOH

cyclopentanecarboxylic acid (PIN)

pyridine-3-carboxylic acid (PIN) nicotinic acid

-COOF



pyrrolidine-1-carboxylic acid (PIN)

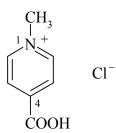
quinoline-1(2H)-carboxylic acid (PIN)

H₃Si-O-SiH₂-COOH disiloxanecarboxylic acid (PIN)

H₂N-NH-COOH

hydrazinecarboxylic acid (PIN) (not carbazic acid) carbonohydrazidic acid (see P-65.2.1.4)

P-65.1.2.2.3 When another group is present that has priority for citation as suffix, for example, a radical anion or cation, or when all carboxylic acid groups cannot be described by a suffix, carboxylic acid groups are indicated by the prefix 'carboxy'.



4-carboxy-1-methylpyridinium chloride (PIN)

•CH₂-CH₂-COOH or -CH₂-CH₂-COOH

2-carboxyethyl (PIN) (radicals and substituent prefixes often have identical names; see P-31.2.1)

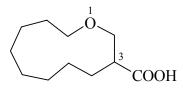
$$\begin{array}{c} CH_2\text{-}COOH \\ 1 & 2 & 4 & 5 & 6 & 7 \\ HOOC\text{-}CH_2\text{-}CH\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}COOH \\ 3 \end{array}$$

3-(carboxymethyl)heptanedioic acid (PIN)

P-65.1.2.3 Seniority order for numbering

When required, numbering is based on the following seniority order:

- (a) fixed numbering of parent hydride (e.g. naphthalene, bicyclo[2.2.2]octane, etc.)
- (b) heteroatoms in rings and chains
- (c) indicated hydrogen [for unsubstituted compounds; a higher locant may be needed at another position to provide for a substituent suffix in accordance with the structural feature (d)].
- (d) principal group named as suffix
- (e) added hydrogen (consistent with the structure of the compound and in accordance with further substitution)
- (f) unsaturation/saturation (ene/yne endings or hydro/dehydro prefixes)
- (g) detachable (alphabetized) prefixes



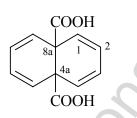
1-oxacycloundecane-3-carboxylic acid (PIN)

$$\overset{1}{\mathrm{CH}_3}\overset{2}{\mathrm{O}}\text{-}\mathrm{CH}_2\text{-}\mathrm{CH}_2\text{-}\mathrm{O}\text{-}\mathrm{CH}_2\text{-}\mathrm{O}\text{-}\mathrm{CH}_2\text{-$$

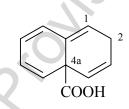
2,5,8-trioxa-11-thiatetradecan-14-oic acid (PIN)

$$\begin{array}{c} \text{CH-CH}_{3} \\ 8 & 7 & 6 & 5 & 4 & 3 \\ \text{CH}_{3}\text{-}\text{CH}_{2}\text{-}\text{CH}_{2}\text{-}\text{CH}_{2}\text{-}\text{CH}_{2}\text{-}\text{CH}_{2}\text{-}\text{C}_{2}\text{-}\text{COOH} \end{array}$$

2-ethylideneoctanoic acid (PIN) [not 2-hexylbut-2-enoic acid; see P-44.3, criterion (b)]



naphthalene-4a,8a-dicarboxylic acid (PIN; see P-53.1) 4a,8a-dihydronaphthalene-4a,8a-dicarboxylic acid



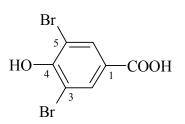
naphthalene-4a(2*H*)-carboxylic acid (PIN; see P-53.1) 2,4a-dihydronaphthalene-4a-carboxylic acid

P-65.1.2.4 Polyfunctional carboxylic acids

Systematic names of substituted carboxylic acids are formed by adding appropriate prefixes, such as 'oxo', 'hydroxy', 'amino', 'imino', 'halo', 'nitro', etc., to the name of the acid. Prefixes are not ranked as functional entities; they are cited in a name in alphabetical order, which is also used to assign lowest locants when required.

Examples:

⁶ ⁵ ⁴ ³ ² ¹ CH₃-CO-CH₂-CH₂-CH₂-COOH 5-oxohexanoic acid (PIN)



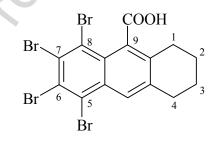
3,5-dibromo-4-hydroxybenzoic acid (PIN)

 ² NH₂
 2-amino-5-nitrobenzoic acid (PIN) (not 5-nitroanthranilic acid; anthranilic acid is not a retained name)

1-hydroxy-3-oxopropane-1,2,3-tricarboxylic acid (PIN) [not 3-hydroxy-1-oxopropane-1,2,3-tricarboxylic acid; lowest locants are attributed to prefixes that are cited first, see P-44.3(m)]

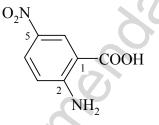
> 4 3 2 1 H₃C-S-CH₂-CH₂-CO-COOH

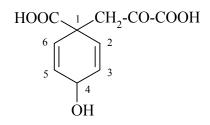
4-(methylsulfanyl)-2-oxobutanoic acid (PIN) [not 4-(methylthio)-2-oxobutyric acid]



5,6,7,8-tetrabromo-1,2,3,4-tetrahydroanthracene-9-carboxylic acid (PIN) (not 1,2,3,4-tetrabromo-5,6,7,8-tetrahydroanthracene-9-carboxylic acid hydro/dehydro prefixes are given lowest possible locants before detachable prefixes)

5 4 3 2 1 H₂N-CH₂-CH₂-CH₂-CH₂-COOH 5-aminopentanoic acid (PIN)





1-(2-carboxy-2-oxoethyl)-4-hydroxycyclohexa-2,5-diene-1-carboxylic acid (PIN) 1-carboxy-4-hydroxy-β-oxocyclohexa-2,5-dienepropanoic acid (a conjunctive name; see P-13.5.2)

OH O

$$1 \ 2 \ 3 \ | \ 5 \ | \ 7 \ 8$$

HOOC-CH=CH-CH=CH-C-CH₂-COOH

4-hydroxy-6-oxoocta-2,4-dienedioic acid (PIN) (not 5-hydroxy-3-oxoocta-4,6-dienedioic acid; unsaturation is senior to detachable prefixes)

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

P-65.1.3 Carboximidic, carbohydrazonic, carbohydroximic and carbohydroxamic acids

P-65.1.3.1 Carboximidic acids

P-65.1.3.1.1 Substitutive nomenclature; suffix mode

The name of an acid in which the carbonyl oxygen atom of a carboxylic acid group has been replaced by =NH is formed by functional replacement nomenclature and the infix 'imid(o)' to modify the 'ic acid' or 'oic acid' ending of the retained name of an acid; or the 'oic acid' or 'carboxylic acid' suffix of a systematic name of an acid, to 'imidic acid' or 'carboximidic acid'. Preferred names of imidic acids are those derived from systematic substitutive preferred IUPAC names of carboxylic acids.

This is a change in the case of formic acid, acetic acid, benzoic acid.

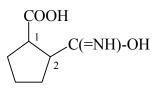
> HC(=NH)-OH CH₃-C(=NH)-OH methanimidic acid (PIN) ethanimidic acid (PIN) formimidic acid acetimidic acid 3 2 4 1 CH3-CH2-CH2-C(=NH)-OH $C_6H_5-C(=NH)-OH$ butanimidic acid (PIN) benzenecarboximidic acid (PIN) benzimidic acid butyrimidic acid 3 HO-C(=NH)-CH₂-CH₂-C(=NH)-OH butanediimidic acid (PIN) succinimidic acid NH || 1 C(=NH)-OH С-ОН C(=NH)-OH cyclohexanecarboximidic acid (PIN benzene-1,2-dicarboximidic acid (PIN) phthalimidic acid

P-65.1.3.1.2 Substitutive nomenclature, prefix mode

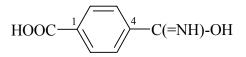
When another group is present that has seniority for citation as principal group, the following prefixes are used.

- the compound prefix 'C-hydroxycarbonimidoyl' is used to denote the acyl group -C(=NH)-OH; the compound prefix name is formed by concatenation based on the simple prefix name carbonimidoyl, -C(=NH)-, derived from carbonimidic acid (see P-65.2.1.5).
- (2) the combination of the prefixes 'hydroxy' and 'imino' at the end of a carbon chain is used in preferred IUPAC names rather than the prefix '*C*-hydroxycarbonimidoyl'.

Note that the italicized letter 'C' is used to avoid potential confusion with N-hydroxy substitution. The name carbonohydroximoyl is not used to generate preferred IUPAC names.



(1) 2-(*C*-hydroxycarbonimidoyl)cyclopentane-1-carboxylic acid (PIN)



(1) 4-(C-hydroxycarbonimidoyl)benzoic acid (PIN)

⁴ ³ ² ¹ HO-C(=NH)-CH₂-CH₂-COOH

(2) 4-hydroxy-4-iminobutanoic acid (PIN)

(1) 3-(C-hydroxycarbonimidoyl)propanoic acid

SH | CH₃-C=N-O-NH-CH₂-S-NH-CH₂-CHO

N-{[({[(2-oxoethyl)amino]sulfanyl}methyl)amino]oxy}ethanimidothioic acid (PIN) (see P-65.1.3.1.1; P-65.1.5.2)

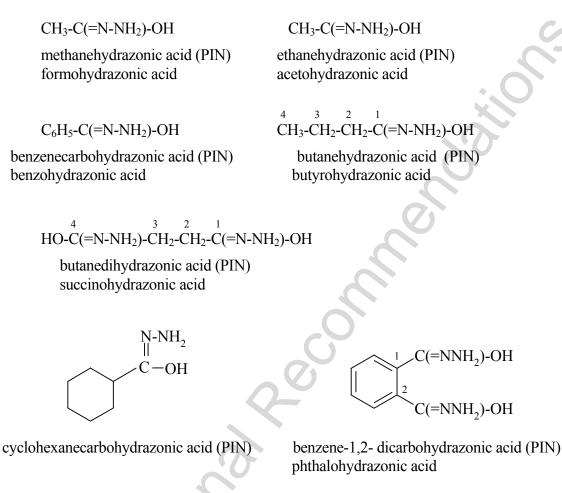
P-65.1.3.2 Carbohydrazonic acids

P-65.1.3.2.1 Substitutive nomenclature; suffix mode

The name of an acid in which the carbonyl oxygen atom of a carboxylic acid group has been replaced by $=NNH_2$ is formed by functional replacement nomenclature. The infix 'hydrazon(o)' is used to modify the 'ic acid' or 'oic acid' ending of the retained name of an acid; or the 'oic acid' or 'carboxylic acid' suffix of a systematic name of an acid is changed to 'hydrazonic acid' or 'carbohydrazonic acid'.

Preferred IUPAC names of hydrazonic acids are those derived from systematic substitutive preferred IUPAC names of carboxylic acids.

This is a change in the case of formic, acetic, and benzoic acids

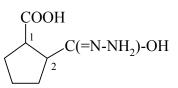


P-65.1.3.2.2 Substitutive nomenclature, prefix mode

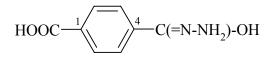
When another group is present that has seniority for citation as principal group, the following prefixes are used:

- the compound prefix 'C-hydroxycarbonohydrazonoyl' is used to denote the acyl group -C(=N-NH₂)-OH; the compound prefix name is formed by concatenation based on the simple prefix name carbonohydrazonoyl, -C(=NNH₂)-, derived from carbonohydrazonic acid (see P-65.2.1.5)]
- (2) the combination of prefixes 'hydroxy' and 'hydrazono' at the end of a carbon chain is used in preferred IUPAC names rather than the prefix '*C*-hydroxycarbonohydrazonoyl'.

Note that the italicized letter 'C' is used to avoid potential confusion with N-hydroxy substitution. Examples:



(1) 2-(*C*-hydroxycarbonohydrazonoyl)cyclopentane-1-carboxylic acid (PIN)



(1) 4-(C-hydroxycarbonohydrazonoyl)benzoic acid (PIN)

 $\begin{array}{c} 5 \\ \text{HO-C}(=\text{N-NH}_2)\text{-}\text{CH}_2\text{-}\text{CH}_2\text{-}\text{CH}_2\text{-}\text{COOH} \end{array}$

(2) 5-hydrazono-5-hydroxypentanoic acid (PIN)

(1) 4-(C-hydroxycarbonohydrazonoyl)butanoic acid

P-65.1.3.3 Carbohydroximic acids

P-65.1.3.3.1 Substitutive nomenclature; suffix mode

Acids in which the carbonyl oxygen atom of a carboxylic acid group has been replaced by =N-OH are named:

- (1) as N-hydroxy derivatives of imidic acids named in P-65.1.3.1
- (2) by modifying the 'ic acid' or 'oic acid' ending of the retained name of an acid to 'hydroximic acid'. The letter 'o' is added for euphony between 'h' and a preceding consonant;
- (3) by using the suffixes 'hydroximic acid' and 'carbohydroximic acid' that are attached to the name of a parent hydride.

Method (1) generates preferred IUPAC names.

Examples:

CH₃-C(=N-OH)-OH

- (1) *N*-hydroxyethanimidic acid (PIN)
- (2) acetohydroximic acid

$$C_6H_5$$
-C(=N-OH)-OH

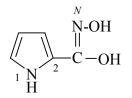
(1) *N*-hydroxybenzenecarboximidic acid (PIN)

(2) benzohydroximic acid

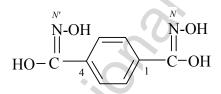
- (2) butyrohydroximic acid
- (3) butanehydroximic acid

$$HO-C(=N-OH)-CH_2-CH_2-C(=N-OH)-OH$$

- (1) N,N'-dihydroxybutanediimidic acid (PIN)
- (2) succinohydroximic acid
- (3) butanedihydroximic acid



- (1) 2-*N*-hydroxy-1*H*-pyrrole-2-carboximidic acid (PIN)
- (3) pyrrole-2-carbohydroximic acid

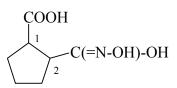


- (1) N,N'-dihydroxybenzene-1,4-dicarboximidic acid (PIN)
- (2) terephthalohydroximic acid

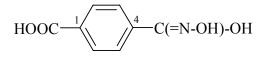
P-65.1.3.3.2 Substitutive nomenclature, prefix mode

When another group is present that has seniority for citation as principal group, the following prefixes are used:

- (1) 'dihydroxycarbonimidoyl' to denote the group -C(=N-OH)-OH;
- (2) the combination of the prefixes 'hydroxy' and 'hydroxyimino' at the end of a carbon chain is used in preferred IUPAC names rather than the prefix 'dihydroxycarbonimidoyl'.



(1) 2-(dihydroxycarbonimidoyl)cyclopentane-1-carboxylic acid (PIN)



(1) 4-(dihydroxycarbonimidoyl)benzoic acid (PIN)

5 4 3 2 1 HO-C(=N-OH)-CH₂-CH₂-CH₂-COOH

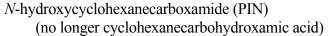
(2) 5-hydroxy-5-(hydroxyimino)pentanoic acid (PIN

(1) 4-(dihydroxycarbonimidoyl)butanoic acid

P-65.1.3.4 Hydroxamic acids have the generic structure R-CO-NH-OH and are named as *N*-hydroxy amides (see P-66.1.1.3.3). The suffixes 'hydroxamic acid' and 'carbohydroxamic acid' are no longer recommended.

Examples:

N-hydroxyacetamide (PIN) (no longer acetohydroxamic acid)



P-65.1.4 Peroxycarboxylic acids

The general methodology for modifying acids expressed by suffixes by functional replacement nomenclature is to use modified suffixes in the same way as for unmodified acids. A major change and simplification, i.e., that suffixes are always modified by infixes, is recommended.

P-65.1.4.1 Peroxycarboxylic acids are named systematically using the following suffixes:

-(C)O-OOH peroxoic acid -CO-OOH carboperoxoic acid

Retained names of peroxy carboxylic acids are modified by the prefix 'peroxy'. Preferred IUPAC names are formed by functional replacement of systematic substitutive names.

This is a change in the case of formic, acetic, and benzoic acids

Examples:

HCO-OOH

methaneperoxoic acid (PIN) peroxyformic acid (not performic acid)

⁶ СН₃-[СН₂]₄-СО-ООН

hexaneperoxoic acid (PIN)

CH₃-CO-OOH

ethaneperoxoic acid (PIN) peroxyacetic acid (not peracetic acid)

C₆H₅-CO-OOH

benzenecarboperoxoic acid (PIN) peroxybenzoic acid (not perbenzoic acid)

cyclohexanecarboperoxoic acid (PIN)

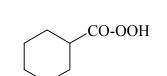
P-65.1.4.2 When another group is present that has priority for citation as a suffix (see seniority of classes, P-41), the following prefixes are used:

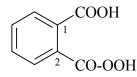
- (1) the functional replacement prefix 'carbonoperoxoyl-' or the compound prefix 'hydroperoxycarbonyl-' is used to denote the acyl group -C(O)-OOH; the compound prefix 'hydroperoxycarbonyl-' is formed by concatenation, on the basis of the simple acyl group 'carbonyl', for >C=O (see P-65.2.1.5); the prefix 'carbonoperoxoyl' is used in preferred IUPAC names, except as noted in (2) below.
- (2) the combination of the prefixes 'hydroperoxy and oxo' at the end of a carbon chain is used in preferred IUPAC names rather than the prefix 'hydroperoxycarbonyl-' or the prefix 'carbonoperoxoyl-'.

