Nomenclature in organic chemistry

Introduction

The great diversity of organic compounds requires the use of a nomenclature allowing a common language in chemistry with the aim of knowing the compounds and differentiating them.

The International Union of Pure and Applied Chemistry (IUPAC) is a scientific organization that has established the rules of nomenclature and revises them periodically.

I/ Nomenclature of alkanes (general formula: C_nH_{2n+2})

These are saturated acyclic HC, their names end with the suffix ane.

1/ Linear alkanes

The names of the first twelve compounds which will later be used in the nomenclature of all other organic compounds are given in the table below.

formula	Name	Formula	Name
CH_4	Méthane	$CH_3-(CH_2)_5-CH_3$	Heptane
CH_3-CH_3	Ethane	$CH_3-(CH_2)_6-CH_3$	Octane
$CH_3-CH_2-CH_3$	Propane	$CH_3-(CH_2)_7-CH3$	Nonane
$CH_3-(CH_2)_2-CH_3$	Butane	$CH_3-(CH_2)_8-CH_3$	Décane
$CH_3-(CH_2)_3-CH_3$	Pentane	$CH_3-(CH_2)_9-CH_3$	Undécane
$CH_3-(CH_2)_4-CH_3$	Hexane	$CH_3-(CH_2)_{10}-CH_3$	Dodécane

Noticed :

Any alkane can be written in the form R—H where $R=C_nH_{2n+1}$ and is called an alkyl radical, the nomenclature of these radicals is obtained from the name of the alkane which derives with replacement of the suffix ane by the suffix yle.

Example:

The radical which derives from propane C_3H_8 is propyl of formula C_3H_7

2/ Branched alkanes

An alkane is said to be branched if it contains at least one tertiary carbon.

Example:

The compound: $CH_3-\mathbf{C}H(CH_3)-CH_3$

has a branched structure (the carbon in bold is tertiary).

The nomenclature of this type of compound obeys the following rules:

• Choose, in the expanded formula, the longest chain which is called Main chain or mother chain.

• Identify the side chains (radicals) that are substituents.

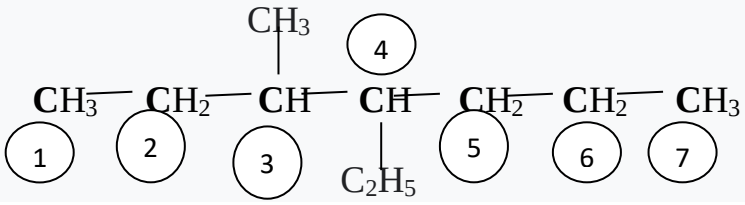
• Number the carbon atoms of the main chain in the direction which makes it possible to establish the sum of the indices assigned to the substituents as the lowest possible sum (the index of the substituent corresponds to the number of the carbon atom of the main chain who wears it).

• Classify the substituents before the name of the HC in alphabetical order and each substituent is preceded by the number of the carbon which carries it.

• Each carbon linked to a substituent has its number surrounded by two hyphens except at the beginning where it is followed by a hyphen.

• In the as where there are identical substituents we use the prefixes di, tri, tetra…etc. (these prefixes are not taken into consideration in the alphabetical arrangement of the substituents).

Example: The name of the compound

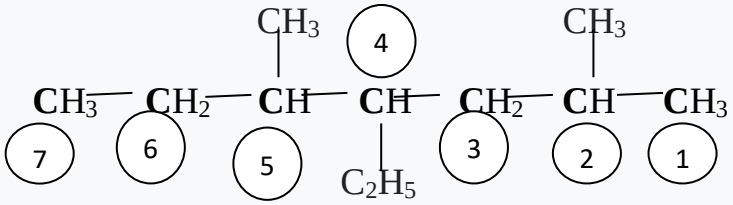


The main chain is made up of seven carbon atoms. Carbon 3 carries the methyl radical and carbon 4 carries the ethyl radical.

