Badji Mokhtar University - Annaba

Faculty of Technology

Department : 2nd Year Sciences and technologies

Organic chemistry

Chapter 2

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Chapter 2 :
Classification of organic functions

Specific objectives :

- Identify and name the main classes of organic compounds.
- Apply IUPAC nomenclature rules to correctly name complex organic compounds.
- Analyze and evaluate the molecular structure to identify the present functional groups.

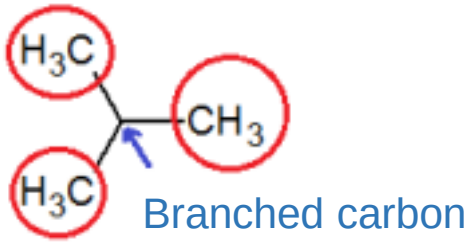
Contents table of chapter 2 :

1- Aliphatic hydrocarbons:

- Alkanes :

Alkanes are compounds composed of carbon and hydrogen atoms. They are also known as saturated hydrocarbons with general formula **CnH2n+2**. To name them, we use the suffix **'ane'** preceded by a prefix derived from the Greek number.

- Branched alkanes : When a carbon atom is linked to at least three carbon atoms, the alkane is said to be branched.

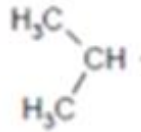
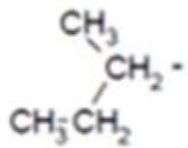
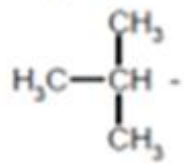
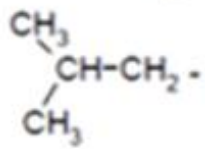


Alkyls : are groups derived from an alkane by the loss of a hydrogen atom. They are named by replacing the suffix **'ane'** with **'yl'**. Alkyls are not considered to be functional groups.

Table 1 : Alkanes naming

n	Prefix	Name	Formula
1	Meth	Methane	CH_4
2	Eth	Ethane	C_2H_6
3	Prop	Propane	C_3H_8
4	But	Butane	C_4H_{10}
5	Pent	Pentane	C_5H_{12}
6	Hex	Hexane	C_6H_{14}
7	Hept	Heptane	C_7H_{16}
8	Oct	Octane	C_8H_{18}
9	Non	Nonane	C_9H_{20}
10	Dec	Decane	$C_{10}H_{22}$
11	Undec	Undecane	$C_{11}H_{24}$
12	Dodec	Dodecane	$C_{12}H_{26}$
13	Tridec	Tridecane	$C_{13}H_{28}$
14	Tetradec	Tetradecane	$C_{14}H_{30}$
15	Pentadec	Pentadecane	$C_{15}H_{32}$
16	Hexadec	Hexadecane	$C_{16}H_{34}$
17	Heptadec	Heptadecane	$C_{17}H_{36}$
18	Octadec	Octadecane	$C_{18}H_{38}$
19	Nonadec	Nonadecane	$C_{19}H_{40}$
20	Eicos	Eicosane	$C_{20}H_{42}$
30	Triacont	Triacontane	$C_{30}H_{62}$
40	Tetracont	Tetracontane	$C_{40}H_{82}$

Table 2 : Naming of some substituants (alkyls)

Substituant :	Name :	Abbreviation :
CH_3-	Methyl	Me
$H_3C—CH_2$-	Ethyl	Et
$CH_3CH_2CH_2$-	Propyl	Pr
	Isopropyl	isoPr or iPr
$CH_3CH_2CH_2CH_2$-	Primary butyl or n-butyl	Bu or nBu
	Secondary butyl or sec-butyl or s-butyl	secBu or sBu
	Tertiary butyl or ter-butyl or tertiobutyl	terBu or tBu
	Isobutyl	isoBu or iBu
C_6H_5-	Phenyl	Ph
C_6H_5 - CH_2-	Benzyl	

The following rules established by IUPAC must be followed when naming branched alkanes.

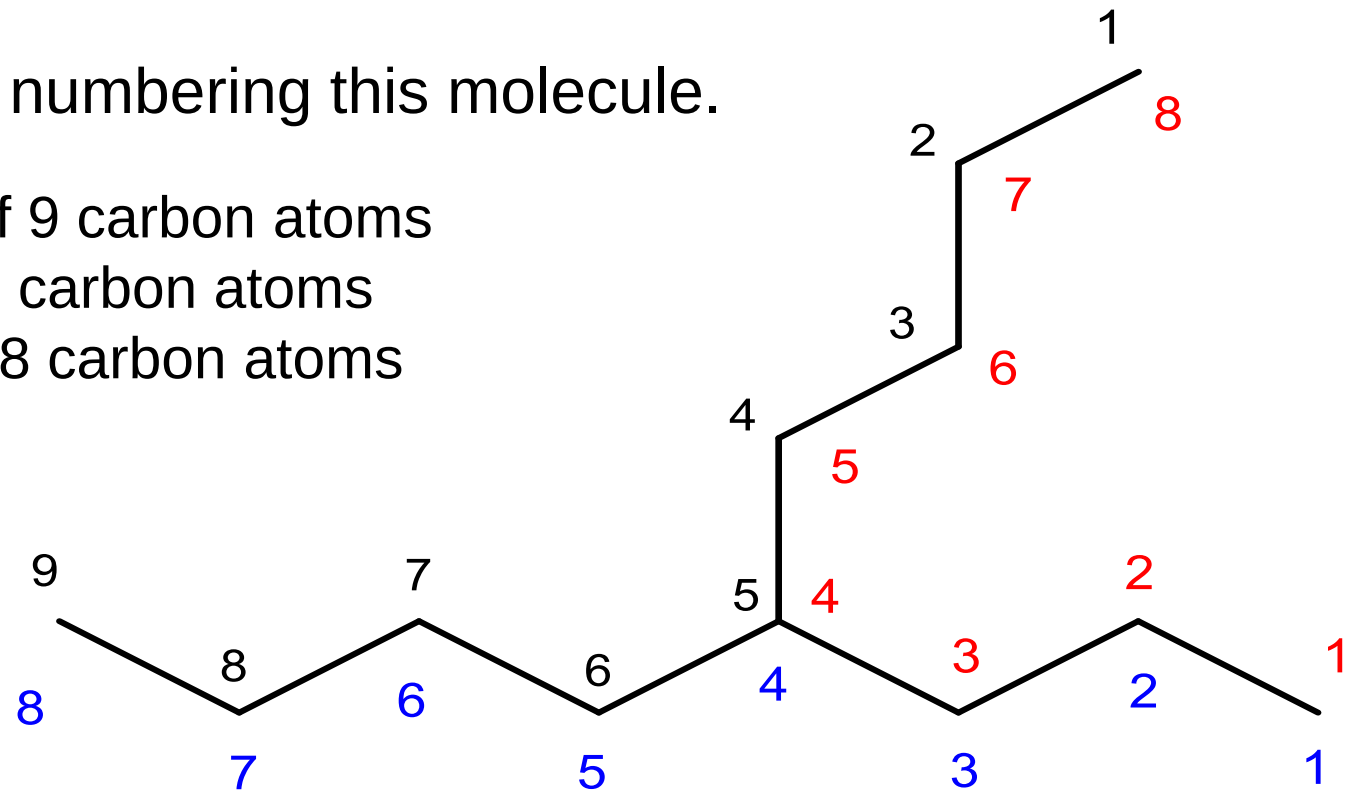
Rule 1:

Find and name the longest chain that can be found in the molecule.

