(....Contd.) ORGANIC CHEMISTRY : BASIC PRINCIPLES AND TECNIQUES

Kumud Bala

Nomenclature of different classes of organic compounds:- compounds of carbon and hydrogen are called hydrocarbons. These are further divided into two classes (i) Saturated (ii) Unsaturated hydrocarbons

1. Saturated hydrocarbons -------Alkanes :Hydrocarbon in which all the carbon atoms are linked to one another by only single bonds are called saturated hydrocarbons. In the IUPAC system, saturated acyclic hydrocarbons are called alkanes. Earlier, they were also called Paraffins (Latin: parum—little; affins—affinity). Since they are relatively inert towards most of the chemical reagent.

General formula: C_nH_{2n+2} where n=1, 2, 3, 4, ... etc. Primary suffix = ane

The IUPAC name of alkanes are obtained by adding the suffix 'ane' to the word root indicating the number of carbon atoms. For example ---- The first four alkanes (CH_4 to C_4H_{10}) have their special names i.e methane , ethane, propane and butane. Names of alkanes containing five or more carbon atoms are obtain by adding prefixes such as pent (five) , hex (six), hept(seven), oct(eight) etc. indicating the number of carbon atoms in the molecule to the suffix 'ane'. The name of an individual alkane is always written as one word. For example:

n	Formula	Common name	IUPAC Name
1	CH_4	methane	methane
2	CH_3CH_3	ethane	ethane
3	$CH_3CH_2CH_3$	propane	propane
4	$CH_3CH_2CH_2CH_3$	n-butane	butane
5	$CH_3CH_2CH_2CH_2CH_3$	n-pentane	pentane
6	$CH_3(CH_2)_4CH_3$	n-hexane	hexane
7	$CH_3(CH_2)_5CH_3$	n-heptane	heptane
8	$CH_3(CH_2)_6CH_3$	n-octane	octane
9	$CH_3(CH_2)_7CH_3$	n-nonane	nonane
10	$CH_3(CH_2)_8CH_3$	n-decane	decane
11	$CH_3(CH_2)_{18}CH_3$		Icosane

Types of Alkanes:- Depending upon the structure of the carbon chain, alkanes are of the following two types

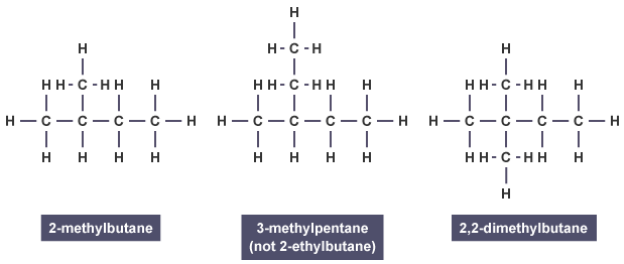
(a) Straight chain alkanes (b) Branched chain alkanes

(a) **Straight chain alkane** :- These alkanes contain straight chains of carbon atoms in their molecules. Alkanes in which no carbon atom is linked to more than two other carbon atoms are called straight chain alkanes.

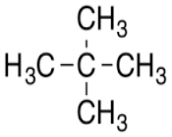
Examples: CH_3-CH_2-CH_2-CH_3 ----------Butane (n-butane, n=normal)

CH_3-CH_2-CH_2-CH_2-CH_2-CH_3 ----------- Hexane (n-hexane)

(b) Branched chain alkanes:- In these alkane the carbon atoms are not arranged in a straight chain . Alkanes in which at least one carbon atom is linked to three or four other carbon atoms are called branched chain alkanes . Examples



(iso-pentane) (neohexane) 2,2,Dimethypropane



(Neo-pentane)

The prefix 'iso' is used when the second carbon of the branched chain alkanes carries one methyl group. The prefix 'neo' is used for those branched chain alkanes which contain a 'quaternary' carbon at the end of the chain.

