Badji Mokhtar University - Annaba

Faculty of Technology

Department : 2nd Year Sciences and technologies

Organic chemistry

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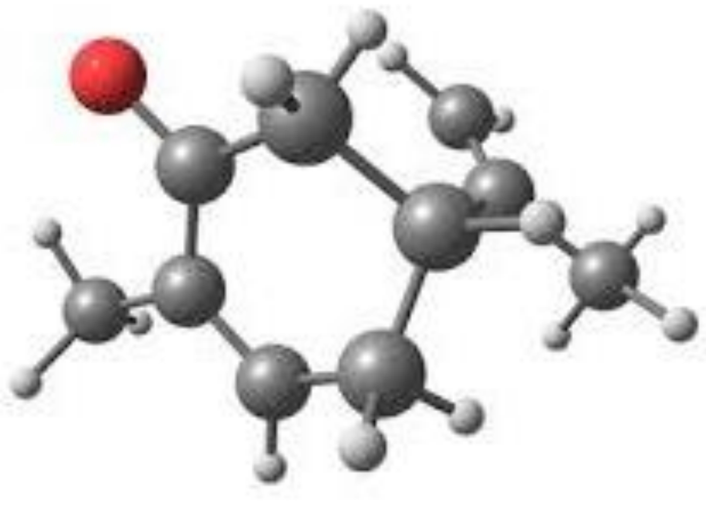
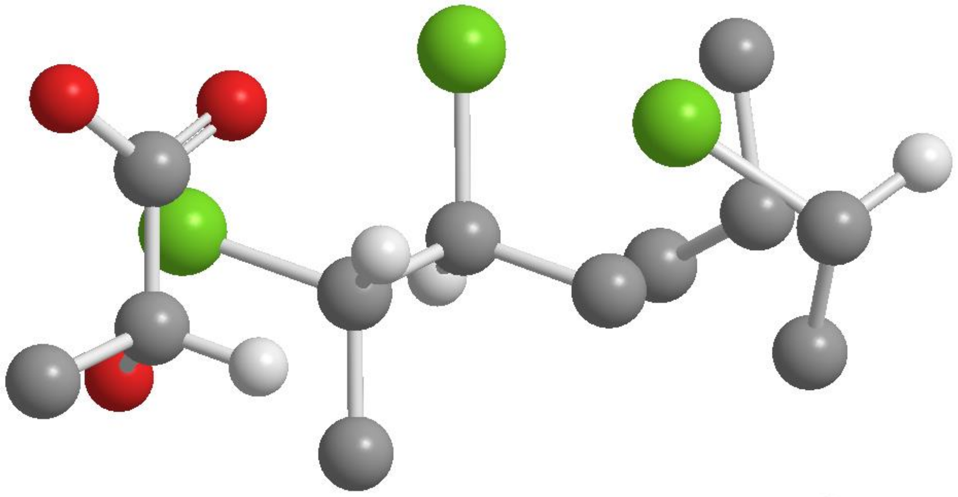
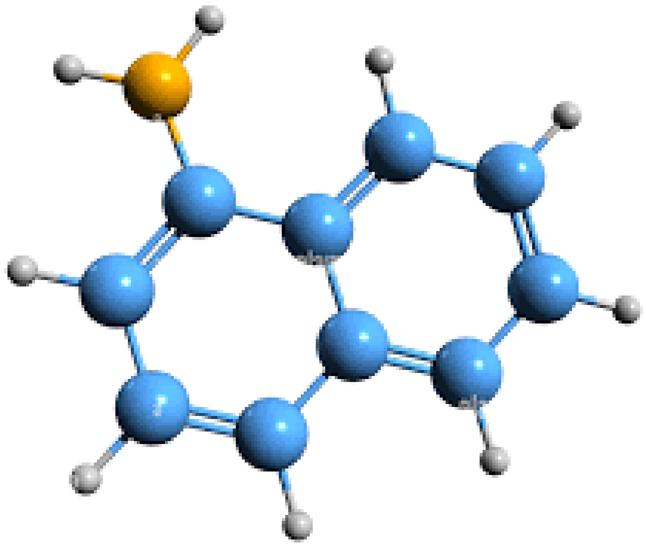
Academic year : 2024/2025

Presentation of the organic chemistry course :

Organic chemistry is a fundamental field that supports a wide range of technical and industrial applications, which is important for the 2^{nd} year science and technology undergraduates students (section: Process Engineering/Petrochemical Industries), who have the aspiration to pursue careers in science and technology, as well as industry sectors such as **petrochemicals** and **pharmaceuticals**.







Contents table :

General objectives :

- In terms of knowledge :

- Identify and name the different families of organic compounds, including alkanes, alkenes, alkynes, alcohols, aldehydes, ketones, carboxylic acids, and amines etc,.
- Use IUPAC naming rules to correctly name complex organic molecules.
- Explain common reaction mechanisms such as substitution, addition, elimination reactions, and molecular rearrangements.

- In terms of practical skills :

- Produce mechanisms for obtaining different functions and the main reactions encountered in organic chemistry.
- Carry out simple organic syntheses in the laboratory using appropriate techniques.

- In terms of attitudes/professional behavior :

- Evaluate the experimental methods used, including the responsible management of chemicals and waste with safety protocols.

Chapter 1 :
Generalities

Specific objectives :

- Identify key concepts such as **sigma** and **pi** bonds, atomic and molecular orbitals.
- Explain the differences between single, double and triple covalent bonds, using molecular models.
- Define the main terms used in organic chemistry, such as functional group and isomerism.
- Interpret the octet rules and the exceptions to these rules for carbon atoms.
- Apply IUPAC nomenclature rules to name saturated and unsaturated hydrocarbons.
- Evaluate bonding models and test their validity.

Contents table of chapter 1 :

1- Study of the carbon atom and its bonds :

1-1- Definition :

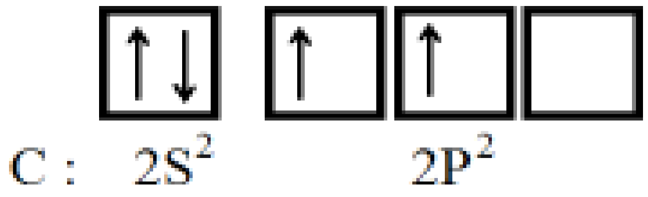
Organic chemistry is a science in chemistry which studies and describes organic compounds based on carbon; it is also known as carbon chemistry. In general, an organic molecule can be written in the form (molecular formula): **CxHyOzNt**...

