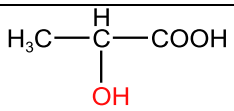
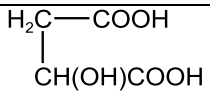
Nomenclature of organic compounds

Introduction :

Principles of nomenclature In early days of organic chemistry, each new compound was given an individual name. Such a name was based on the source, some property, or some other trivial reason. Thus formic acid, HCOOH, was so named as it was obtained by distillation of red ants (Latin, *formica* = ants). The structure of many of these compounds was not known at that time. An ordinary name given to a compound without reference to its structure is called a **Common Name** or **Trivial name.**

Examples :

S. NO.	ORGANIC COMPOUND	TRIVIAL NAME	SOURCE
1	CH_3OH	Wood spirit or Methyl spirit	Obtained by estructive distillation of wood
2	NH_2CONH_2	Urea	Obtained from urine
3	CH_4	Marsh gas (fire damp)	It was produced in marshy places
4	CH_3COOH	Vinegar	Obtained from Acetum (Vinegar)
5		Oxalic acid	Obtained from oxalis plant
6	HCOOH	Formic acid	Obtained from formicus [Red ant]
7		Lactic acid	Obtained from sour mild
8		Malic acid	Obtained from apples
9	$CH_3CH_2CH_2COOH$	Butyric acid	Obtained from butter
10	$CH_3(CH_2)_4COOH$	Caproic acid	Obtained from goats

With the rapid growth of organic chemistry, the number of compounds increased fantastically (now about 6 million). It became impossible to give common names to such a large number of compounds. In 1957, the *International Union of Pure and Applied Chemistry* evolved a

scheme for giving systematic names to organic compounds on the basis of structure. This is known as the **IUPAC System.** One organic compound can have only one IUPAC name.

.*IUPAC* system has set rules for :

- naming organic molecules from their structures.
- write its structural formula from name of a compound

The IUPAC system is much the same for all classes of orgamc compounds. IUPAC rules for naming alkanes are given below.

- Primary prefixe : It defines substituent & position of substituent.
- Secondary prefixe : is used simply to distinguish cyclic from acyclic compounds 'cyclo, bicyclo….)
- PCC : parent carbon chaine, It is the basic unit of the name. It tells the number of carbon atoms present in the principal chain
- Primary Suffix : A primary suffix is always added to the word root to indicate position (locant), nature and number of unsaturated bonds.
- Secondary suffix : secondary suffix is always added to the primary suffix to indicate the nature of the principal functional.

Procedure for naming an organic compound :

1. Select principal fonctionel groupe
2. Select the parent carbon chaine (PCC)
3. Number the PCC
4. Write the name as single worde

NB: all the atoms or groups of atoms connected to this chain, except the principal function, are considered as substituent.

