petroleum chemistry

Chemical engineering department

Al-Mustaqbal-college

First class

second semester

Lecture two

By

Asst. lect. Ban Ali Hassan

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Lecture two

The IUPAC Naming (nomenclature) System

- How to Name Organic Compounds

We will use the nomenclature (systematic) system for alkanes and cycloalkanes as a demonstration of how to systematically name organic compounds. The system used to name alkanes forms the basis for naming all organic compounds.

The general approach is as follows :

The name given to any compound containing a chain of carbon atoms consists of three parts;

- The **root** of the name which appears in the middle (this is further divided into the carbon chain designation and the infix),
- The **prefix** which appears at the start; and
- The **suffix** which appears at the end.

- **The three parts of the name are linked together as shown below:**

Prefix---Root---Suffix

Each part will be described, and then some examples examined to show how organic compound nomenclature works**.**

1. The Root
This is divided into two sections – the **chain designation** and the **infix**.
The **chain designation** tells us the number of carbon atoms contained in the **longest continuous carbon chain** in the molecule. This is based upon the Table given below.

For example if the longest continuous C chain is four the chain designation is but-, if it is eight it is oct-

Table 1. Table of chain designation and corresponding number of carbons. The prefix cyclo- is added to these chain designations if the carbons exist in ring formation.

Chain Designation	No. of C Atoms
meth-	1
eth-	2
prop-	3
but-	4
pent-	5
hex-	6
hept-	7
oct-	8
non-	9
dec-	10

The **infix** tells us the **nature of the carbon bonds.** This is based on the system shown in the table below.

Table 2: The infix and corresponding nature of carbon-carbon bonds.

Infix	Nature of Carbon-Carbon Bonds
-an-	only single bonds
-en-	one or more double bonds
-yn-	one or more triple bonds
-yl	attached group (not part of main carbon chain)

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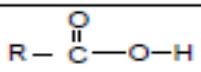
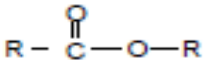
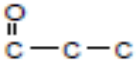
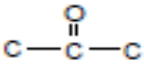
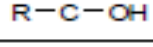
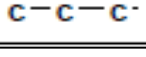
2. The Suffix

This tells us the class of compound to which the substance belongs. It is derived from the most important functional group in the molecule. The suffixes listed in the table below are given in their order of importance, the most important at the top, the least at the bottom. If more than one functional group is in the molecule, it is assigned to that class which has the more important functional group. In organic chemistry this is based upon the amount of oxygen and hydrogen in the functional group. **Essentially the more oxygen and the less hydrogen the more important the functional group.**

Table 3: The suffix and the corresponding class of organic compound.

Suffix	Class of Compound
-oic acid	alkanoic acid 
-oate	ester 
-al	alkanal 
-one	alkanone 
-ol	alkanol 
-e	hydrocarbon 

3. The Prefix

This **tells us the other atoms and groups of atoms attached to the main carbon chain**. It may be single species such as halogen atoms, carbon chains smaller than the main carbon chain, or even rings of carbon atoms.

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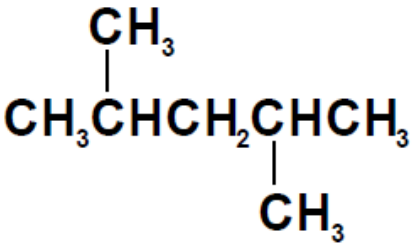
Prefix---Root---Suffix

Note: In naming, **dashes** are used to separate numbers and letters; **commas** are only used to separate numbers from other numbers. Names are given in **one piece**; there are no gaps between the pieces except when specifically stated in the naming system.

Some examples of the naming system are given below.

Example 1 :



To name this compound

1a. First count the longest continuous carbon chain – in this case 5.

Therefore the chain designation is **pent-.**

1b. As the molecule contains only single bonds to the carbon and hydrogen atoms the infix is **an-**.

Therefore the root of the name is **pentan-**.

2. Next add the suffix. As this molecule is a hydrocarbon the suffix is just **-e**.

Therefore the root plus suffix is **pentane**.

Finally we must list the attached groups as prefixes. In this case there are two groups attached to the main carbon chain. They are both single carbon groups. When naming carbon chains that are attached to the main carbon chain, the same naming conventions are used as in determining the root of the name for carbon designation, but the infix **-yl** is employed to distinguish attached chains from the main carbon chain.

In this case the attached groups have only one carbon atom so the chain designation is **meth-**, whilst the infix is **-yl**.

Therefore the attached groups are referred to as **methyl** groups.

3. If there is any ambiguity as to the position of the attached groups they must be numbered. The numbering and listing system has the following rules.

1. the longest continuous carbon chain is numbered such that the most important functional group is given the lowest number.
2. the attached groups are listed in alphabetical order.
3. the number of the carbon atom from the main chain to which the group is attached is placed in front of the name for the group and a hyphen placed between them.
4. if there is more than one type of group attached then the pre-prefixes listed below are used to state how many of each attached group is present .

Table 4*:* The pre-prefix and the corresponding number of attached groups.