Type of carbon and hydrogen atoms in alkanes:--- The carbon atoms in an alkane molecule may be classified into four types as

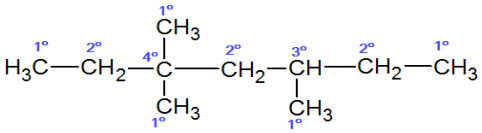
(i) Primary (1°) –A carbon atom attached to one other carbon atom is called a primary carbon atom and is designated as 1° carbon.

(ii) Secondary (2°) – A carbon atom attached to two other carbon atoms is called a secondary carbon atom and designated as 2° carbon.

(iii) Tertiary (3°)—A carbon atom attached to three other carbon atoms is called a tertiary carbon atom and (3°) carbon .

(iv) Quaternary (4°) – A carbon atom attached to four other carbon atoms is called quaternary carbon atom and designated as (4°) carbon.

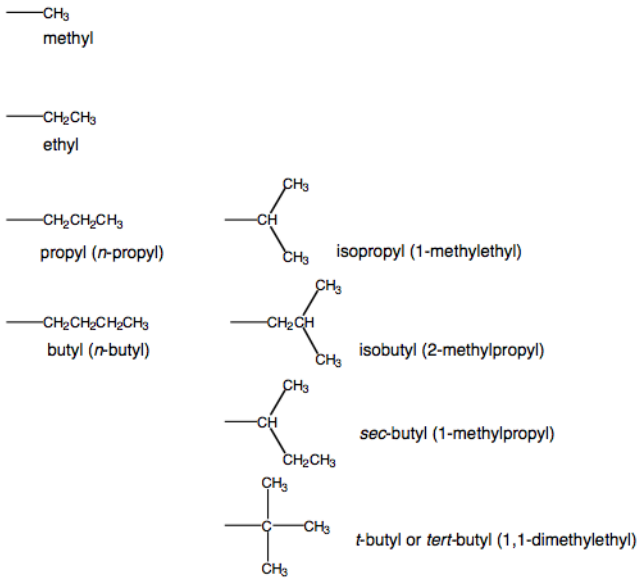
The hydrogen atoms attached to 1°,2°, 3° carbon atoms are called primary , secondary and tertiary hydrogen atoms . It may be noted that there is nothing like quaternary hydrogen since a quaternary carbon does not carry any hydrogen.



Alkyl group:--The removal of one hydrogen atom from the molecule of an alkane gives an alkyl group, represented by the letter R

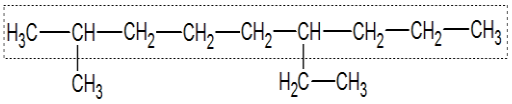
Alkane--ane + yl= Alkyl

General formula for alkyl = C_nH_{2n+1} where n =1, 2, 3, 4, etc. for example

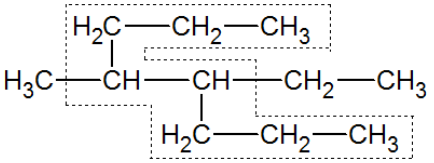


Rules for IUPAC nomenclature for branched chain alkanes

1. **Longest chain rule**—Select the longest continuous chain of carbon atoms as the parent chain, while all other carbon atoms which are not included in the parent chain are called branched chain alkane or side chains or substituents. The branched chain alkane is then named as a derivative of the parent chain. It may be noted that the longest chain may or may not be straight but it must be continuous. For example

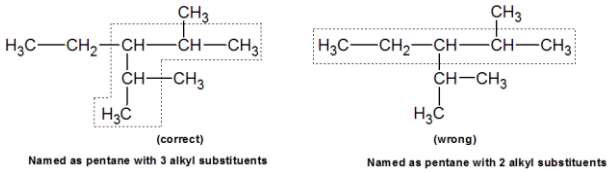

(I)

(longest chain contains nine carbon atoms and it is a derivative of nonane)

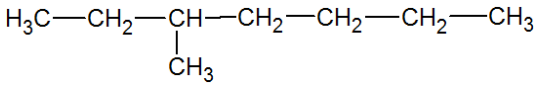

(II)