1-2- Carbon atom and its bonds :

Carbon has 6 electrons, 6 protons and 6 neutrons, and is represented by : $^{12}_{6}C$

- Its electronic configuration can be written as : **1s2 2s2 2p2**

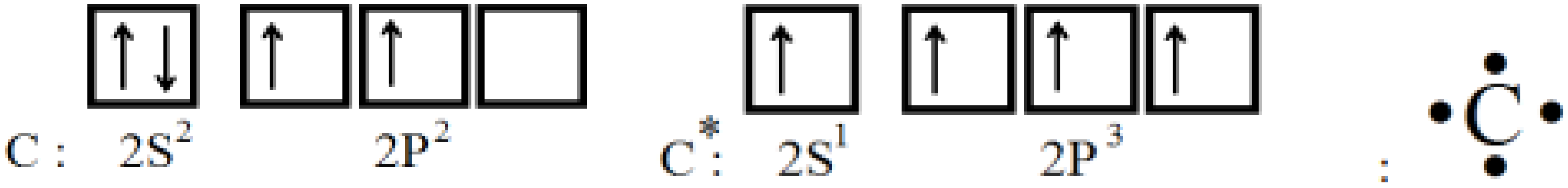
- Its representation is :



1-3- Types of bonds :

These bonds are totally covalent and not ionic, unlike inorganic compounds. In terms of bonding, carbon can bond with most of the atoms in the periodic table. In particular, there is the possibility of carbon-carbon bonds via single, double or triple bonds.

$$H_3C-CH_3 \quad , \quad H_2C=CH_2 \quad , \quad HC\equiv CH$$

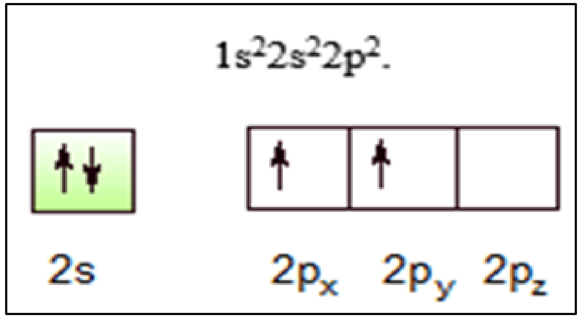


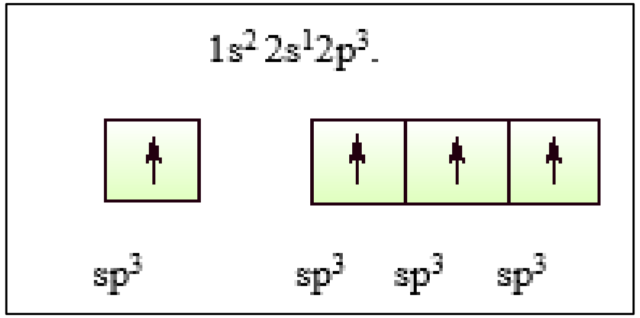
- Hybridization theory, or valence bond theory :

This theory was developed in the 1930s, describe the chemical bonding that had great success in organic chemistry, because it gives explanation of experimental facts that were completely incomprehensible by LEWIS's theory, such as the existence of s and p bonds.

- « sp3 » hybridization :

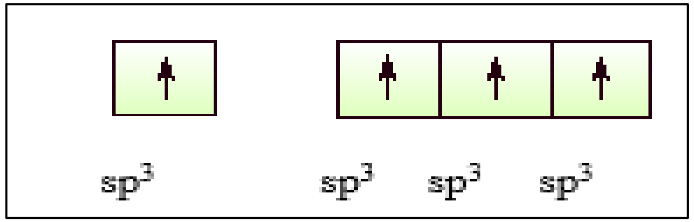
We will start with an example that illustrates the general method: the methane molecule, CH_4.



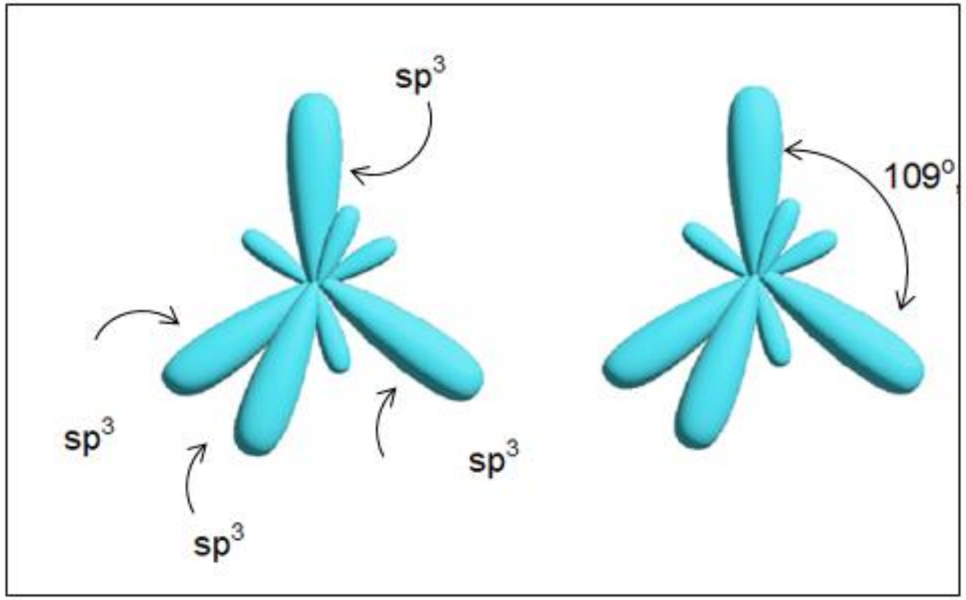


1 atomic orbital 2s + 3 atomic orbitals 2p → 4 hybridized atomic orbitals « sp3 »