According to the given rules, the compound is named:

4-ethyl-3-methyl heptane

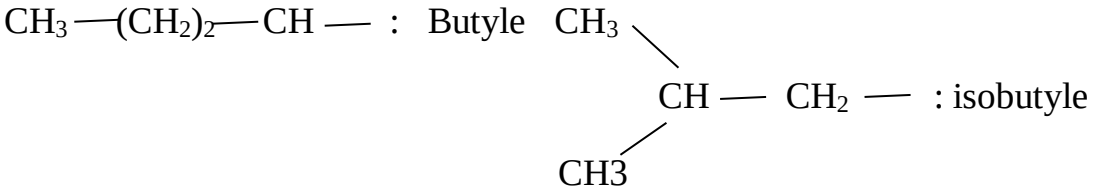
Example: Case of identical substituents

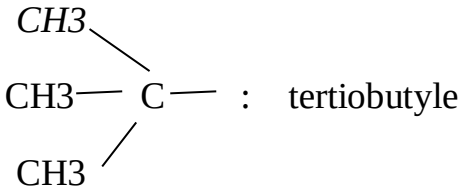


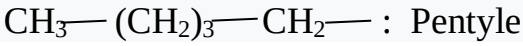
According to the given rules, the compound is named:

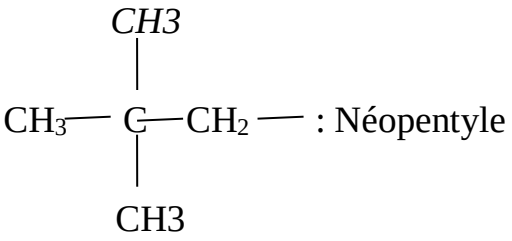
4-éthyle-2-méthyle-5-méthyle heptane **or**4-éthyle-2,5-diméthyle heptane

Note: Special radical names









Noticed :

In the alphabetical arrangement the prefixes iso, tertio and neo are not taken into consideration.

II/ Nomenclature of unsaturated acyclic HC

1/ Alkenes :general formula C_nH_{2n}

These are the HC having a double bond. Their names are formed from the alkane of the same skeleton by replacing the ending ane with ene.

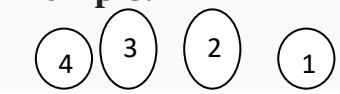
The nomenclature rules for this type of compound are:

• Find the longest carbon chain containing the double bond.

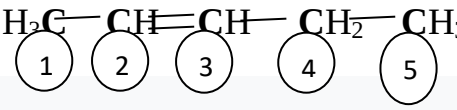
• The position of the double bond in the main chain is indicated by an index placed before the ene ending giving the number of the first unsaturated carbon atom.

• The smallest index is assigned to the double link, thus giving the numbering direction of the main chain.

Example:



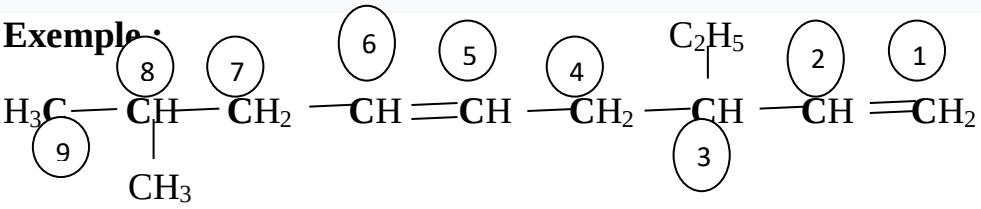
$H_3C-CH_2-CH=CH_2$ named : But-1-ène ou Butène



$H_2C-CH=CH-CH_2-CH_3$ named : Pent-2-ène

• In the case where there is more than one double bond, we use the endings diene, triene…..

Exemple :



$H_3C-CH(CH_3)-CH_2-CH=CH-CH_2-CH(C_2H_5)-CH=CH_2$

3-Ethyl-8-Methyl nona-1,5-diène

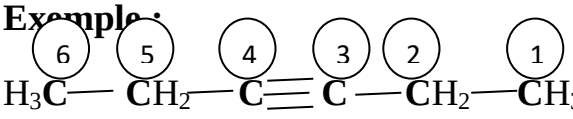
2/ Alkynes: general formula C_nH_{2n-2}

These are the HC having a triple bond. Their names are formed from the alkane of the same skeleton by replacing the ending ane with yne.