Examples:

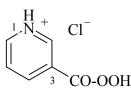
HOO-CO-[CH₂]₄-COOH

- (2) 6-hydroperoxy-6-oxohexanoic acid (PIN)
- (1) 5-carbonoperoxoylpentanoic acid
 - 5-(hydroperoxycarbonyl)pentanoic acid

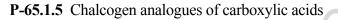




- (1) 2-carbonoperoxoylbenzoic acid (PIN) 2-(hydroperoxycarbonyl)benzoic acid
- (2) monoperoxyphthalic acid (see P-65.1.4.1)



(1) 3-carbonoperoxoylpyridin-1-ium chloride (PIN)3-(hydroperoxycarbonyl)pyridin-1-ium chloride



P-65.1.5.1 Functional replacement in systematic names of carboxylic acids.

Replacement of oxygen atom(s) of a carboxylic acid group by another chalcogen is indicated by the affixes 'thio', 'seleno', and 'telluro'. These names do not differentiate between tautomeric forms of mixed chalcogen acids; such nonspecificity may be shown in a structure such as:

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$$C \begin{cases} O \\ B \\ S \end{cases}$$
 or $-C \{O/S\}H$

In names, tautomeric groups in mixed chalcocarboxylic acids, such as -CO-SH or -CS-OH, -S(O)-SH or -S(S)-OH, are distinguished by prefixing italic element symbols, such as *O* or *S*, respectively, to the term 'acid', for example, thioic *S*-acid for -(C)O-SH and carbothioic *O*-acid for -CS-OH. Normally, these locants are omitted, because the exact position of chalcogen atoms is not known in acids; such letter locants are principally used in naming esters.

When the position of chalcogen atoms is undetermined, the prefix for the unmodified acid, i.e. 'carboxy' for -COOH, is used and modified by functional replacement using prefixes, as in 'thiocarboxy' for $-C{O/S}H$, and is enclosed in parentheses to avoid the possibility of ambiguity. The order of seniority of these suffixes is fully described in Section P-43.

When the position of chalcogen atoms is known, combinations of prefixes such as 'hydroxy- and sulfanylidene-' and 'sulfanyl- and oxo-' are used in acyclic compounds; compound prefixes such as '[hydroxy(carbonothioyl)]-' and '(sulfanylcarbonyl)-' are used in cyclic compounds, as appropriate (see P-64.6.1). The compound prefixes are formed by concatenation using simple acyl prefixes derived from carbonic acids (see P-65.2.1.5)

The seniority order between acids and acids modified by functional replacement is discussed in P-43 and expressed in Tables 4.3 and 4.4. In presence of unmodified acids cited as suffix, modified acids are cited as prefixes.

Examples:

CH₃-CH₂-CH₂-CH₂-CH₂-CS-OH

hexanethioic *O*-acid (PIN)

CH₃-CH₂-CH₂-CH₂-CH₂-C{S/Se}H hexaneselenothioic acid (PIN)

CH₃-CH₂-CH₂-CH₂-CH₂-CSe-SH hexaneselenothioic *S*-acid (PIN)

H{S,O}C-CH₂-CH₂-CH₂-CH₂-C{O/S}H hexanebis(thioic) acid (PIN)

CH₃-CH₂-CH₂-CH₂-CH₂-C{O/Se}H

hexaneselenoic acid (PIN)

HSSC-CH₂-CH₂-CH₂-CH₂-CS-SH

hexanebis(dithioic) acid (PIN)

CS-SH

piperidine-1-carbodithioic acid (PIN)

cyclohexanecarboselenothioic Se-acid (PIN)

-SeH

 $5^{4} + 3^{2} + 1^{1}$ H{S/O}C-CH₂-CH₂-CH₂-CH₂-CH₂-COOH 5-(thiocarboxy)pentanoic acid (PIN) 4 3 2 1 HS-CO-CH₂-CH₂-COOH

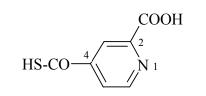
4-oxo-4-sulfanylbutanoic acid (PIN) 4-(sulfanylcarbonyl)propanoic acid

HO-C(=S)-CH₂-CH₂-COOH 4-hydroxy-4-sulfanylidenebutanoic acid (PIN)

HO-CS 4 N 1

4-[hydroxy(carbonothioyl)]pyridine-2-carboxylic acid (PIN)

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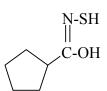
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4-(sulfanylcarbonyl)pyridine-2-carboxylic acid (PIN)

CH₃-CH₂-C(=NH)-SH

CH₃-CH₂-CH₂-C(=NNH₂)-SeH butanehydrazonoselenoic acid (PIN)

propanimidothioic acid (PIN)



N-sulfanylcyclopentanecarboximidic acid (PIN)

N-OH || C-SeH

N-hydroxycyclohexanecarboximidoselenoic acid (PIN)

 $\begin{array}{c}
 NH_2 \\
 | 2 1 \\
 CH_3-CH_2-S-C=CH-CS-SH
\end{array}$

3-amino-3-(ethylsulfanyl)prop-2-enedithioic acid (PIN)

P-65.1.5.2 Functional replacement in retained names of carboxylic acids

Preferred names of chalcogen analogues of monocarboxylic acids are formed using the suffixes 'thioic acid', 'selenoic acid', 'telluroic acid' or 'carbothioic acid', 'carboselenoic acid', 'carbotelluroic acid' and names of appropriate parent hydrides, even in the case of formic acid, acetic acid and benzoic acid.

This is a change in the case of formic, acetic, and benzoic

Chalcogen analogues of monocarboxylic acids with retained names may also be named by placing the prefix 'thio', 'seleno' or 'telluro' in front of the name of the acid.

Chalcogen analogues of dicarboxylic acids are named systematically; retained names are not used to name chalcogen analogues of dicarboxylic acids.

The symbols *O*, *S*, *Se* and *Te* are used to specify the structure of the acid, as indicated in P-65.1.5.1).

Examples:

CH₃-CS-OH

ethanethioic *O*-acid (PIN) thioacetic *O*-acid C₆H₅-C{O,Se}H

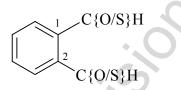
benzenecarboselenoic acid (PIN) selenobenzoic acid

HCO-SH

methanethioic *S*-acid (PIN) thioformic *S*-acid

⁴ ³ ² ¹ H{S,O}C-CH₂-CH₂-CH₂-COOH

3-(thiocarboxy)butanoic acid (PIN) (not thioglutaric acid)



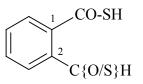
benzene-1,2-dicarbothioic acid (PIN) (not 1,2-dithiophthalic acid)

HOO CO-SeH

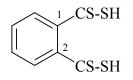
4-(selanylcarbonyl)benzoic acid (PIN) (not 1-selenophthalic *Se*-acid)

4 3 2 1 HS-CO-CH₂-CH₂-COOH

4-oxo-4-sulfanylbutanoic acid (PIN) (not thiosuccinic acid)



2-(thiocarboxy)benzenecarbothioic S-acid (PIN) (not 1,2-dithiophthalic S-acid)



benzene-1,2-dicarbodithioic acid (PIN) (not tetrathiophthalic acid)

P-65.1.5.3 Functional replacement in peroxycarboxylic acids.

Peroxy acid suffixes can be modified by S , Se, and Te using functional replacement nomenclature. Italic prefixes in front of the term 'acid' are used for specificity, where necessary (see Table 4.3; for more suffixes modified by functional replacement and their seniority order). Preferred names are all formed by using appropriate suffixes and parent hydrides, even in the case of derivatives of formic acid, acetic acid, and benzoic acid.

This is a change in the case of formic, acetic, and benzoic acids

Examples:

–(C)O-OSH	(thioperoxoic) OS-acid
–(C)Se-SSH	(dithioperoxo)selenoic acid
-CO-SOH	carbo(thioperoxoic) SO-acid
-CS-OOH	carboperoxothioic acid
-COS ₂ H	dithiocarboperoxic acid (location of sulfur atom unknown)

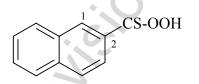
The recommended suffixes, and their seniority order, are fully discussed in Section P-43.

Examples:

CH₃-CO-OSH

C₆H₅-CO-SOH

ethane(thioperoxoic) *OS*-acid (PIN) (not peroxythioacetic *OS*-acid) benzenecarbo(thioperoxoic acid) SO-acid (PIN) (not peroxothiobenzoic SO-acid)



naphthalene-2-carboperoxothioic acid (PIN) (not peroxythio-2-naphthoic acid)

Compound prefixes, such as 'sulfanyloxy' and 'oxo' and 'hydroxysulfanyl' and 'sulfanylidene' at the end of acyclic chains are used to generate preferred IUPAC names.

Appropriate prefixes constructed by concatenation based on simple acyl groups derived from carbonic and related acids (see P-65.2.1.5) are also used in preferred IUPAC names. Letter locants such as *SO* and *OS* are required to specify the structures of thioperoxy groups (see also P-63.3.2.1).

Prefixes derived by functional replacement nomenclature have only limited use because there is no accepted method to unambiguously describe precise structures of thioperoxy groups.

4-sulfanylidene-4-(sulfanyloxy)butanoic acid (PIN)
3-[(SO-thiohydroperoxy)carbonothioyl]propanoic acid (see P-63.3.2.1) (not 3-carbono(thioperoxo)thioylpropanoic acid; ambiguous name)

 $HOS_2C\text{-}CH_2\text{-}CH_2\text{-}COOH$

3-(dithiocarboperoxoyl)acetic acid (PIN) (location of sulfur atoms unknown)

HOS-CO COOH

4-[(hydroxysulfanyl)carbonyl]cyclohexanecarboxylic acid] (PIN) 4-[(*OS*-thiohydroperoxy)carbonyl]cyclohexanecarboxylic acid

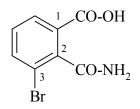
P-65.1.6 Amic, anilic and aldehydic acids

Amic acids are compounds containing a carboxy (–COOH) and a carboxamide (–CONH₂) group; similarly, anilic and aldehydic acids include a carboxy group and a carboxanilide (–CO-NH- C_6H_5) or formyl (–CHO) group, respectively. The endings 'amic acid', 'anilic acid' and 'aldehydic acid' can only be used in general nomenclature to name modified dicarboxylic acids having retained names. Preferred IUPAC names are all formed systematically using preferred names of acids and appropriate prefixes.

P-65.1.6.1 Amic acids

P-65.1.6.1.1 When a dicarboxylic acid has a retained name (see P-34.4.1) and when one of its carboxy groups is replaced by a carboxamide group $-\text{CO-NH}_2$, the resulting structure is called an amic acid and, in general nomenclature, may be named by replacing the ending 'ic acid' of the name of the dicarboxylic acid by the ending 'amic acid'. Although substitution may not be allowed on the parent acid, it is allowed on nitrogen atoms of the corresponding amic acid and is denoted in names by a *N* locant.

The prefix 'carbamoyl' is preferred to 'aminocarbonyl' to name amic acids systematically. The combination of the prefixes 'amino' and 'oxo' is used for describing the $-CO-NH_2$ at the end of an acyclic chain resulting in preferred IUPAC names



3-bromo-2-carbamoylbenzoic acid (PIN) 2-(aminocarbonyl)-3-bromo-benzoic acid

> ⁴ ³ ² ¹ H₂N-CO-CH₂-CH₂-COOH

4-amino-4-oxobutanoic acid (PIN)3-carbamoylpropanoic acid3-(aminocarbonyl)propanoic acidsuccinamic acid

CO-N(CH, HOO

4-(dimethylcarbamoyl)benzoic acid (PIN) 4-[(dimethylamino)carbonyl]benzoic acid *N*,*N*-dimethylterephthalamic acid

P-65.1.6.2 Anilic acids

N-Phenyl derivatives of amic acids are called 'anilic acids' and are named by changing the 'amic acid' ending to 'anilic acid'. Substitution on the nitrogen atom is indicated by the locant *N*, even if no substitution is allowed on the parent acid. Anilic acids may also be named as *N*-substituted amic acids.

The combination of the prefixes 'anilino' or 'phenylamino' and 'oxo' is used for describing $-CO-NH-C_6H_5$ at the end of an acyclic chain resulting in preferred IUPAC names

Examples:

5 4 C₆H₅-NH-CO-CH₂-CH₂-COOH

5-anilino-5-oxopentanoic acid (PIN) 5-(phenylamino)-5-oxopentanoic acid 4-(phenylcarbamoyl)butanoic acid *N*-phenylglutaramic acid glutaranilic acid

CO-OH NO₂ CO-NH

2-[(4-nitrophenyl)carbamoyl]benzoic acid (PIN)N-(4-nitrophenyl)phthalamic acid (not 4'-nitrophthalanilic acid; substitution of phthalanilic acid not

allowed, except on the nitrogen atom)

P-65.1.6.3 Aldehydic acids

When a dicarboxylic acid has a retained name (see P-34.4.1) and when one of its carboxy groups is replaced by a formyl group, –CHO (see P-65.2.2.5), the resulting structure is called an aldehydic acid and, in general nomenclature, may be named by replacing the ending 'ic acid' of the name of the dicarboxylic acid by the ending 'aldehydic acid'. Systematically constructed names are preferred IUPAC names for aldehydic acids derived from all dicarboxylic acids. The prefix 'formyl' is used in preferred IUPAC names, except for a –CHO group at the end of an acyclic chain, which is designated by the prefix 'oxo'.

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Examples:

HOOC CHO

4-formylbenzoic acid (PIN) terephthalaldehydic acid

```
<sup>4</sup> <sup>3</sup> <sup>2</sup> <sup>1</sup>
OHC-CH<sub>2</sub>-CH<sub>2</sub>-COOH
```

4-oxobutanoic acid (PIN) 3-formylpropanoic acid succinaldehydic acid

P-65.1.7 Acyl groups derived from carboxylic and related acids

P-65.1.7.1 Definitions and name construction

P-65.1.7.1.1 Definition.

Carboacyl groups are R-CO-, -OC-R-CO-, or -OC-R-[R'-CO- $]_x$ -R''-CO- groups and their functional replacement analogues, where R, R' and R'' are chains, rings, or ring systems, derived from carboxylic acids by the removal of the hydroxy group from each carboxylic acid group that is expressed by the suffix, and x = 1,2,3, etc..

P-65.1.7.1.2. Carboacyl groups.

The name of a monovalent or divalent carboacyl groups derived by removal of the –OH group from each carboxy group of a carboxylic acid or functional replacement analogue denoted by an 'oic acid' or 'ic acid suffix or having a trivial name is derived from the name of the corresponding acid by changing the 'oic acid' or 'ic acid' ending to 'oyl' or 'yl'. The general rule that the ending of all acyl group prefixes be 'oyl', proposed years ago, has not been regularly followed. This rule is fully implemented in these recommendations, but some traditional exceptions are maintained.

Carboacyl groups derived from acids named by means of the suffix 'carboxylic acid' are named by changing the suffix 'carboxylic acid' to 'carbonyl'. Acyl groups derived from functional replacement analogues are named by changing the suffixes 'carbothioic acid' to 'carbothioyl' (and

likewise for the selenium and tellurium analogues); 'carboximidic acid' to 'carboximidoyl'; 'carbohydrazononic acid' to 'carbohydrazonoyl'l; and 'carbohydroximic acid' to 'carbohydroximidoyl'.

P-65.1.7.2 Acyl groups derived from carboxylic acids having retained names used as preferred names (see P-55.4.3.1)

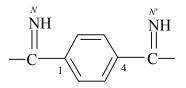
P-65.1.7.2.1 Acyl groups from the carboxylic acids described in P-65.1.1.1.

Examples:

CH ₃ -CO–	acetyl (PIN) ethanoyl	HCO-	formyl (PIN) methanoyl	
C ₆ H ₅ -CO–	benzoyl (PIN) benzenecarbonyl			

P-65.1.7.2.2 Acyl groups corresponding to the imidic, hydrazonic, and hydroximic, and hydroxamic acids described in P-65.1.3.

- ()	ethanimidoyl (PIN) acetimidoyl	HC(=NH)-	methanimidoyl (PIN) formimidoyl
C ₆ H ₅ -C(=NH)-	benzenecarboximidoyl (PIN) benzimidoyl)	
CH ₃ -C(=NNH ₂)-	methanehydrazonoyl (PIN) formohydraznoyl		
CH ₃ -C(=NNH ₂)-	ethanehydrazonoyl (PIN) acetohydrazonoyl		
C ₆ H ₅ -C(=N-OH)-	N-hydroxybenzenecarboxim	nidoyl (PIN)	
	N-hydroxybenzimidoyl		
\mathbf{O}	benzenecarbohydroximoyl		



benzene-1,4-dicarboximidoyl (PIN) terephthalimidoyl

P-65.1.7.2.3 Chalcogen analogues of acyl groups corresponding to carboxylic acids with retained names are named systematically by the infixes of functional replacement nomenclature; these names are preferred IUPAC names.

Examples:

CH ₃ -CSe-	ethaneselenoyl (PIN) selenoacetyl	HCS-	methanethioyl (PIN) thioformyl
C ₆ H ₅ -CS-	benzenecarbonothioyl (PIN) thiobenzoyl	5	

P-65.1.7.3 Acyl groups derived from acids with names retained for use only in general nomenclature.

P-65.1.7.3.1 Traditional names are maintained for acyl groups derived from acids having retained names for use only in general nomenclature (see P-55-4.3.2); no substitution is allowed. The rule of having acyl groups ending in 'oyl' is applied, with certain exceptions that end in 'yl'. The following exceptions below are limiting. Preferred IUPAC names are systematic substitutive names.

P-65.1.7.3.2 Acyl groups derived from imidic, hydrazonic, hydroximic acids with retained names for use only in general nomenclature are named by changing the 'ic acid' ending of the names described in P-65.1.3 into 'oyl'.