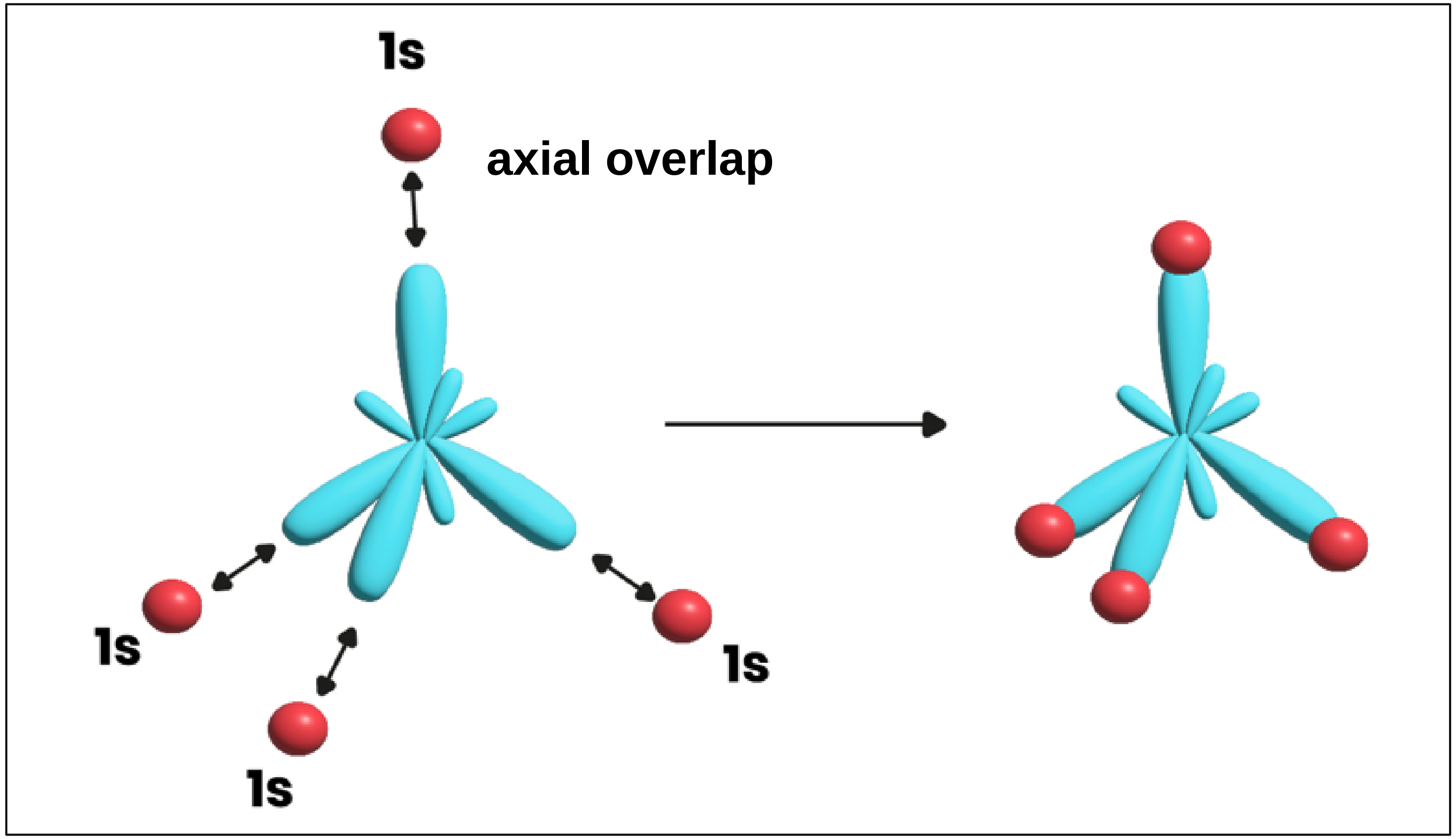
The four electrons that were in the two sub-shells 2s and 2p are now uniformly distributed in each of the four **sp3 hybridized atomic orbitals**. This uniform distribution of the four electrons is justified by the equivalence of the four chemical bonds in the methane molecule.

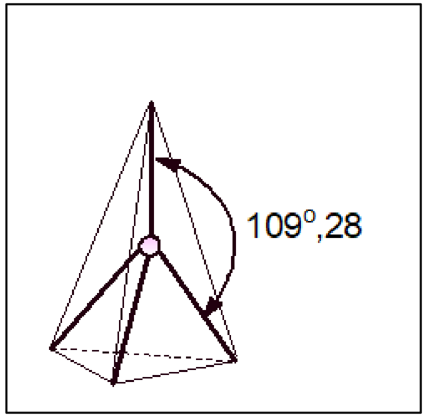


The four hybridized sp3 orbital, will be arranged in four directions at angles of 109°28' from each other.



Each **sp3 hybrid atomic orbital** unites with a **1s atomic orbital** from a hydrogen atom carrying a single electron.





Tetrahedral structure

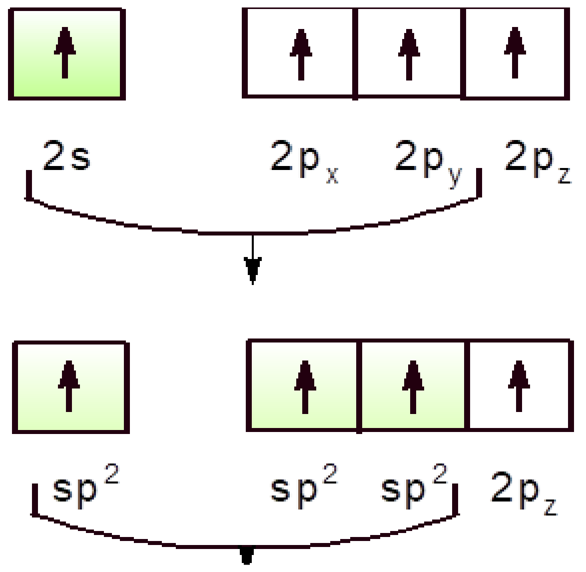
- **“ sp2 “ hybridization :**

The example will be illustrated by the ethylene molecule C_2H_4. We will work on one of the two carbon atoms in the molecule. By symmetry, we will then work on the second one.

By writing the electronic configuration of the carbon atom in its **hybridized state : 1s2 2s1 2p3**, we hybridize the following atomic orbitals of the carbon atom: **2s, 2px** and **2py**.

The **2pz** orbital is **left unhybridized** .

1 atomic orbitals 2s + 2 atomic orbitals 2p =>
3 hybridized atomic orbitals « sp2 »



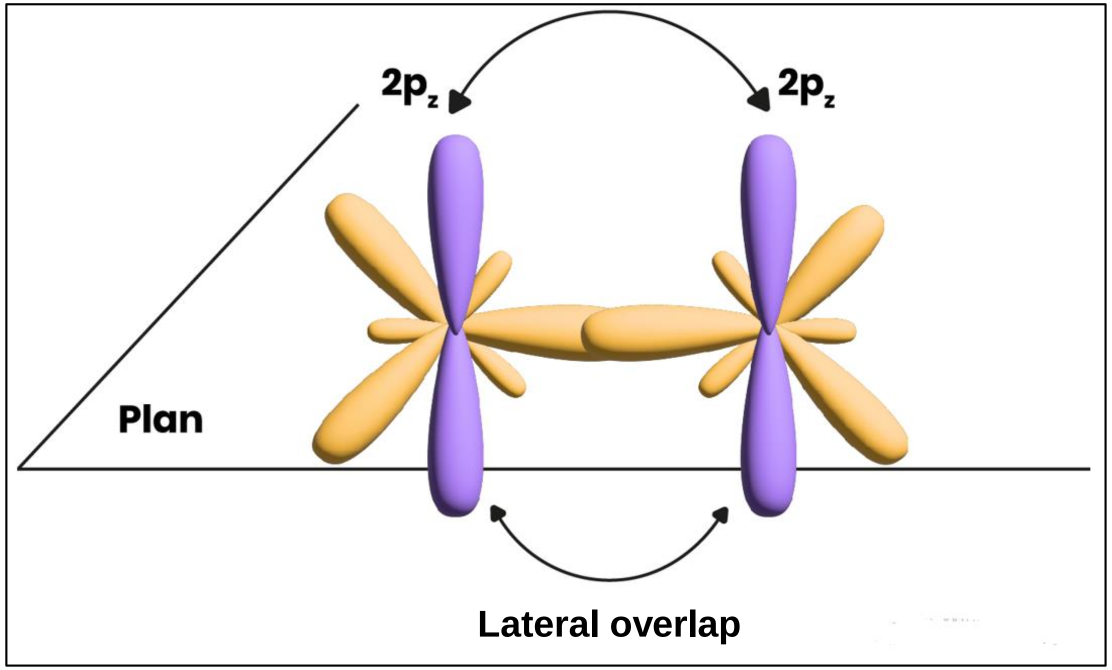
3 hybridized atomic orbitals « sp2 »