(Longest chain contains eight carbon atoms and it is a derivative of octane)

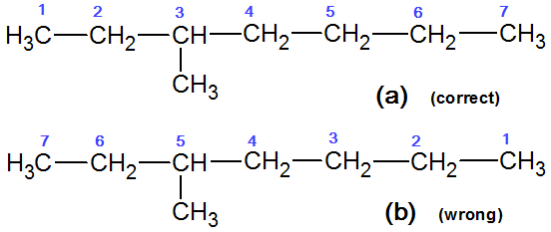
2. **Rule for larger number of side chains** :--If two chains of equal length are possible , select the one with the larger number of side chains . For example-



3. **Lowest number rule** :- Number the carbon atoms of the parent chain as 1, 2, 3, 4,etc.Starting from that end which gives the lowest possible number to the carbon atom carrying the substituent. For example, in the compound given below-

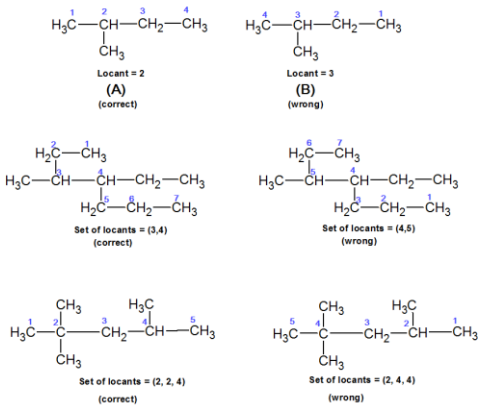


The numbering can be done in two different ways (a) and (b). The numbering of the carbon chain as given in the structure (a) is correct since it gives a lowest number i.e. 3 to the substituent i.e. methyl group while the numbering as given in structure (b) is wrong since it gives a higher number i.e. 5 to the substituent.



The number that indicates the position of the substituent on the parent chain is called the positional number or the locant. Thus, the correct locant for the methyl side chain in structure (a) is 3.

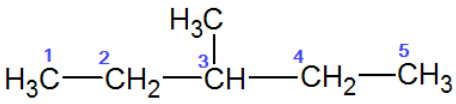
4. **Lowest set of locants rule**:- When two or more substituents are present , the lowest set of locants rule is applied . According to this rule , when two or more different sets of locants containing the same number of terms is possible ,then that set of locants is the lowest which when compared term by term with other sets , each in order of increasing magnitude ,has the lowest term at first point of difference. For deciding the lowest set of locants, the carbon atom of the parent chain are numbered from all possible direction and a locant assigned to each substituent from each direction. The set of locants from each direction is then compared term by term till the first point of difference is reached. That set of locants is preferred which has a lower number at the first point of difference. That is why this rule is also sometimes called as First point of difference. For example



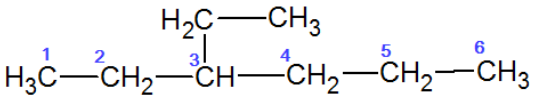
Out of two sets of locants (3,4) and (4,5) in example no.2, the first set is lower and hence preferred because the first term i.e.3 in the first set (3,4) is lower than the first term i.e.4 in the second set (4,5) .

5. **Name of the branched chain alkane**:- Prefix the name of the substituent (i.e. the alkyl groups.) to the name of the parent alkane and indicate its position (on the parent chain) by writing before it the number of the carbon atom carrying the substituent. The name of the substituent is separated from its locant by a hyphen (-).The final name of the alkane is always written as one word. The name of the compound is written in the following sequence.