I. Hydrocarbons :

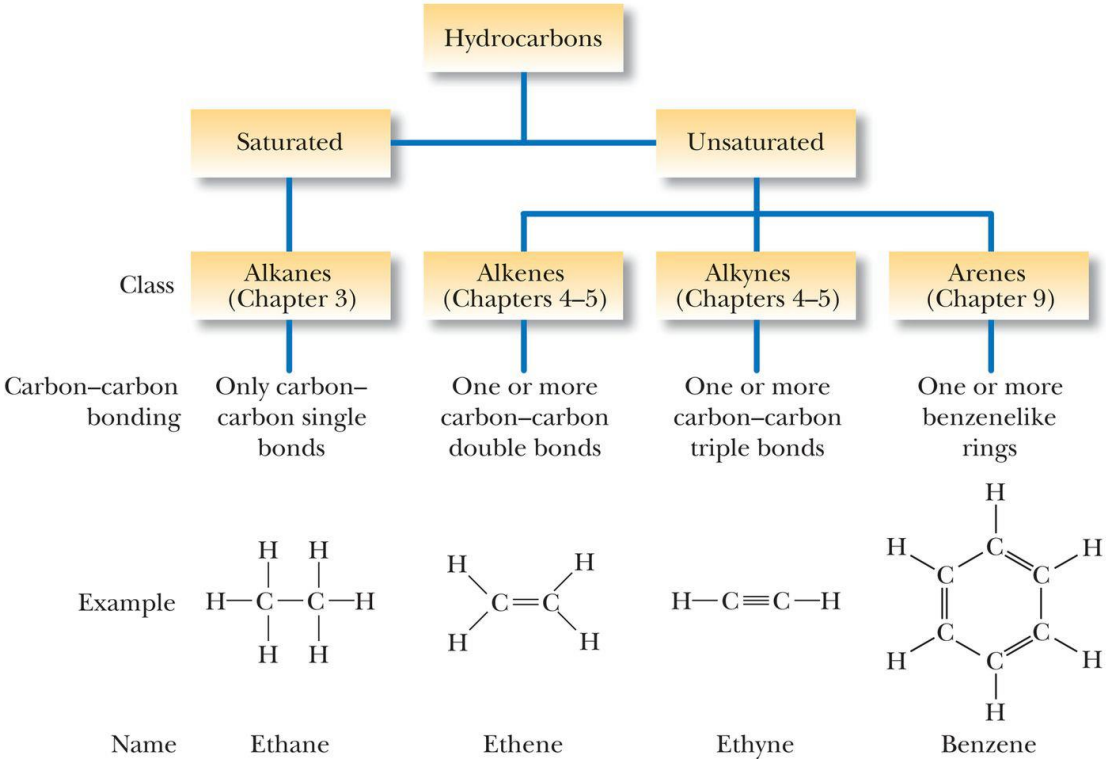


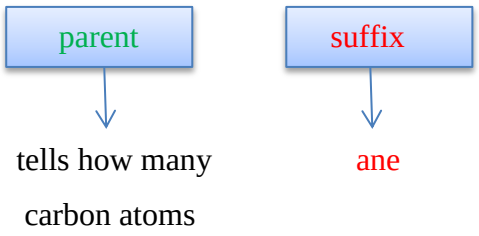
Figure 1 : The Four Classes of Hydrocarbons

I.1. acycliques satureted hydrocarbures (alkane) : Alkanes have the general formula C_nH_{2n+2}

a. **linear (**Straight **) alkanes** :

We'll soon see that these alkane names form the basis for naming all other organic compounds, so at least the first ten should be memorized.

The first four (n=1-4) Straight-chain alkanes are called methane, ethane, propane and butane whose names have historical roots. After this, the alkanes are named based on Greek numbers followed by the ending "-ane". The first twelve members are given in Table 1.

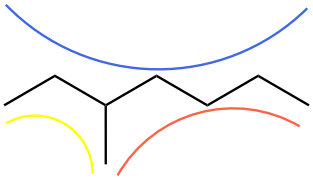


Example :

Tableau 2 : names of linear alKanes

Nombre de carbones	USF	Nom	Nombre de carbones	USF	Nom
1	Méth	méthane	11	undéc(a)	undécane
2	Eth	ethane	12	dodéc(a)	dodécane
3	Prop	propane	13	tridéc(a)	tridécane
4	But	butane	14	tétradéc(a)	tétradécane
5	Pent	pentane	20	eicos(a)	eicosane
6	Hex	hexane	30	triacont(a)	triacontane
7	Hept	heptane	50	pentacont(a)	pentacontane
8	Oct	octane	100	hect(a)	hectane
9	Non	nonane	120	eicosahect(a)	eicosahectane
10	Déc	décane	132	dottriacontahet(a)	dottriacontahetane

b. Branched alkanes :

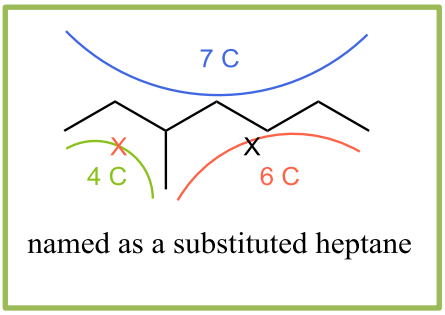


The branched acyclic alkanes have several chains, for a systematic chemical naming it is necessary to proceed the following rules :

détermination de PCC :