Example:

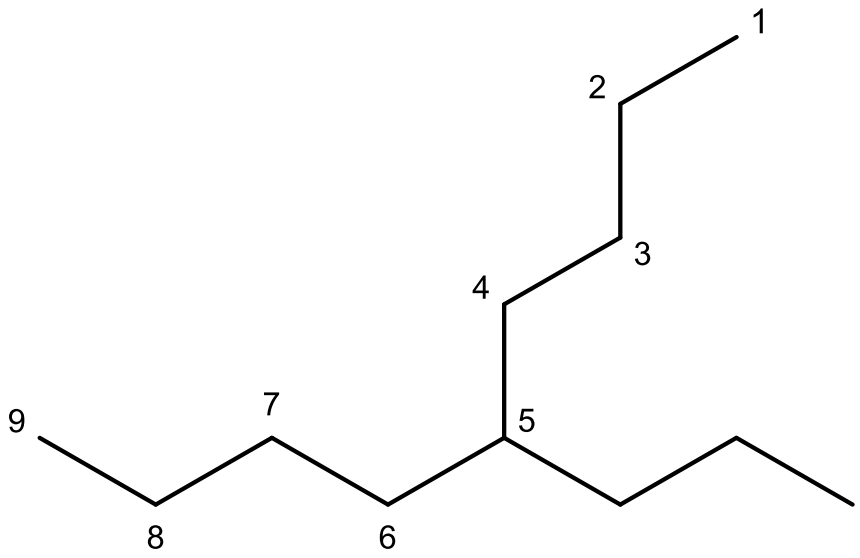
There are three **‘03’** ways of numbering this molecule.

- Chain 1 in **black** : composed of 9 carbon atoms
- Chain 2 in **red** : composed of 8 carbon atoms
- Chain 3 in **blue** : composed of 8 carbon atoms



In this case, the main carbon chain contains 9 carbon atoms: shown in black on the figure. The rest of the grafted chains will be considered as radical.

The name given to a molecule takes the following form : **nonane**



Rule 2:

Name all the carbon groups grafted onto the longest chain as alkyl substituents or radicals (see rule 4).

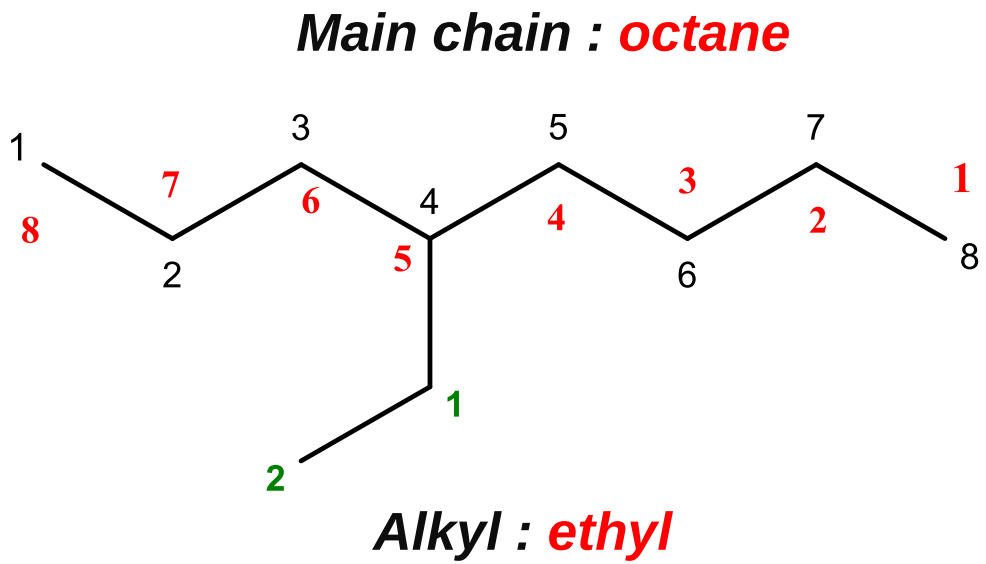
Rule 3:

Number the longest chain starting with the end closest to a substituent (radical), if two numberings are possible, choose the one that leads to the lowest index for branching.

Example : in the figure below, the main chain can be numbered in both directions.

From left to right (in **black**) : the radical is in **position 4** .

From right to left (in **red**) : the radical is in **position 5**.

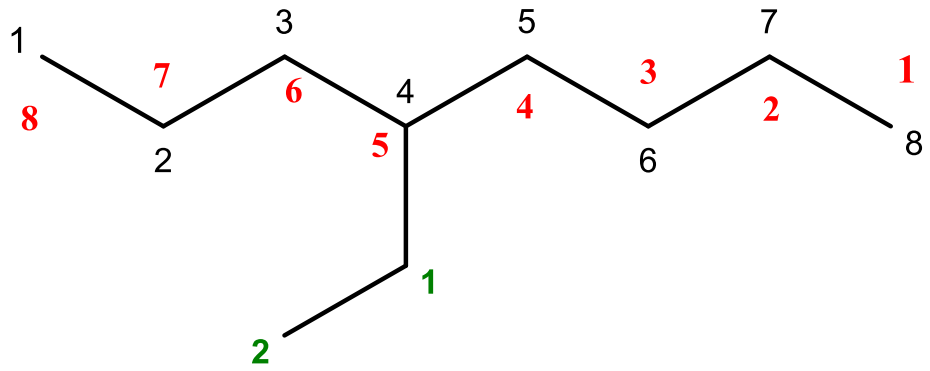


We therefore choose position 4

Rule 4 :

Radicals always have a **‘yl’** ending and are placed before the main chain preceded by their position on that chain.

Here, it's a 2-carbon radical in position 5 on the nonane, so it's a: **4-ethylnonane** .



Rule 5 : If the main carbon chain carries several radicals, the position of each radical is designated by an appropriate number and name.

- The sum of the indices of all the radicals is counted, and the one giving the lowest sum is kept.

Identical radicals are preceded by indices: di, tri, tetra, penta, hexa, hepta, octo, nona or deca, to indicate their number.

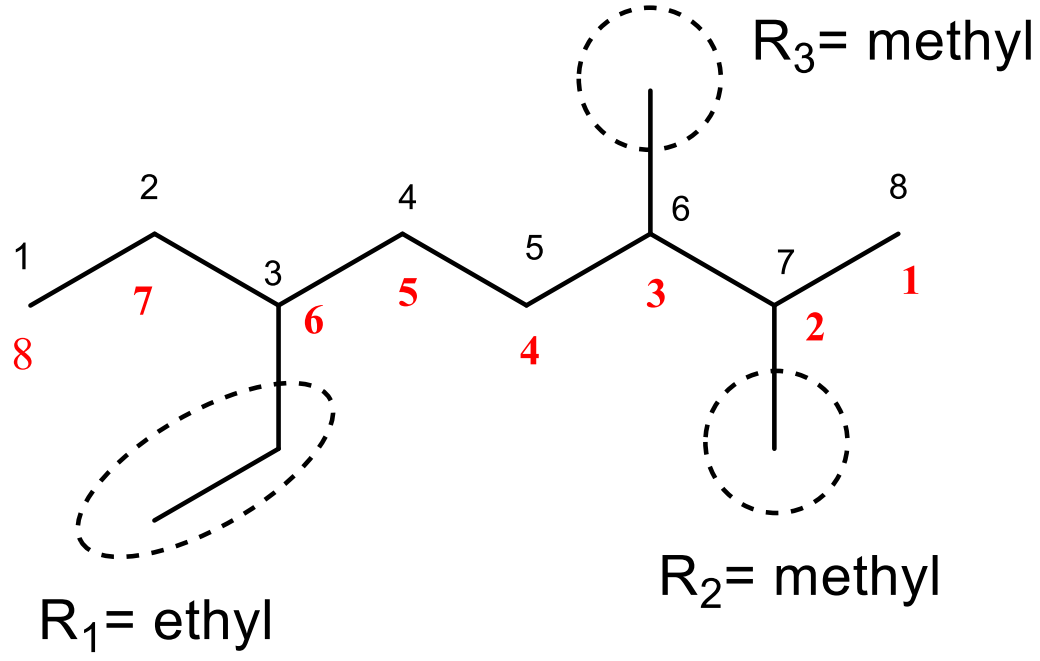
The radicals are written in alphabetical order. Prefixes such as ‘sec-’, ‘tert-’, and the indices ‘di, tri, tetra, penta, hexa, hepta, octo, nona or deca’ **are not taken into account** in the alphabetical arrangement.

Example:

The main carbon chain is composed of 8 carbons and carries 3 radicals (two methyl and one ethyl).

According to the red numbering they are linked to carbons 2-methyl, 3-methyl and 6-ethyl, hence the sum 2+3+6=11.

Following the black numbering, they are linked to the 3-ethyl, 6-methyl and 7-methyl carbons, giving a sum of 3+6+7=16.



The name of this compound is as follows **:** **6-ethyl-(2,3)-*di*methyloctane**

2 . Alkenes

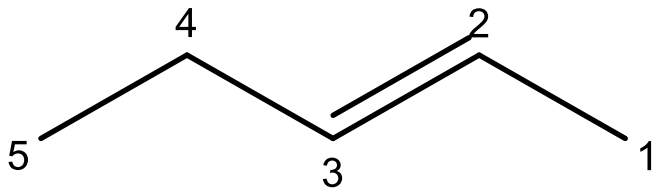
These are hydrocarbons with at least one carbon-carbon double bond, their formula is C_nH_{2n}.

To name alkenes, we main chain which is made up of number of carbons in the longest carbon chain, and a **suffix (ene)** which designates the double bond preceded by its position.

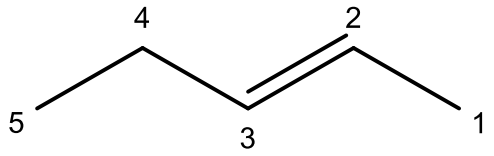
Example: the following alkene has 5 carbons, so its **prefix is 'pent'**.

The C=C double bond is in position 2, so it is :

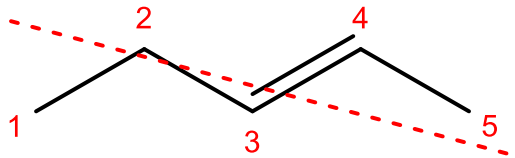
pent-2-ene



Note1. You must number from the carbon in the chain closest to the C=C double bond.



TRUE

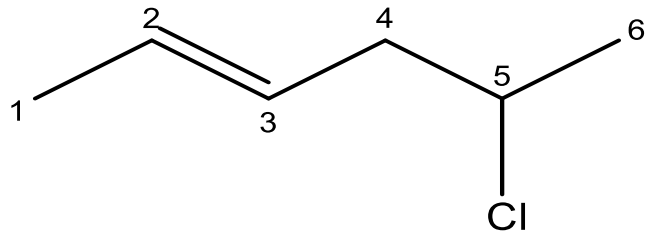


FALSE

Note 2 :

The parent chain is numbered so that multiple bonds have the lowest numbers (double and triple bonds have priority over alkyl and halo substituents).

Example:

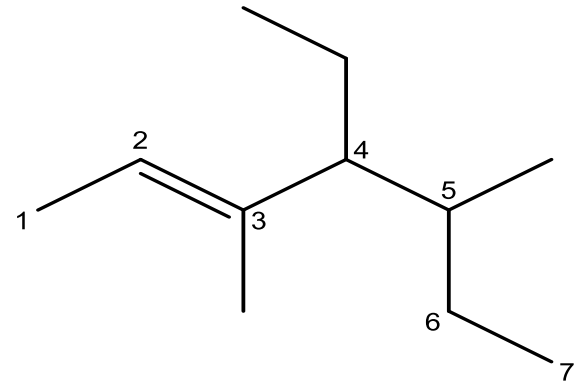


5-chlorohex-2-ene

- Branched alkenes

The double bond has priority in the numbering of the carbon chain and must therefore have the lowest index.

Example :



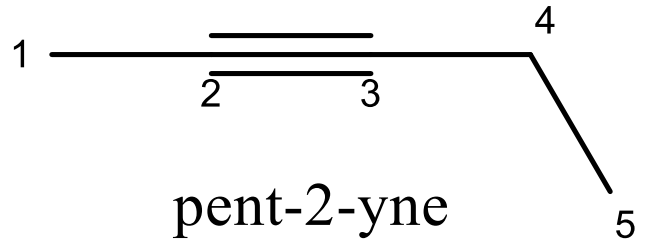
4-ethyl-3,5-dimethylhept-2-ene

3 . Alkynes

These are hydrocarbons with at least one carbon-carbon triple bond, their formula is **C_nH_{2n-2}**.