Each of these hybridized orbitals therefore contains an electron. The way in which three electrons are distributed in space on a planar geometry with an angle of 120° between each of the chosen directions.

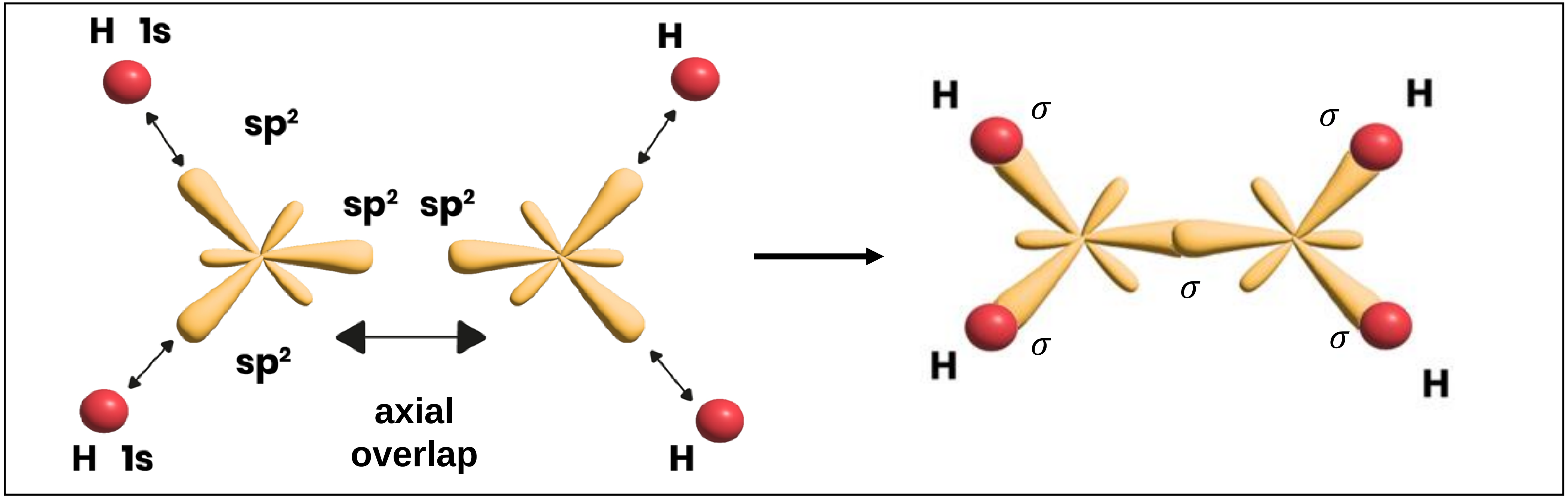
As the **2pz orbital is not affected by the hybridization** of the three previous orbitals, it occupies a direction **perpendicular** to the plane in which the three sp2 hybrid orbitals are located. This orbital also contains an electron.

Between the two non-hybridized atomic orbitals 2pz: the fusion between these two atomic orbitals 2pz is a **lateral overlap**.

Lateral overlap with the 2pz atomic orbital gives the " pi " bond. The ethylene molecule thus has the following form :

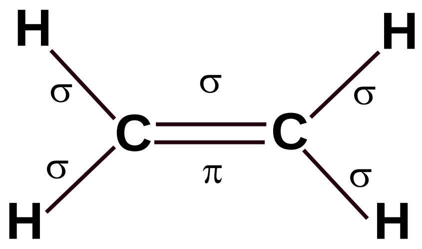


To complete the construction of the ethylene molecule, we finally create four CH bonds. Where the four molecular orbitals, of type ‘s’, between a **sp2 hybrid atomic orbital** of the carbon and a **1s atomic orbital** coming from a hydrogen atom.



Between the two sp2 hybrid atomic orbitals : axial fusion, we create what is known as an ‘sigma bond’.