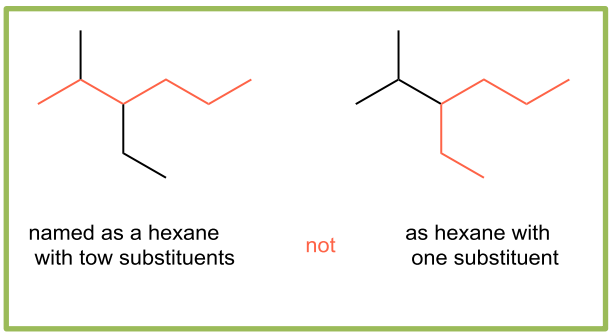
Select the longest carbon chain containing maximum number of carbon and this longest carbon chain is also called parent carbon chain (PCC).

y Longest carbon chain not always straight.



If two or more carbon chain contains same number of carbon

then PCC is considered which has more number of substituents.

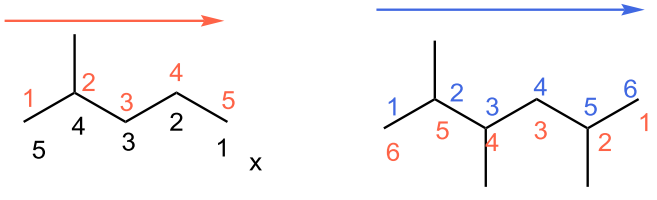


Number of PCC :

Numbering of parent carbon chain is done by lowest locant rule.

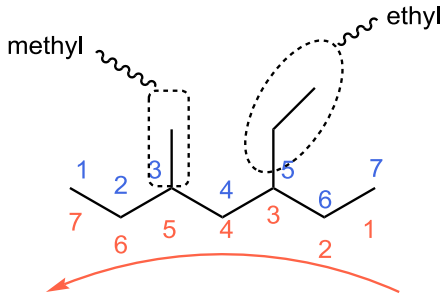
- Lowest Locant Rule : According to this rule numbering is done in such a way so that substituent will get lowest number.

Examples :



2,3,5 not 2,4,5

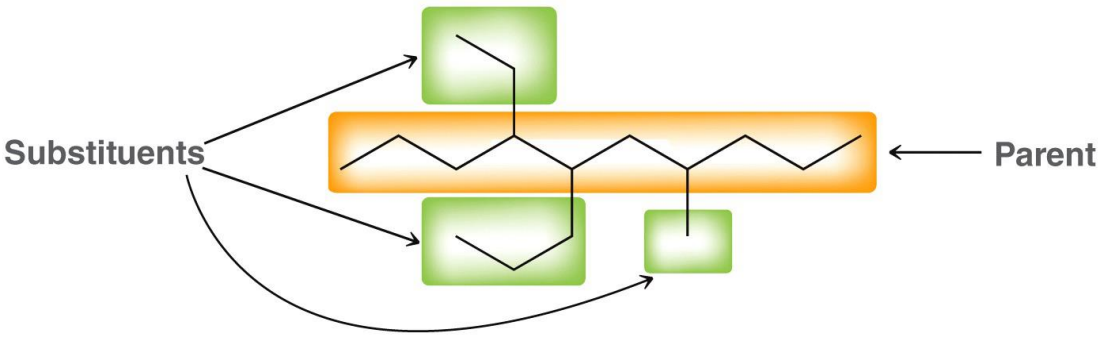
If two or more substituents are present on parent carbon chain and they get same number from either side during numbering then numbering is done by alphabetical order.



