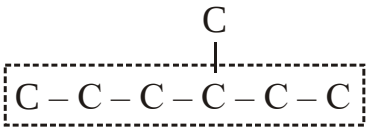
Carbon & its Compounds
Rules for IUPAC nomenclature of organic compounds

➢ Rules for IUPAC nomenclature of organic compounds

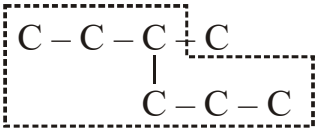
There are certain (following) rule for naming a complex organic molecule according to IUPAC system. These rules are illustrated below.

1. **Longest Chain Rule :** The first step for naming an organic compound is to select the longest continuous chain of carbon atoms which may or may not be horizontal (straight). This is called the parent chain or main chain, and other carbon chains attached to it are known as side chains. On the basis of the number of carbon atoms present in the parent chain, the parent hydrocarbon is determined. For example, if the parent chain contains six carbon atoms, the compound is considered to be a derivative of hexane.

Example : The structure I has the longest chain of six carbon atoms present in a straight line; therefore it is said to be a derivative of hexane. On the other hand, in structure II the straight chain has only four or three carbon atoms while the longest possible chain may have as many as six carbon atoms (zig-zig chain).



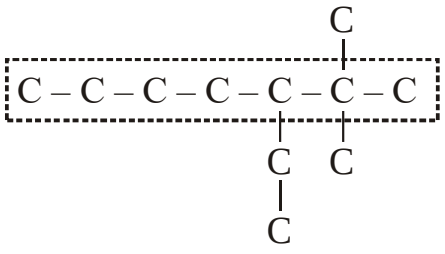
I
(Longest chain, straight)



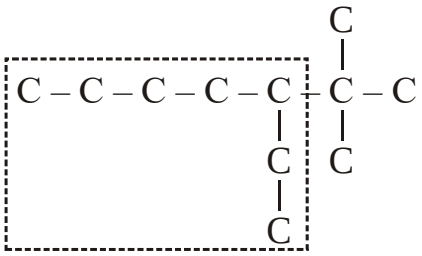
II
(Longest chain, zig-zig)

Therefore, both the structures are the derivatives of hexane.

In case a molecule contains two equally long carbon chains, the one carrying larger number of side chains is selected. For example, structure A and B have carbon chains of equal lengths (C_7), but the one carrying three substituents is selected.

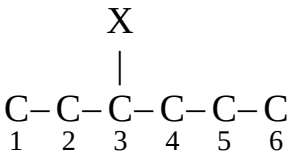


(A)
Straight parent chain of C_7
with three side chains (correct)

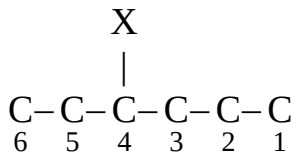


(B)
Zig-zig parent chain of C_7
with only one side chains (incorrect)

2. **Lowest number of lowest sum rule :** The carbon atom of longest carbon chain is numbered as 1, 2, 3, 4, ... etc. starting from the end that gives the lowest possible number to the substituent. For example, in structures A and B numbering may be done in two ways;



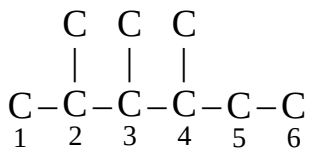
Substituent at C_3(A)
(Correct)



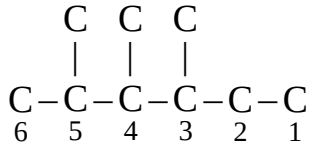
Substituent at C_4 (B)
(Incorrect)

In one case (A), the substituent is assigned position 3 while in other case (B), it is assigned position 4. Hence the former, being smaller, is correct. The number that locates the position of a substituent is known as locant. Thus the locant for X in the above correct structure is 3.

In case, the parent chain has two or more substituents, numbering must be done in such a way that the sum of the locants on the parent chain is the lowest possible. Thus in following structures A and B numbering may be done in two ways: in one (A), the sum of locants is 9 while in other (B), it is 12, hence the former is correct while the latter is wrong.

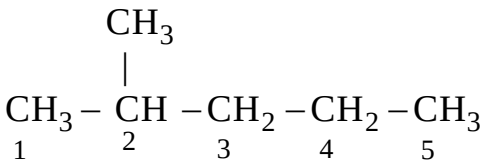


Sum of locants : $2 + 3 + 4 = 9$ (A)
(Correct)



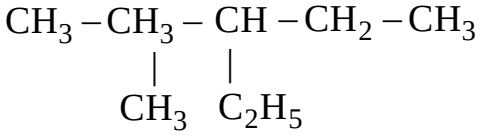
Sum of locants : $3 + 4 + 5 = 12$ (B)
(Incorrect)

3. **Name of the complex alkane :** The name of the substituent is prefixed to the name of the parent hydrocarbon and its position on the main chain is indicated by writing the locant before the prefix. A hypen (–) is inserted between the locant and the substituent name. The final name is always written as one word. Thus the following compound is written as 2-methylpentane.



