

NOMENCLATURE OF ORGANIC COMPOUND

The word 'nomenclature' refers to the way we name organic compounds. There are two naming systems:

- (a) Trivial or Common System
- (b) IUPAC System of Nomenclature

Trivial or Common System

This system names organic compounds based on where they come from or certain characteristics. For example, citric acid is named after the source it comes from, which is citrus fruits. Formic acid got its name because it was first obtained from red ants, and in Latin, the word for ant is formica. Some of these names are still used today. While some common names may be a bit hard to remember, they are sometimes used when the IUPAC name is too long.

Some Common Names Based and Source

| S.No. | Compound | Common Name | Source |
|-------|----------------------------------------------------------------------------------------------------------------------------------------|------------------------|----------------------------------|
| 1 | CH ₄ | Marsh gas (Free damp) | Marshy places |
| 2 | CH ₃ OH | Wood spirit (Carbinol) | Destructive distillation of wood |
| 3 | CH ₃ CH ₂ OH | Grain alcohol | Grain |
| 4 | $\text{NH}_2 - \underset{\text{O}}{\underset{\parallel}{\text{C}}} - \text{NH}_2$ | Urea (Carbamide) | Urine |
| 5 | HCOOH | Formic acid | Formica (Red ants) |
| 6 | CH ₃ COOH | Acetic acid | Acetum (Vinegar) |
| 7 | HOOC-COOH | Oxalic acid | Oxalis plant |
| 8 | $\text{CH}_3 - \underset{\text{OH}}{\underset{ }{\text{CH}}} - \text{COOH}$ | Lactic acid | Lactam (Milk) |
| 9 | CH ₃ CH ₂ CH ₂ COOH | Butyric acid | Butter |
| 10 | $\begin{array}{c} \text{HO} - \text{CH} - \text{COOH} \\ \\ \text{HO} - \text{CH} - \text{COOH} \end{array}$ | Tartaric acid | Tamarind |
| 11 | $\begin{array}{c} \text{HO} - \text{CH} - \text{COOH} \\ \\ \text{CH}_2 - \text{COOH} \end{array}$ | Malic acid | Malum (Apple) |
| 12 | $\begin{array}{c} \text{CH}_2 - \text{COOH} \\ \\ \text{HO} - \text{CH} - \text{COOH} \\ \\ \text{CH}_2 - \text{COOH} \end{array}$ | Citric acid | Citron (Lemon) |

Some Frequently Used Common Names (To Be Remember)

| S.No. | Common Name | Structure Formula |
|-------|--------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 1 | Isooctane | $ \begin{array}{c} \text{CH}_3 \\ \\ \text{CH}_3 - \text{CH} - \text{CH}_2 - \text{C} - \text{CH}_3 \\ \quad \quad \\ \text{CH}_3 \quad \quad \text{CH}_3 \end{array} $ |
| 2 | Triptane | $ \begin{array}{c} \text{CH}_3 \\ \\ \text{CH}_3 - \text{CH} - \text{C} - \text{CH}_3 \\ \quad \\ \text{CH}_3 \quad \text{CH}_3 \end{array} $ |
| 3 | Ethylene | $\text{H}_2\text{C} = \text{CH}_2$ |
| 4 | Acetylene | $\text{HC} \equiv \text{CH}$ |
| 5 | Allylene | $\text{HC} \equiv \text{C} - \text{CH}_3$ |
| 6 | Crotonyl Ene | $\text{CH}_3 - \text{C} \equiv \text{C} - \text{CH}_3$ |
| 7 | Allene | $\text{CH}_2 = \text{C} = \text{CH}_2$ |
| 8 | Ketene | $\text{CH}_2 = \text{C} = \text{O}$ |
| 9 | Acetone or Dimethyl Ketone | $ \begin{array}{c} \text{CH}_3 - \text{C} - \text{CH}_3 \\ \\ \text{O} \end{array} $ |
| 10 | Paraldehyde | $ \begin{array}{c} \text{CH}_3 \\ \\ \text{CH}_3 - \text{C} - \text{CHO} \\ \\ \text{CH}_3 \end{array} $ |
| 11 | Chloral | $\text{Cl}_3\text{C} - \text{CHO}$ |
| 12 | Acrolein or Acryl aldehyde | $\text{CH}_2 = \text{CH} - \text{CHO}$ |
| 13 | Acetophenone or Methyl phenyl Ketone | $ \begin{array}{c} \text{CH}_3 - \text{C} - \text{C}_6\text{H}_5 \\ \\ \text{O} \end{array} $ |
| 14 | Benzophenone or Diphenyl Ketone | $ \text{C}_6\text{H}_5 - \text{C} - \text{C}_6\text{H}_5 \\ \\ \text{O} $ |

| | | |
|----|------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 15 | Pinacol | $ \begin{array}{c} \text{CH}_3 \quad \text{CH}_3 \\ \quad \\ \text{CH}_3 - \text{C} - \text{C} - \text{CH}_3 \\ \quad \\ \text{OH} \quad \text{OH} \end{array} $ |
| 16 | Pinacolone | $ \begin{array}{c} \text{CH}_3 \\ \\ \text{CH}_3 - \text{C} - \text{C} - \text{CH}_3 \\ \quad \\ \text{O} \quad \text{CH}_3 \end{array} $ |