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Examples:

CH₃-CH₂-C(=NH)-

propionimidoyl propanimidoyl (PIN) CH₂=CH-C(=NNH₂)-

acrylohydrazonoyl prop-2-enehydrazonoyl (PIN)

-(HN=)C-CH₂-CH₂-C(=NH)succinimidoyl

butanediimidoyl (PIN)

P-65.1.7.3.3 Chalcogen acyl groups derived acids with retained names corresponding to acids used only in general nomenclature are described by prefixes expressing functional replacement

Names of acyl groups derived from monocarboxylic acids are modified by prefixes expressing functional replacement by =S, =Se, and =Te. Acyl group prefixes corresponding to dicarboxylic acids are formed systematically, in accordance with Rule P-65.1.7.4.

Examples:

CH₃-CH₂-CS– thiopropionyl propanethioyl (PIN) CH2=CH-CSe-

selenoacryloyl prop-2-eneselenoyl (PIN)

P-65.1.7.4 Acyl groups derived from systematically named carboxylic acids

P-65.1.7.4.1 The name of a monovalent or divalent acyl group formed by removal of the -OH group from each carboxy group of a carboxylic acid denoted by an 'oic acid' suffix is derived from the name of the corresponding acid by changing the ending 'oic acid' to 'oyl'. Names of acyl groups derived from carboxylic acids modified by functional replacement are all denoted by the ending 'oyl'.

Examples:

³ ² ¹ CH₃-CH₂-CO– propanoyl (PIN) propionyl

¹⁰ 1 -OC-[CH₂]₈-COdecanedioyl (PIN)

> 4 3 2 1 CH₃-CH₂-CH₂-C(=NH)– butanimidoyl (PIN) butyrimidoyl

³ ² ¹ CH₃-CH₂-CS-

propanethioyl (PIN) thiopropionyl

³ ² ¹ -C(=NH)-CH₂-C(=NH)propanediimidoyl (PIN)

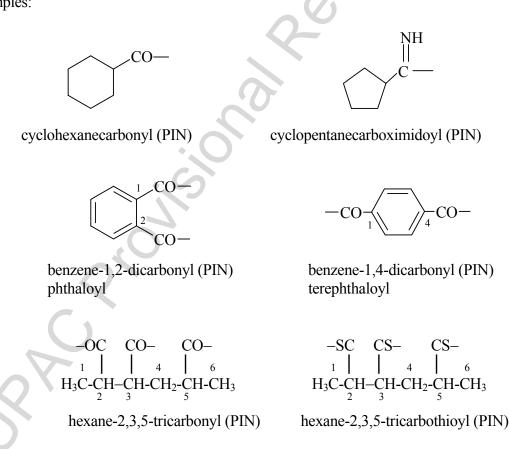
malonimidoyl (PIN)

⁴ ³ ² ¹ -CS-CH₂-CH₂-CS-

butanebis(thioyl) (PIN) (not dithiosuccinyl)

P-65.1.7.4.2 Acyl groups derived from an acid named by means of the suffix 'carboxylic acid' are named by changing the 'carboxylic acid' suffix to the suffix 'carbonyl'. Similarly, the suffix 'carbothioic acid' is changed to 'carbothioyl'; the suffix 'carboselenoic acid' is changed to 'carbotelluroic acid' is changed to 'carbotelluroic' is changed to 'carbotelluroyl'; the suffix 'carbotelluroyl'; the suffix 'carbotylic acid' is changed to 'carbotelluroyl' and the suffix 'carbohydrazonic acid' is changed to 'carbohydrazonic' is changed

Examples:



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P-65.1.7.4.3 Acyl groups derived from dicarboxylic acids with retained names modified by functional replacement by =S, =Se, and =Te are formed systematically, as described in P-65.1.7.4.2. Examples:

4 3 2 1 -CS-CH₂-CH₂-CSbutanebis(thioyl) (PIN) (not dithiosuccinyl)

benzenedicarbothioyl (PIN) (not dithiophthaloyl)

P-65.1.8. Formic acid

For organic nomenclature, formic acid is considered to be a monocarboxylic acid (see P-65.1). It is a retained name and treated like acetic acid; it can be functionalized leading to salts, esters, and anhydrides, and forms an acyl group that is used as a substituent group. Functional replacement analogues are named systematically, for example, methanethioic acid and methanimidic acid. The hydrogen atom attached to carbon is substitutable under specific conditions that are described in P-65.1.8.1, P-65.1.8.2, and P-65.1.8.3

P-65.1.8.1 Substitution of the hydrogen atom of formic acid by the following atoms or groups leads to preferred IUPAC names derived from carbonic acid by functional replacement nomenclature (see P-65.2.1.4):

Examples:

Cl-COOH

HS-COOH

carbonochloridic acid (PIN) chloroformic acid

carbonothioic acid (PIN) (not sulfanylformic acid)

P-65.1.8.2 Substitution of the hydrogen atom of formic acid by $-NHNH_2$ leads to a structure named by the suffix carboxylic acid attached to the parent hydride hydrazine (see P-68.3.1.2).

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Example:

H₂N-NH-COOH

hydrazinecarboxylic acid (PIN) carbonohydrazonic acid (see P-65.2.1.4) (not carbazic acid)

P-65.1.8.3 Substitution of the hydrogen atom of formic acid is permitted when substituent groups are different from those cited in P-65.1.8.1.

Example:

O₂N-COOH

nitroformic acid (PIN)

65.1.8.4 Acyl groups derived from formic acid are formed as described in P-65.1.7.1 and compound prefixes are formed in accordance with the structure of the substituent group. The hydrogen atom present in the group formyl, -CHO, is substitutable under the same conditions as those described in P-65.1.8.1 to P-65.1.8.2 for formic acid.

Examples:

Cl-CO-

carbonochloridoyl (PIN) (not chloroformyl)

carbonobromidothioyl (PIN) [not bromo(thioformyl)]

HCO-O-

HCO-S-

formyloxy (PIN)

formylsulfanyl (PIN)

P-65.2 Carbonic, cyanic, oxalic, and the polycarbonic acids

Carbonic acid, cyanic acid, oxalic acid, and the polycarbonic acids are a group of functional parent compounds different from carboxylic acids; these acids have no hydrogen atom(s) to be used in substitutive nomenclature.

The following acids classified as mononuclear carbon acids, have retained names that are preferred IUPAC names:

carbonic acid HO-CO-OH (PIN) cyanic acid HO-CN (PIN)

The following acids are di- or polynuclear carbon acids, have retained names that are preferred **IUPAC** names:

Br-CS-

polycarbonic acids	HO-[CO-O] _{<i>n</i>} -H $n = 4 - 5$; higher homolog	gues are named by
	skeletal replac	cement ('a')
	nomenclature	
tricarbonic acid	HO-CO-O-CO-O-CO-OH (PIN)	
dicarbonic acid	HO-CO-O-CO-OH (PIN)	

The decreasing order of seniority of the carbon acids as indicated in Section P-41 is: polycarbonic acids > tricarbonic acid > dicarbonic acid > oxalic acid > carbonic acid > cyanic acid

HO-OC-CO-OH (PIN)

- P-65.2.1 Carbonic acidP-65.2.2 Cyanic acidP-65.2.3 Oxalic acidP-65.2.4 Di- and polynuclear acids

oxalic acid

P-65.2.1 Carbonic acid

The nomenclature of chalcogen analogues and derivatives of carbonic acid is based on functional replacement of one oxygen in –OH groups or of the doubly bonded oxygen atom, =O, indicated by infixes. Substitution of formic acid is not recommended for generation of these names.

P-65.2.1.1 The contracted name 'carbamic acid' (from carbonamidic acid), for H_2N -CO-OH, is retained and is the preferred IUPAC name .

Examples:

(CH₃)₂N-COOH

dimethylcarbamic acid (PIN)

 CH_{3} $|_{N'}$ $CH_{3}-CH_{2}-N-C(=NH)-OH$

N-ethyl-N-methylcarbamimidic acid (PIN)

H2N-CH2-CH2-NH-CO-O-CH2-CH(OH)-CH3

2-hydroxypropyl *N*-(2-aminoethyl)carbamate (PIN)

P-65.2.1.2 Functional replacement in carbonic acid and carbamic acid by -OO-, -S-, -Se-, and -Te- is expressed by the infixes 'peroxo', 'thio', 'seleno', 'telluro'. In names, tautomeric groups in mixed chalcocarbonic acids, such as HO-CO-SH or HO-CS-OH, are distinguished by prefixing italic element symbols, such as *S* or *O*, respectively, to the term 'acid '; the italic symbols *OS* and *SO* are used for peroxy acids

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> H₂N-CS-OH carbamothioic *O*-acid (PIN)

H₂N-CO-SeH carbamoselenoic *Se*-acid (PIN)

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HO-CO-SH

carbonothioic *S*-acid (PIN) (not sulfanylformic acid) HSe-CO-SeH

carbonodiselenoic Se,Se-acid (PIN)

HS-CS-SH (PIN)

carbonotrithioic acid

carbamoperoxoic acid

H₂N-CO-OOH (PIN

HO-CO-OOH (PIN)

carbonoperoxoic acid

HOO-CO-OOH (PIN) carbonodiperoxoic acid

HO-CO-OSH

carbono(thioperoxoic) OS-acid (PIN)

HOS-CO-OSH

carbonobis(thioperoxoic) OS,SO-acid (PIN)

H₂N-C(=NH)-OSH

carbamimido(thioperoxoic) OS-acid (PIN)

P-65.2.1.3 Functional replacement of =O in carbonic acid and carbamic acid by =NH and =N-NH₂ is expressed by the infixes 'imido' and 'hydrazono' and of oxygen in -OH groups in the resulting acids by chalcogen atoms is expressed by infixes, as in P-65.1.1.5.1.2.

Italic letter locants N, N', etc. are used to designate substitution on nitrogen atoms.

Examples:

HO-C(=NH)-OH carbonimidic acid (PIN)

HO-C(=N-NH₂)-OH

carbonohydrazonic acid (PIN)

H₂N-C(=NH)-OH carbamimidic acid (PIN)

HS-C(=NH)-OH carbonimidothioic acid (PIN) $H_2N-C(=NH)-SH$ carbamimidothioic acid (PIN)

carbonohydrazonodiselenoic acid (PIN)

HSe-C(=N-NH₂)-SeH

P-65.2.1.4 Functional replacement (see P-67) of one of the -OH groups of carbonic acid by various atoms or groups is expressed by the following infixes: fluorido, -F; chlorido, -Cl; bromido, -Br; iodido, -I; azido, $-N_3$; amido, $-NH_2$; cyanido, -CN; isocyanido, -NC; isocyanatido, -NCO; isothiocyanatido, -NCS; isoselenocyanatido, -NCSe; isotellurocyanatido, -NCTe.

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Italic letter locants N, N', etc. are used to designate substitution on nitrogen atoms.

Replacement by the -NHNH₂ group results in hydrazinecarboxylic acid and related derivatives (see P-68.3.1.2.4).

Examples:

H₂N-CO-OH

carbamic acid (PIN) (not carbonamidic acid) H₂N-C(=NH)-OH

carbamimidic acid (PIN) (not carbonamidimidic acid)

H₂N-CO-SH

carbamothioic *S*-acid (PIN)

H₂N-C(=NH)-SeH

carbamimidoselenoic acid (PIN)

Cl-CO-OH

NC-CO-OH

carbonochloridic acid (PIN)

carbonocyanidic acid (PIN)

N₃-CO-OH

SCN-CO-OH

carbonazidic acid (PIN)

carbonisothiocyanatidic acid (PIN)

H₂N-NH-CO-OH

hydrazinecarboxylic acid (PIN; see P-68.3.1.2.4) (not carbonohydrazonic acid; acids expressed by suffixes are senior to carbonic acid analogues)

P-65.2.1.5 Acyl groups derived from carbonic and related acids

Acyl groups are derived from carbonic and related acids, including functional replacement analogues, by the removal of one or two hydroxy groups from the acid. They are named in accordance with the methodology described in P-65.1.7. Names are formed in two ways:

(1) Names may be formed by changing the -ic or -oic acid ending of the name of the acid to -yl or -oyl, respectively. Names of acyl groups ending in -yl are exceptions to the

general rule (see P-65.1.7). This method is the traditional method that consists in removing the two hydroxy groups from carbonic acid or its analogues; it is now recommended to be used also when only one hydroxy group is present in an acid. It is also recommended that divalent acyl groups, such as 'carbonyl' represent only the 'diyl' type of substituent prefix in which the two free valences are divergent (symbols CO < or - CO-). Substituent prefixes in which both free valences are attached to the same atom are named by substitutive nomenclature, for example, =CO is named oxomethylidene (see P-65.2.1.7)

(2) Names may be formed by a concatenation operation, i.e., by adding appropriate monovalent substituent groups to divalent acyl groups such as 'carbonyl', 'carbonothioyl', and 'carbonimidoyl' formed by method (1).

Names formed by method (1) are preferred IUPAC names; they are preferred to other names for acyl groups, including the use of prefixes rather than infixes or names formed by full or partial concatenation.

Examples:

НО-СО-ОН

carbonic acid (PIN)

HO-CS-OH

carbonothioic O,O-acid (PIN)

carbonothioyl (PIN) thiocarbonyl

-CS-

-CO-

carbonyl (PIN)

HO-C(=NH)-OH carbonimidic acid (PIN) -C(=NH)carbonimidoyl (PIN)

HO-C(=NNH₂)-OH carbonohydrazonic acid (PIN) -C(=NNH₂)-

carbonohydrazonoyl (PIN)

H₂N-CO-OH carbamic acid (PIN)

H₂N-CS-OH carbamothioic *O*-acid (PIN) carbamoyl (PIN) aminocarbonyl

H₂N-CO-

 H_2N -CS-

carbamothioyl (PIN) aminocarbonothioyl

> H₂N-C(=NH)-OH carbamimidic acid (PIN)

H₂N-C(=NH)– carbamimidoyl (PIN) aminocarbonimidoyl

Cl-CO-

chlorocarbonyl

carbonochloridoyl (PIN)

Cl-CO-OH

carbonochloridic acid (PIN)

NC-CO-OH carbonocyanidic acid (PIN) NC-CO– carbonocyanidoyl (PIN) cyanocarbonyl

Br-CS-OH carbonobromidothioic *O*-acid (PIN)

carbonobromidothioyl (PIN) bromocarbonothioyl

Br-CS-

Cl-C(=NH)-OH carbonochloridimidic acid (PIN) Cl-C(=NH)-

carbonochlorimidoyl (PIN) *C*-chlorocarbonimidoyl

НОО-СО-ОН

carbonoperoxoic acid

НОО-СО-

carbonoperoxoyl (PIN) hydroperoxycarbonyl

P-65.2.1.6 The prefix 'carboxy' and related prefixes.

The prefix 'carboxy' for –COOH is a retained prefix. Chalcogen analogues are named by functional replacement nomenclature provided that it is not necessary to specify the location of the chalcogen atom. Specification of chalcogen atoms is accomplished by compound prefixes formed by concatenation.

Examples:

-COSH or -CSOH

thiocarboxy (PIN)

sulfanylcarbonyl (PIN)

HS-CO-

HS-CS-

dithiocarboxy (PIN) sulfanylcarbonothioyl

HOOC-O-

carboxyoxy (PIN)

carboxysulfanyl (PIN)

HOOC-S-

HOOC-NH-

HS-CO-O-(sulfanylcarbonyl)oxy (PIN)

carboxyamino (PIN)

P-65.2.1.7 Chalcogen analogues of the 'carbonoperoxoyl' prefix, -CO-OOH, are named in two ways.:

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(1) by compound prefixes formed by concatenation;

(2) by thiohydroperoxy prefixes using the italic prefixes SO- or OS-, as necessary.

Method (1) leads to preferred IUPAC names.

Examples:

HOS-CSe-

(hydroxysulfanyl)carbonoselenoyl (PIN) (*OS*-thiohydroperoxy)carboselenoyl

HS-O-CO-O-

=C=0

=C=S

[(sulfanyloxy)carbonyl]oxy (PIN) [(SO-thiohydroperoxy)carbonyl]oxy HOS-CO- or HSO-CO-

carbono(thioperoxoyl) (PIN) (thiohydroperoxy)carbonyl

HSS-CO-O-

(disulfanylcarbonyl)oxy (PIN) (dithiohydroperoxycarbonyl)oxy

P-65.2.1.8 Names of non-acyl substituent groups derived from carbonic acid

Acyl groups derived from carbonic acid and carbonic acids modified by functional replacement are divalent groups with the two free valences belonging to the 'diyl' type, such as CO<. When the two free valences are of the 'ylidene' type, =C=O for example, names of acyl groups are no longer used to designate such groups; systematic substitutive names are used instead.

Examples:

oxomethylidene (PIN)

sulfanylidenemethylidene (PIN) thioxomethylidene

=C=NHiminomethylidene (PIN)=C=N-NH2hydrazinylidenemethylidene (PIN)
hydrazonomethylidene

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P-65.2.2 Cyanic acid

Cyanic acid is the retained name for NC-OH. The functional replacement name based on carbonic acid would be carbononitridic acid, but this name has not been used and is not recommended. Cyanic acid is classified as an acid, thus generating anhydrides (see P-65.7.2) and esters (see P-65.6.3.2).

Functional replacement by –OO–, –S–, –Se–, and –Te–, is expressed by the appropriate functional replacement prefix. This exception to the use of infixes in the functional replacement nomenclature applied to the mononuclear noncarboxylic acids carbonic acid and formic acid is necessary to maintain well entrenched traditional names and their related isocyanates, such as isothiocyanates.

Prefixes derived from cyanic acid are 'cyano' for -CN and 'cyanato' for -O-CN, 'thiocyanato' for -S-CN, 'selenocyanato' for -Se-CN, and 'tellurocyanato' for -Te-CN.