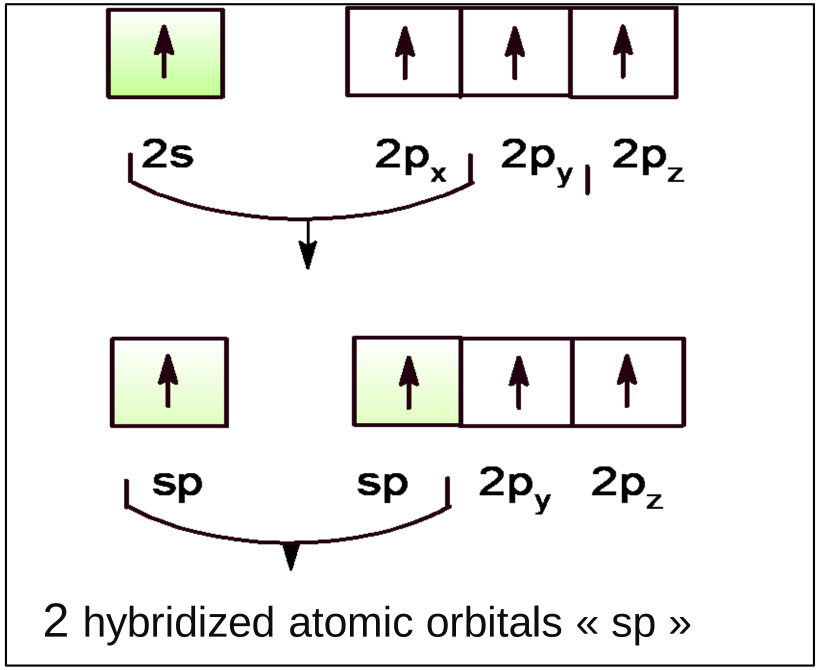
5 sigma bonds and 1 pi bond



- **« sp » hybridization :**

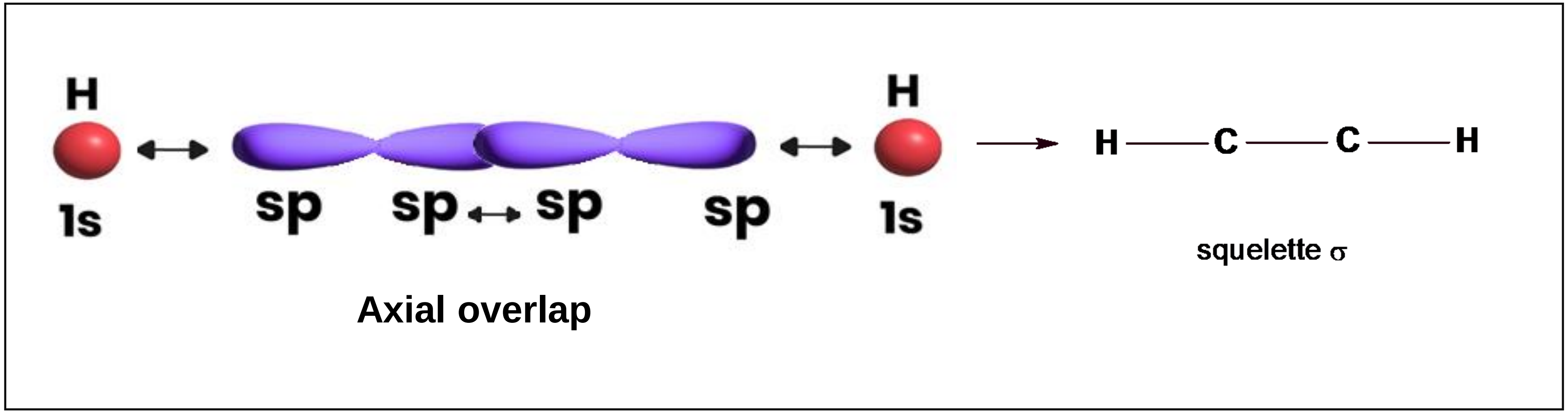
Let's take the example of the acetylene molecule **C_2H_2**. The electronic configuration of the carbon will be the same as for methane and ethylene: **$1s^2\ 2s^1\ 2p^3$**. On this basis, the **2s** atomic orbital with the **2p** atomic orbital for each carbon atom **are hybridized**. We therefore leave two atomic orbitals for each carbon atom, the **2py** and **2pz** atomic orbitals **non hybrized**.

1 atomic orbitals 2s + 1 atomic orbital 2p => 2 hybridized atomic orbitals « sp »



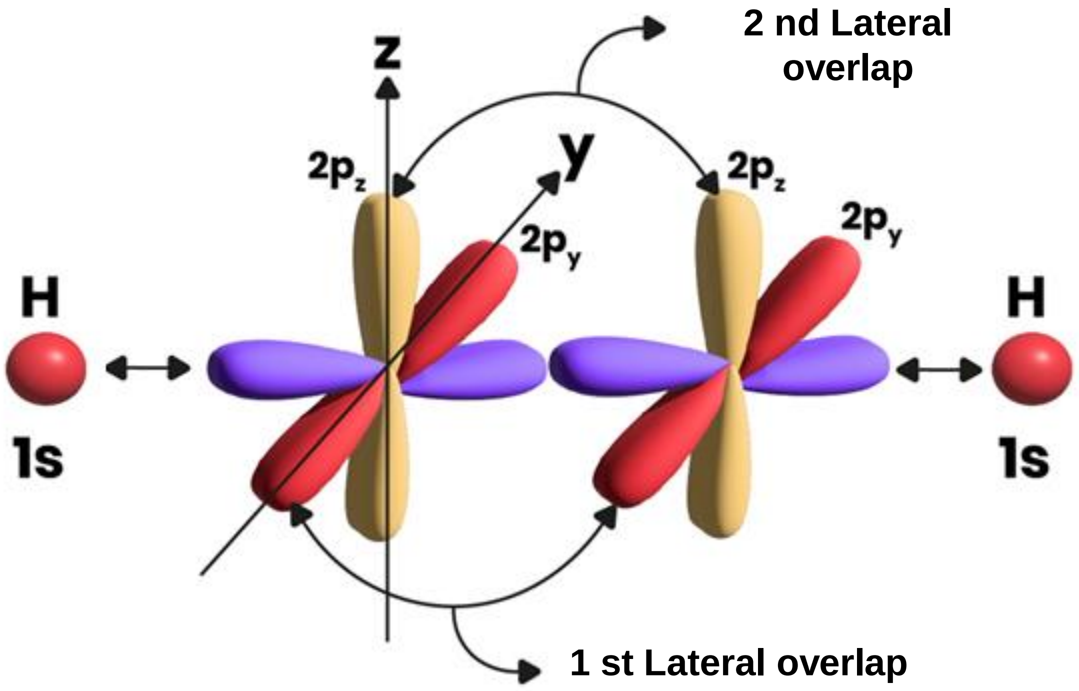
The acetylene molecule is therefore constructed by :

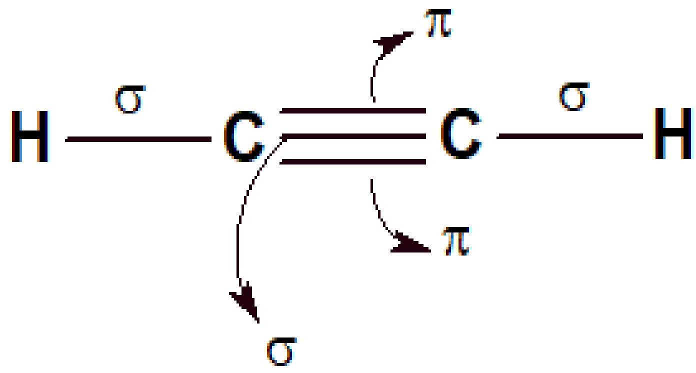
1. An axial overlap of two ‘sp’ hybrid orbitals on each carbon atom. This produces an ‘sigma’ bond between the two carbon atoms. The CH bonds are obtained by axial overlapping the other sp hybrid atomic orbitals of the carbon and the 1s atomic orbitals of the hydrogens.



2. A **lateral overlap** of **two non-hybridized orbitals 2py**, of each carbon atom creates a **pi-type bond** between the two carbon atoms.

3. A **second lateral overlap** between the two **non-hybridized** atomic orbitals **2pz** from C_1 and C_2 , creates the second **pi-type bond** between the two different carbon atoms.