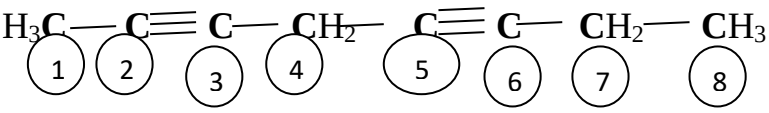
• The rules of nomenclature are identical to those used with alkenes and the position of the triple bond imposes the direction of numbering of the main chain.

• In the case where there is more than one triple bond, we use the endings diyne, triyne…..

Exemple :



Hex-3-yne



Oct-2,5-diyne

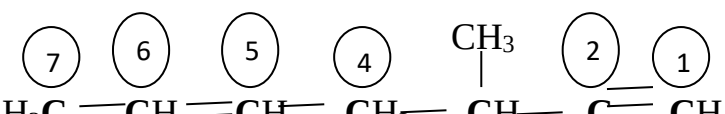
3/ Compounds containing double and triple bonds

The nomenclature of this type of compound is done according to the rules:

• Find the longest chain containing the maximum number of double and triple bonds, if two chains have the same number of establishments we choose the one which contains the most carbon atoms and if the numbers of carbon atoms are equal we chooses the one with the most double bonds.

• The direction of numbering is done in such a way as to assign the lowest indices to the unsaturations even if this favors the triple bond. In the case where there is a tie, we choose the direction which assigns the lowest index to the double bond.

Exemple :



3-Methyl Hept-5-ène-1-yne 3-Methyl Hept-5,1-enyne

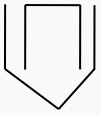
III/ Nomenclature of cyclic and aromatic HC

1/ Monocyclic hydrocarbons

• HC which do not have side chains are named by preceding the name of the acyclic hydrocarbon having the same carbon number.

Example :

Cyclobutane



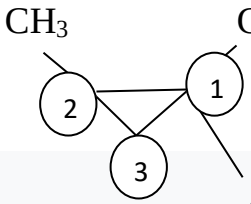
Cyclopent-1,3-diene

• In the case where there is a side chain (simple or complex substituents)

• **Case of single substituents**: The cycle is considered as the main chain

and the substituents are named according to the IUPAC rules.

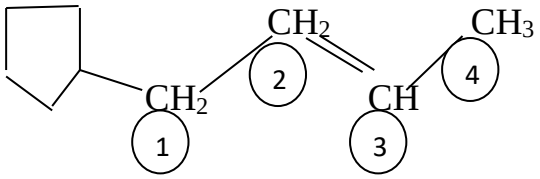
Example :



1,1,2-trimethyl cycloproane

• **Case of complex substituents**: In this case the IUPAC rules are applied, that is to say the main chain is the longest chain which contains the functional group if it exists, the unsaturation if it exists and the maximum number of substituents.

Example :

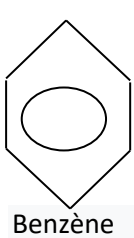


1-Cyclopentyl But-2-ène

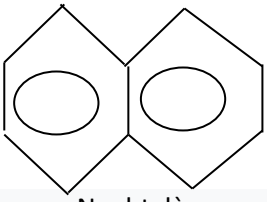
2/ Aromatic Hydrocarbons

The generic name for aromatic HC is arena.

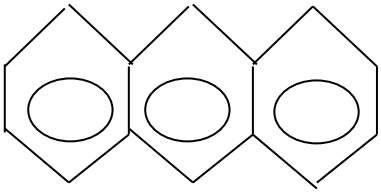
• **Case of unsubstituted aromatic HC**



Benzène



Naphtalène



Anthracène

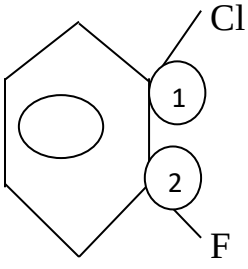
• **Case of substituted aromatic HC**

In this case the nomenclature obeys the rules:

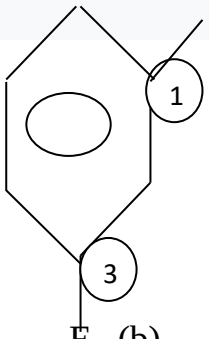
Rule 1: The substituted derivatives of benzene are named by numbering the atoms of the cycle from 1 to 6 in such a way that all the indices associated with the substituents are as low as possible by preceding the word benzene with prefixes and indices corresponding to the various substituents.