(position of substituent) as prefixes, (word root) , primary suffix. Example:

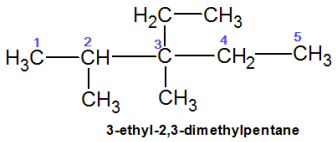


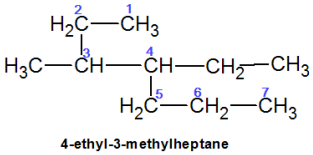
prefix is methyl and it is at carbon no. 3 in the parent chain , word root is 'pent' and primary suffix is 'ane'. Hence the name is 3-methylpentane



Prefix is ethyl and it is at carbon no. 3 in the parent chain, word root is 'hex' and primary suffix is 'ane' . Hence the name is 3-ethylhexane

6. **Alphabetical order of the side chain** :-When two or more alkyl groups (side chain) are present on the parent chain, each alkyl group prefixed by its positional number is arranged in alphabetical order





(Irrespective of its positional number) before the name of the parent alkane. For example

It may be noted here that while deciding the alphabetical order of the various alkayl groups, prefixes 'iso' and 'neo' are consider to the part of the fundamental name of the alkyl group while the prefixes 'sec' and 'tert' are not. For example:

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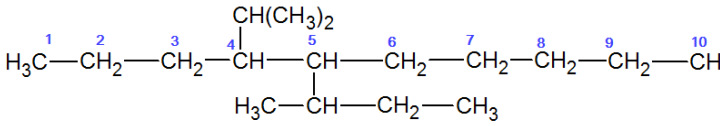
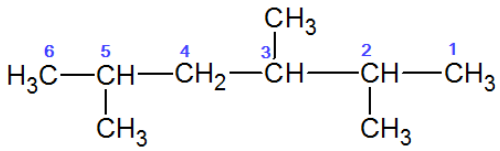
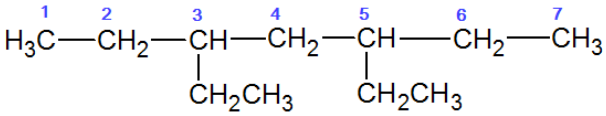


5-sec-butyl-4-isopropyldecane

7. **Naming the same alkyl group at different position**: When the same alkyl group occurs more than once on the parent chain at different positions, the positional number of each alkyl group is separated by commas and suitable prefixes such as di (for two), tri (for three), tetra (for four), etc. are attached to the name of the alkyl group. However the prefixes di, tri, etc. are not considered while deciding the alphabetical order of the alkyl group. For example



2,3,5-trimethylhexane



3,5-diethylheptane

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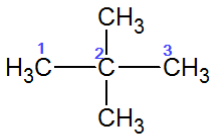
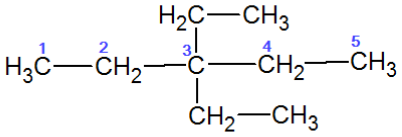
If the same alkyl group occurs twice on the same carbon atom, its positional number is also repeated twice. For example

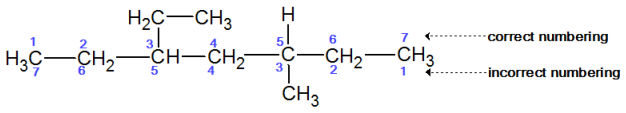


2,2-dimethylpropane

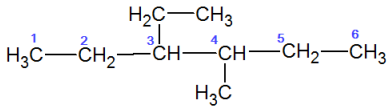


3,3-diethylpentane

8. **Numbering of different alkyl groups at equivalent position: I**f two different alkyl groups are present at equivalent positions, the numbering of the parent chain is done in such a way that the alkyl group which comes first in the alphabetical order (written first in the name) gets the lower number.