To name alkynes, we use a prefix which is also made up of a numerical root (number of carbons in the longest carbon chain) and a **suffix (yne)** which refers the triple bond preceded by its position.

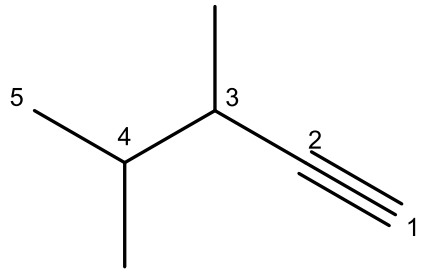
Example:



pent-2-yne

The same rules as for the alkenes apply to the alkynes. The triple bond takes priority in the numbering of alkyl .

Example:

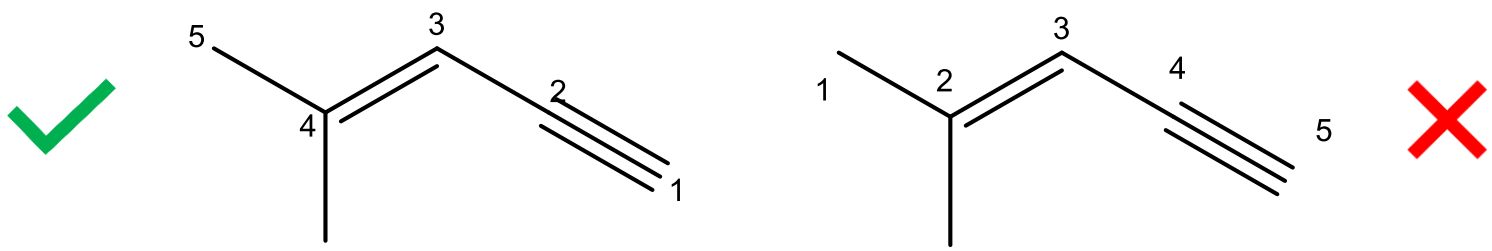


3,4-dimethylpent-1-yne

Double and triple bonds in the same molecule

In the IUPAC naming system, a hydrocarbon containing both a double and a triple bond is called an **alkenyne**.

The chain is numbered from the end closest to either of these two functional groups, in such a way as to have the lowest sum of indices.



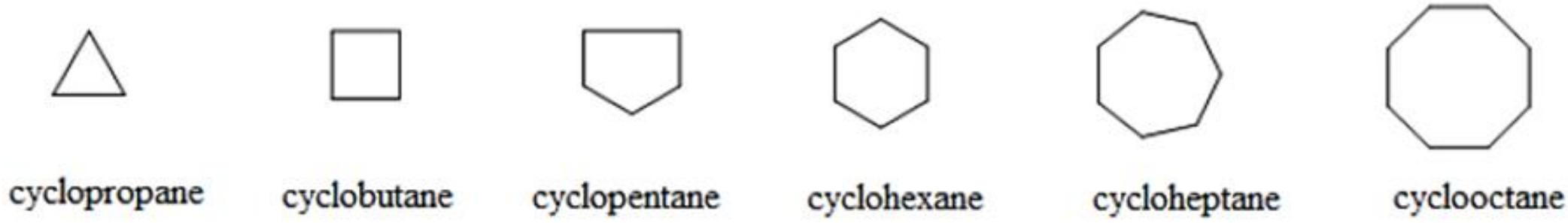
4-methylpent-3-en-1-yne

When the double and triple bonds are at equal distances at the ends, the double bond is given the lowest index.

4- Cyclic compounds :

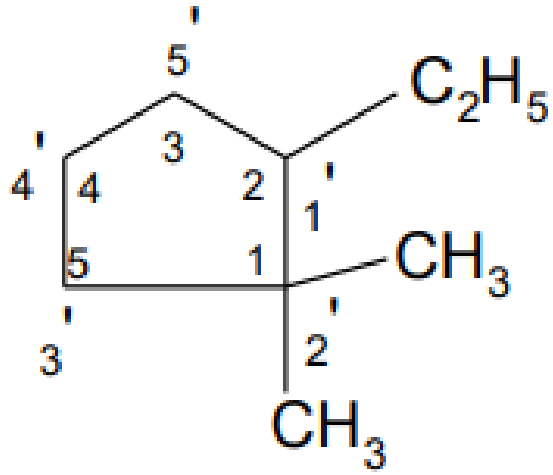
- Saturated cyclic hydrocarbons or cyclanes:

Saturated hydrocarbons with a ring are called cyclanes or cycloalkanes (C_nH_{2n}), their name is derived from that of the alkane with the same number of carbon atoms, preceded by the prefix cyclo.



When the cyclane is poly-substituted, it is numbered by giving the number 1 to the substituent listed first in alphabetical order and continuing along the ring,

so that the substituent listed second in alphabetical order has the lowest index. Also in such a way as to have the lowest sum of indixes.



Example :

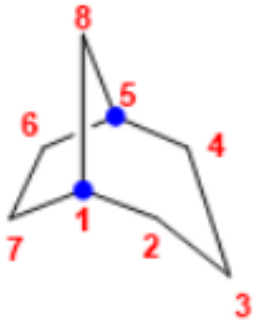
the lowest index : **2'+2'+1'= 5**

1+1+2= 4

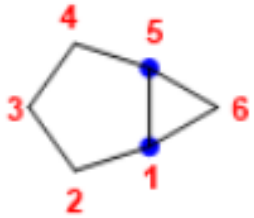
⇒ The adapted name : **2-ethyl-1,1-dimethyl cyclopentane**

For bicyclanes, their names take the name of the linear alkane of the same carbon number preceded by the prefix bicyclo. After this prefix, the number of carbon atoms in each of the 3 bridges is placed in square brackets, the atoms in the ring are numbered starting from one bridgehead, numbering first the longest chain leading to the other bridgehead, continuing by numbering the middle chain back to the first bridgehead and then ending with the shortest.