Rule 2: The prefixes O-(ortho) instead of 1,2-, m-(meta) instead of 1,3- and p-(para) instead of 1,2- are used.

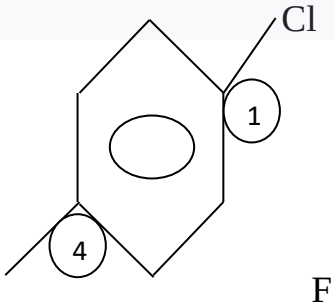
Example:



(a)



(b)



(c)

(a) : 1-Chloro-2-Fluoro Benzène **or** O-Chlorofluoro Benzène

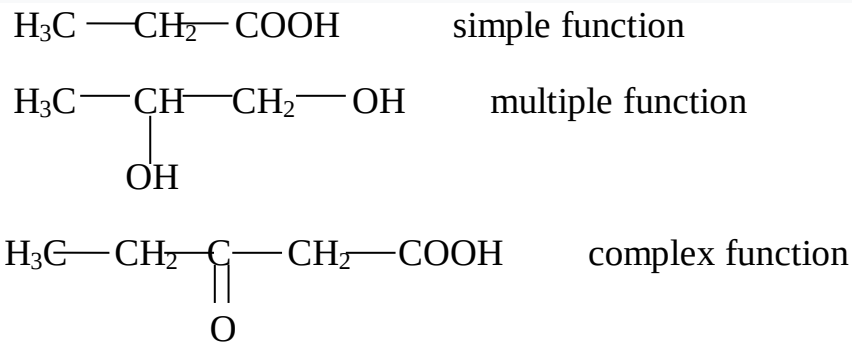
(b) : 1-Chloro-3-Fluoro Benzene **or** m-Chlorofluoro Benzène

(c) : 1-Chloro-4- Fluoro Benzene **or** p- Chlorofluoro Benzène

IV/ Nomenclature of organic functions

An organic compound can contain one, two or more identical functional groups (compound with multiple functional groups) as well as it can contain several different groups (compound with complex functional groups).

Example :



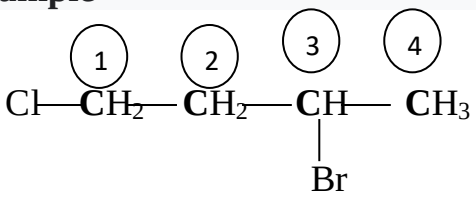
1/ Halogenated derivatives

The halogens are: Fluorine F, chlorine Cl, bromine Br and iodine I. They are designated by the symbol X. A derivative is said to be halogenated if it contains at least one C-X bond.

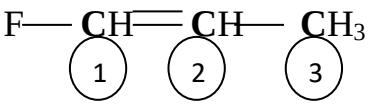
To name this type of compound we apply the rule:

The name of HC is preceded by the prefixes fluoro, chloro, bromo or iodo which are in turn preceded by position indices corresponding to the carbon atom of the main chain with which the halogen is linked.

Example



3-Bromo-1-Chloro Butane



1-Fluoro prop-1-ène

Noticed :

If all the hydrogens in the molecule are replaced by a halogen, we precede the halogen prefix with per.

Example :

H_3C——CH_3 Ethane F_3C—— CF_3 Perfluoro éthane

2/ Alcohols

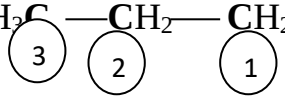
The general formula for alcohols is R—OH where OH is the hydroxyl group.

To name these compounds, we follow the rules:

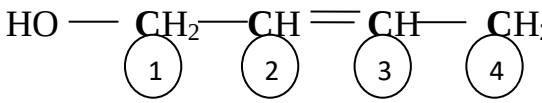
• We follow the name of the corresponding HC by the suffix ol preceded by the position index of the function.

