Nomenclature of polyfunctional group organic compounds

A nomenclature dilemma: what do you do when there's MULTIPLE functional groups Which suffix do we use?





Family	as Prefix	as Suffix
Carboxylic acid	carboxy-	-oic acid -carboxylic acid
Acid anhydride	<i>alkanoyl</i> oxycarbonyl-	-oic anhydride -carboxylic anhydride
Ester	alkoxycarbonyl-	<i>alk</i> yl -oate <i>alk</i> yl -carboxylate
Acid halide	halocarbonyl-	-oyl <i>hal</i> ide -carbonyl <i>hal</i> ide
Amide	carbamoyl-	-amide -carboxamide
Nitrile	cyano-	-nitrile -carbonitrile
Aldehyde	oxo- formyl- methanoyl-	-al -carbaldehyde
Ketone	oxo- <i>alkan</i> oyl-	-one

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1] Carboxylic acid

Case (I) Suffix "1"

If the carbon of carboxyl group is being inclusive in the longest chain "main chain" numbering, then the letter e in alkane chain is replaced by oic acid



Hexanoic acid

(Z)2-Heptenoic acid

How to name compound with two carboxy groups?

If the compound has two carboxylic groups then it is known as dioic acid and named as...dioic acid through replacing the letter e by dioic acid



Some common di carboxylic acids





2,6-Naphthalenedicarboxylic acid

Phthalic acid

OH

Case (II) Suffix "2"

If the carbon of the carboxyl group is not counted but still having the most priority, then it is named as cyclic system followed by carboxylic acid Examples:-



Examples for some common carboxylic acids



benzoic acid



Toluic acid



o-phthalic acid



Anisic acid



Salicylic acid

2] Ester

Case (I) Suffix "1"

If the carbon of carboxyl group is being inclusive in the longest chain "main chain" numbering, then the letter e in alkane chain is replaced by oate (N.B:the group that is attached to oxygen atom forming the ester must come first before all substituents)

(E) Phenyl-2-hexenoate

Ethyl heptanoate

Case (II) Suffix "2"

If the carbon of the carboxy ester group is not counted but still having the most priority, then it is named as Name of cyclic system followed by carboxylate.

Examples:-



Ethyl cyclopentanecarboxylate





Ethyl 2,3,5-triamino-4,6-di-tert-butyl-8-mercaptocyclooctanecarboxylate

Case III "Prefix"

If there is a functional group which has more priority than the ester; that means the ester is substituent. In this case the ester is named as alkoxycarbonyl or aroxycarbonyl taking into your account that the carbon of carboxylate is not inclusive in numbering the longest chain.



5-Ethoxycarbonylpentanoic acid



(E)-4-Phenoxycarbonyl-3-butenoic acid



Aspirin Or 2-Acetoxybenzoic acid Or O-Acetyl salicylic acid

3] Acid Halide

Case (I) Suffix "1"

If the carbon of carbonyl group is being inclusive in the longest chain "main chain" numbering, then the letter e in

alkane chain is replaced by oyl halide.



Butanoyl chloride



(2E,4E)--2,4-Hexadienoyl bromide



Case (II) Suffix "2"

If the carbon of the carbonyl halide group is not counted but still having the most priority, then it is named as Name of cyclic system followed by carbonylhalide Examples:-



Cyclopentanecarbonyl bromide



1,3-Cyclohexadienecarbonyl chloride



3,5-diamino-2,8-dimercapto-6-methylcyclooctanecarbonyl chloride 13

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Case III "Prefix"

If there is a functional group which has more priority than the acid halid; that means the acid halide is a substituent. In this case the acid halide is named as halo carbonyl taking into your account that the carbon of carbonyl halide is not inclusive in numbering the longest chain.



5-Acetyl-2-Chlorocarbonyl-3-formyl-4-methoxycarbonyl-benzoic acid

4-Amides

Case (I) Suffix "1"

If the carbon of amido group is being inclusive in the longest chain "main chain" numbering, then the letter e in alkane chain is replaced by amide.