IUPAC System of Nomenclature

The IUPAC System of Nomenclature was created because remembering all the common names for the vast number of organic compounds was challenging. A set of rules was needed to give a systematic name to each organic compound, making them easy to identify. That's when the IUPAC (International Union of Pure and Applied Chemistry) system of nomenclature was introduced. Under the IUPAC system, the name of an organic compound is structured in a systematic way, providing clarity in identification.

Format for IUPAC name

| | | | | | | | | |
|---------------------------|---|----------|---|------------------------------------------------|---|----------------------|---|------------------------------------------------------------|
| s-prefix | + | p-prefix | + | word root | + | p-suffix | + | s-suffix |
| Substituents with locants | | cyclo | | Alk word according to carbon in parent C chain | | -ane -ene -yne | | According to main functional group given in priority table |

- (a) **Locant:** - Locants are separated by (,) comma.
- Locants and alphabets are separated by hyphen (-). [2, 3-dimethyl pentane]
 - di, tri, iso, neo and cyclo are neither separated by comma nor by hyphen

- (b) **Prefix:** - According to substituents.

Prefix (es) are written in alphabetical order before root word.

prefix ← $\left\{ \begin{array}{l} 1^\circ \text{ or p - prefix} \\ 2^\circ \text{ or sec. - prefix} \end{array} \right.$

Cyclo is 1^o prefix and used for cyclic compound.

2^o prefix is used for substituents and written before 1^o prefix.

For acyclic compounds: 2^o prefix + Root word + 1^o Suffix + 2^o suffix.

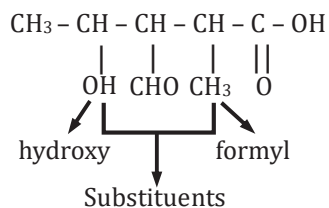
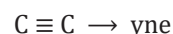
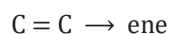
| Substituents | Prefix |
|----------------------------------|----------------|
| -R | Alkyl group |
| -X (F, Cl, Br, I) | Halo |
| -O, -N=O | Nitrite |
| -CH ₂ OH | Hydroxy methyl |
| -NHC ₂ H ₅ | Ethyl amino |

| Substituents | Prefix |
|-------------------------------------------------------------------------------------|---------------|
| -OR | Alkyl group |
| $\begin{array}{c} \text{O} \\ \parallel \\ -\text{N} \searrow \text{O} \end{array}$ | Nitro |
| -N=O | Nitroso |
| -CH ₂ Cl | Chloro methyl |

(c) **Word root:** - According to number of carbons in parent C-chain.

| Number of carbons | Root Word |
|-------------------|-----------|
| 1 | Meth |
| 2 | Eth |
| 3 | Prop |
| 4 | But |
| 5 | Pent |
| 6 | Hex |
| 7 | Hept |
| 8 | Oct |
| 9 | Non |
| 10 | Dec |
| 11 | Undec |
| 12 | Dodec |
| 13 | Tridec |

(d) **Primary suffix:** - According to saturation and unsaturation.



(e) **Secondary Suffix:** - According to senior most of F. G.
3-Formyl-4-hydroxy-2-methyl pentatonic acid

IUPAC Nomenclature of Alkanes

Straight Chain Hydrocarbons

Straight chain hydrocarbons are named using a word root and primary Suffix.

Word Root

It serves as the fundamental part of the name and indicates how many carbon atoms are in the main chain of the organic molecules. This main chain is the longest continuous sequence of carbon atoms that includes the functional group, following the common names of alkanes.

| Number of Carbon Atoms | Word root | Number of Carbon Atoms | Word root |
|------------------------|-----------|------------------------|-----------|
| C ₁ | Meth | C ₇ | Hept |
| C ₂ | Eth | C ₈ | Oct |
| C ₃ | Prop | C ₉ | Non |
| C ₄ | But | C ₁₀ | Dec |
| C ₅ | Pent | C ₁₁ | Undec |
| C ₆ | Hex | C ₁₂ | Dodec |




Primary Suffix

It shows the type of bonds between carbon atoms in the principal/parent chain (whether they are single, double, or triple bonds).

Iupac Nomenclature of Saturated Unbranched Hydrocarbon

Iupac name = Word Root + Primary Suffix

Ex.

| | | | |
|-----------------------------------------------------------------------------------|----------------|---|-------------|
| CH ₄ | Meth + ane | = | Methane |
| CH ₃ – CH ₃ | Eth + ane | = | Ethane |
| CH ