BP 202T - PHARMACEUTICAL ORGANIC CHEMISTRY - I

UNIT: 1 CLASSIFICATION, NOMENCLATURE & ISOMERISM

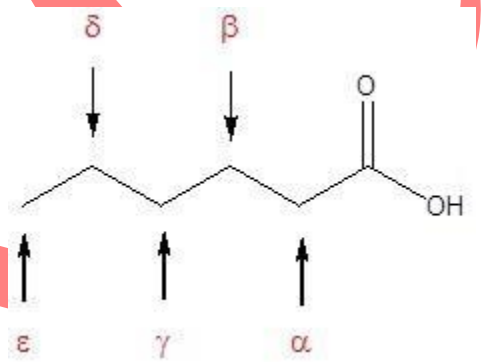
CLASS: 4

TOPIC: IUPAC NOMENCLATURE OF CARBOXYLIC ACID & ITS DERIVATIVES

Carboxylic acids are the compounds which contain carboxyl group (-COOH) attached to the organic molecule.

The IUPAC system of nomenclature assigns a characteristic suffix to these classes. The **–e** ending is removed from the name of the parent chain and is replaced **-anoic acid**. Since a carboxylic acid group must always lie at the end of a carbon chain, it is always is given the #1 location position in numbering and it is not necessary to include it in the name.

Many carboxylic acids are called by the common names. These names were chosen by chemists to usually describe a source of where the compound is found. In common names of aldehydes, carbon atoms near the carboxyl group are often designated by Greek letters. The atom adjacent to the carbonyl function is alpha, the next removed is beta and so on.



Formula	Common Name	Source	IUPAC Name
HCO_2H	formic acid	ants (L. formica)	methanoic acid
CH_3CO_2H	acetic acid	vinegar (L. acetum)	ethanoic acid

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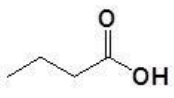
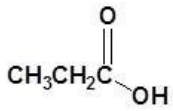
$CH_3CH_2CO_2H$	propionic acid	milk (Gk. protus prion)	propanoic acid
$CH_3(CH_2)_2CO_2H$	butyric acid	butter (L. butyrum)	butanoic acid
$CH_3(CH_2)_3CO_2H$	valeric acid	valerian root	pentanoic acid

Formula	Common Name	Source	IUPAC Name
$CH_3(CH_2)_4CO_2H$	caproic acid	goats (L. caper)	hexanoic acid
$CH_3(CH_2)_5CO_2H$	enanthic acid	vines (Gk. oenanthe)	heptanoic acid
$CH_3(CH_2)_6CO_2H$	caprylic acid	goats (L. caper)	octanoic acid
$CH_3(CH_2)_7CO_2H$	pelargonic acid	pelargonium (an herb)	nonanoic acid
$CH_3(CH_2)_8CO_2H$	capric acid	goats (L. caper)	decanoic acid

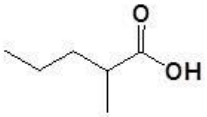
Example (Common Names Are in Red)



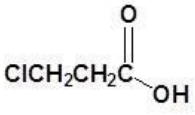
Butanoic acid
(Butyric Acid)



Propanoic acid
(Propionic Acid)



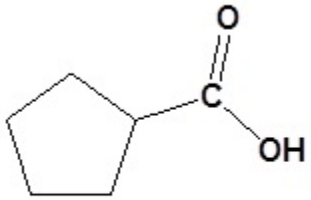
2-Methylpentanoic acid
(β-Methylvaleric acid)



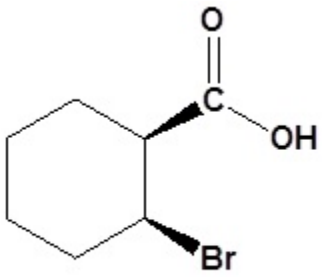
3-Chloropropanoic acid
(γ-Chloropropionic acid)

Naming carboxyl groups added to a ring

When a carboxyl group is added to a ring the suffix **-carboxylic acid** is added to the name of the cyclic compound. The ring carbon attached to the carboxyl group is given the #1 location number.



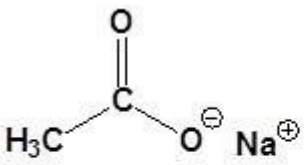
Cyclopentanecarboxylic acid



Cis-2-Bromocyclohexanecarboxylic acid

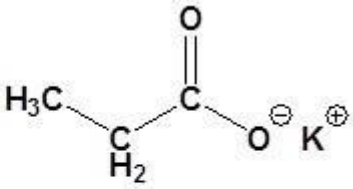
NAMING CARBOXYLATES

Salts of carboxylic acids are named by writing the name of the cation followed by the name of the acid with the **–ic acid** ending replaced by an **–ate** ending. This is true for both the IUPAC and Common nomenclature systems.



Sodium ethanoate

(Sodium Acetate)

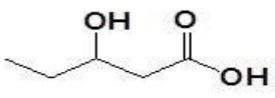


Potassium Propanoate

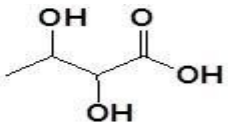
(Potassium propionate)

Naming carboxylic acids which contain other functional groups

Carboxylic acids are given the highest nomenclature priority by the IUPAC system. This means that the carboxyl group is given the lowest possible location number and the appropriate nomenclature suffix is included. In the case of molecules containing carboxylic acid and alcohol functional groups the OH is named as a hydroxyl substituent. However, the **l** in hydroxyl is generally removed.

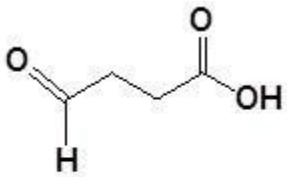


3-Hydroxypentanoic acid

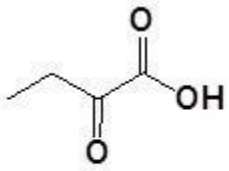


2,3-Dihydroxybutanoic acid

In the case of molecules containing a carboxylic acid and aldehydes and/or ketones functional groups the carbonyl is named as a "Oxo" substituent.

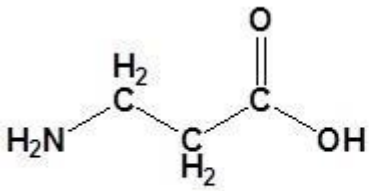


4-Oxobutanoic acid

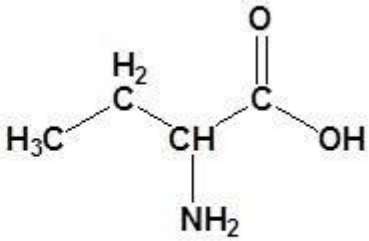


2-Oxobutanoic acid

In the case of molecules containing a carboxylic acid an amine functional group the amine is named as an "amino" substituent.



3-Aminopropanoic acid

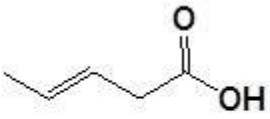


2-Aminobutanoic acid

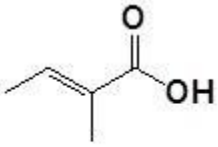
When carboxylic acids are included with an alkene the following order is followed:

(Location number of the alkene)-(Prefix name for the longest carbon chain minus the -ane ending)-(an –enoic acid ending to indicate the presence of an alkene and carboxylic acid)

Remember that the carboxylic acid has priority so it should get the lowest possible location number. Also, remember that cis/tran or E/Z nomenclature for the alkene needs to be included if necessary.



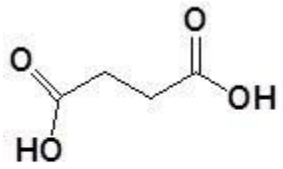
Trans-3-pentenoic acid



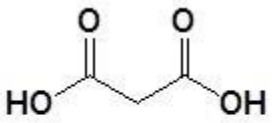
(E)-2-Methyl-2-butenoic acid

Naming dicarboxylic acids

For dicarboxylic acids the location numbers for both carboxyl groups are omitted because both functional groups are expected to occupy the ends of the parent chain. The ending **–dioic acid** is added to the end of the parent chain.



Butanedioic acid

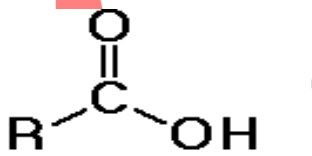


Propanedioic acid

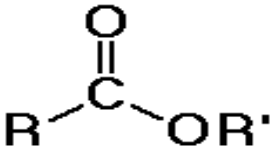
CARBOXYLIC ACI D DERIVATIVES:

Compounds in which the hydroxyl part of the carboxyl group is replaced with various other groups

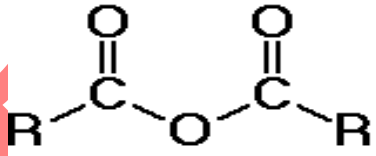
1. Esters
2. Amides
3. Acid halides
4. Acid Anhydrides