• If the compound contains more than one OH group we use the suffix diol, triol…etc.

Example :



Prop-1-ol ou propanol



But-2-ène-1,4-diol

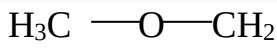
3/ Oxide ethers

Their general formula is R O R (symmetric) or R O R' (asymmetric).

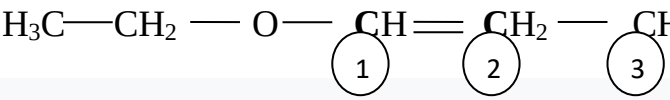
The nomenclature of this type of compound is as follows:

• We determine a base name which is that of the HC corresponding to the priority R group, that is to say which contains the greatest number of carbons or an unsaturation or a function. The RO alkoxy group which contains the other R' is considered as a substituent.

Example :



méthoxy éthane



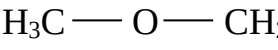
éthoxy propène

Noticed :

We can assimilate the oxide ethers by preceding the names of the groups R and R' with the terms oxide of……

Example :

oxyde de diéthyle



oxyde d'éthyle et de méthyle

4/ Amines

Amines are divided into three classes:

Primary amines of general formula: R —NH2

Secondary amines of general formula: R—NH—R'

Tertiary amines of general formula: R—N(R")—R'

The nomenclature of amines

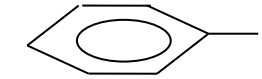
Primary amines:

They are named by adding the amine ending to the R group.

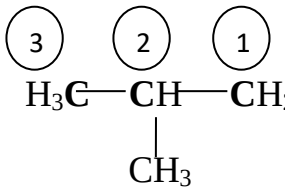
If R is branched, the main chain must contain the carbon linked to —NH2 and which has the index 1.

Example :

$H_3C—CH_2—NH_2$ éthylamine



NH_2 Phénylamine



$H_3C—CH(CH_3)—CH_2—NH_2$ 2-méthyle propylamine

Secondary and tertiary amines:

If: R= R' case of secondary amines or R= R'= R" case of tertiary amines.

Amines are named as primary amines preceded by the prefixes di or tri.

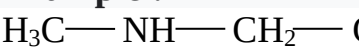
Example :

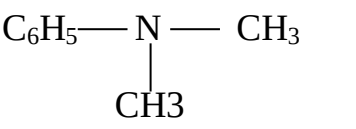
$H_3C—CH_2—NH—CH_2—CH_3$ diéthylamine

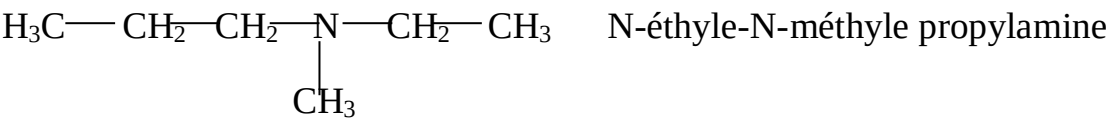
$H_3C—N(CH_3)—CH_3$ triméthylamine

If the radicals are not identical, the amines are considered derivatives of the primary amine which has the longest or most complex R group and the names of the other groups are placed in front of that of the primary amine by doing so. precede with the letter N.

Example :


N-méthyle éthylamine

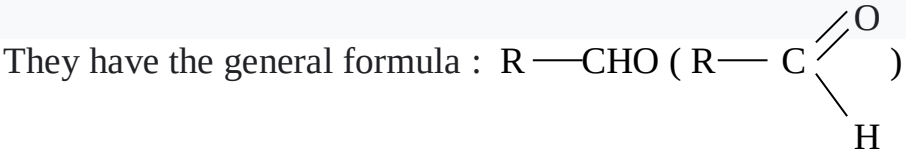

N,N-diméthyle phénylamine


N-éthyle-N-méthyle propylamine

Noticed :

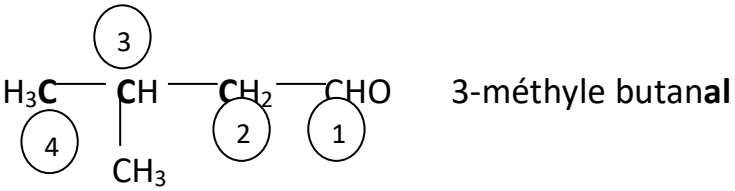
When the amine function does not have priority, the NH2 group is called amino.