Acetylene molecule

3 sigma bonds and 2 pi bonds

1-4- Organic compounds formulas :

Organic compounds can be represented in different ways, using different types of formulas: a molecular formula, an empirical formula, a general formula, a structural formula, a displayed formula and a skeletal formula.

1- Molecular formula

A molecular formula gives the actual number of atoms of each element in a molecule.

Examples :

- Ethane has the molecular formula C_2H_6 : the molecule is made up of 2 carbon atoms and 6 hydrogen atoms.
- Pentene has the molecular formula C_5H_{10} : the molecule is made up of 5 carbon atoms and 10 hydrogen atoms.
- 1,4-dibromobutane has the molecular formula $C_4H_8Br_2$: the molecule is made up of 4 carbon atoms, 8 hydrogen atoms and 2 bromine atoms.
- 1,3-dichloropropane has the molecular formula $C_3H_6Cl_2$: the molecule is made up of 3 carbon atoms, 6 hydrogen atoms and 2 chlorine atoms.

The molecular formula is insufficient to define a compound, as it does not specify how the atoms are linked.

2- Structural formula :

We can simplify the writing of a structural formula by another simpler formula, by avoiding representing certain bonds, such as CH, OH. The semi-developed formulae in the previous examples can be represented as follows :

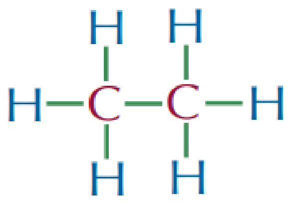
Examples :

- Ethane has the structural formula CH_3-CH_3 .
- Pent-1-ene has the structural formula CH_3-CH_2-CH_2-CH=CH_2 .
- 1,4-dibromobutane has the structural formula Br-CH_2-CH_2-CH_2-CH_2-Br.
- 1,3-dichloropropane has the structural formula Cl-CH_2-CH_2-CH_2-Cl.

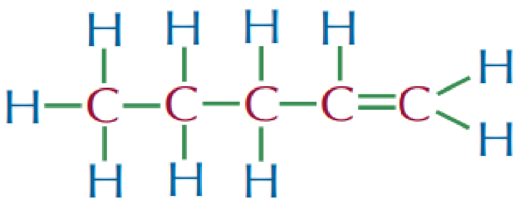
3- Displayed formula :

A displayed formula shows how all the atoms are arranged, and all the bonds between them.

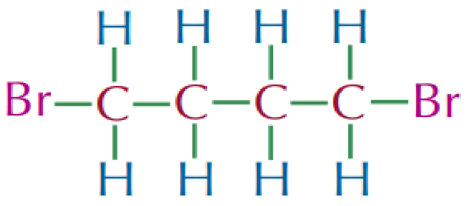
Displayed formula of ethane:



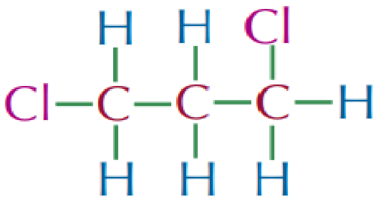
Displayed formula of pent-1-ene:



Displayed formula of 1,4-dibromobutane:



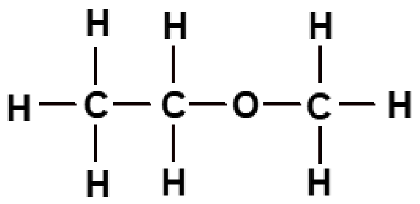
Displayed formula of 1,3-dichloropropane:

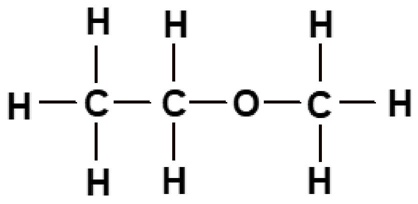


Also the displayed formula is used to distinguish between isomers.

Example:

These two compounds, which have the same gross formula **C_3H_8O**, have different structural formulas:





4- The skeletal formula :

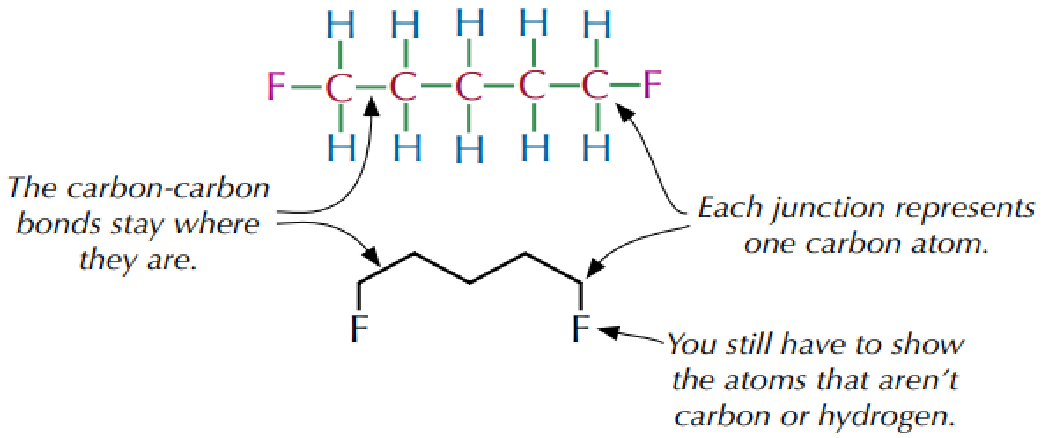
The simplified structure is the most schematic representation of the carbon skeleton. It shows the bonds of the carbon skeleton only, with any functional groups.

Examples :

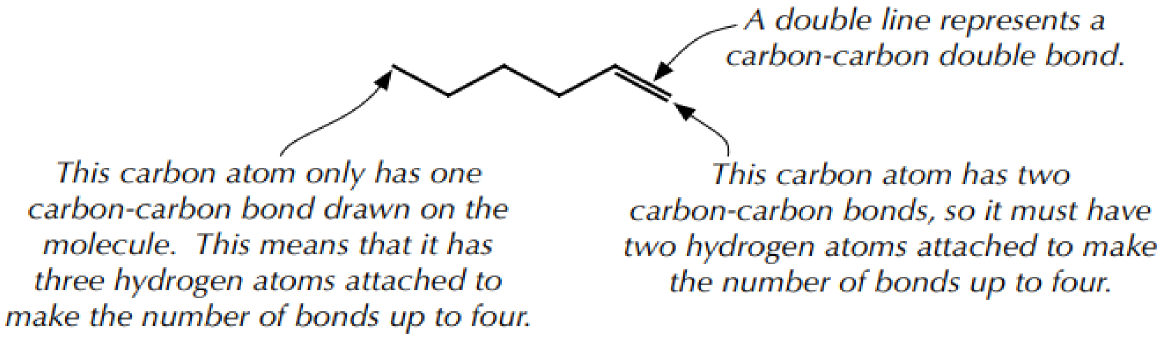
The hydrogen and carbon atoms that are part of the main carbon chain aren’t shown. This is handy for drawing large complicated structures, like cyclic hydrocarbons.