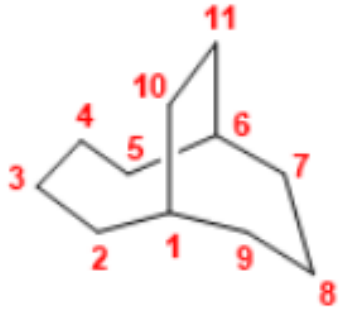
Examples:



Bicyclo[3.2.1]octane



Bicyclo[3.1.0]hexane



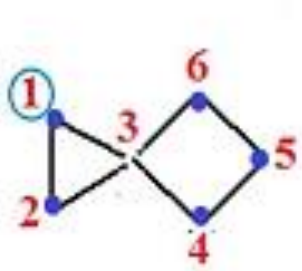
Bicyclo[4.3.2]undécane

- Spiro compounds :

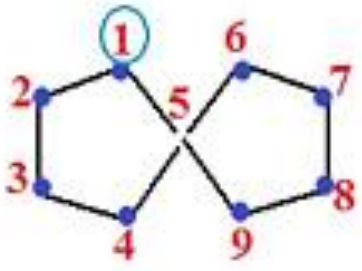
An organic spiro compound is composed of two rings bonded by a single carbon (a spiro atom or node). To name spiro compounds, start with the **prefix ‘spiro’** followed by a pair of **square brackets**, inside which are **two numbers separated by dots**. These numbers indicate the number of atoms in the long ring, then in the short ring, **without calculating** the **carbon of the node**.

For numbering, the carbon atom adjacent to the node atom is numbered 1, the small ring is numbered, then the large ring, passing through the spiro node. If the two rings are identical, the functions are numbered with the lowest indices, followed by the substituents.

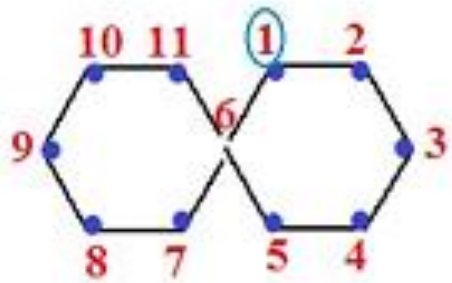
Examples :



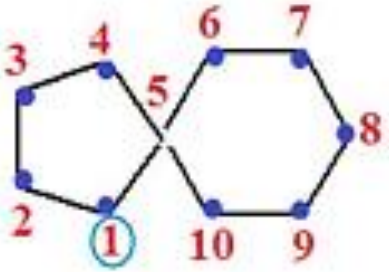
Spiro[3.2]hexane



Spiro[4.4]nonane



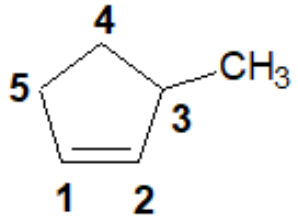
Spiro[5.5]undecane



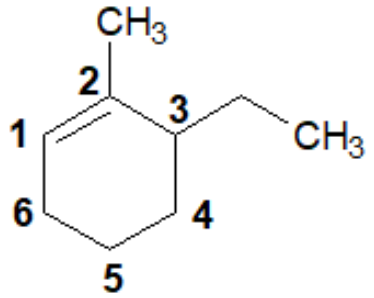
Spiro[5.4]decane

- Cyclenes

Example :



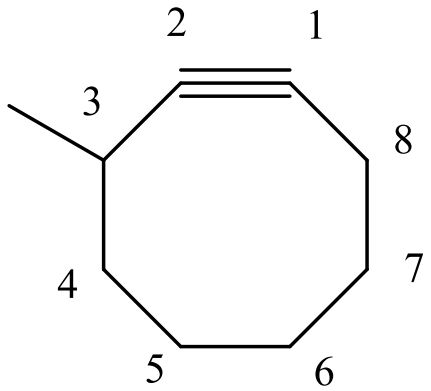
3-methylcyclopentene



3-ethyl-2-methylcyclohexene

- Les cyclynes

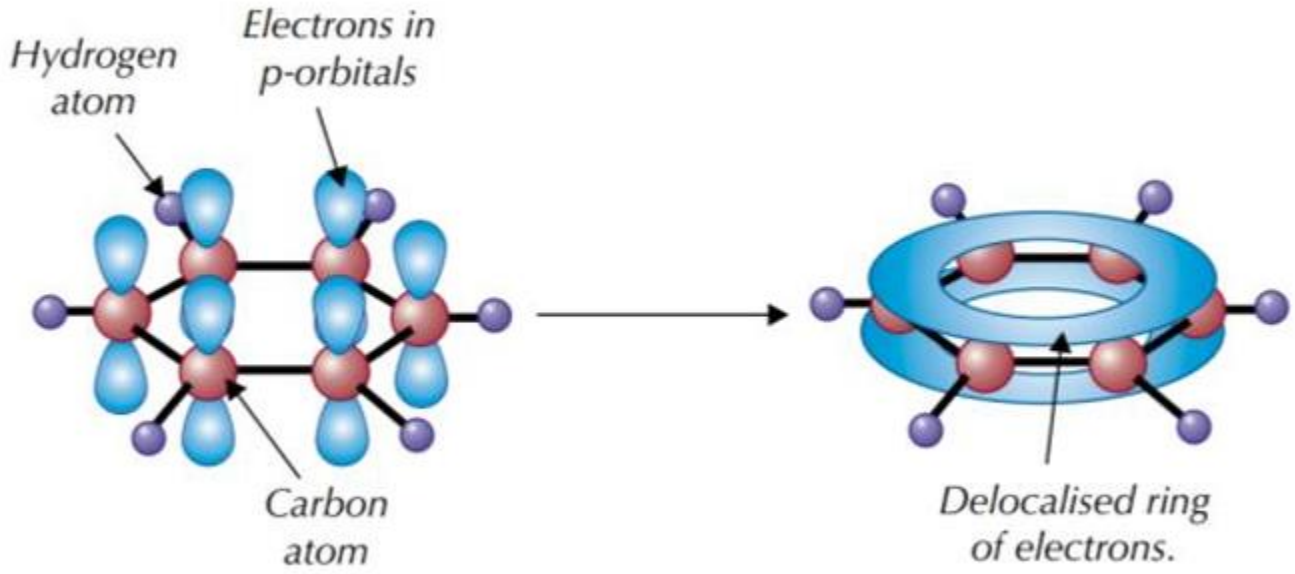
Example :



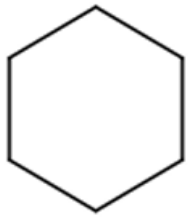
3-methylcyclooct-1-yne

- Aromatic compounds :

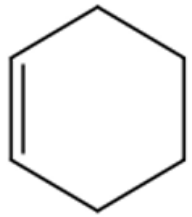
Aromatic compounds are molecules such as benzene whose atoms form particularly stable cyclic and flat structures.



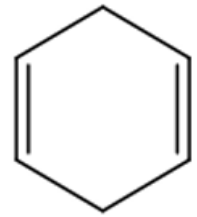
Hückel's rule can be used to predict the aromaticity of a molecule: if a cyclic molecule has **4n+2 π** electrons, it is considered to be an aromatic molecule (the number 'n' must be an integer 0, 1, 2, 3, 4, ... etc.).