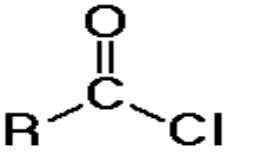
carboxylic acid



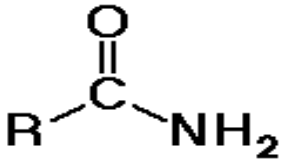
ester



acid anhydride



acid chloride
or acyl chloride



amide

nitrile

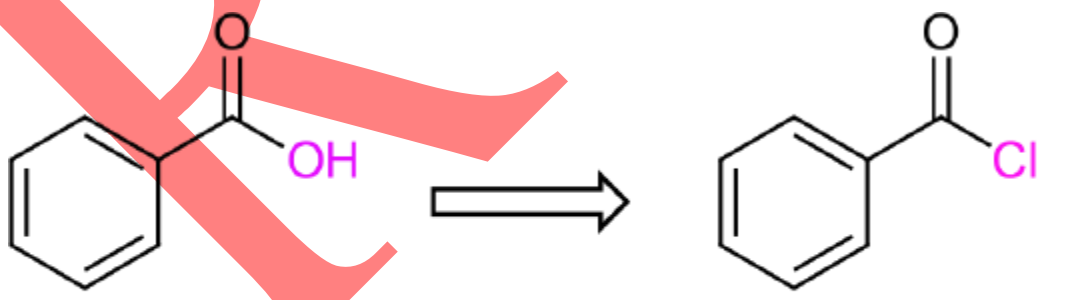
ACID HALIDES

- The nomenclature of acid halides starts with the name of the corresponding carboxylic acid.
- If the corresponding carboxylic acid has an **–oic acid** or **–ic acid** ending it is removed and replaced with the ending **-oyl** followed by the first syllable of the name of the halogen along with an **–ide** ending.
- However there are a number of specific exceptions where IUPAC allows the ending **-yl** to be used instead.

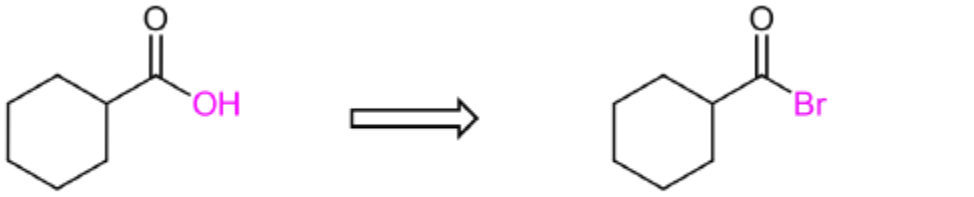
Examples:

1. formic ⇒ formyl,
2. acetic ⇒acetyl,
3. propionic ⇒propionyl
4. butyric ⇒butyryl
5. oxalic ⇒ oxalyl
6. succinic ⇒ succinyl.

- When the corresponding acid includes a **-carboxylic acid** ending, it is removed and replaced with the ending **-carbonyl.** This is followed by the first syllable of the name of the halogen along with an **–ide** ending
- The carbonyl carbon is given the #1 location number. The acid halide functional group is assumed to be on the end of the parent chain, so it is not necessary to include the functional group location number in the name



Benzoic Acid **Benzoyl Chloride**



Cyclopentanecarboxylic Acid Cyclopentanecarbonyl Bromide

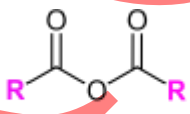
ACID ANHYDRIDES:

Nomenclature of Anhydrides, RCO_2COR'

An anhydride functional group results when two carboxylic acids combine and lose water (anhydride = without water). The names of anhydrides come from the names of the two combined carboxylic acids.

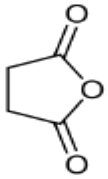
The carbonyl carbon is given the #1 location number on both chains. The anhydride functional group is assumed to be on the end of the each parent chain, so it is not necessary to include the functional group location number in the name.

Symmetrical anhydrides made from unsubstituted carboxylic acids and cyclic anhydrides made from dicarboxylic acids are named based on their corresponding carboxylic acid. The ending **-acid** is replaced with **-anhydride**. This is true for both the IUPAC and common nomenclature. An anhydride is symmetrical when it is acyclic and the acyl R groups are the same.



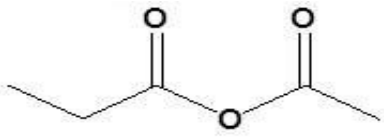
Symmetrical Anhydride

Example:



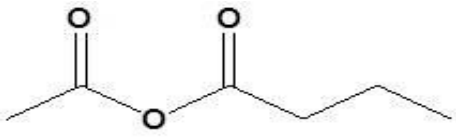
Succinic Anhydride

An unsymmetrical anhydride is created from two different carboxylic acids. For unsymmetrical anhydrides, name both acids *alphabetically* with a space between them. Then add the end word **anhydride**.