The carbon atoms are found at each junction between bonds and at the end of bonds. Each carbon atom has enough hydrogen atoms attached to make the total number of bonds from the carbon up to four.

Displayed and skeletal formulas of 1,5-difluoropentane:

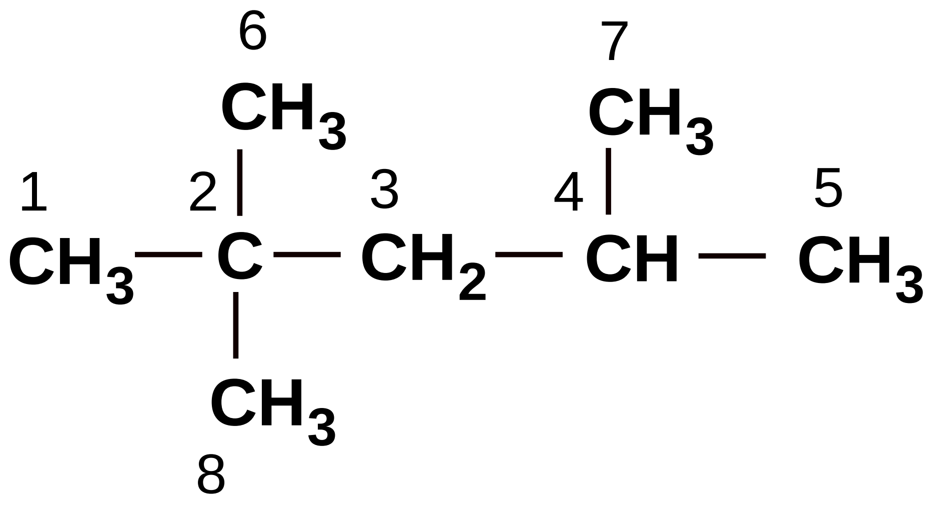


Skeletal formula of hex-1-ene:



1-5- Classification of carbon atoms

- The atoms numbered **C1, C5, C6, C7** and **C8** are linked / bonded to a single carbon atom and are said to be primary.
- The atom numbered **C3** bonded to two carbon atoms is called secondary.
- The atom numbered **C4** bonded to three carbon atoms is called tertiary.
- The atom numbered **C2** bonded to four carbon atoms is quaternary.

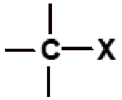
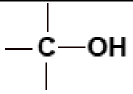
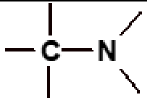
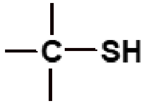
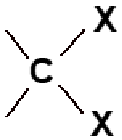
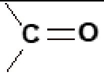
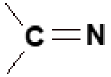
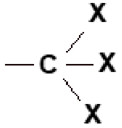
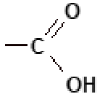


2- Functions and nomenclature of organic compounds :

2-1- Chemical functions / Functional groups :

A chemical function or functional group is the atom or group of atoms that characterizes a family of organic compounds and determines all its properties and chemical reactivity.

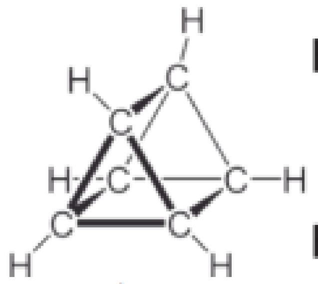
The main functions are classified according to the nature of the mineral heteroatom (O, N, S, X) and the number of bonds these heteroatoms have with carbon.

Function	Halogen	Oxygen	Nitrogen	Sulphur
Monovalent		 alcohol	 amine	 thiol
Divalent		 Ketones and aldehyde	 imine	
Trivalent		 Carboxylic acid	 nitrile	

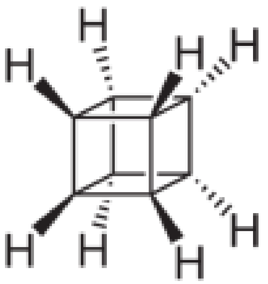
2-2- Naming:

In previous times, the names of organic compounds were given in relation to :

- Their origins (Formic acid: ants; Citranol: lemon; Cumene: cumin; Menthol: menth; ....).
- Their geometric form : (Prismane : C_6H_6 ; Cubane :C_8H_8 ; …..)

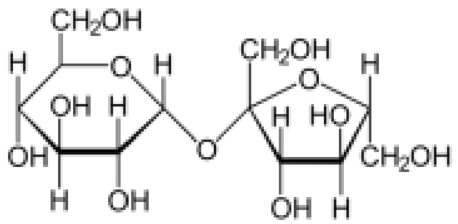


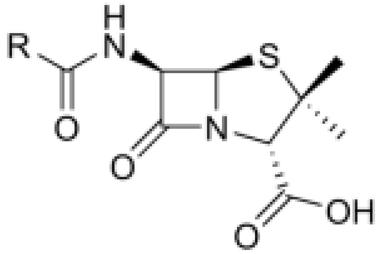
Prismane



Cubane

- Their complex names : Sucrose; Penicillin

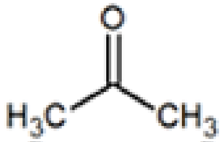
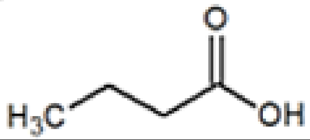
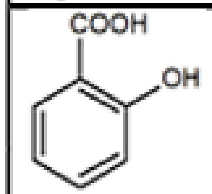
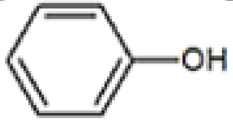




Chemists have therefore thought of establishing universal and systematic rules for naming any organic compound. There are several methods for naming an organic compound:

- **Ordinary, common, trivial or commercial nomenclature**
- **IUPAC's systematic and scientific nomenclature**