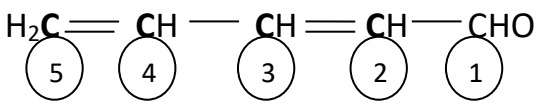
5/ Aldehydes

They have the general formula : 

The name of an acyclic aldehyde is formed by adding the ending al (dial, trial, etc.) to the name of the corresponding HC. The carbon in the CHO group must always take the number 1.

Example :

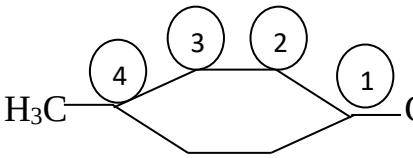

3-méthyle butan**al**



Penta-2,4-dien**al**

Cyclic aldehydes in which the function is linked directly to the ring are named by adding the ending carbaldehyde to the ring name.

Example :



4-méthyle cyclohexane carbaldéyde

Noticed :

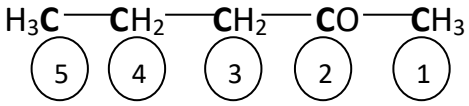
When the aldehyde function is not a priority, the CHO group is called formyl.

6/ Ketones

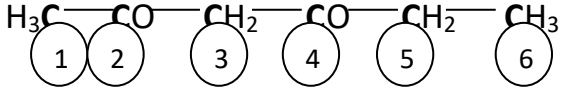
Ketones have the general formula: R CO R (symmetric) or R CO R' (mixed).

The name of a ketone is formed by adding the ending one, preceded by the position index of the carbon of the CO group to that of the corresponding HC. The main chain is the longest chain which contains the carbon of the CO group.

Example :



Penta-2-**one**



Héxa-2,4-di**one**

If the groups R and R' are simple, we can also name the ketones by following their names in alphabetical order with the word ketone.

Example :

H_3C— CO —CH_2— CH_3 éthyle méthyle cétone

Noticed :

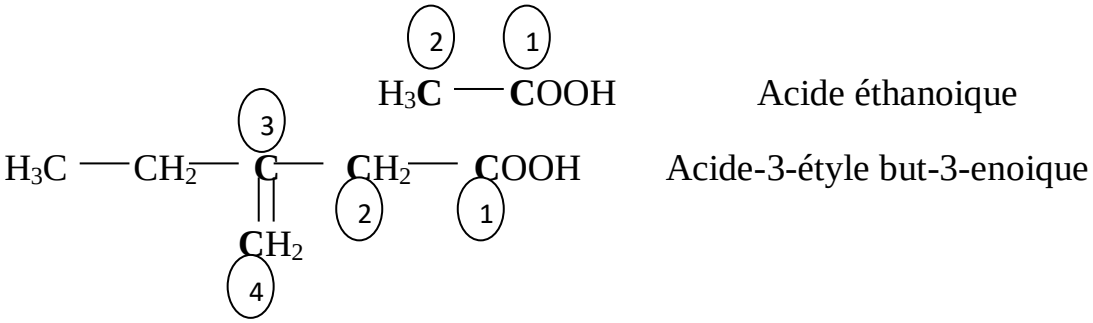
When the function is not a priority, the **CO** group is called **oxo**.

7/ Carboxylic acids

These are the compounds containing the carboxyl group COOH.

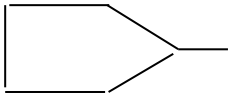
In the acyclic series, the acids are named by following the name of the corresponding HC with the oic ending (dioic, trioic, etc.) and by preceding the word acid. The carbon in the COOH group always bears number 1 because the acid function has the highest priority (see table…..).

Example :



In the cyclic series, the acids whose function is directly linked to the cycle are named by following the word acid with the name of the corresponding cyclic HC to which the carboxylic suffix is added.

Example :



Acide cyclopentane carboxylique