Ethanoic propanoic anhydride

(Acetic propionic anhydride)

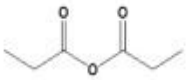


Butanoic ethanoic anhydride

(Acetic butyic anhydride)

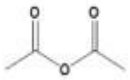
The acid anhydride functional group results when two carboxylic acids combine and lose water (anhydride = without water). Symmetrical acid anhydrides are named like carboxylic acids except the ending **-acid** is replaced with **-anhydride**. This is true for both the IUPAC and Common nomenclature.

Symmetrical anhydrides



Propanoic anhydride

(Propionic anhydride)

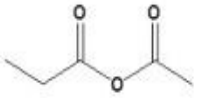


Ethanoic anhydride

(Acetic anhydride)

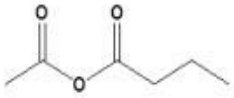
Unsymmetrical acid anhydrides

Unsymmetrical acid anhydrides are named by first naming each component carboxylic acid alphabetically arranged (without the word acid) followed by spaces and then the word anhydride.



Ethanoic propanoic anhydride

(Acetic propionic anhydride)

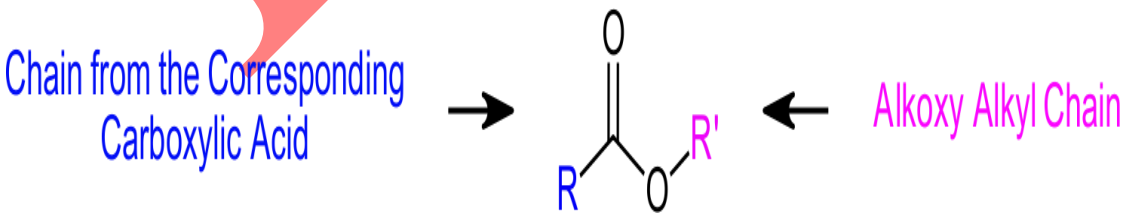


Butanoic ethanoic anhydride

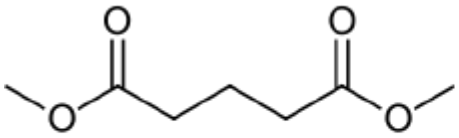
(Acetic butyic anhydride)

Nomenclature of Esters: (RCO_2R)

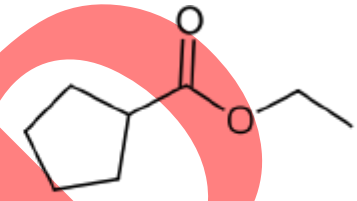
Esters consist of two distinctly different carbon chains which need to be named separately. One carbon chain is from the corresponding carboxylic acid and the other chain, attached to the singly bonded oxygen, is called the alkoxy alkyl chain.



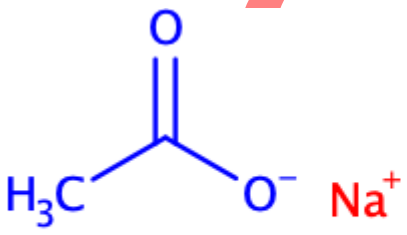
Esters are named as if the alkoxy alkyl chain is a substituent **(Prefix + yl)**. This is followed bythe name of the corresponding carboxylic acid part of the ester with **-ic acid** or **-oic acid** replacedwith the ending **–ate**. The carbonyl carbon is given the #1 location number. The carbonyl functional group is assumed to be on the end of the parent chain, so it is not necessary to include the functional group location number in the name.