Examples:

NC-SeH

selenocyanic acid (PIN)

peroxycyanic acid (PIN)

NC-OOH

NC-SS-

NC-SS-CN

cyanodisulfanyl (PIN) (not thiocyanatosulfanyl)

disulfanedinitrile

NC-CH₂-COOH

2-cyanoacetic acid (PIN)

NC-S-CH₂-CH₂-COOH 3-thiocyanatopropanoic acid (PIN)

P-65.2.3 Oxalic acid, HO-CO-CO-OH

The name 'oxalic acid' is retained and is the preferred IUPAC name. This acid belongs to the group of polynuclear oxoacids having a direct link between central atoms (see P-67.2 and also Rule I-9.7.2, ref. 14).

P-65.2.3.1. Retained names for acids related to oxalic acid are as follows:

H₂N-CO-CO-OH

oxamic acid (PIN) (contraction of oxalamic acid) amino(oxo)acetic acid

OHC-CO-OH oxaldehydic acid (PIN) (contraction of oxalaldehydic acid) oxoacetic acid

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P-65.2.3.2 Functional replacement nomenclature using only prefixes to designate the replacement of –OH or =O is used to name derivatives other than those in P-65.2.3.1.

P-65.2.3.2.1 General methodology
P-65.2.3.2.2 Replacement by -OOH, -S-, =S, -Se-, =Se, -Te-, =Te, =NH and =NHNH₂
P-65.2.3.2.3 Replacement by halides and pseudohalides
P-65.2.3.2.4 Replacement by -NH₂ and -NHNH₂

P-65.2.3.2.1 General methodology

Prefixes are used to indicate the replacement of oxygen atoms by other groups generally listed as replacing groups (see P-16). The two carbon atoms are numbered and the locants are used to indicate the position of the replacing atoms or groups cited as prefixes.

P-65.2.3.2.2 Replacement by -OO-, -S-, =S, -Se-, =Se, -Te-, =Te, =NH and =NHNH₂

Functional replacement of oxygen atom(s) is denoted by prefixes, i.e., peroxy, -OO-; thio, -S- or =S; seleno, -Se- or =Se; telluro, -Te- or =Te; imido, =NH, and hydrazono =NHNH₂ (see P-15.5). The position of each replaced oxygen atom is denoted by the appropriate numerical locant. When necessary, letter locants *O*, *S*, *Se*, and *Te* are used before the acid term, as appropriate, to designate the position of a chalcogen atom in the -OH group rather than the =O group. Numerical locants are used in front of the letter locants *O*, *S*, *Se*, and *Te*, as needed.

Italic letter locants N, N', etc. are used to designate substitution on nitrogen atoms of imido and hydrazono groups.

Examples:

$\rm CO_3SH_2$

thiooxalic acid (PIN)

H(S/O)C-CO-OH 1- thiooxalic acid (PIN) ¹² HS-CO-CO-OH 1-thiooxalic *S*-acid (PIN)

¹² HS-CS-CO-OH

1,1-dithiooxalic acid (PIN)

¹² HO-CS-CO-SH 1,2-dithiooxalic *O*,*S*-acid (PIN)

1 2 HS-CS-CO-SH

1,1,2-trithiooxalic *S*-acid (PIN)

2 1 OHC-CO-SH

1-thiooxaldehydic S-acid (PIN) 2-oxoethanethioic S-acid

> 1 N2 HO-C(=NH)-CO-OH imidooxalic acid (PIN)

HO-C(=NNH₂)-CO-OH hydrazonooxalic acid (PIN)

N' $HO-C(=NH)-C(=NNH_2)-OH$

1-hydrazono-2-imidooxalic acid (PIN)

1 2 HS-CS-CS-SH

tetrathiooxalic acid (PIN)

SHC-CO-OH

2-thiooxaldehydic acid (PIN 2-thioxoacetic acid

> N HO-C(=NH)-C(=NH)-OH diimidooxalic acid (PIN)

$$\frac{1}{1} \frac{N}{N} \frac{2}{2} \frac{N'}{N'}$$
HO-C(=NNH₂)-C(=NNH₂)-OH
dihydrazonooxalic acid (PIN)

2 HS-CO-C(=NH)-OH 1-imido-2-thiooxalic S-acid

P-65.2.3.2.3 Replacement by halides and pseudohalides

The prefixes bromo for -Br, chloro for -Cl, fluoro for -F, and iodo for -I, azido for -N₃, cyano for -CN, isocyano for -NC, cyanato for -NCO, isocyanato for -OCN, isothiocyanato for -SCN (and similarly for other chalcogen analogues) are used to indicate functional replacement (see P-15.5).

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Examples:

Br-CO-CO-OH

bromooxalic acid (PIN) (not 2-bromo-2-oxoacetic acid)

2 1 Cl-CS-COOH 2-chloro-2-thiooxalic acid(PIN) (not 2-chloro-2-thioxo-acetic acid)

2 1 SCN-CO-CO-OH

(isothiocyanato)oxalic acid (PIN) (not 2-isocyanato-2-oxoacetic acid)

NC-CO-COOH cyanooxalic acid (PIN) (not 2-cyano-2-oxoacetic acid) P-65.2.3.2.4 Replacement by -NH₂ and -NHNH₂

The prefixes amido for $-NH_2$ and hydrazido for $-NHNH_2$ are used with oxalic acid in functional replacement nomenclature. The name oxamic acid is retained for the amic acid H₂N-CO-COOH. Italic letter locants *N*, *N'*, etc. are used to designate substitution on nitrogen atoms. Functional replacement prefixes are used to indicate replacement of =O in oxamic acid.

Examples:

N 2 1 H₂N-CO-CO-OH oxamic acid (PIN) amidooxalic acid (not 1-amino-2-oxoacetic acid) ^{N' N' 1 2} H₂N-NH-CO-CO-OH

hydrazidooxalic acid (PIN) (not 2-hydrazino-2-oxoacetic acid)

 $^{N 1}_{H_2N-C(=NH)-C(=NH)-OH}$

diimidooxamic acid (PIN) (not 2-amino-1-iminoacetic acid) 1-hydrazido-2-imidooxalic acid (PIN) (not 2-hydrazino-2-iminoacetic acid)

H₂N-NH-CO-C(=NH)-OH

 2 1 H₂N-CO-CS-OH

1-thiooxamic *O*-acid (PIN) 2-amido-1-thiooxalic *O*-acid (not 2-amino-2-oxothioacetic *O*-acid) H_2N -CS-CO-OH

2-thiooxamic acid (PIN) (not 2-amino-2-thioxoacetic acid)

P-65.2.3.3. Substituent groups cited as prefixes

The acyl groups oxalyl, oxalo, oxamoyl, and oxaldehydoyl are retained as preferred IUPAC names for use as substituent prefixes but not for naming acid halides, amides, and hydrazides, etc. (see P-65.5.1.2; P-66.1.5.5; P-66.3.5.1). Concatenation and functional replacement prefixes are used with oxalyl to form preferred IUPAC names of derivatives.

Examples:

-0C-CO-

oxalyl (PIN) ethanedioyl dioxoethane-1,2-diyl НО-СО-СО-

oxalo (PIN) carboxycarbonyl (not carboxyformyl) (not hydroxy(oxo)acetyl)

(not 2-hydraz

N' N' 1

2 1 Cl-CO-CO-

chlorooxalyl (PIN) 2-chloro-1,2-dioxoethyl

H₂N-CO-CO-

oxamoyl (PIN) (not carbamoylcarbonyl) (not carbamoylformyl) (not amino(oxo)acetyl)

HOOC-CS-

1-thiooxalo (PIN) (not carboxycarbonothioyl)

HO-CS-CO-

2-hydroxy-2-thiooxalyl (PIN) [not (hydroxycarbonothioyl)carbonyl]

2 1 Cl-CO-CS-

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2-chloro-1-thiooxalyl (PIN) 2-chloro-2-oxo-1-thioxoethyl

НСО-СО-

oxaldehydoyl (PIN) hydrooxalyl (not formylcarbonyl)

$H{O/S}C-CO-$

2-thiooxalo (PIN) [not (thiocarboxy)carbonyl]

HS-CS-CS-

trithiooxalo (PIN) (not dithiocarboxycarbonothioyl)

HOOC-CO-CH₂-COOH

2-oxaloacetic acid (PIN) 3-carboxy-3-oxopropanoic acid (not 4-hydroxy-3,4-dioxobutanoic acid)

HOOC-CO COOH

3-oxalobenzoic acid (PIN) 3-(carboxycarbonyl)benzoic acid

НООС-СО-О-

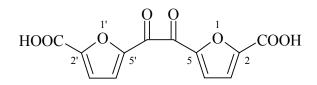
oxalooxy (PIN) (carboxycarbonyl)oxy [not carboxyformyl)oxy] [not [hydroxy(oxo)acetyl]oxy]

HOOC-CO-NH-

oxaloamino (PIN) (carboxycarbonyl)amino [not carboxyformamido] [not [hydroxy(oxo)acetyl]amino] HOOC-CO-S– oxalosulfanyl (PIN) (carboxycarbonyl)sulfanyl [not (carboxyformyl)sulfanyl] HOOC-CS-S-

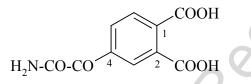
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1-thiooxalylsulfanyl (carboxycarbonothioyl)sulfanyl [not carboxythioformyl)sulfanyl] [not [hydroxy(oxo)ethanethioyl]sulfanyl



[not [hydroxy(oxo)acetyl]sulfanyl]

^{5,5&#}x27;-oxalyldi(furan-2-carboxylic acid) (PIN) 5,5'-oxalyldi-(2-furoic acid)



4-oxamoylbenzene-1,2-dicarboxylic acid (PIN) 4-oxamoylphthalic acid

P-65.2.4 Di- and polycarbonic acids

Di- and polycarbonic acids belong to the series of homopolynuclear acids, whose central atom is carbon. Their generic formula is HO-[CO-O]_n-H, where *n* is 2, 3, 4, etc. They are named by adding a multiplying prefix corresponding to the number of carbon atoms to the name 'carbonic acid'. The structure is numbered consecutively from one end to the other, starting from and ending at a carbon atom:

Examples:

HO-CO-O-CO-OH

dicarbonic acid (PIN)

```
1 2 3 4 5
HO-CO-O-CO-O-CO-OH
```

tricarbonic acid (PIN)

P-65.2.4.1 Functional replacement for di- and polynuclear carbon acids

P-65.2.4.1.1 General methodology P-65.2.4.1.2 Replacement by -OO-, -S-, =S, -Se-, =Se, -Te-, =Te, =NH, and =NHNH₂

> P-65.2.4.1.3 Replacement by halides and pseudohalides P-65.2.4.1.4 Replacement by -NH₂ and -NHNH₂ groups.

P-65.2.4.1.1 General methodology

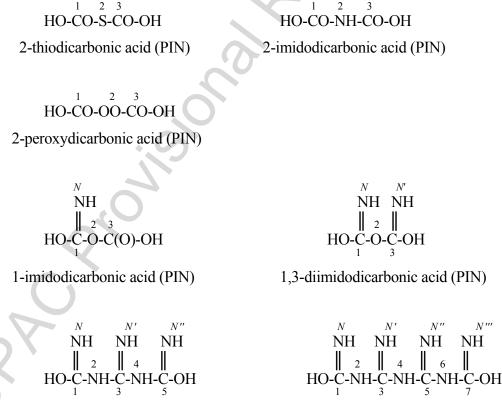
Nomenclature for functional analogues of the polycarbonic acids follows the principles for naming polynuclear inorganic oxo acids (see P-67). Prefixes are used to indicate functional replacement and the chain is numbered consecutively from one end to the other, starting from and ending at a carbon atom. These prefixes are listed in Table 4.2; they are cited in alphabetical order in front of the retained name of the polyacid, with appropriate locants as required.

P-65.2.4.1.2 Replacement by -OO-, -S-, =S, -Se-, =Se, -Te-, =Te, -NH-, =NH, and =NHNH₂

Functional replacement of oxygen atom(s), -OH, =O, -O-, is denoted by prefixes, i.e., peroxy for -OO-; this for -S- or =S; seleno for -Se- or =Se; telluro for -Te- or =Te; imido for -NH- or =NH, and hydrazono for =NHNH₂. The position of each replaced oxygen atom is denoted by the appropriate numerical locant.

Italic letter locants N, N', etc. are used to designate substitution on nitrogen atoms that are not anhydride linkages.

Examples:



1,2,3,4,5-pentaimidotricarbonic acid (PIN) 1,2,3,4,5,6,7-heptaimidotetracarbonic acid (PIN)

 $N^{\prime\prime\prime}$

NH

³ ² ¹ HO-CO-O-CO-OOH 1-peroxydicarbonic acid (PIN)

HOO-CO-O-CO-OOH 1,3-diperoxydicarbonic acid (PIN)

HS-CS-S-CS-SH

2 3

1

When necessary, letter locants O, S, Se, and Te are used, as appropriate, to designate the position of a chalcogen atom replacing oxygen in -OH or =O groups. Numerical locants are used in front of the letter locants O, S, Se, and Te placed before the term 'acid' as needed.

Examples:

1,1,3,3-tetrathiodicarbonic acid (PIN)

pentathiodicarbonic acid (PIN)

1,3-dithiodicarbonic acid (PIN; the location of the sulfur atoms is unknown)

¹ ² ³ HS-CO-O-CO-SH 1 2 3 HO-CS-O-CS-OH

1,3-dithiodicarbonic 1-O,3-O-acid (PIN)

1,3-dithiodicarbonic 1-*S*,3-*S*-acid (PIN)

~

Compound substituent groups may have to be used to name chalcogen analogues when the location of chalcogen atoms is not known.

Examples:

H{O/S}C-O-CO-SH

[(thiocarboxy)oxy]formothioic S-acid (PIN)

H{O/S}C-O-CS-OH

[(thiocarboxy)oxy]formothioic O-acid (PIN)

P-65.2.4.1.3 Replacement by halides and pseudohalides

Prefixes bromo for -Br, chloro for -Cl, fluoro for -F, and iodo for -I, azido for $-N_3$, isocyano for -NC, isocyanato for -NCO (and chalcogen analogues) are used to indicate functional replacement.

Examples:

¹ ² ³ Cl-CO-O-CO-OH chlorodicarbonic acid (PIN)

OCN-CO-NH-CO-OH

1-isocyanato-2-imidodicarbonic acid (locants are used to avoid ambiguity)

P-65.2.4.1.4 Replacement by NH₂ and NHNH₂ groups

The prefixes amido and hydrazido are used to indicate functional replacement by $-NH_2$ and $-NHNH_2$ groups, respectively. Italic letter locants *N*, *N'*, etc. are used to designate substitution on nitrogen atoms that are not anhydride linkages.

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Examples:

1 2 3 H₂N-CO-S-CO-OH

1-hydrazido-2,4-diimidotricarbonic acid (PIN)

1-amido-2-thiodicarbonic acid (PIN)

P-65.2.4.1.5 Substituent groups derived from polycarbonic acids

со-о-соон

Names of substituent groups are formed by substitution or concatenation as required.

Examples:

HOOC-O-CO-

HS-CS-S-CS-

(carboxyoxy)carbonyl (PIN) (carboxyoxy)formyl

COOH

[(dithiocarboxy)sulfanyl]carbonothioyl (PIN) [(sulfanylcarbonothioyl)sulfanyl]carbonothioyl [sulfanyl(thiocarbonyl)sulfanyl](thiocarbonyl) [not (dithiocarboxy)sulfanyl]thioformyl]

2-[(carboxyoxy)carbonyl]benzoic acid (PIN)

P-65.3 Sulfur, selenium, and tellurium acids with chalcogen atoms directly linked to a parent hydride.

P-65.3.0 Introduction. The following acids are discussed in this section:

R-SO ₃ H	sulfonic acids	R-SO ₂ H	sulfinic acids
R-SeO ₃ H	selenonic acids	$R-SO_2H$	seleninic acids
R-TeO ₃ H	telluronic acids	R-TeO ₂ H	tellurinic acids

Table 6.1 Suffixes and prefixes used to denote sulfur, selenium, and tellurium acids with chalcogen atoms directly linked to a parent

Group	Suffix	Prefix
SO ₂ -OH	sulfonic acid	sulfo
SO-OH	sulfinic acid	sulfino
SeO ₂ -OH	selenonic acid	selenono
SeO-OH	seleninic acid	selenino
TeO ₂ -OH	telluronic acid	tellurono
TeO-OH	tellurinic acid	tellurino

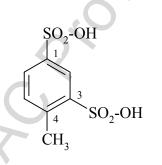
P-65.3.1 Substitutive nomenclature, suffix mode, for sulfonic, sulfinic, etc., acids

Sulfonic, sulfinic, etc., acids are named substitutively by adding an appropriate suffix listed in Table 6.1 to the name of a parent hydride name. Multiplying prefixes 'di', 'tri', 'tetra', etc. are used to denote multiplicity of suffixes.

Examples:

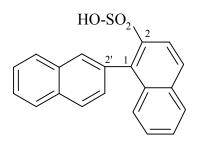
C₆H₅-SO₂-OH

benzenesulfonic acid (PIN)



4-methylbenzene-1,3-disulfonic acid (PIN) (not toluene-2,4-disulfonic acid) SO-OH 4 3 1 1 CH₃-CH₂-CH-CH₃

butane-2-sulfinic acid (PIN)



[1,2'-binaphthalene]-2-sulfonic acid (PIN)

P-65.3.1.1 Modification by functional replacement

Oxygen atoms of a suffix acid may be replaced by -OO- and/or other chalcogen analogues, -Sor =S, -Se- or =Se, -Te- or =Te, =NH and =N-NH₂ by functional replacement nomenclature. The general methodology is to modify the suffixes by infixes and use them in systematic substitutive nomenclature in the way prescribed for unmodified suffixes. If necessary, names are formed in accordance with the order of seniority, unmodified acids followed by -OO- > S > Se > Te. This seniority is fully exemplified in Section P-43 and in Appendix 1.

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P-65.3.1.2 Peroxy acids

The suffixes given in Table 6.1 are modified by the infix 'peroxo' and used as such in substitutive nomenclature as illustrated by the following suffixes.