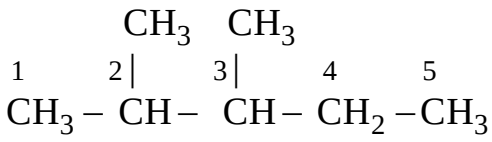
2–Methylpentane

4. **Alphabetical order of sides chains :** In case two or more alkyl groups (side-chains) are attached to the parent chain, these are prefixed in alphabetic order, e.g.

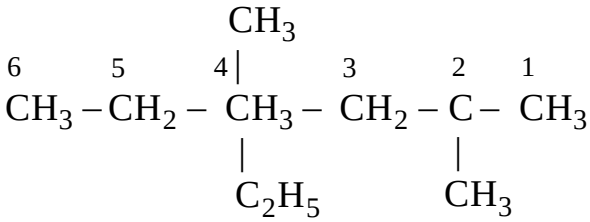


3–Ethyl–2methylpentane and not as
2–Methyl-3-ethylpentane

5. **If a substituent is present two or more times :** This is indicated by the prefix di-,tri-, tetra-, etc. added to the substituent. The different locants of the substituents are separated by commas. For example,

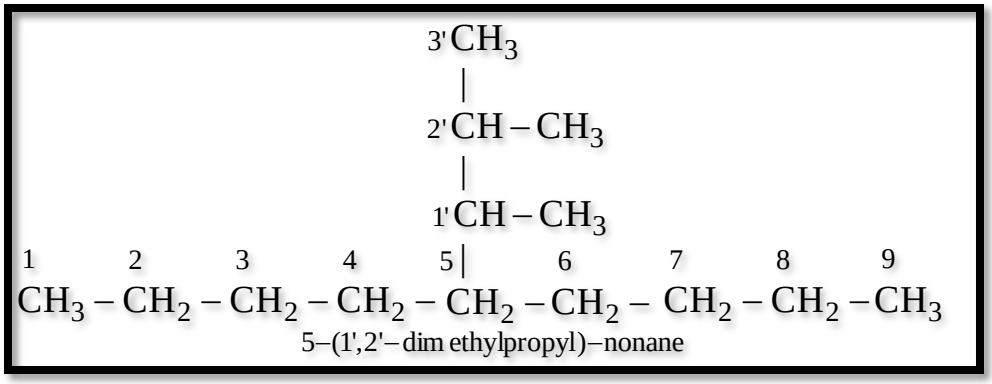


2,3–Dimethylpentane



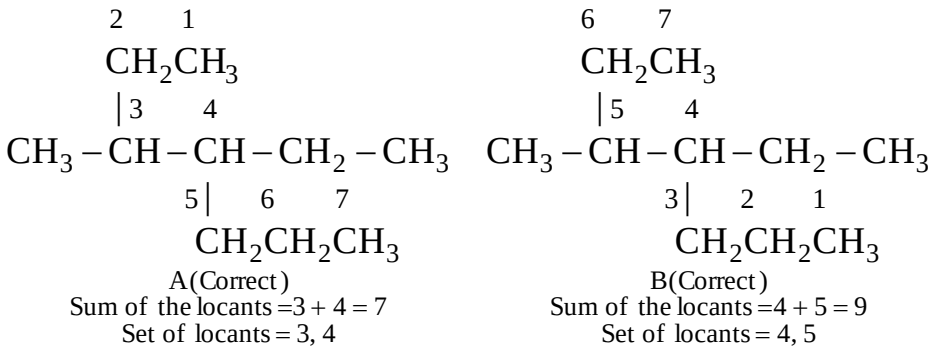
4–Ethyl–2,4–Dimethylhexane

6. **Naming the complex substituent:** In case the substituent on the parent chain is complex (i.e. it has itself branched chain) then it is named as a substituted alkyl group and its carbon chain is numbered from the carbon atom attached to the main chain. The name of this complex substituent is written in bracket to avoid confusion with the numbers of the main chain. e.g.,



When two or more substituents are present, the carbon atoms of parent chain are numbered in such a way that the set of locants is the lowest. This is called lowest set of locants rule.

In accordance with the above rules, the carbon atoms of the alkanes given below should be numbered as shown in structures A and not as in structures B.