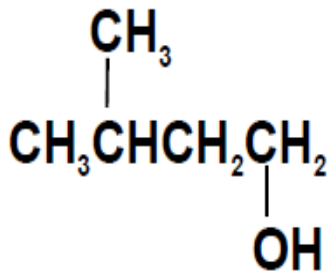
Pre-Prefix	Number of Attached Groups
di-	two
tri-	three
tetra-	four
penta-	five
hexa-	six

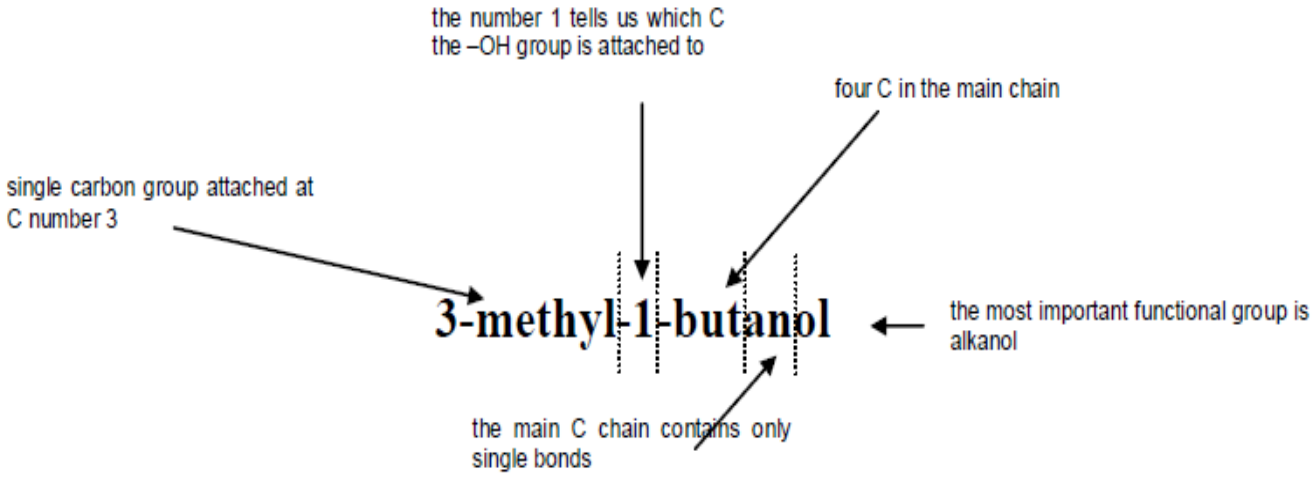
Using the above conventions the attached groups in our example would be 2,4-dimethyl-, because the one carbon groups are attached to carbons two and four of the main chain and the pre-prefix **di-** is used as there are two of them.

So the full name is 2,4-dimethylpentane.

Example 2 :

For the structure





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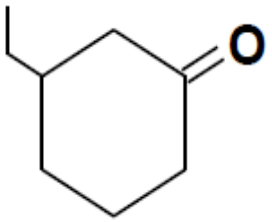
Example 3 :

For the structure



6C atoms in a ring

main C chain has only single bonds

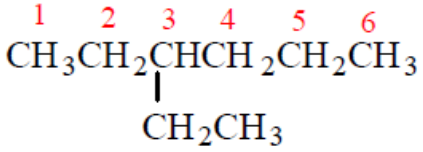
3-ethylcyclohexanone

2 C group attached to C number 3

most important functional group is alkanone

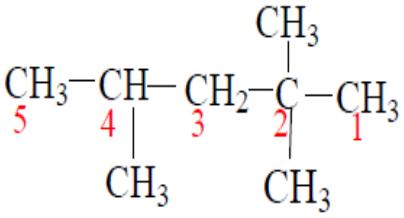
Examples :

1-



3-Ethyl hexane

2-



2-2-4-Trimethylpentane

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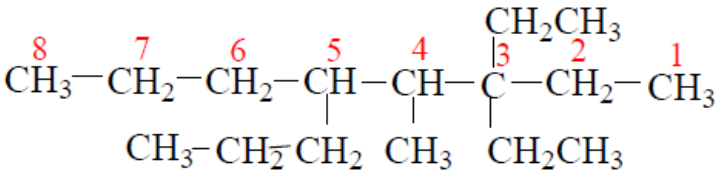
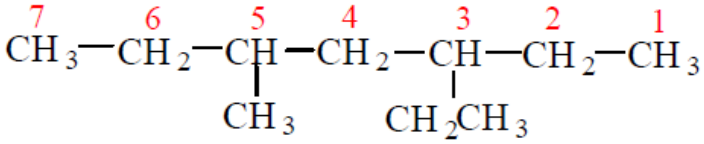
3-



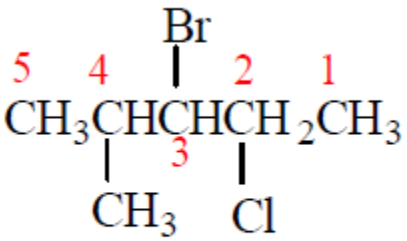
3,3-Diethyl-4-methyl-5-n-propyloctane

4-



3-Ethyl-5-Methylheptane

5-



3-Bromo-2-chloro-4-methylpentane

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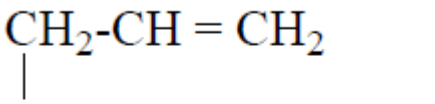
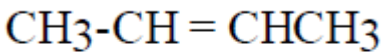
6-



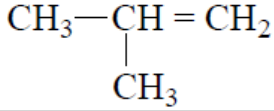
3-Chloro -l- Propene

7-



2-Butene

8-

Ethylene	$CH_2=CH_2$	Ethane	CH_3CH_3
Propylene	$CH_3-CH=CH_2$	Propane	$CH_3CH_2CH_3$
Butylene	$CH_3CH_2CH=CH_2$		
2-Butylene	$CH_3CH=CHCH_3$	n-Butane	$CH_3CH_2CH_2CH_3$
Isobutylene		Isobutane