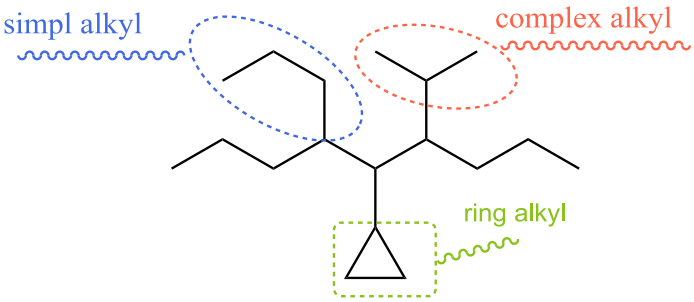
Write the name :

a. Identify and number the substituents. Then cite them in alphabetical orde

Rad_1 Rad_2….Rad_n PCC ane



- Substitutents are the Alkyl Groups, they can be simpl, complex or ring alkyl groups



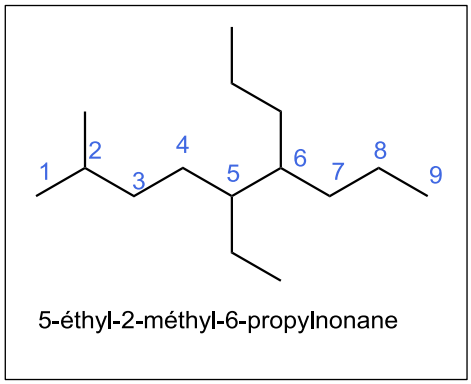
- An alkyl group is formed by removmg one hydrogen atom from an alkane.
- The symbol R-is often used to represent an alkyl group. The grouping R-.

➢ Alkyl types :

- simpl alkyl:

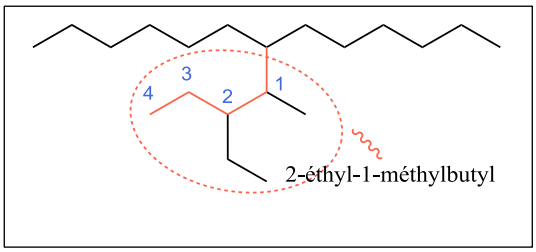
Alkyl groups are named by dropping *-ane* from the name of the corresponding alkane, and adding the ending-y/.

Alkane - ane + yl = Alkyl



- **Complex alky groups**

(those which are branched themselves) are named as if they were alkanes, but the name ends in ***-yl*** and
is enclosed in parenthesis. The carbon from which the substituent atttaches to the main chain is automatically number



- ring alkyl

A ring can be either a parent chain or a substituent depending on the number of carbons, the name of cycloalkyl is formed by attached the prefixe cyclo to the name of acyclic alkyl withe the same number of carbons

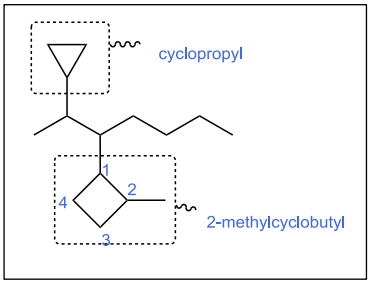
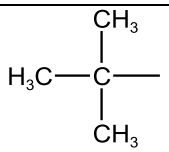
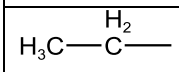
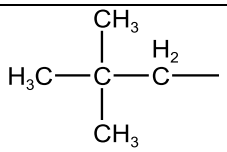
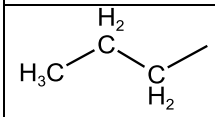
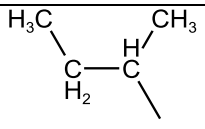
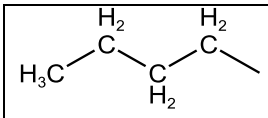
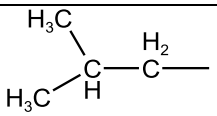
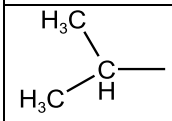
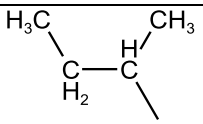


Table2 : name of alkyl groups

H_3C-	Méthyl		1,1-diméthylpropyl (tertiobutyl)
	Ethyl		2,2-diméthylpropyl (néopenthyl)
	Propyl		1-méthylpropyl