Thus, according to the lowest sum rule, the numbering of the carbon chain should be done from right to left but according to the lowest set of locants rule, the numbering should be done from left to right. To overcome such an ambiguity, the IUPAC nomenclature recommends that the lowest set of locants rule should be preferred over the lowest sum rule.

Illustration 2

Give IUPAC name of the following compounds

W.R. = Word root, P.S. = Primary suffix, S.S. = Secondary suffix

1. $H_3C — CH_2 – CH_2 —OH$

Word root - Prop; Primary suffix - ane

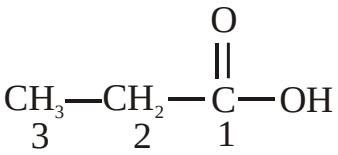
Functional group (Secondary suffix) = l-position of OH group in carbon chain

Hence IUPAC Name is, **1- Prop + ane - e + ol = 1-propanol**

2. $CH_3 —CH_2 — CH = CH_2$

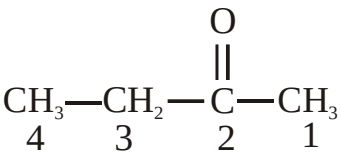
Word Root - but Primary Suffix = ene Position - 1

Name: **1-Butene**

3. 

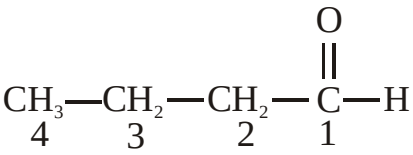
W.R. - Prop, P.S. = ane Secondary Suffix = Oic acid

Position - 1 Name: **Propanoic Acid**

4. 

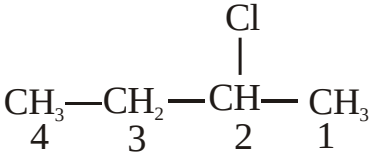
W.R. = But. P.S. = ane S.S. = one Position-2

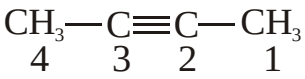
Name: **2-Butanone**

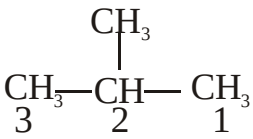
5. 

W.R. = But., P.S. = ane, S.S. = al Position-1

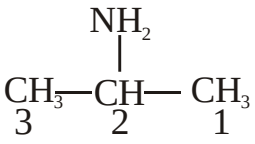
Name : **Butanal**

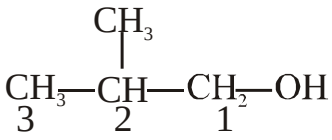
6.  **2- Chlorobutane**

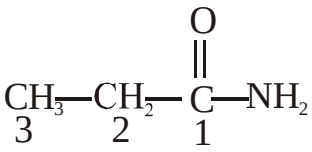
7.  **2 - Butyne**

8. 

2- Methyl propane or Methyl propane

9.  **2- Propanamine**

10.  **2-Methyl-1-propanol**

11.  **Propanamide**

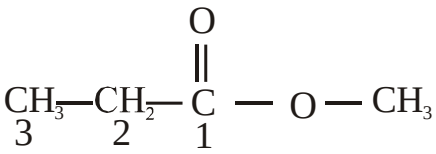
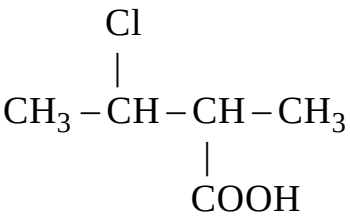
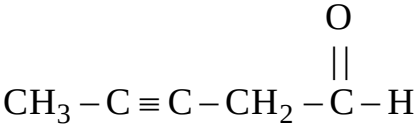
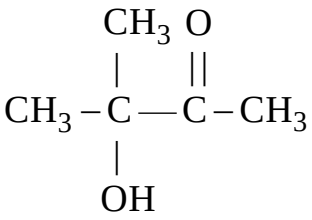
12.  **Methyl propanoate**

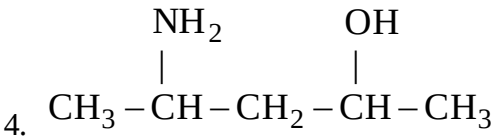
Illustration 3

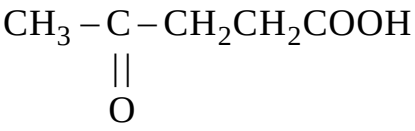
Write IUPAC names of following compound:

1. 

2. 

3. 

4. 

5. 

Solution

1. 3-chloro-2-methylbutan-1-oic acid
2. Pent-3-yn-1-al
3. 3-Hydroxy-3-methylbutan-2-one
4. 4-Aminopentane-2-ol
5. 4-Oxopentanoic acid