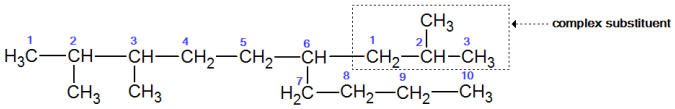


3-ethyl-5-methylheptane



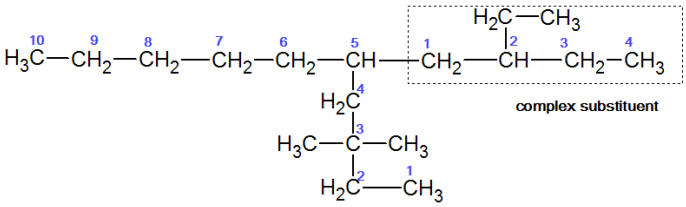
3-ethyl-4-methylhexane

9. **Numbering of complex substituent:** In case the substituent on the parent chain is complex i.e. (it has branched chain) , it is named as a substituted alkyl group by numbering the carbon atom of this group attached to the parent chain as 1. The name of such a substituent is always enclosed in brackets to avoid confusion with the numbers of the parent chain. For example—



2,3-dimethyl-6-(2-methylpropyl)decane

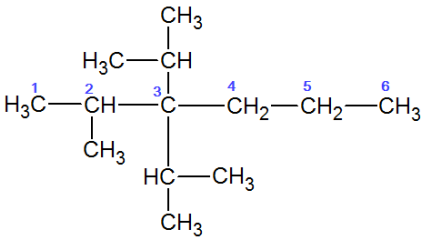
If two complex substituent are of equal length, then the complex substituent with larger number of alkyl groups forms a part of the longest carbon chain while the other one is considered the real complex substituent. For example—



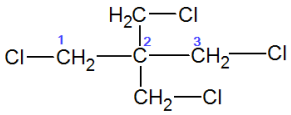
5-(2-ethylbutyl)-3,3-dimethyldecane (Correct)

5-(2,2-dimethylbutyl)-3-ethyldecane (Incorrect)

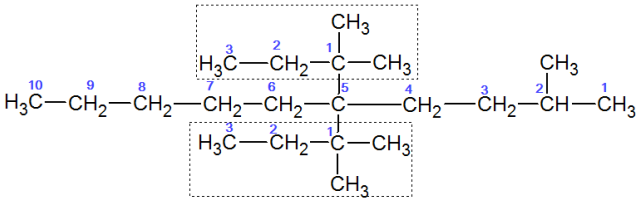
If the same complex substituent occurs more than once on the parent chain at different positions prefixes bis (for two), tris(for three) , tetrakis(for four), pentakis(for five) etc. are used before the name of the complex substituent. For example-



2-methyl-3,3-bis(1-methylethyl)hexane



1,3-dichloro-2,2-bis(chloromethyl)propane



5,5-bis(1,1-dimethylpropyl)-2-methyldecane

ASSIGNMENT

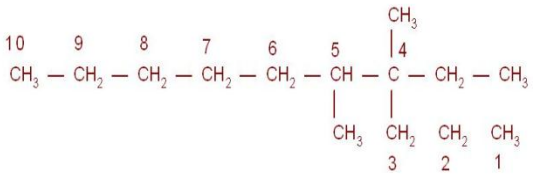
1. The common name of the compound $CH_3CH_2C(CH_2)_3$ is :
[A] Trimethylpropane [B] Neopentane [C] Neohexane [D] 2,2-Dimethyl butane.

2. How many primary carbon atoms are present in a 2,2,4-trimethylpentane?
[A] four [B] one [C] six [D] five.

3. Which one of the following IUPAC names is correct? [A] 2-methyl-3-ethylpentane [B] 2-ethyl-3-methylpentane [C] 3-ethyl-2-methylpentane[D] 3-methyl-2-ethylpentane .

4. The compound having one isopropyl group is [A] 2,2,3 ,3-tetramethylpentane [B] 2,3-dimethylpentane [C] 2,2,3-trimethylpentane [D] 2-methylpentane.

5. What is the correct IUPAC name of the following compound?



[A] 3,4-dimethyl-3-n-propylnonane [B] 4,5-dimethyl-4-ethyldecane

[C] 6,7-dimethyl-7-n-propylnonane [D] 6,7-dimethyl-7-ethyldecane

Answers to the above Assignment : 1. [C] 2. [D] 3. [B] 4.[D] 5. [B]

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