-SO₂-OOH

sulfonoperoxoic acid

Examples:

C₆H₅-TeO-OOH

methanesulfonoperoxoic acid (PIN)

benzenetellurinoperoxoic acid (PIN)

P-65.3.1.3 Modification by other chalcogen atoms

Suffixes are modified by the infixes 'thio', for -S- or =S, 'seleno', for -Se - or =Se, and 'telluro', for -Te - or = Te, and used as such. Tautomers are denoted by symbols S, Se and Te placed in front of the term 'acid', to express positions of chalcogen atoms when known. The infixes 'thioperoxo', 'selenoperoxo', etc. are used to indicate functional replacement in peroxy acids.

-SO₂-SH

sulfonothioic S-acid

-SO₂-OSH

sulfono(thioperoxoic) OS-acid

-Se(=S)-OH

-SeO-OOH

seleninoperoxoic acid

seleninothioic O-acid

-TeO-SeSH

tellurino(selenothioperoxoic) SeS-acid

Examples:

 CH_3 - CH_2 - CH_2 - $S{O,Se}H$

propane-1-sulfonoselenoic acid (PIN)

CH₃-CH₂-S(O)(S)-OH ethanesulfonothioic *O*-acid (PIN) CH₃-CH₂-Se(=S)-OH

ethaneseleninothioic O-acid (PIN)

CH₃-CH₂-S(=NH)₂-OH

ethanesulfonodiimidic acid (PIN)

P-65.3.1.4 Imidic and hydrazonic acids derived from sulfonic, sulfinic, etc., acids

Imidic acids and hydrazonic acids derived from sulfonic, sulfinic, etc., acids are named by using suffixes such as 'sulfinimidic acid' for -S(O)(=NH)-OH, 'sulfonohydrazonic acid' for $-S(O)(=NNH_2)-OH$. The prefix 'di' is used to indicate the replacement of two oxygen atoms (=O) in sulfonic acids, for example, 'sulfonodiimidic acid' for $-S(=NH)_2-OH$, Suffixes are listed in Table 4.3 and in Appendix 1.

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Examples:

CH₃-S(=NH)-OH

methanesulfinimidic acid (PIN)

C₆H₅-Se(=NH)₂-OH

benzeneselenonodiimidic acid (PIN)



benzenesulfonohydrazonic acid (PIN) naphthalene-2-selenonohydrazonimidothioic acid (PIN)

P-65.3.1.5 Hydroximic and hydroxamic acids derived from sulfonic, sulfinic, etc., acids

Hydroximic acids and hydroxamic acids derived from sulfonic, sulfinic, etc., acids are named as *N*-hydroxysulfonimidic acids and *N*-hydroxysulfonamides, etc. (see P-66.1.1.2), respectively. Examples:

СH₃-S(O)(=N-OH)-OH

N-hydroxymethanesulfonimidic acid (PIN)

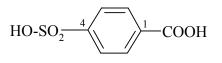
CH₃-CH₂-CH₂-SO-NH-OH

N-hydroxypropanesulfonamide (PIN)

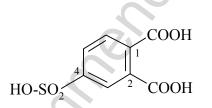
P-65.3.2 Substitutive nomenclature, prefix mode for sulfonic, sulfinic, etc., acids

P-65.3.2.1 When another group is also present that has seniority for citation as principal group (see P-41, P-42, P-43), or when all groups cannot be expressed as suffixes, organic oxoacids of sulfur, selenium or tellurium are named by adding to the name of the parent compound the appropriate prefix given in Table 6.1. These prefixes can be modified by prefixes designating chalcogen atoms in functional replacement nomenclature when the position of the chalcogen atom is not known or when it is not desirable to indicate such position.

Examples:



4-sulfobenzoic acid (PIN)



4-sulfobenzene-1,2-dicarboxylic acid (PIN) 4-sulfophthalic acid

$$HO-SO_2-CH_2-CH_2-CH_2-CH_2-O-S-CH_2-O-CH_2-CH_2-CH_2-SO_2-OH$$

4-({[(3-sulfopropoxy)methyl]sulfanyl}oxy)butane-1-sulfonic acid (PIN)

HO-SO-CH₂-COOH sulfinoacetic acid (PIN) HOOC-CH₂-CH₂-SeO₂-OH

3-selenonopropanoic acid (PIN)

H{O,S}S-CH₂-CH₃-SO₂-OH

2-(thiosulfino)ethane-1-sulfonic acid (PIN)

P-65.3.2.2 Acyl groups derived from sulfonic, sulfinic, etc., acids and their functional replacement analogues

P-65.3.2.2.1 Acyl sulfonic, sulfinic, selenonic, seleninic, telluronic, and tellurinic groups, R- EO_x , $-O_xE$ -R- EO_x , or $-O_xE$ -R- $[R'-EO_x-]$ -R"- EO_x , where E = S, Se, or Te, x = 1 or 2, and R, R', and R" are chains, rings, or ring systems, and their functional replacement analogues are groups derived by the removal of the hydroxy group from each sulfonic, sulfinic, or related selenium or tellurium acid group that is expressed as the principal characteristic group by an appropriate suffix.

P-65.3.2.2.2 Names for acyl groups derived from sulfonic and sulfinic acids, and their Se and Te counterparts, by removal of the -OH group from each sulfonic, sulfinic, etc. acid expressed as a suffix are formed by changing the 'ic acid' ending of the suffix to 'yl'. When the suffix is modified by functional replacement nomenclature, the ending of the corresponding acyl group is 'oyl'.

Examples:

> C₆H₅-SO₂benzenesulfonyl (PIN)

CH₃-SeO– methaneseleninyl (PIN)

CH₃-CH₂-S(O)(S)– ethanesulfonothioyl (PIN) C_6H_5 -S(Se)-

benzenesulfinoselenoyl (PIN)

CH₃-CH₂-S(=NH)– ethanesulfinimidoyl (PIN)

P-65.3.2.3 Substituent groups formed by concatenation

When the name of an acyl group cannot be derived directly from that of the acid expressed by a suffix, a concatenation procedure is used. For this procedure names of divalent mononuclear acyl groups are required. Acyl groups corresponding to sulfuric and sulfurous acids and the corresponding selenium and tellurium acids are formed from the acids by subtracting all -OH groups from the parent acid. The names used in the nomenclature of organic compounds are as follows:

-SO ₂ -	sulfonyl (PIN) sulfuryl	-SO-	sulfinyl (PIN) thionyl
-SeO ₂ -	selenonyl (PIN)	-SeO-	seleninyl (PIN)
-TeO ₂ -	telluronyl (PIN)	-TeO-	tellurinyl (PIN)

These acyl groups are modified by infixes in functional replacement nomenclature to indicate replacement by '=S', '=Se', '=Te', '=NH', and '=N- NH_2 '.

Examples:

-S(=O)(=S)-sulfonothioyl (PIN)-S(=S)(=S)-sulfonodithioyl (PIN)-S(=NH)-sulfinimidoyl (PIN) $-Se(=O)(=NNH_2)-$ selenonohydrazonoyl (PIN)-Se(=S)(=NH)-selenonimidothioyl (PIN)

Prefixes denoting characteristic groups can then be attached to these divalent acyl group names. The prefix 'hydro-' for H can also be used. This traditional method generates preferred IUPAC names. Names of acyl groups derived directly from the names sulfuric acid and sulfurous acid, and their Se and Te congeners, are inappropriate because of ambiguity and incompleteness (see P-67.1.4.4.1). The name sulfamoyl for H₂N-SO₂- is a retained name used as a preferred IUPAC name

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Examples:

CH₃O-SO₂– methoxysulfonyl (PIN)

 H_2N - SO_2 -

sulfamoyl (PIN) aminosulfonyl

CH₃-CO-O-SO₂-

(acetyloxy)sulfonyl (PIN)

CH₃-O-S(=NH)– S-methoxysulfinimidoyl (PIN)

Cl-S(O)-

H-SO-

hydrosulfinyl (PI

chlorosulfinyl (PIN)

H-SeO₂-

hydroselenonyl (PIN)

HO-SO₂-O-

sulfooxy

 $-S-SO_2-S-$

sulfonylbis(sulfanediyl)

-O-SO-O-

sulfinobis(oxy)

P-65.3.4 Polyfunctional compounds

Polyfunctional compounds are named in accordance with the general order of seniority of suffixes described in Sections P-41 and P-43, and also in Appendix 1. When required, numbering is based on the following seniority order:

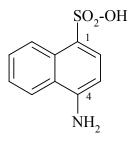
- (a) fixed numbering of parent hydride (e.g. naphthalene, bicyclo[2.2.2]octane, etc.)
- (b) heteroatoms in rings and chains
- (c) indicated hydrogen [for unsubstituted compounds; a higher locant may be needed at another position to provide for a substituent suffix in accordance with the structural feature (d)].

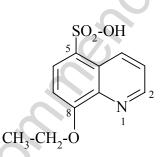
- (d) principal group named as suffix
- (e) added hydrogen (consistent with the structure of the compound and in accordance with further substitution)
- (f) unsaturation/saturation (ene/yne endings or hydro/dehydro prefixes)

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(g) detachable (alphabetized) prefixes

Examples:



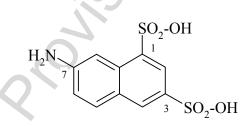


8-ethoxyquinoline-5-sulfonic acid (PIN)

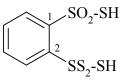
4-aminonaphthalene-1-sulfonic acid (PIN)



8-hydroxy-5,7-dinitronaphthalene-2-sulfonic acid (PIN)



7-aminonaphthalene-1,3-disulfonic acid (PIN)



2-(trithiosulfo)benzene-1-sulfonothioic *S*-acid (PIN)

DRAFT 7 October 2004

P-65.4. Acyl groups as substituent groups

P-65.4.1 General methodology

Acyl group nmaes that are described in preceding sections are used unchanged to denote substituent groups. Thus, the traditional way of using acyl groups derived from acyclic carboxylic acids to name ketones, pseudokeones and heterones is maintained (see P-64.4 for more examples).

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This is a change in the case of acyl groups derived from carboxylic acids named by the suffix 'carboxylic acid' and for sulfonic, sulfinic, etc., acids; the traditional concatenation method denoting the parent hydride by a prefix is no longer recommended.

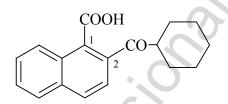
Examples:

COOH CO-CH₂

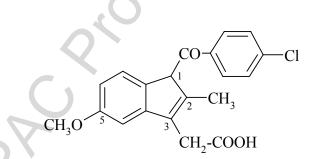
COOH SO₂-CH₃

2-acetylbenzoic acid (PIN) 2-methanesulfonylbenzoic acid (PIN)

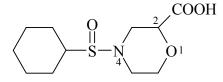
[not 2-(methylsulfonyl)benzoic acid]



2-cyclohexanecarbonylnaphthalene-1-carboxylic acid (PIN) [not 2-(cyclohexylcarbonyl)naphthalene-1-carboxylic acid]



2-[1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1*H*-inden-3-yl]acetic acid (PIN)

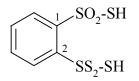


4-cyclohexanesulfinylmorpholine-2-carboxylic acid (PIN) [not 4-(cyclohexylsulfinyl)morpholine-2-carboxylic acid]

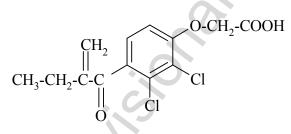
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SO₂-CH₂-CH₂-CH₃

propane-1-sulfonylbenzene (PIN) [not (propylsulfonyl)benzene]



2-(trithiosulfo)benzene-1-sulfonothioic S-acid (PIN)



2-[2,3-dichloro-4-(2-methylidenebutanoyl)phenoxy]acetic acid (PIN)

P-65.5 Acyl halides and pseudohalides

- P-65.5.1 Acyl halides from suffix acids
- P-65.5.2 Acyl pseudohalides from suffix acids
- P-65.5.3 Acyl halides and pseudohalides from carbonic, oxalic, cyanic and the polycarbonic acids
- P-65.5.3 Acyl halides and pseudo halides as substituent groups

P-65.5.1 Acyl halides from suffix acids

P-65.5.1.1 Acid halides in which hydroxy groups of all acid groups expressed as the suffix denoting the principal characteristic group (carboxylic, sulfonic, sulfinic, selenonic, etc. acids) have been replaced by halogen atoms (F, Cl, Br, and I) are named by citing the name of the acyl group (see P-65.1.7) followed by the name(s) of the specific class(es) as a separate word(s), in alphabetical order, each preceded by a multiplicative prefix, as needed.

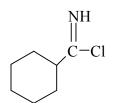
The names formyl, acetyl, and benzoyl are retained.

Names of acid halides are functional class names (see Table 6.2)

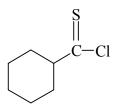
Halide		Prefix	Pseudoh	alides	Prefix
–F	fluoride	fluoro	-N ₃	azide	azido
-Cl	chloride	chloro	-CN	cyanide	cyano
–Br	bromide	bromo	-NC	isocyanide	isocyano
-I	iodide	iodo	-NCO	isocyanate	isocyanato
			-NCS	isothiocyanate	isothiocyanato
		5	-NCSe	isoselenocyanate	isoselenocyanato
			-NCTe	isotellurocyanate	isotellurocyanato
mples: ² CH ₃ -(1 CO-Cl	НСО-Е	ßr	654 CH ₃ -CH-CH	³ ² ¹ 2-CH ₂ -CH ₂ -CO-
acetyl chl	oride (PIN)	formyl brom	nide (PIN)	hexanoyl	fluoride (PIN)
3					

Table 6.2. Halides and pseudohalides

 (\mathbf{Z})



cyclohexanecarbonimidoyl chloride (PIN)



cyclohexanecarbothioyl chloride (PIN)

Cl-CO-CH₂-CO-Cl

propanedioyl dichloride (PIN) malonyl dichloride SO-Cl

benzenesulfinyl chloride (PIN)

SeO-(

benzeneseleninyl chloride (PIN)

Br-O₂S-CH₂-CH₂-SO₂-Br ethane-1,2-disulfonyl dibromide (PIN)

Cl-CC CO-C

benzene-1,4-dicarbonyl dichloride (PIN) terephthaloyl dichloride

P-65.5.2 Acyl pseudohalides from suffix acids

P-65.5.2.1 Acyl pseudohalides in which hydroxy groups of all acid groups expressed as the suffix denoting the principal characteristic group (carboxylic, sulfonic, sulfinic, selenonic, etc. acids) have been replaced by pseudohalogen groups (N₃, CN, NC, NCO, NCS, NCSe, NCTe) are named by citing the name of the acyl group (see P-65.1.7) followed by the name(s) of the class(es) as separate words, preceded by a multiplicative prefix, as needed. When a choice has to be made, the senior pseudohalide group is chosen in accordance with the decreasing order of seniority: N₃ > CN > NC > NCO > NCS > NCSe > NCTe. Halogen atoms are senior to pseudohalogen groups.

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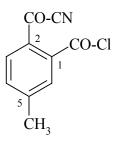
The names formyl, acetyl, and benzoyl are retained.

Examples:

> ⁴ ³ ² ¹ H₃C-CH₂-CH₂-CO-CN butanoyl cyanide (PIN) butyryl cyanide

butanedioyl isocyanate isocyanide (PIN)

4-(2-isocyanato-2-oxoethyl)benzenecarbothioyl cyanide (PIN)



2-(carbonocyanidoyl)-5-methylbenzoyl chloride (PIN) 2-(cyanocarbonyl)-5-methylbenzoyl chloride

P-65.5.3 Acyl halides and pseudohalides from carbonic, cyanic, oxalic, and the polycarbonic acids

P-65.5.3.1 Acyl groups derived from carbonic acid, carbamic acid, and related acids, such as 'carbonyl' from carbonic acid and 'carbamoyl' from carbamic acid, are used to form the names of the corresponding acyl halides.

Examples:

Cl-CO-Cl carbonyl dichloride (PIN)

H₂N-CO-I carbamoyl iodide (PIN) Br-CO-Cl

carbonyl bromide chloride (PIN) (not carbonobromidic chloride) N-methylcarbonazidimidoyl fluoride (PIN)

NC-CO-Cl

carbonocyanidoyl chloride (PIN)

H₂N-CO-NCO

N₃-C-F

carbamoyl isocyanate (PIN)

N-CH₃

P-65.5.3.2 The acyl group names oxalyl and oxalo from oxalic acid and oxamoyl from oxamic acid are **not** used to form preferred IUPAC names for acid halides and halogenoids; however, oxalyl and oxamoyl may be used in general nomenclature, but not oxalo. Names for acyl halides derived from oxalic acid, oxamic acid, and the polycarbonic acids are formed by using the name of the acid followed by the name(s) of the halides.

Examples:

HO-CO-CO-Cl oxalic (mono)chloride (PIN)

Cl-CO-CO-Cl

oxalic dichloride (PIN) oxalyl chloride

Cl-CO-O-CO-Cl

dicarbonic dichloride (PIN)

H₂N-CO-CO-Br

oxamic bromide (PIN) oxamoyl bromide

ONC-CO-CO-Br

oxalic bromide isocyanate (PIN) oxalyl bromide isocyanate

Cl-CO-O-CO-Br dicarbonic bromide chloride (PIN)

¹ ² ³ Cl-CO-NH-CO-Cl imidodicarbonic dichloride (PIN)

 $\begin{array}{c} 1 & N & 2 & 3 & 4 & 5 \\ \text{Cl-C}(=\text{NH})\text{-NH-CO-S-C}(\text{S})\text{-Br} \end{array}$

1,2-diimido-4,5-dithiotricarbonic 1-chloride 5-bromide (PIN)

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SCN-CO-CO-NCS

oxalic diisothiocyanate (PIN) oxalyl diisothiocyanate

OCN-CO-O-CO-NCO

dicarbonic diisocyanate (PIN) oxalyl diisocyanate

P-65.5.3.3 Acyl halides and pseudohalides from cyanic acid are formed in two ways:

(1) as acyl halides or pseudohalides of carbononitridic acid

(2) by citing the name of the halide or pseudohalide after the name of the acid:

Method (1) generates preferred IUPAC names.