Aetamide Or Ethanamide



Benzamide

Primary amides

are named by changing the name of the acid by dropping the -oic acid endings and adding –amide (or e is replaced by amide). The carbonyl carbon is given the #1 location number. It is not necessary to include the location number in the name because it is assumed that the functional group will be on the end of the parent chain.



 \mathbf{M}_{2}

Butanamide

decanamide

Secondary amides

are named by using an upper case N to designate that the alkyl group is on the nitrogen atom. Alkyl groups attached to the nitrogen are named as substituents. The letter N is used to indicate they are attached to the nitrogen.





N-Tertbutyloctanamide

Tertiary amides

are named in the same way as secondary amides, but with two N's or *N,N*-Di.....if N is bonded to similar group or substituent

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N-Allyl-*N*-isopropyloctanamide

N,N-dimethylheptanamide

Case (II) Suffix "2"

If the carbon of the amido group is not counted but still having the most priority, then it is named as Name of cyclic system followed by carboxamide. Examples:-





2-Hydroxy--3,4-dioxo *N*,*N*dimethylcyclobutanecarboxamide

2-*Tert*-butoxy-3-phenylcyclopropane carboxamide

Case III "Prefix"

If there is a functional group which has more priority than the amide; that means the amide is substituent and the carbonyl of amide is directly bonded to the main longest chain; in this case it is named as carbamoyl.





(E)4-Phenylcarbamoyl-but-3-enoic acid

While if the amide group is bonded to the main chain by nitrogen atom; then it is named as alkanoylamino or alkanamido.



4-Acetylamino-2-diisobutylcarbamoyl-5-formylamino-cyclohexanecarboxylic acid OR

4-Acetamido-2-diisobutylcarbamoyl-5-formamido-cyclohexanecarboxylic acid

5] Nitrile

Case (I) Suffix "1"

If the carbon of nitrile group is being inclusive in the longest chain "main chain" numbering, then after the alkane just add the word nitrile (alkane nitrile)

Propanenitrile

NC

(2E,4E)--2,4-Hexadienenitrile



Case (II) Suffix "2"

If the carbon of the nitrile group is not counted but still having the most priority, then it is named as Name of cyclic system followed by carbonitrile Examples:-





2-Ethyl-3,4-dioxocyclobutanecarbonitrile

2,3-Diphenylcyclo propanecarbonitrile



4,4-Dimethyl-2,6-diphenoxycycloheptanecarbonitrile

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Case III "Prefix"

If there is a functional group which has more priority than the nitrile; that means the nitrile is substituent. In this case the nitrile is named as cyano taking into your account that the carbon of CN group is not inclusive in numbering the longest chain.



6-Benzyl-4-cyano-1-hydroxy-3- methoxycycloheptanecarboxylic acid

6-Aldehydes

Case (I) Suffix "1"

If the carbon of carbonyl group is being inclusive in the longest chain, then, then the letter <u>"e"</u> of alkane chain is replaced by <u>al</u>. Example;



6,7-Epoxy-3-hydroxy-4- mercapto-2- heptenal

Note:-If there are two aldehyde groups in the compound; then it is Known as dial.

Examples;





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Case (II) Suffix"

If the carbon of the carbaldehyde group is not counted but still having the most priority, then it is named as Name of cyclic system followed by the word carbaldehyde. Examples;





Case III "Prefix"

If there is a functional group which has more priority than the aldehyde; that means the aldehyde is a substituent. In this case, the aldehyde is named as:-

<u>1] Oxo :-</u>

taking into your account that the carbon of carbaldehyde is counted and being inclusive in numbering of the longest chain.



(2Z,4Z)6-Oxo-2,4-hexadienoic acid



Methyl-2,3-epoxy-5-oxopentanoate

2- Formyl (CHO)

taking into your account that the carbon of carbaldehyde is not counted and being exclusive in numbering of the longest chain.