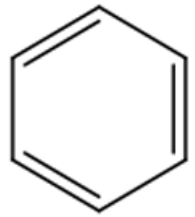
π electrons = 0
4n+2 = 0 , so: n = -1/2
Non aromatic



π electrons = 2
4n+2 = 2 , so: n = 0
Aromatic



π electrons = 4
4n+2 = 4 , so: n = 1/2
Non aromatic



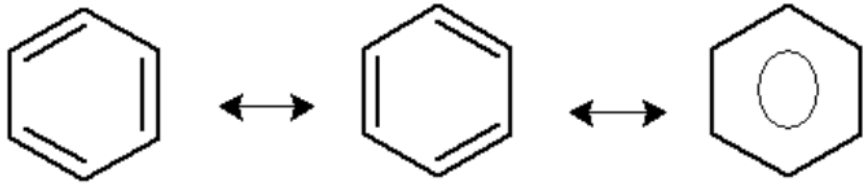
π electrons = 6
4n+2 = 6 , so: n = 1
Aromatic

- Benzenic hydrocarbons:

These molecule contain one or more benzene rings, the simplest being benzene C_6H_6 , the basic name of these compounds is generally ‘benzene’, has six delocalized electrons. Under normal conditions, benzene is a colorless liquid with a characteristic odor, volatile, highly flammable and carcinogenic.

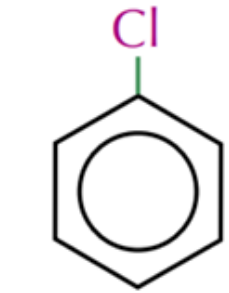
This system is represented by a shape of hexagon in which three double bonds alternate with three single bonds. The six bonds are of identical length, intermediate between the lengths of the single and double bonds. The six carbon atoms are sp2 hybridized.

The IUPAC naming convention is ‘benzene’, according to structural analyses, this compound is **not considered** to be an **alkene**, so it **cannot** be named **cyclohexa1,3,5-triene.**

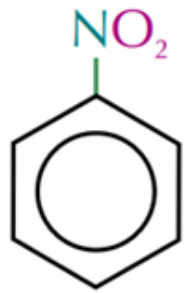


To name a monosubstituted benzene compound, name the substituent followed by the name **‘benzene’.**

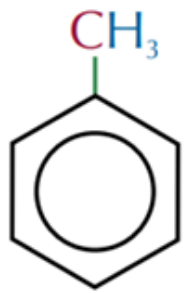
Examples :



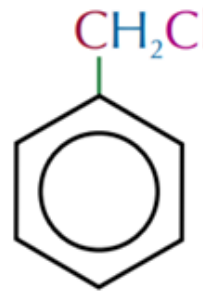
Chlorobenzene



Nitrobenzene



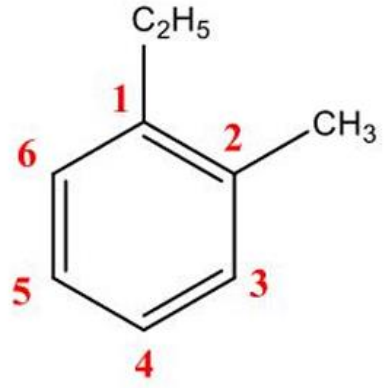
Methylbenzene



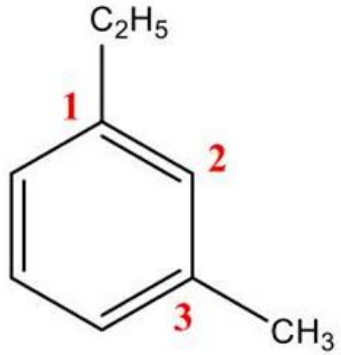
Chloromethylbenzene

To name a poly-substituted benzene compound, name the substituents then name the main function followed by the name ‘benzene’.

The position of the substituents in the benzene ring is indicated by the terms **meta**, **ortho** and **para** or (o, m and p) in relation to the main function in benzene.



1-ethyl-2-methylbenzene
o-ethylmethylbenzene



1-ethyl-3-methylbenzene
m-ethylmethylbenzene

1-ethyl-4-methylbenzene
p-ethylmethylbenzene

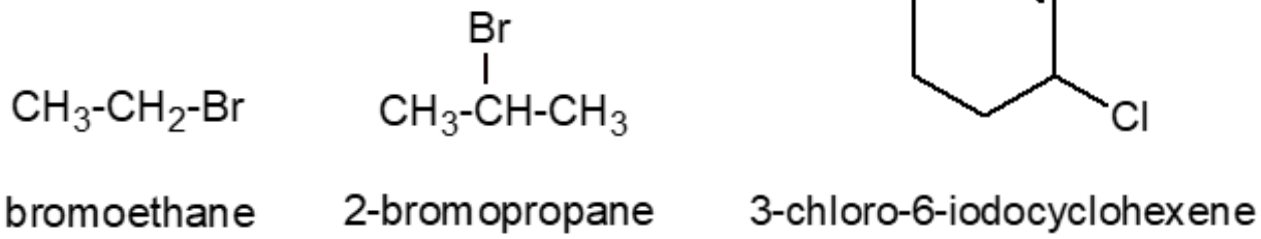
5- Main functional groups :

Haloalkanes RX :

X : is a hydrogen atom **Cl, Br, I, F.** These molecules containing one or more chlorine, bromine, iodine or fluorine atoms. Their name begins with the prefix **‘chloro’**, **‘bromo’**, **‘iodo’** or **‘fluoro’** added to the name of the alkane with the same number of carbon atoms.

The halogen is considered to be a substituent attached to the alkane skeleton.

Examples :



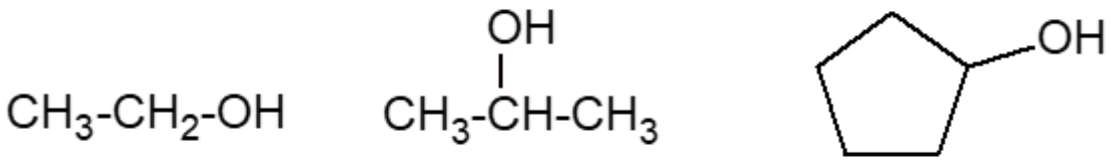
bromoethane 2-bromopropane 3-chloro-6-iodocyclohexene

Alcohols R-OH :

The name of the alcohol is derived from the longest chain containing the OH substituent. To locate the positions along the chain, each carbon atom is numbered, starting with the end closest to the **OH group**.

The names of the other substituents attached to the chain are added to the **alkanol** substrate as prefixes.