	Butyl		2-méthylpropyl (isobutyl)
	1-méthyléthyl (isopropyl)		1-méthylpropyl

2. Write out the name as a single word:

- ✓ hyphens (-) separate prefixes
- ✓ commas (,) separate numbers
- ✓ Substituents are listed in alphabetical order

Note :

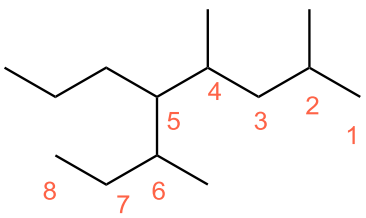
- ➢ If two or more identical substituents are present use the multiplicative prefixes:

Nombre	**Radical simple**	**Radical complexe**
2	di	Bis
3	tri	Tris
4	tétra	Tétrakis
5	penta	Pentakis
6	hexa	Hexakis

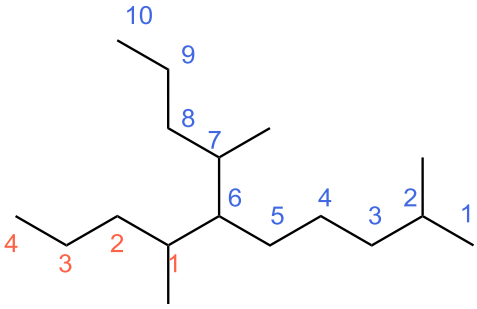
- ➢ Ignore multiplicative prefixes *as in alphabetizing.*

- ➢ When the multiplicative prefixes (di, tri, tetra,…)write in parentheses (complixe alkyles)are conssiderred alphabeticaly.
- ➢ Iso- and neo are part of the alkyl group name and are used for alphabetizing. sec- and tert- are not included in the alphabetical order.

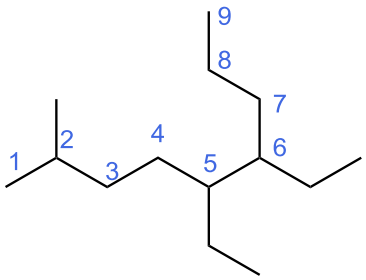
Exemples :



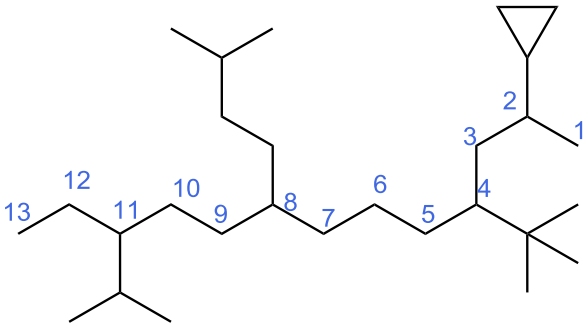
2,4,6-triméthyl-5-ropyloctane



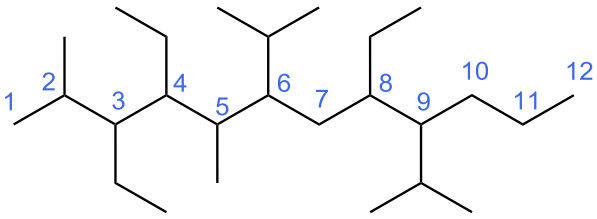
6-(1-methylbutyl)-1,7-dimethyldecane



5,6-diethyl-2-methylnonane

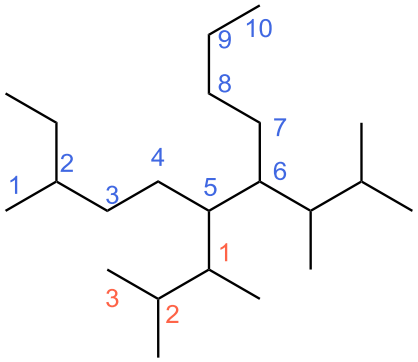


2-cyclopropyl-8-isobutyl-11-isoprppyl
-4-tetiobutyltridecane



3,4,8-triéthyl-6,9-bisisobutyl

-2,5-diméthyldodécane



5,6-bis(1,2-dimethylpropyl)-2-ethyldecane