(3Z)3-Formyl-3-heptenedinitrile

2,3-Diformylbutandioic acid



2-Formyl-3-nitro-benzoic acid

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<u>3- Oxoalkyl</u>

taking into your account that the carbon of carbaldehyde is not counted and being exclusive in numbering of the side chain. Examples;





4-(3-Oxo-propyl)-heptanedioic acid

3-Bromo-2-formyl-4-(6-oxo-hexyl)-benzoic acid

Some well-known aldehydes



Cinnamaldehyde





Salicylaldehyde

Benzaldehyde



Formaldehyde

о-Сно

Anisaldehyde



Acetaldehyde

7] Ketone

Case (I) Suffix "1"

If the carbon of carbonyl group is being inclusive in the longest chain, then the letter "e" of alkane chain is replaced by one.





4-Mercapto-3- hexanone

2.3-Epoxy-4isopropylcyclohexanone

Note:-If are two ketone groups in the compound; then it is Known as dione, then use the prefix; trione, tetraone, pentaone.....etc. Examples :-



2,4,6-Heptantrione



1,2,3,5-Cyclohexantetraone

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3,3-Dimethoxy-2,4-pentandione

Case (II) Suffix "2"

If the ketone has the priority and not counted as a chain; it is named as the case of ether (alkylalkyl ketone or aryl aryl ketone or alkyl aryl ketone) looks like ether naming.

Examples:-







Diphenyl ketone "Benzophenone"

Methylphenyl ketone ''Acetophenone'' Cyclopropylphenyl ketone

Case III "Prefix"

If there is a functional group which has more priority than the ketone; that means the ketone is a substituent. In this case the ketone is named as :-

1] Oxo taking into your account that the carbon of carbonyl is counted and being inclusive in numbering of the longest chain.



2,3,4,5-Diepoxy-6-oxoheptanal

NH₂

3,5-Dioxo hexanamide

2] Alkanoyl or aroyl

taking into your account that the carbon of ketone is not counted and being exclusive in numbering of the longest chain.



2-Benzoylcyclopropanecarbonitrile



4-Butanoylbenzoic acid



3-Hydroxy-4-propanoyl cyclopentanecarbaldehyde

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Common Names of Carboxylic Acids



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8] Amine

Case (I) Suffix "1"

Amines are named as alkanamines or alkylamine. The –e in the alkane name of the longest chain is changed to –amine or it can be named as alkyl or arylamine.

Primary Amines





1-Propanamine or 1-Propylamine

3-Butenamine or 3-Butenylamine



Cyclohexanamine or Cyclohexylamine

Secondary and Tertiary Amines

In a secondary or tertiary amine. The longest alkane chain is numbered. Each alkyl group bonded to the N atom is named as a N-alkyl group.

N-methylpropan-1-amine or N-methyl-1-propylamine

N-propyl-3-butenamine or N-propyl-3-butenamine



N-isopropylcyclohexanamine or N-isopropylcyclohexylamine



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Case (II) Suffix "2"

Another sort of nomenclature; it looks like the ether one. Alky-alkylamine, arylalkylamine or arylarylamine

Hexylpropylamine





Hexylphenylamine

Prefix:-

If amine is un-substituted (NH₂) then it is named as amino; if it is primary; alkylamino or aryl amino is it is secondary and dialkyl or diarylamino.....as follow





3-Benzylaminohexanoic acid

4-Allylmethylaminodecanoicacid



4-Diethylamino-decanoyl chloride

Applications



N-Cyclohexyl-N-cyclopentyl -3-butenamide

2]



N,*N*-Dibenzylbenzamide



N-(4-Hydroxy-phenyl)-acetamide or Paracetamol





2-Carbamoyl-3-formyl-cyclopropane carboxylic acid





3-(4-Amino-2-formyl-3,6-diisopropyl-phenyl)propanoyl bromide



(E) Ethyl-7-Bromocarbonyl-3,4-epoxy -6-heptenoate



Benzyl-2-tertbutyl-4-oxobutanoate

10]



(3E,5Z) Methyl -5-(Allylcyclopentylamino) -8-carbamoyl--3,5-octadienoate







5-(Ethylmethylcarbamoyl)-2-(hexanoylmethylamino) -4-phenoxy-cyclohexanecarboxylic acid