Examples :

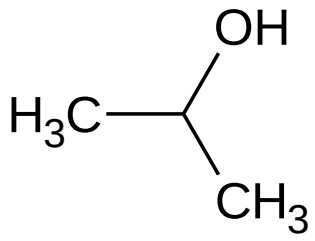


ethanol propan-2-ol cyclopentanol

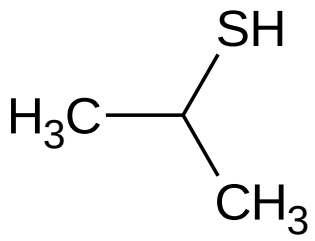
Thiols:

The sulfurated analogues of alcohols, **R-SH**, are called thiols. The suffix thiol is added to the name of the alkane, giving the name **alkanethiol**. The SH group is referred to as **sulfanyl** or **mercapto** when it loses priority to another substituent present in the molecule, such as the OH group of an alcohol.

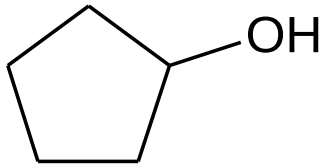
Examples :



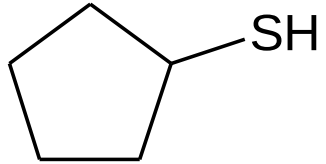
propan-2-ol



propane-2-thiol



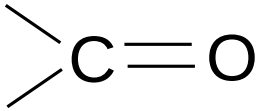
cyclopentanol



cyclopentanethiol

Aldehydes ketones:

Aldehydes and ketones are compounds with the functional group :

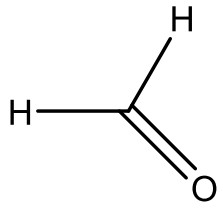


- Aldehydes :

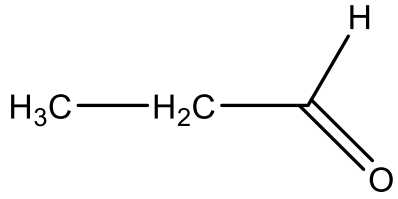
The systematic names of aldehydes are obtained by considering them as derivatives of alkanes, with the **-e** ending of this latter replaced by **-al**. Thus an **alkane** becomes an **alkanal**.

- The chain containing substituents is numbered by giving the number 1 to the carbonyl carbon.
- Cyclic aldehydes are described as carbaldehydes.

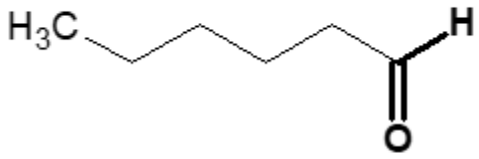
Examples :



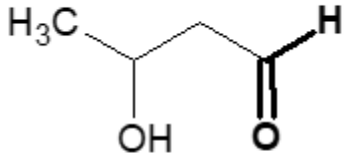
methanal is knowen as formaldehyde



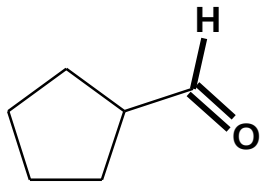
propanal is knowen as acetaldehyde



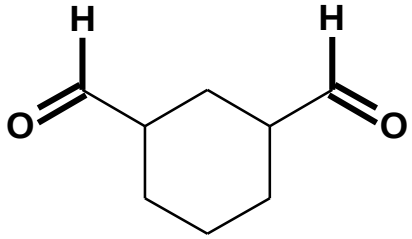
hexanal



3-hydroxybutanal



cyclopentane**carbaldehyde**

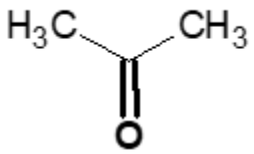


cyclohexane-**1,3-dicarbaldehyde**

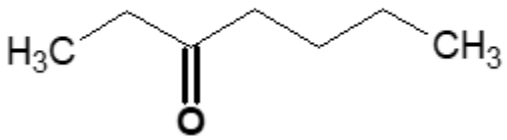
- Ketones:

Ketones are called **alkanones**, the **-e** ending of the alkane name being replaced by **-one**. The chain is numbered so as to give the lowest possible number to the C=O carbonyl. Ketones inserted into a ring are called **cycloalkanones**.

Examples :



propanone



heptan-3-one

Carboxylic acids :

Like other organic compounds, many carboxylic acids have been given a variety of common names that are frequently found in the literature (see table below).

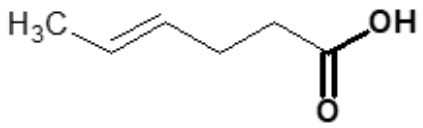
The IUPAC system creates the names of carboxylic acids by replacing the **-e** in the name of the alkane with **-oic** followed by the word : **acid**. The **alkanoic acid** chain is numbered by assigning number 1 to the carboxylic carbon and positioning all the substituents along the longest carbon chain, including the **-COOH** group.

Table 3: Common and systematic names and natural sources of carboxylic acids

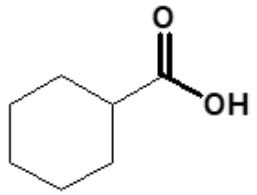
Structure	IUPAC name	Common name	Natural sources
HCOOH	methanoïc acid	formic acid	ants
CH_3COOH	ethanoïc acid	acctic acid	vinegar
CH_3CH_2COOH	propanoïc acid	propionic acid	milk products
$CH_3CH_2CH_2COOH$	butanoïc acid	butyric acid	butter
$CH_3(CH_2)_3COOH$	Pentanoïc acid	Valeric acid	valerian root
$CH_3(CH_2)_4COOH$	hexanoïc acid	caproïc acid	goat's smell

Cyclic acids are known as cycloalkanecarboxylic acids. In these compounds it is the carbon to which the carboxyl functional group is attached that takes the number 1.

Examples :



Hex-4-enoic acid



cyclohexanecarboxylic acid

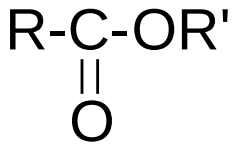
Dicarboxylic acids:

Dicarboxylic acid is known as **alkandioic acid**.