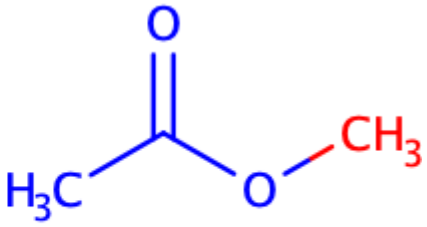
Dimethyl glutarate



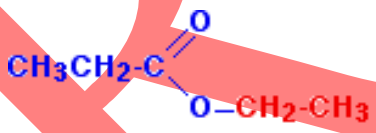
Ethyl cyclopentanecarboxylate



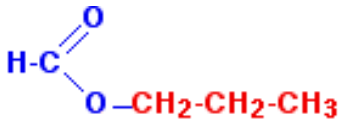
sodium ethanoate



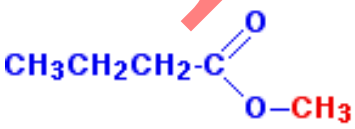
methyl ethanoate



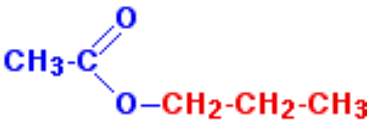
ethyl propanoate



propyl methanoate



methyl butanoate



propyl ethanoate

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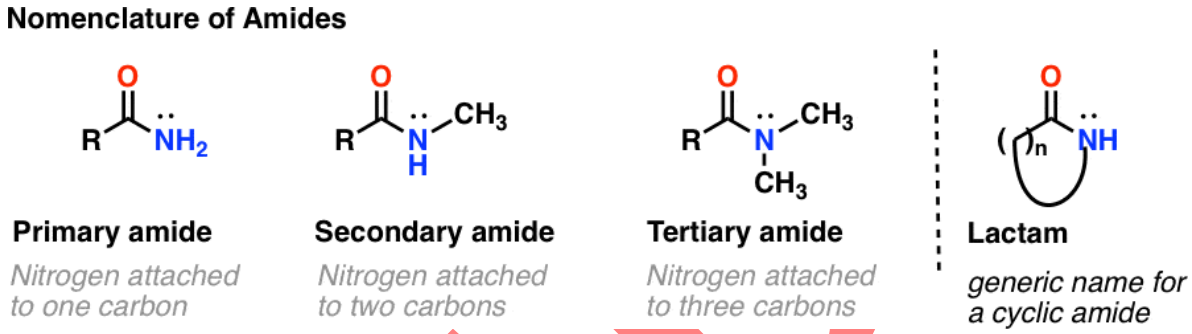
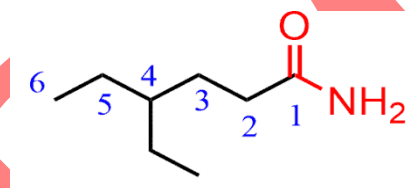
Assistant professor

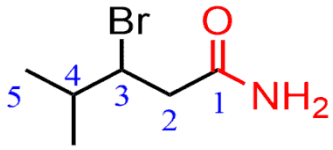
AMIDES:



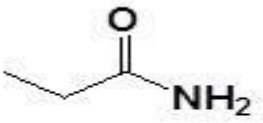
Primary amides ($RCONH_2$) are named by changing the name of the corresponding acid by removing the **-oic acid** or **-ic acid** endings and adding **-amide**. Amides derived from a cyclic carboxylic acid have the **-carboxylic acid** ending replaced with **-carboxamide**. The carbonyl carbon is given 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.



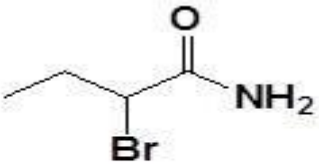
4-ethylhexanamide



3-bromo-4-methylpentanamide



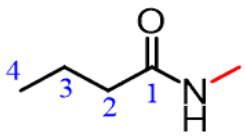
Propanamide



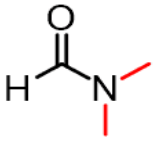
2-Bromobutanamide

Secondary (RCONHR') and tertiary (RCONR'R") amides are named by using an upper case N to designate that the alkyl groups are attached to the nitrogen atom. These alkyl groups are name as substituents **(Prefix + yl)**.

Naming Secondary and Tertiary Amides

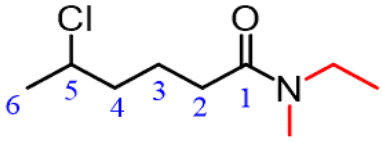


N-methylbutyramide

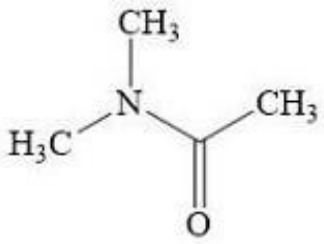


DMF - a common solvent

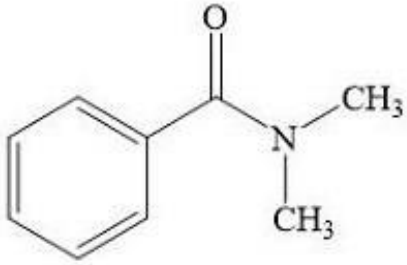
N,*N*-dimethylformamide



5-chloro-*N*-ethyl-*N*-methylhexanamide



N,N-Dimethylacetamide



N,N-Dimethylbenzamide