Examples:

NC-Cl

NC-N₃

carbononitridic chloride (PIN) cyanic chloride

carbononitridic azide (PIN) cyanic azide

P-65.5.3 Acyl halides and pseudo halides as substituent groups

When another group is present that has priority for citation as principal group or when attached to another substituting group, an acyl halide or pseudohalide is expressed:

(1) by a prefix formed from the name of the acid;

- (2) by a compound prefix composed of a halo or halogeno prefix and an appropriate bivalent acyl group, such as 'sulfonyl', for example, fluorosulfonyl;
- (3) at the end of an acyclic carbon chain by a prefix denoting the halide or pseudohalide group and the prefix 'oxo', or a chalcogen analog of oxo, such as thioxo.

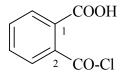
Method (1) leads to preferred IUPAC names when the suffix '-carboxylic acid' is used to name the corresponding acid; method (3) generates preferred IUPAC names for acyclic carbon chains.

Seniority for numbering follows that for acids, for which see P-65.1.2.3 or P-65.3.4.

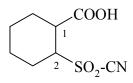
Examples:



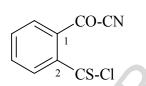
(3) 3-chloro-3-oxopropanoic acid (PIN)(1) (carbonochloridoyl)acetic acid



- (1) 2-(carbonochloridoyl)benzoic acid (PIN)
- (2) 2-chlorocarbonylbenzoic acid



- (1) 2-(cyanosulfonyl)cyclohexane-1-carboxylic acid (PIN)
- (2) 2-sulfurocyanidoylcyclohexane-1-carboxylic acid



- (1) 2-(carbonochloridothioyl)benzoyl cyanide (PIN)
- (2) 2-(chlorocarbonothioyl)benzoyl cyanide

Br-CO-CO-CH₂-COOH

- (3) 4-bromo-3,4-dioxobutanoic acid (PIN)
- (2) 3-(bromooxalyl)acetic acid

Br-CO-O-CO-CH₂-COOH

(3) 3-[(carbonobromidoyl)oxy]-3-oxopropanoic acid (PIN)

P-65.6 Salts and esters

P-65.6.1 General methodology

Neutral salts and esters are both named using the name of the anion derived from the name of the acid. Anion names are formed by changing an '-ic acid' ending of an acid name to '-ate' and an '- ous acid' ending of an acid name to '-ite'. Then, salts are named using the names of cations, and esters the names of organyl groups, cited as separate words in front of the name of the anion.

P-65.6.2 Salts

P-65.6.2.1 Neutral salts of acids are named by citing the name of the cation(s) followed by the name of the anion (see P-7) as a separate word. Different cations are cited in alphabetical order. Formation of salts is a functionalization and not a substitution. Thus, all retained names, both those used as preferred IUPAC names and those used only for general nomenclature can be used without restriction. This rule applies equally to acids expressed by suffixes and carbonic, cyanic, oxalic, and the polycarbonic acids.

Examples:

 $CH_3-CH_2-CH_2-COO^- K^+$

potassium butanoate (PIN) potassium butyrate

 $(CH_3-COO^-)_2 Ca^{2+}$

calcium diacetate (PIN)

K⁺ [–] OOC-CH₂-CH₂-COO[–] Na⁺

potassium sodium butanedioate (PIN) potassium sodium succinate CH₃-CH₂-CS-S⁻ Na⁺ sodium propanedithioate (PIN) sodium dithiopropionate

C₆H₅-SO-O⁻ Na⁺

sodium benzenesulfinate (PIN)

NH4^{+ -} OOC-CH₂-CH₂-CH₂-CH₂-COO⁻ K⁺

ammonium potassium hexanedioate (PIN) ammonium potassium adipate

 $C(O)O_2^{2-} 2Na^+$

disodium carbonate (PIN)

P-65.6.2.2 Acid salts

P-65.2.2.1 Acid salts of polybasic organic acids and organic derivatives of polybasic inorganic oxo acids are named in the same way as the neutral salts, the remaining acid hydrogen atom(s) being indicated by the word 'hydrogen' (preceded by a numerical prefix, 'di', 'tri', etc., as appropriate) inserted as a separate word between the name(s) of the cation(s) and the name of the anion. When required, cations are cited in names in alphabetical order. Anionic substitutents, such as $-COO^-$, $-SO_3^-$, $-SO_2^-$, are described by the prefix names 'carboxylato', 'sulfonato', and 'sulfinato', respectively, and similarly for the corresponding selenium and tellurium acids.

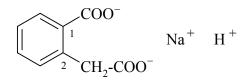
Examples:

HOOC-[CH₂]₅-COO⁻ K⁺

potassium hydrogen heptanedioate (PIN)

HOOC-CH₂-CH₂-COO⁻ NH₄⁺

ammonium hydrogen butanedioate (PIN) ammonium hydrogen succinate



sodium hydrogen 2-(carboxylatomethyl)benzoate (PIN)

COO H^+ Na^+ K OOC-CH2-CH-CH2-COO

potassium sodium hydrogen propane-1,2,3-tricarboxylate (PIN)

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 $HO-CO-O^- Na^+$

 $CH_3-P(O)(O^-)_2 K^+ H^+$

sodium hydrogen carbonate (PIN) potassium hydrogen methylphosphonate (PIN)

P-66.6.2.2.2 In the nomenclature of inorganic chemistry (I-8.5.2, ref. 14), the term 'hydrogen' is written directly in front of the name of the anion, without a space, to indicate that it is part of the anion.

Example:

 $P(O)(O^{-})_3$ Na⁺ 2 H⁺ sodium dihydrogenphosphate

P-65.6.3 Esters, lactones and related compounds.

P-65.6.3.1 Definitions P-65.6.3.2 Esters P-65.6.3.3 Esters of acids modified by functional replacement P-65.6.3.4 Pseudoesters P-65.6.3.5 Cyclic esters P-65.6.3.6 Acylals

P-65.6.3.1 Definitions

Esters of oxoacids are organic compounds formally derived from an oxoacid, and an alcohol, phenol, heteroarenol, or enol by a formal loss of water from an acidic hydroxy group of the former and an hydroxy group of the latter. By extension, they are 'acyl' derivatives of alcohols, etc. Alcohols, phenols, enols, heteroarenols, ynols are hydroxy compounds in which one or more hydroxy groups are attached to (a) carbon atoms.

A new class, 'pseudoesters', is recommended. It includes compounds having the generic group formula $-E(=O)_x(OZ)$ and chalcogen analogues where x = 1 or 2 and Z is not a carbon atom but another element such as Si, Ge, B, Al, N, P, S, Se. Pseudoesters are ranked as esters in the seniority order of classes (see P-41).

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P-65.6.3.2 Esters

P-65.6.3.2.1 Fully esterified acids are systematically named by placing the name(s) of the organyl group(s) (alkyl, aryl, etc.) in front of the name of the anion as separate word(s); they are cited in alphabetical order when more than one. When required, locants are cited at the front of the organyl groups. (For the endings 'ate' and 'ite', see P-65.6.1.). This rule applies equally to carboxylic, sulfonic, sulfinic, etc. acids, the other carbon acids, i. e., carbonic, oxalic, cyanic, and the polycarbonic acids and their replacement analogues.

Examples:

CH₃-CO-O-CH₃ ethyl acetate (PIN) H₃CO-OC-CH₂-CO-O-CH₂CH₃

ethyl methyl propanedioate (PIN) ethyl methyl malonate

ethane-1,2-diyl diacetate (PIN)

CH₃-O-CO-CO-CH₃

dimethyl oxalate (PIN)

1,4-phenylene acetate dichloroacetate (PIN)4-(acetyloxy)phenyl dichloroacetate

HCO-O-CH₂-CO-CH₃

methylene acetate formate (PIN)

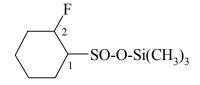
H₃C-CH₂ SO₂-OCH₃

methyl 4-ethylbenzenesulfonate (PIN)

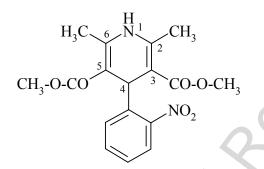
ethyl cyclohexanecarboxylate (PIN)

$$\overset{4}{\text{CH}_{3}}\overset{3}{\text{-CH}}\overset{2}{\text{CH}_{2}}\overset{1}{\text{-CH}}(\text{CO-O-CH}_{2}\text{CH}_{3})_{2}$$

1,1-diethyl 3-methyl butane-1,1,3-tricarboxylate (PIN)



trimethylsilyl 2-fluorocyclohexanesulfinate (PIN)



dimethyl 2,6-dimethyl-4-(2-nitrophenyl)-1,4-dihydropyridine-3,5-dicarboxylate (PIN)

P-65.6.3.2.2 When, in an ester another group is present that has priority for citation as a suffix or when all ester groups cannot be described by the above methods, an ester group is indicated by prefixes such as 'acyloxy' for the group R-CO-O–, or 'alkyloxy-…oxo' or 'alkyloxycarbonyl' for the group –CO-OR'.

The systematic name 'acetyloxy' is preferred to the contracted name 'acetoxy' that may be used in general nomenclature.

Seniority for numbering follows that for acids, for which see P-65.1.2.3 or P-65.3.4.

Examples:

 3 2 1 [CH₃CH₂-O-CO-CH₂CH₂-N⁺(CH₃)₃] Br⁻

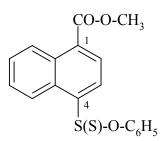
(3-ethoxy-3-oxopropyl)-*N*,*N*,*N*-trimethylazanium bromide (PIN) [2-(ethoxycarbonyl)ethyl]-*N*,*N*,*N*-trimethylammonium bromide

 3 2 1 2 1 C_{6} H_{5} -CO-O- CH_{2} CH_{2} -COO CH_{2}

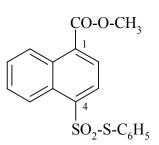
3-(benzoyloxy)propanoic acid (PIN)

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2-(acetyloxy)ethanesulfonic acid (PIN) 2-acetoxyethanesulfonic acid



methyl 4-(phenoxysulfinothioyl)naphthalene-1-carboxylate (PIN)



methyl 4-[(phenylsulfanyl)sulfonyl]naphthalene-1-carboxylate (PIN)

$$\begin{array}{c|c} H_{3}C & O-CO-O-CH_{2}-CH_{3} \\ 5 & 4 & \parallel & \mid & 1 \\ CH_{3}-C-C-C-CH-CO-O-CH_{2}CH_{3} \\ & \mid & 3 \\ H_{3}C \end{array}$$

ethyl 2-[(ethoxycarbonyl)oxy]-4,4-dimethyl-3-oxopentanoate (PIN)

4-{[(methoxyoxalyl)oxy]methyl}phenyl formate (PIN)

{4-[(methoxycarbonyl)oxy]phenyl} methyl methyl oxalate (PIN) (not 4-{[(methoxyoxalyl)oxy]methyl}phenyl methyl carbonate; oxalic acid preferred to carbonic acid)

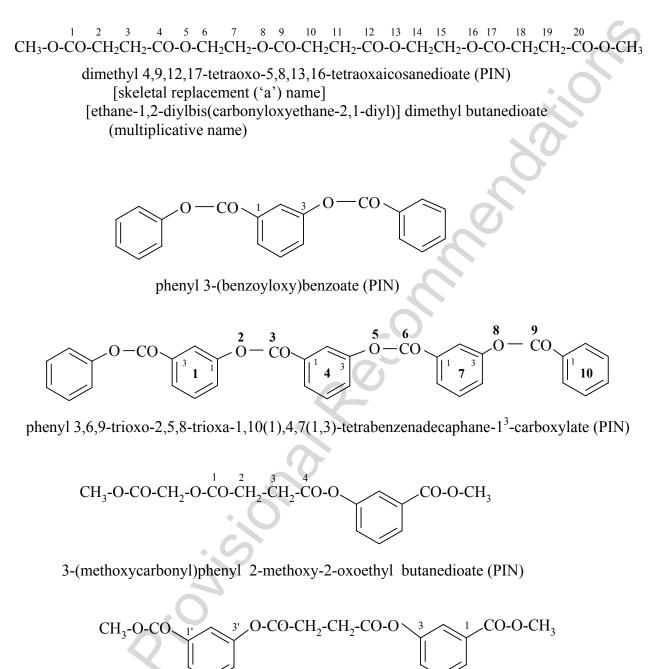
P-65.6.3.2.3 Polyesters, i.e., esters between two or more acids, are named as described in P-65.6.3.1.1, then by using substitutive nomenclature, multiplicative nomenclature, skeletal ('a') replacement nomenclature, or phane nomenclature when the specific conditions are fulfilled.

Examples:

¹ ² ³ ⁴ CH₃-O-CO-CH₂CH₂-CO-O-CH₂CH₂-O-CO-CH₃ 2-(acetyloxy)ethyl methyl butanedioate (PIN) 2-acetoxyethyl methyl butanedioate Н₃С-О-СО-СО-С O-CO-CO-O-CH, 1,4-phenylenebis(methyl oxylate) (PIN) 4-[(methoxyoxalyl)oxy]phenyl methyl oxalate; (multiplicative name preferred to substitutive name) O-CO-CO-O-CH₃ H₂C-CH₂-O-CO-CO-O

4-[(ethoxyoxalyl)oxy]phenyl methyl oxalate (PIN) (not ethyl 4-[(methoxyoxalyl)oxy]phenyl oxalate

¹ ² ³ ⁴ ^{4'}
^{4'} CH₃-O-CO-CH₂-CH₂-CH₂-CO-O-CH₂-CH₂-CO-O-CH₂-CH₂-O-CO-CH₃
²-(acetyloxy)ethyl methyl 4,4'-[ethane-1,2-diylbis(oxy)]bis(4-oxobutanoate) (PIN)
²-({4-[2-(acetyloxy)ethoxy]-4-oxobutanoyl}oxy)ethyl methyl butanedioate
²-(acetyloxy)ethyl 2-[(4-methoxy-4-oxobutanoyl)oxy]ethyl butanedioate] (multiplicative name preferred to substitutive name, see P-51.2)



dimethyl 3,3'-[butanedioylbis(oxy)]dibenzoate (PIN)

P-65.6.3.2.4 Partial esters of polybasic acids and their salts are named by the procedure for neutral esters and acid salts; the components present are cited in the order, cation, organyl group, hydrogen, anion. Numerical locants and italic element symbols (see P-65.6.3.3.1) are added as necessary to provide specificity. The numbering of the polybasic acid is retained when the hydrogen method is applied to retained names.

Examples:

CH₃-CH₂-O-CO-CH₂-CH₂-COO⁻ Na⁺

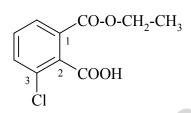
sodium ethyl succinate (PIN)

3 2 1 CH₃-CH₂-S-CO-CH₂-CH₂-C{O/S}

lithium 1-S-ethyl butanebis(thioate) (PIN)

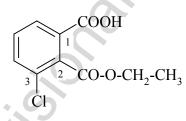
 K^+ H^+

potassium 3-ethyl hydrogen 2-hydroxypropane-1,2,3-tricarboxylate (PIN) potassium 5-ethyl hydrogen citrate



CH₃-CH₂-O-CO-CH₂-C(OH)-CH₂-COO⁻

1-ethyl hydrogen 3-chlorobenzene-1,2-dicarboxylate (PIN) 1-ethyl hydrogen 3-chlorophthalate



2-ethyl hydrogen 3-chlorobenzene-1,2-dicarboxylate (PIN) 2-ethyl hydrogen 3-chlorophthalate

4 3 2 CH₃-[CH₂]₃-O-CO-CH₂-CH₂-CH(CH₃)-COOH

5-butyl hydrogen 2-methylpentanedioate

5 4 3 2 1CH₃-CH₂-CH₂-CH₂-O-CO-CH₂-CH₂-C-COOH O-CO-CH₂

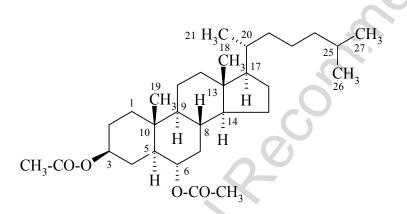
5-butyl hydrogen 2-(acetyloxy)-2-methylpentanedioate (PIN)

P-65.6.3.2.5 In the context of preferred IUPAC names, substitutive nomenclature is preferred over functional class nomenclature.

Examples:

CH₃-CO-C COOH

4-(acetyloxy)benzoic acid (PIN) 4-hydroxybenzoic acid acetate



 5α -cholestane- 3β , 6α -diyl diacetate (PIN) 5α -cholestane- 3β , 6α -diol diacetate

P-65.6.3.3 Esters of acids modified by functional replacement

P-65.6.3.3.1 With the exception of retained names, polycarbonic acids, oxalic acid, and cyanic acid that are described in P-65.6.3.3.3, names of esters are all derived from acids modified by functional replacement whose substitutive names are systematically formed, as indicated in sections P-65.1.3 to P-65.1.7.

Structural specification for esters of thio-, seleno- or tellurocarboxylic acids, thio-, seleno-, or tellurosulfonic acids and sulfinic acids and their peroxy analogues is provided by the appropriate italic element symbol, such as *S*, *O*, or *SO*, prefixed to the name of the organyl group.