Table 4: Common and systematic names of some dicarboxylic acids

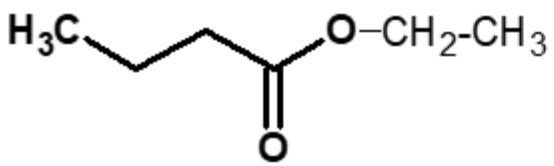
Structure	IUPAC name	Common name
HOOC-COOH	Ethandioic acid	oxalic acid
HOOC-CH_2-COOH	Propanedioic acid	malonic acid
HOOC-$(CH_2)_2$-COOH	Butanedioc acid	succinic acid
HOOC-$(CH_2)_3$-COOH	Pentanedioic acid	glutaric acid
HOOC-$(CH_2)_4$-COOH	Hexanedioic acid	adipic acid
HOOC-CH=CHCOOH	But-2-ènedioic-cis acid But-2-ènedioic-trans acid	maleic acid fumaric acid

Esters

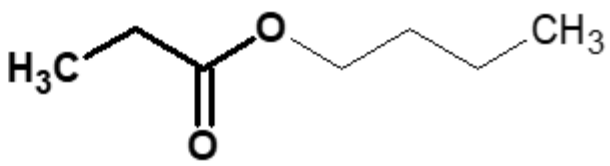
Esters have the general formula : 

An ester results from the ‘grafting’ reaction between an alcohol and a carboxylic acid (**RCO-OR'**). The name is that of : the name of **the alkyl group derived** from the name of the **alcohol** + the **alkanoate group** (derived from the name of the **acid**) .

Examples :



Ethyl butanoate



Butyl propanoate

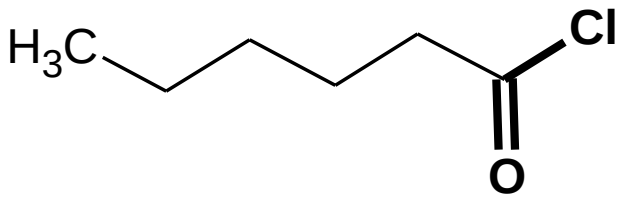
Acid halides :

The change of the OH group in a carboxylic acid to a halogen X produces an acid halide, **R-CO-X**. Since RCO groups are known as **acyl** groups, these compounds are also called **acyl halides**.

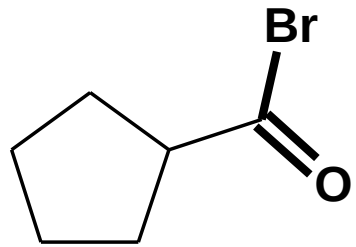
The names of acyl groups are derived from those of acids by replacing the **-oic** ending with the **-oyl** ending. Acyl groups derived from **cycloalkanecarboxylic acids** are named by replacing the **-xylic** end with the **-nyl** end.

Also they are named by preceding the name of the **acyl group** with the words **fluoride**, **chloride**, **bromide** or **iodide**.

Examples :



Hexanoyl chloride

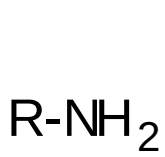


cyclopentaecarbonyl bromide

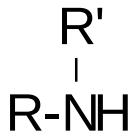
Amines :

Amines are named by adding the **amine ending** to the name of the hydrocarbon chain (by replacing the final **-e** of the alkane with **amine**).

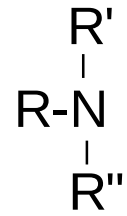
Amines are classified as follows:



primary amine

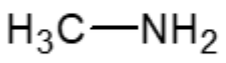


secondary amine

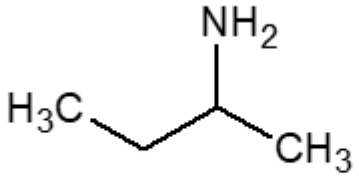


tertiary amine

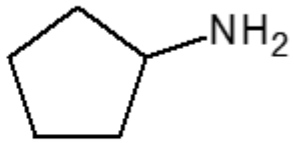
Examples :



methanamine



butan-2-amine

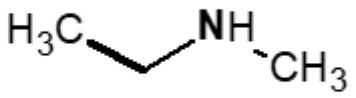


cyclopentanamine

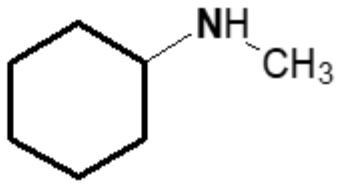
For secondary and tertiary amines, the most important alkyl substituent on the nitrogen is chosen to form the name of the basic : **alkanamine** , and the other group(s) are named as substituent(s) **following the letter(s) N- (N,N'-).**

Examples :

Secondary amine

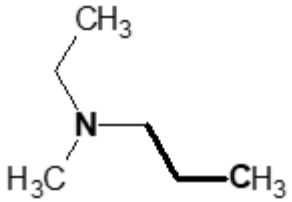


N-methyl**ethanamine**

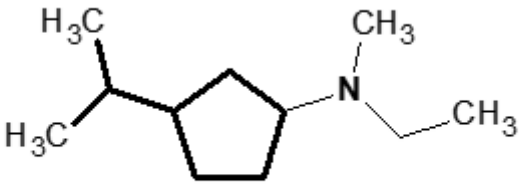


N-methyl**cyclohexanamine**

Tertiary amine

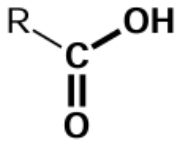
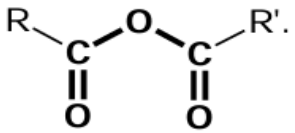
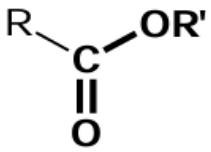
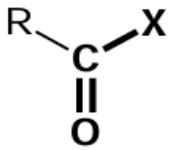
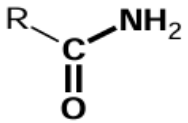


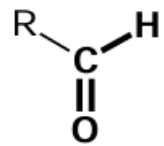
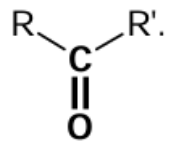
N-ethyl-*N*-methyl**propan-1-amine**



N-ethyl-*N*-methyl-**3-isopropylcyclopentanamine**

Table 2: Classification of chemical functions in descending order of priority

Class	Formula	Prefix	Suffix
Carboxylic Acids		Carboxy-	…..oic acid ….. carboxylic acid
Sulphonic Acids		Sulfo-	…….sulphonic acid
Acid Anhydrides		-	…….Acid anhydride
Esters		Alk-oxycarbonyl-	… ... alkyl oate … ... alkyl carboxylate
Acyl Halides		Halocarbonyl-	... Oyl halide ….Carbonyl halide
Amides		Carbamoyl-	…amide …carboxamide

Nitriles	R—**C≡N**	Cyano-	…nitrile …carbonitrile
Aldehydes		Formyl-	…al …carbaldehyde
Ketones		Oxo-	…one
Alcohols	R—**OH**	Hydroxy-	…ol
Thiols	R—**SH**	Mercapto-	…thiol
Amines	R—**NH_2**	Amino-	…amine
Alkynes	R-C≡C-R’	-	…….yne
Alkenes	R-C=C-R’	-	……ene

Chapter 3 :