Table 1: Trivial and IUPAC names of some organic compounds

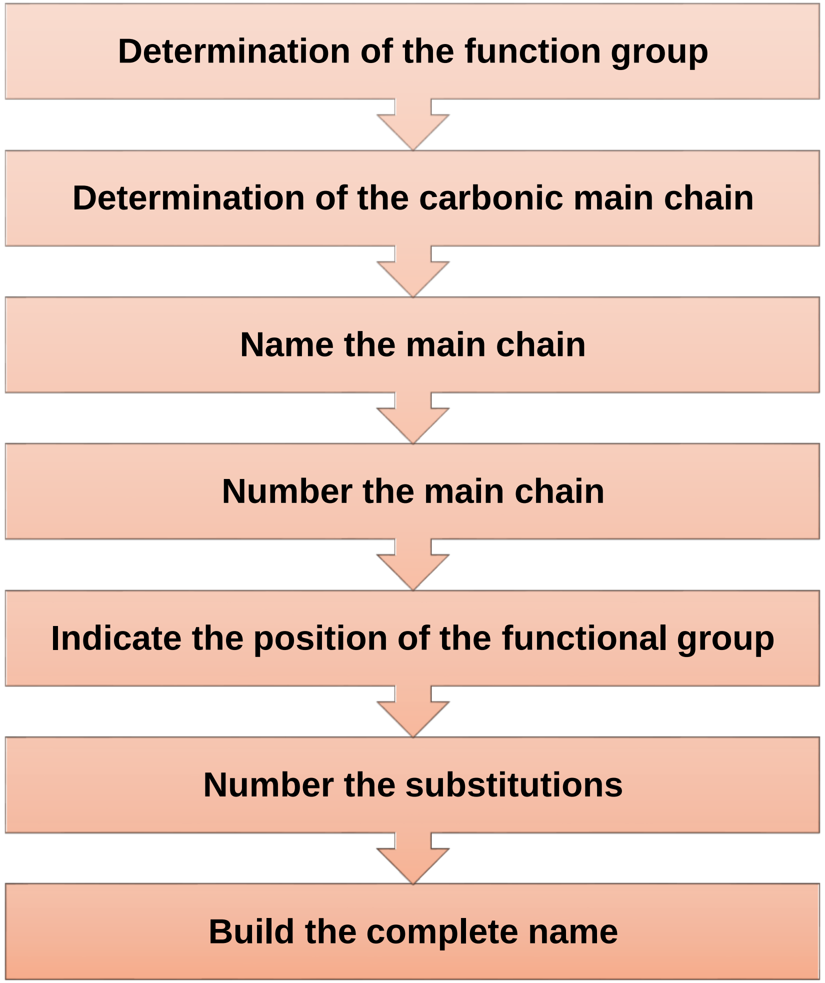
Formula	Trivial name	IUPAC name
$HCOOH$	Formic acid	Methanoic acid
$CH_3\text{-}COOH$	Acetic acid	Ethanoic acid
$CHCl_3$	Chloroform	Trichloromethane
$C_2H_5\text{-}OH$	Ethylic alcohol Ordinary alcohol	Ethanol
$CH_2(OH)\text{-}CH_2(OH)$	Glycol Ethyleneglycol	Ethan-1,2-diol
$CH_2(OH)\text{-}CH_2(OH)\text{-}CH_2(OH)$	Glycerine Glycerol	Propan-1,2,3-triol
	Acetone	Propanone
	Butyric acid	Butanoic acid
	Salicylic acid	2-hydroxybenzoic acid
	Phenic acid	Phenol

Systematic naming :

The International Union of Pure and Applied Chemistry (IUPAC) is the agreed authority for the development of the adopted rules of the naming, symbols and terminology of chemical elements and their derivatives.

Because of the large number of structures present in organic chemistry, it is essential to have an unambiguous description and name for the molecule. The two concepts that appear in this definition need to be defined:

- The carbon chain
- The function



The carbon chain is the assembly of carbon atoms linked together in the molecule, while the function is an atom or group of atoms that gives the molecule an important property.

The name given to a molecule therefore takes the following form [2] :

Prefix(es)* + *main chain name* + *suffix(es)* + *terminal suffix

- The '**Main chain name**' corresponds to the number of carbon atoms in the main chain.

- The **prefix** or **prefixes** which precede the main chain name identify the substituents of the main chain; these substituents are either characteristic groups other than the main group (alkyls) which do not belong to the main chain.

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[2] : cours de chimie organique par : A. SAFER , fac de chimie usto/ L2 GP

- The **suffix** or **suffixes** immediately preceding the terminal suffix should be called ‘saturation or unsaturation suffixes’. If the main chain has only **single bonds** between carbons, this suffix is **‘ane’** ; it will be **‘ene’** if the main chain includes a **C=C double bond** or **‘yne’** if there is a **C≡C triple** bond.

- If there is a chemical function, there is a **terminal suffix**. The terminal suffix therefore characterizes the main **functional group**.

- Finally, **indexes** indicating the positions on the main chain : substituents, multiple bonds and the main group should be placed in the prefixes, suffixes and main suffix respectively.

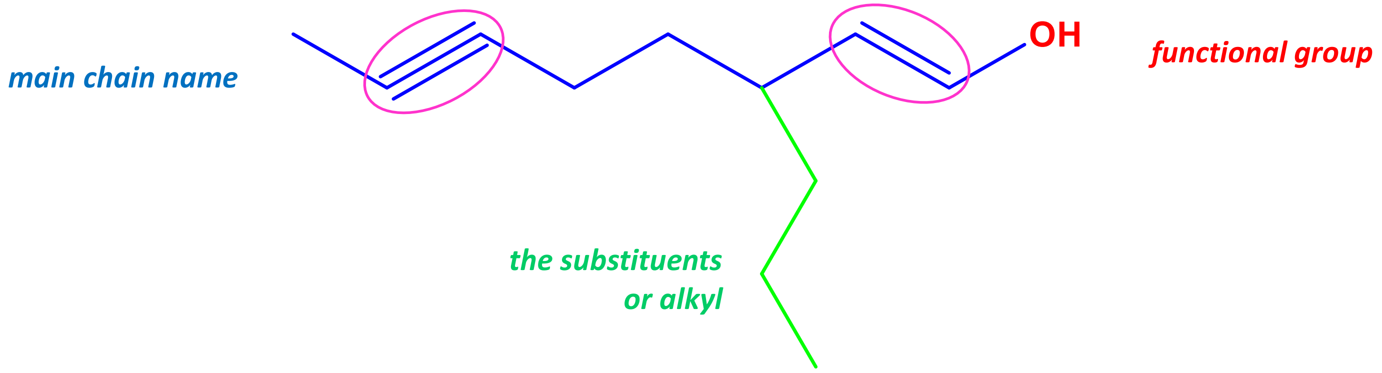
In general, an IUPAC name will have three essential characteristics :

a. A base indicating a major chain or ring of carbon atoms found in the molecular structure.

b. A suffix (ending) or other element designating functional groups that may be present in the compound.

c. Names of substituent groups (prefix), other than hydrogen, which complete the molecular structure.

Example :



Prefix(es) + main chain name + suffix(es) + terminal suffix

Chapter 2