Examples:

CH₃-[CH₂]₄-CO-S-CH₂-CH₃ S-ethyl hexanethioate (PIN)

CH₃-C(=NH)-O-CH₃

methyl ethanimidate (PIN) methyl acetohydroximate CH₃-[CH₂]₄-CSe-O-CH₂-CH₃ *O*-ethyl hexaneselenoate (PIN)

 CH_3 - CH_2 - $C(=N-NH_2)$ -O- C_2H_5

ethyl propanehydrazonate (PIN) ethyl propionohydrazonate

$C_6H_5-C(=NH)-S-CH_3$

methyl benzenecarboximidothioate (PIN)

HC(=N-SH)-S-CH₂-CH₃

ethyl *N*-sulfanylbenzenecarboximidothioate (PIN)

C₆H₅-CO-S-O-CH₃

SO-methyl benzene(carbothioperoxoate) (PIN)

CH₃-CH₂-SO₂-O-S-C₂H₅ OS-ethyl ethanesulfono(thioperoxoate) (PIN)

In the presence of a characteristic group having seniority for citation as suffix, an ester group is indicated by appropriate prefixes in accordance with the type of attachment of the substituent group, such as 'acylsulfanyl' for the group –S-CO-R, or 'alkylsulfanylcarbonothioyl', or alkylsulfanyl)...sulfanylidene' for the group –CS-SR. Examples:

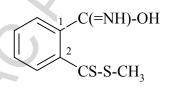
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 CH_3 -S-C(=S)-CH₂-CH₂-CO-SH

4-(methylsulfanyl)-4-sulfanylidenebutanethioic S-acid

2-[(ethanimidoyl)selanyl]benzene-1-carboximidic acid (PIN)



2-[(methylsulfanyl)carbonothioyl]benzene-1-carboximidic acid

P-65.6.3.3.2 Esters of carbonic acid, oxalic acid, cyanic acid, and the polycarbonic acids modified by functional replacement.

P-65.6.3.3.2.1 Names of acids modified by functional replacement are used to generate preferred IUPAC names of corresponding esters. Element symbols *O*, *S*, etc. and locants are used to designate the location of organyl groups.

Examples:

¹ ² ³ ⁴ ⁵ CH₃-S-CO-O-CO-O-CH₂-CH₃ 1-methyl 5-ethyl 1-thiodicarbonate (PIN)

CH₃-S-CS-O-CH₃ *O*,*S*-dimethyl carbonodithioate (PIN)

¹² CH₃-S-CO-CO-S-CH₃ *S,S*-dimethyl 1,2-dithiooxlate (PIN)

CH₃-O-CS-C(=NH)-S-CH₂-CH₃ S-ethyl O-methyl 1-imido-1,2-dithiooxalate (PIN)

² ¹ CH₃-S-CO-CS-S-CH₂-CH₃ 1-ethyl 2-methyl 1,1,2-trithiooxalate

(CH₃)₂CH-S-CN propan-2-yl thiocyanate

P-65.6.3.3.2.2 In the presence of a characteristic group having seniority for citation as suffix, an ester group is indicated by appropriate prefixes in accordance with the type of attachment of the substituent group.

Examples:

 $CH_3\text{-}S\text{-}CS\text{-}CO\text{-}O\text{-}CH_2\text{-}CS\text{-}SH$

2-{[(methylsulfanyl)-2-thiooxalyl]oxy}ethanedithioic acid (PIN)

NC-S-CH₂-CH₂-CO-S-CH₂-CH₃

S-ethyl 3-(cyanosulfanyl)propanethioate (PIN)

2-*O*-{4-[(methoxy-1-thiooxalyl)oxy]phenyl} *O*-methyl 1-thiooxalate (PIN) (not 1-*O*-{4-[(methoxy-2-thiooxalyl)oxy]phenyl} methyl 1-thiooxalate; 1-thiooxalyl is senior to 2-thiooxalyl)

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(4-{[(methylsulfanyl)-1-imido-2-thiooxalyl]oxy}phenyl)methyl methyl tetrathiooxalate (PIN)

P-65-6.3.4 Pseudoesters

Compounds having the generic formula R-CO-O-E, where E is not a carbon atom, belong to this class. Functional class names are constructed in the manner used for esters.

P-65.6.3.4.1 When E, in R-CO-O-E, is a nitrogen, phosphorus, arsenic, silicon, germanium, boron, or a chalcogen atom, pseudoesters are named as esters, unless other names must be selected in accordance with the seniority order of classes, in decreasing order: salts > acids > anhydrides > esters.

Examples:

trimethylsilyl acetate (PIN)

 CH_3 - CH_2 - SO_2 -S- $Ge(CH_3)_3$

S-(trimethylgermyl) ethanesulfonothioate (PIN)

-O-CO-CH₂

borinan-1-yl acetate (PIN)

(CH₃-CO-O)₃-B

triacetic boric trianhydride (PIN)

-O-CO-C₆H₅

phosphinan-1-yl benzoate (PIN)

H₂P-O-CO-CH₃ acetic phosphinous anhydride (PIN)

> CH₃-CO-O-SSS-CH₃ methyltrisulfanyl acetate (PIN)

> > (CH₃)₂N-O-CO-CH₃

O-acetyl-*N*,*N*-dimethylhydroxylamine (PIN) (hydroxylamine is a retained preferred IUPAC name; see P-68.3.1.1.1)

CH₃-CO-O-P(CH₃)₂

acetic dimethylphosphinous anhydride (PIN; see P-67.1.3.2)

P.65.6.3.4.2 For compounds where E is an element belonging to Group 16, see also P-68.4.

P-65.6.3.5 Cyclic esters

Compounds that may be considered as derived from a hydroxy carboxylic acid or hydroxy sulfonic acid by loss of water intramolecularly are classified as 'lactones' and 'sultones', respectively. For these compounds heterocyclic names are preferred IUPAC names. Names derived from corresponding hydroxy acids are not recommended, but may be used in general nomenclature.

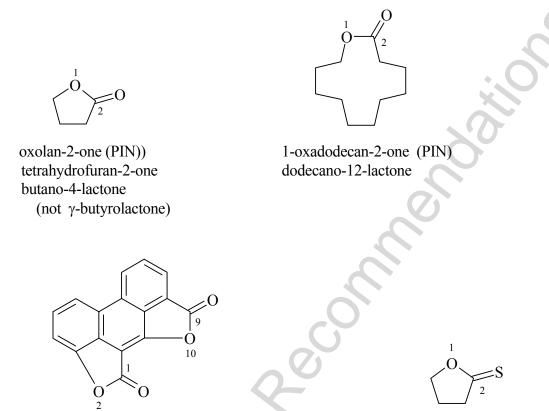
P-65.6.3.5.1 Lactones.

Intramolecular esters of hydroxy carboxylic acids are 'lactones' and are named in two ways.

- (1) as heterocyclic pseudoketones by adding the suffix 'one', 'e', etc. to the name of the heterocyclic parent [Hantzsch-Widman names are used for monocycles with up to ten ring members; names for saturated heterocycles are used when the system is fully saturated; otherwise, names are based on mancude heterocycles; skeletal replacement ('a') nomenclature is used for monocyclic lactones having more than ten ring atoms].
- (2) by changing the 'ic acid' ending of a systematic 'oic acid' name for the nonhydroxylated parent acid to 'lactone', and inserting a locant designating the position of the hydroxy group between the 'o' and 'lactone'.

Method (1) gives preferred IUPAC names.

Examples:

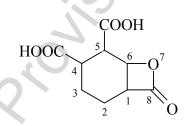


phenanthro[1,10-*bc*:9,8-*b*'*c*']difuran-1,9-dione (PIN) phenanthrene-1,10:9,8-dicarbolactone

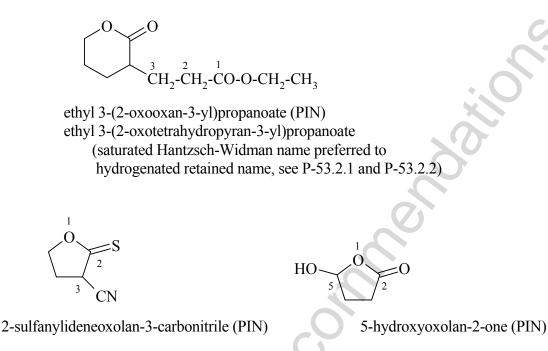
oxolane-2-thione (PIN)

A lactone, as a pseudoketone, ranks lower in the seniority of classes than an acid or an ester, but higher than an alcohol, amine, or imine.

Examples:



8-oxo-7-oxabicyclo[4.2.0]octane-4,5-dicarboxylic acid (PIN) 2-oxohexahydro-2*H*-benzooxete-5,6-dicarboxylic acid (to be a preferred ring fusion name, there must be a fusion site and two five membered rings, see P-52.5.2.1)



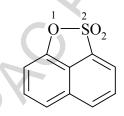
P-65.6.3.5.2 Sultones and sultines are cyclic esters of hydroxy sulfonic acids and sulfinic acids, respectively.

P-65.6.3.5.2.1 Sultones and sultines may be named in three ways:

- (1) as heterocyclic heterones;
- (2) by citing the term 'sultone' or 'sultine' denoting the cyclic –O-SO₂– or –O-SO– group after the name of the appropriate parent hydride preceded by a pair of locants describing the points of attachment of the sulfonyl or sulfinyl group and the oxygen atom, respectively; the locant of the sulfonyl or sulfinyl 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 sultone or sultine rings.
- (3) as heterocycles according to functional class names using the class name 'oxide'

Method (1) gives preferred IUPAC names.

Examples:



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



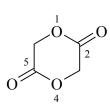
3-methyl-1, $2\lambda^6$ -oxathiane-2,2-dione (PIN) pentane-2,5-sultone 3-methyl-1,2-oxathiane 2,2-dioxide



 $1,2\lambda^4$ -oxathiolan-2-thione (PIN) 1,2-oxathiolane 2-thiooxide

P-65.6.3.5.3 Lactides are cyclic esters derived by multiple esterification between two (or more) molecules of a hydroxy acid and are named as heterocyclic compounds.

Examples:



1,4-dioxane-2,5-dione (PIN)

tribenzo[*b,f,j*][1,5,9]-trioxacyclododecin-6,12,18-trione (PIN) (not trisalicylide)

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CO 6

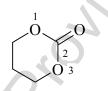
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P-65.6.3.5.4 Other cyclic esters derived from different hydroxy acids or from polybasic acids and polyhydroxy compounds are named as heterocycles.

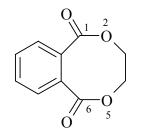
Examples:



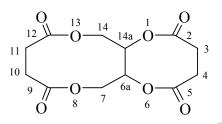
1,3-dioxan-2-one (PIN)



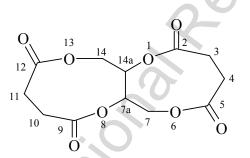
 $1,3,2\lambda^5$ -dioxaphosphepan-2-one (PIN)



3,4-dihydro-2,5-benzodioxepin-1,6-dione (PIN) 3,4-dihydrobenzo[*f*]dioxepin-1,6-dione



octahydro-1,6,8,13-tetraoxacycloocta[10]annulene-2,5,9,12-tetrone (PIN)



octahydro-1,6,8,13-tetraoxanonalene-2,5,9,12-tetrone (PIN)

P-65.6.3.6 Acylals

Acylals are a class of compounds with the general structures R-CH(O-CO-R')₂, R'C(OCOR")₂, etc. Specific compounds are named as esters.

Example:

² ¹ CH₃-CH(O-CO-CH₂-CH₂-CH₃)₂ ethane-1,1-diyl dipropanoate (PIN)

(traditionally ethylidene dipropanoate)

P-65.7 Anhydrides and their analogues

P-65.7.0 Introduction

- P-65.7.1 Symmetric anhydrides
- P-65.7.2 Mixed anhydrides
- P-65.7.3 Cyclic anhydrides
- P-65.7.4 Thioanhydrides and analogues
- P-65.7.5 Peroxyanhydrides and chalcogen analogues
- P-65.7.6 Diacyl derivatives of trioxidane and chalcogen analogues
- P-65.7.7 Polyanhydrides
- P-65.7.8 Polyfunctional anhydrides

P-65.7.0 Introduction

Anhydrides are compounds consisting of two acyl groups bonded to the same oxygen atom, i.e., acyl-O-acyl. Symmetric and mixed anhydrides have identical and different acyl groups, respectively. The central oxygen atom can be replaced by chalcogen atoms, a peroxy group and its chalcogen analogues, and by three consecutive oxygen atoms or any combination of three chalcogen atoms.

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Polyanhydrides and polyfuctional anhydrides are also described in this Section.

P-65.7.1 Symmetric anhydrides

Symmetric anhydrides of monobasic acids, substituted or unsubstituted, are named by replacing the term 'acid' of an acid name by the class name 'anhydride'.

Examples:

CH₃-CO-O-CO-CH₃

acetic anhydride (PIN)

C₆H₅-CS-O-CS-C₆H₅

benzenecarbothioic anhydride (PIN) (thiobenzoic) anhydride (PIN)

(CH₃-CH₂-CH₂-CH₂-CH₂-CO)₂O hexanoic anhydride (PIN)

CH₃-CH₂-CS-O-CS-CH₂-CH₃

(propanethioic) anhydride (PIN) (thiopropionic) anhydride

cyclohexanecarboxylic anhydride (PIN)

benzenesulfonic anhydride (PIN)

(Cl-CH₂-CO-O)₂O chloroacetic anhydride (PIN)

2 1 (Cl-CH₂-CH₂-SO)₂O

2-chloroethanesulfinic anhydride (PIN)

P-65.7.2 Mixed anhydrides

Anhydrides derived from different monobasic acids are named by citing the names of the two acids, substituted or unsubstituted, without the class name 'acid' in alphabetical order, followed by the class name 'anhydride' as a separate word.

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Examples:

CH₃-CO-O-CO-CH₂-CH₃

acetic propanoic anhydride (PIN)

C₆H₅-CO-O-CS-CH₃

benzoic ethanethioic anhydride (PIN) benzoic thioacetic anhydride C_6H_5 -SO-O-SO₂-CH₂-CH₃

benzenesulfinic ethanesulfonic anhydride (PIN)

acetic chloroacetic anhydride (PIN)

$$Cl-CH_2-CO-O-SO_2$$
 NO_2

chloroacetic 4-nitrobenzene-1-sulfonic anhydride (PIN)

Mixed anhydrides with carbonic acid, cyanic acid, and inorganic acids are named as anhydrides. Terms such as 'monoanhydride' are used with di-, tri- or tetrabasic acids to specify the appropriate number of anhydride linkages.

Examples:

CH₃-CO-O-CN

acetic cyanic anhydride (PIN)

HO-B(O-CO-CH₃)₂ acetic boric dianhydride (PIN) (see also P-65.7.7) C₆H₅-CO-O-PH₂ benzoic phosphinous anhydride (PIN)

CH₃-CO-O-CO-CH₂-Cl

P-65.7.3 Cyclic anhydrides

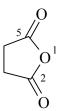
Cyclic anhydrides formed from two acid groups attached to the same parent hydride structure are named in two ways:

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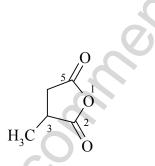
- (1) as heterocyclic pseudoketones;
- (2) by changing the class term 'acid' to 'anhydride' in the systematic or retained name of the dibasic acid.

Method (1) generates preferred IUPAC names

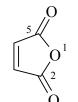
Examples:



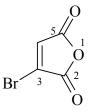
oxolane-2,5-dione (PIN) 3,4-dihydrofuran-2,5-dione butanedioic anhydride succinic anhydride



3-methyloxolane-2,5-dione (PIN) 3-methyl-3,4-dihydrofuran-2,5-dione 2-methylbutanedioic anhydride methylsuccinic anhydride



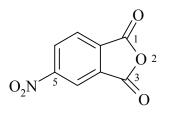
furan-2,5-dione (PIN



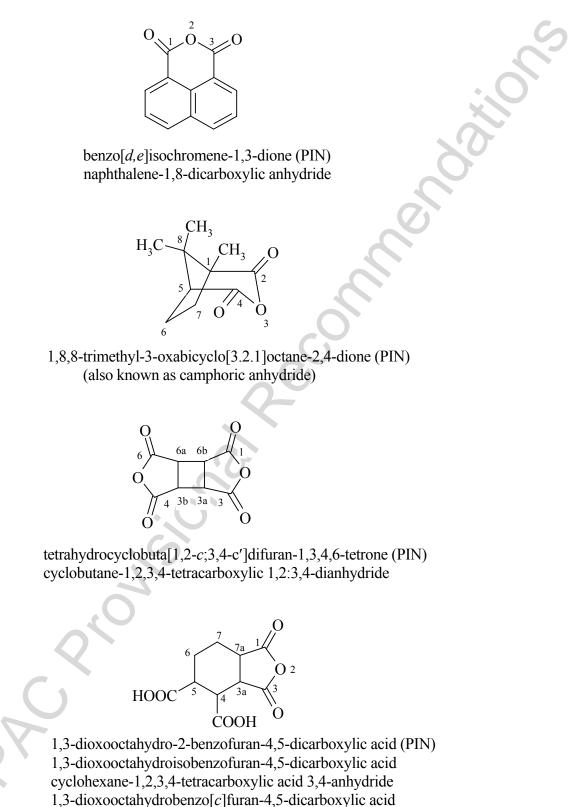
3-bromofuran-2,5-dione (PIN) bromomaleic anhydride

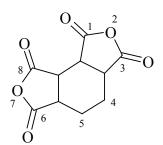


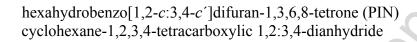
2-benzofuran-1,3-dione (PIN) isobenzofuran-1,3-dione benzo[*c*]furan-1,3-dione phthalic anhydride



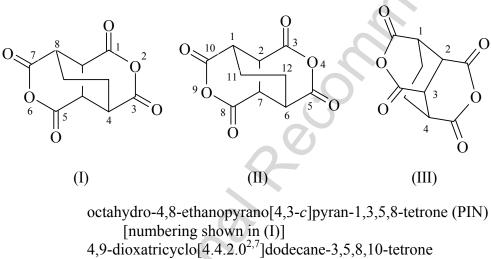
5-nitro-2-benzofuran-1,3-dione (PIN)
5-nitroisobenzofuran-1,3-dione
4-nitrophthalic anhydride
5-nitrobenzo[*c*]furan-1,3-dione







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[numbering shown in (II)] cyclohexane-1,2,3,4-tetracarboxylic 1,3:2,4-dianhydride [numbering shown in (III)]

P-65.7.4 Thioanhydrides and analogues

Chalcogen analogues of anhydrides having the general structure -CO-X-CO-, -CO-X-CS-, or -CS-X-CS-, where X is -S -, -Se -, or -Te -, are named using the class names 'thioanhydride', 'selenoanhydride' or 'telluroanhydride', respectively.

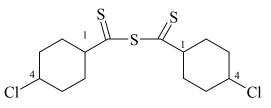
Examples:

C₆H₅-CO-S-CO-C₆H₅

benzoic thioanhydride (PIN)

CH₃-CH₂-SO₂-S-CS-C₆H₅

ethanesulfonic benzenecarbothioic thioanhydride (PIN) ethanesulfonic thiobenzoic thioanhydride



4-chlorocyclohexane-1-carbothioic thioanhydride (PIN)

CH₃-CO-Se-CO-CH₃

acetic selenoanhydride (PIN)

The various unsymmetrical thioanhydrides derived from acetic propanoic anhydride are named as follows.

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CH₃-CO-O-CO-CH₂-CH₃

acetic propanoic anhydride (PIN) acetic propionic anhydride

CH₃-CO-O-CS-CH₂-CH₃

acetic propanethioic anhydride (PIN) acetic thiopropionic anhydride

CH₃-CO-S-CO-CH₂-CH₃

CH₃-CS-O-CO-CH₂-CH₃

acetic propanoic thioanhydride (PIN) acetic propionic thioanhydride ethanethioic propanoic anhydride (PIN) propionic thioacetic anhydride

CH₃-CS-O-CS-CH₂-CH₃ ethanethioic propanethioic anhydride (PIN) thioacetic thiopropionic anhydride

CH₃-CS-S-CS-CH₂-CH₃

ethanethioic propanethioic thioanhydride (PIN) thioacetic thiopropionic thioanhydride

CH₃-CH₂-CS-Se-CO-CH₃

acetic propanethioic selenoanhydride (PIN) acetic thiopropionic selenoanhydride

CH₃-CS-S-CO-CH₂-CH₃

ethanethioic propanoic thioanhydride (PIN) propionic thioacetic thioanhydride

P-65.7.5 Peroxyanhydrides and chalcogen analogues

Peroxyanhydrides, R-CO-OO-CO-R or R-CO-OO-COR', are named by replacing the term 'acid' of an acid or two different acids by the class name 'peroxyanhydride'.

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Example:

CH₃-CO-OO-CO-CH₃

acetic peroxyanhydride (PIN)

Related anhydrides, in which the junction between two acyl groups is of the type -SS- -OS-, -SSe-, etc. are named as 'dithioperoxyanhydrides', 'thioperoxyanhydrides, 'selenothioperoxyanhydrides', etc.. When it is necessary to specify the position of the chalcogen atoms between two unsymmetrically substituted acyl groups or two different acyl group, the acyl group name is preceded by a the appropriate italicized capital element symbols indicating its attachment.

Examples:

CH₃-CO-S-O-CO-CH₃

CH₃-CO-S-O-CO-CH₂-CH₃

acetic thioperoxyanhydride (PIN)

S-acetic *O*-propanoic thioperoxyanhydride (PIN)

CH₃-CO-SS-CO-CH₃

acetic dithioperoxyanhydride (PIN)

P-65.7.6 Acyclic structures with three or more chalcogen atoms linking two acyl groups

P-65.7.6.1 Acyclic monoanhydrides named as pseudo ketones

Anhydrides derived from peroxy acids and their chalcogen analogues are named substitutively as pseudoketones (see P-64.3). Multiplicative names are preferred when the conditions for their use are fulfilled (see P-15.3).

Examples:

¹" ¹ CH₃-CO-OOO-CO-CH₃

1,1'-trioxidanediylbis(ethan-1-one) (PIN)

 CH_3 -CO-SSSS-CO- CH_2 - CH_3

1-(acetyltetrasulfanyl)propan-1-one (PIN)

CH₃-CO-S-O-S-CO-CH₃

1,1'-dithioxanediylbis(ethan-1-one) (PIN)

CH₃-CO-OO-S-CO-CH₃

1-[(acetylperoxy)sulfanyl]ethan-1-one (PIN)

P-65.7.6.2 Acyclic monoanhydrides are named by skeletal replacement ('a') nomenclature when the conditions for its use are fulfilled (see P-15.4).

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Example:

¹ ² ³ ⁴ ⁵ ⁶ ⁷ ⁸ CH₃-CO-O-Te-Se-S-CO-CH₃

3-oxa-6-thia-5-selena-4-telluraoctane-2,7-dione (PIN)

P-65.7.7 Polyanhydrides

Di- and trianhydrides have two and three –CO-O-CO– groups, respectively. They are named in different ways, depending on the general structure of the system.

P-65.7.7.1 Linear polyanhydrides

Linear polyanhydrides are formed by a continuous succession of anhydride linkages resulting from the elimination of water between two or more monobasic acids, called 'exterior acids' and one or more dibasic acids, called 'interior acids'. They are named in the following way.

P-65.7.7.1.1 When interior acids are identical and symmetrical, exterior acids may be identical or different. Names are formed by citing the names of the characteristic part of acids, in alphanumerical order, as separate words followed by the term 'anhydride' preceded by a multiplying prefix denoting the number of anhydride linkages. Identical acids are named by using the appropriate multiplying prefixes.

Examples:

CH₃-CO-O-CO-CH₂-CH₂-CO-O-CO-CH₃

diacetic butanedioic dianhydride (PIN)

CH₃-CO-O-SO₂-CH₂-SO₂-O-CO-CH₂-CH₃

acetic methanedisulfonic propanoic dianhydride (PIN)

CH₃-CH₂-CO-O-CO-CH₂-CH₂-CO-O-CO- CH₂-CH₂-CH₃ butanedioic butanoic propanoic dianhydride (PIN)

CH₃-CO-O-CO-CH₂-CH₂-CO-O-CO-CH₂-CH₂-CO-O-CO-CH₂-CH₃

acetic dibutanedioic propanoic trianhydride (PIN)

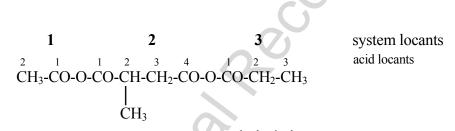
$CH_3\text{-}CO\text{-}O\text{-}CO\text{-}CH_2\text{-}CO\text{-}O\text{-}CO\text{-}CH_2\text{-}CO\text{-}O\text{-}CO\text{-}CH_3$

diacetic butanedioic propanedioic trianhydride (PIN)

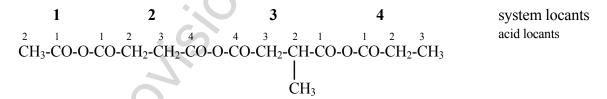
P-65.7.7.1.2 When the conditions required in P-65.7.7.1.1 are not fulfilled, the following methods are used.

P-65.7.7.1.2.1 Acid residues constituting the polyanhydride are numbered consecutively alphanumerically and denoted by locants called 'system locants'. Each acid residue is numbered systematically; these locants are called 'acid locants'. Names are formed by citing the names of the acid residues in alphanumerical order of their 'system locants' followed by the term 'anhydride', which is preceded by the appropriate multiplying prefix denoting the number of anhydride linkages. This anhydride term is preceded by composite locants (formed by the system locant and the 'acid locant' cited as a superscript for each anhydride linkage) indicating the anhydride junctions, in a manner similar to that used in Phane Nomenclature (P-26.4.3) and ring assembly nomenclature (see P-29.3). If there is a choice of locants for interior acid residues, lowest locants are assigned in the order of the 'system locants'.

Examples:



acetic 2-methylbutanedioic propanoic $(1^1, 2^1; 2^4, 3^1)$ -dianhydride (PIN)



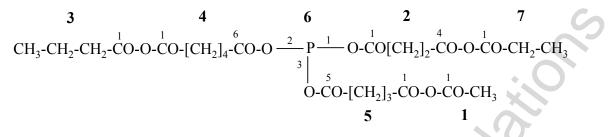
acetic butanedioic 2-methylbutanedioic propanoic $(1^{1}, 2^{1}: 2^{4}, 3^{4}: 3^{1}, 4^{1})$ -trianhydride (PIN)

not

system locants acid locants

acetic butanedioic 2-methylbutanedioic propanoic (1¹,2⁴:2¹,3⁴:3¹4¹)-trianhydride

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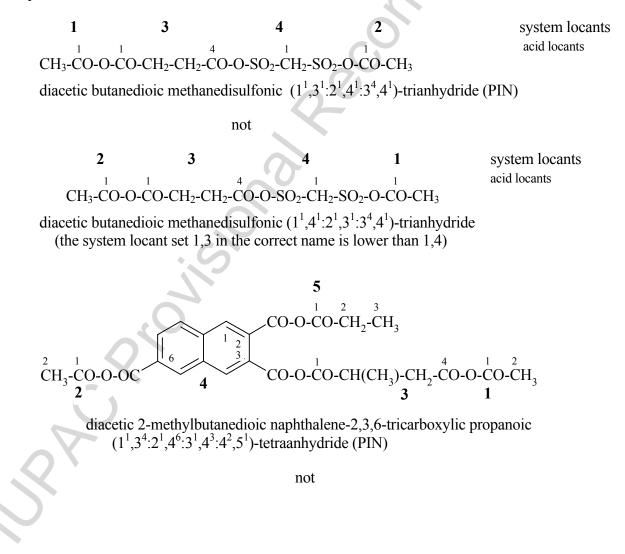


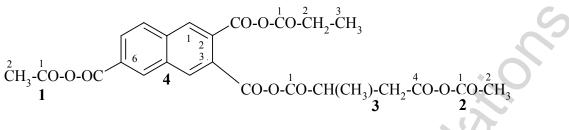
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acetic butanedioic butaneoic hexanedioic pentanedioic phosphoric propanoic $(1^1, 5^1: 2^1, 6^1: 2^4, 7^1: 3^1, 4^1: 4^6, 6^2: 5^5, 6^3)$ -hexaanhydride (PIN)

P-65.7.7.1.2.2 If there is choice in numbering involving system locants and acid locants, lowest locants are assigned to system locants so as to have the lowest locant set at the first point of difference.

Examples:

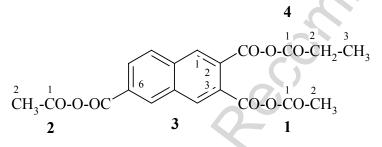




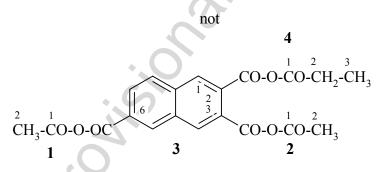
diacetic 2-methylbutanoic naphthalene-2,3,6-tricarboxylic propanoic $(1^1,4^6:2^1,3^4:3^1,4^3:4^2,5^1)$ -tetraanhydride (the system locant set 1,3 in the correct name is lower than 1,4)

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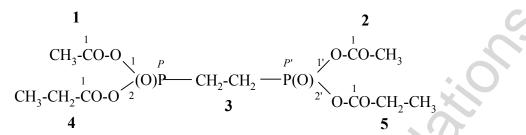
P-65.7.7.1.2.3 If a further choice is still possible because of a lack of difference between system locants, lowest locants are assigned so as to have the lowest set of locants in the order of citation. Example:



diacetic naphthalene-2,3,6-tricarboxylic propanoic (1¹,3³:2¹,3⁶:3²,4¹)-trianhydride (PIN)

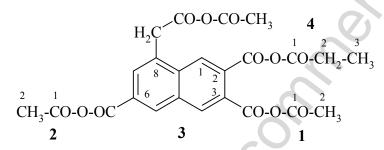


diacetic naphthalene-2,3,6-tricarboxylic propanoic $(1^1,3^6:2^1,3^3,3^2,4^1)$ -trianhydride (the set of locants $1^1,3^3:2^1,3^6:3^2,4^1$ is lower than $1^1,3^6:2^1,3^3,3^2,4^1$)



diacetic P,P'-ethane-1,2-diylbis(phosphonic) dipropanoic $(1^1,3^1:2^1,3^1:3^2,4^1:3^2',5^1)$ -tetraanhydride (PIN)

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1,2-diacetic 3-{8-[2-(acetyloxy)-2-oxoethyl]naphthalene-2,3,6-tricarboxylic} propanoic $(1^1,3^3:2^1,3^6:3^2,4^1)$ -trianhydride (PIN)

P-65.7.7.3 Chalcogen analogues of polyanhydrides

When chalcogen atoms are present in polyanhydrides, names are formed in different ways as follows.

P-65.7.7.3.1 When all anhydride linkages are identical, such as -CO-S-CO-, names are formed by using the class name, for example, 'thioanhydride', preceded by the multiplying prefixes 'bis', 'tris', etc.

Example:

diacetic butanedioic bis(thioanhydride) (PIN)

P-65.7.7.3.2 When mixed anhydride linkages are present, the usual seniority order established for chalcogen atoms, O > S > Se > Te, is used to determine the senior anhydride linkage. This senior anhydride is chosen as the basis of the name and other anhydride linkages are named substitutively. Example:

acetic 5-(acetylsulfanyl)-5-oxopentanoic anhydride (PIN) acetic 4-[(acetylsulfanyl)carbonyl]butanoic acid

P-65.7.7.3.3 When the chalcogen atom replaces an oxygen atom in a carbonyl group, i.e. >C=S, thiocarboxylic acids and thioacyl groups are used in the manner described for anhydrides and polyanhydrides.

Examples:

CH₃-CS-O-CO-CH₂-CH₂-CO-O-CO-CH₃

acetic butanedioic ethanethioic dianhydride (PIN)

CH₃-CO-O-CS-CH₂-CH₂-CS-O-CO-CH₃

diacetic butanebis(thioic) dianhydride (PIN)

CH₃-CO-O-CS-CH₂-CH₂-CS-S-CS-CH₃

acetic 4-(ethanethioylsulfanyl)-4-thioxobutanethioic anhydride (PIN)

P-65.7.7.4 Skeletal replacement ('a') nomenclature and phane nomenclature.

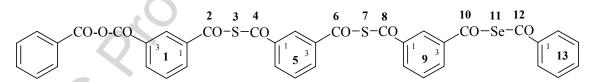
P-65.7.7.4.1 Skeletal replacement ('a') nomenclature is used when four hetero units are present in acyclic anhydrides and other conditions are fulfilled (see P-15.4 and P-65.7.7.3.2) Example:

 $CH_{3}\text{-}CO\text{-}O\text{-}CO\text{-}CH_{2}\text{-}O\text{-}CH_{2}\text{-}CO\text{-}S\text{-}CS\text{-}CH_{2}\text{-}O\text{-}CH_{2}\text{-}CS\text{-}S\text{-}CO\text{-}[CH_{2}]_{2}\text{-}CO\text{-}O\text{-}CO\text{-}CH_{3}$

5,13-dioxo-7,11-dithioxo-3,9-dioxa-6,12-dithiahexadecane1,16-dioic diacetic anhydride (PIN)

P-65.7.7.4.2 Phane nomenclature is used when the conditions for its use are fulfilled (see P-25.5 and P-65.7.7.3.2).

Example:



benzoic 2,4,6,8,10,12-hexaoxo-3,7-dithia-11-selena-1,13(1),5,9(1,3)tetrabenzenatridecaphane-1³-carboxylic anhydride (PIN)

P-65.7.8 Polyfunctional anhydrides

In the seniority of classes, acids are senior to anhydrides, and anhydrides are senior to esters and other classes (see P-41).

P-65.7.8.1 In presence of an acid, anhydrides are expressed by prefixes denoting the different components of the anhydride.

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Examples:

OH | 4 3 2 1 CH₃-CO-O-P(O)-O-CO-CH₂-CH₂-COOH

4-{[(acetyloxy)hydroxyphosphoryl]oxy}-4-oxobutanoic acid (PIN)

OH | CH₃-CO-O-CO-CH₂-CH₂-CO-O-P(O)-OH

{[4-(acetyloxy)-4-oxobutanoyl]oxy}phosphonic acid (PIN)

CH₃-CO-O-CS-CH₂-CH₂-COOH

4-(acetyloxy)-4-sulfanylidenebutanoic acid (PIN) 4-(acetyloxy)-4-thioxobutanoic acid

P-65.7.8.2 Nomenclature for assemblies of identical units is used when symmetry requirements for its use are fulfilled.

Example:

HOOC-CH₂-CH₂-CO-O-CO-CH₂-CH₂-CO-O-CO-CH₂-CH₂-COOH 4,4'-[butanedioylbis(oxy)]bis(4-oxobutanoic acid) (PIN)

P-65.7.8.3 Anhydride nomenclature is applied when esters and other lower ranking characteristic groups are present.

Examples:

O-CH₃

CH₃-CO-O-P(O)-O-CO-CH₃

diacetic (methyl dihydrogen phosphate) dianhydride (PIN)

$CH_3\text{-}CS\text{-}S\text{-}CO\text{-}CH_2\text{-}CH_2\text{-}CO\text{-}O\text{-}CH_3$

ethanethioic (4-methoxy-4-oxobutanoic) thioanhydride (PIN) (methyl hydrogen butanedioate) thioacetic thioanhydride

CH₃-CO-O-CO-CH₂-CN acetic 2-cyanoacetic anhydride (PIN)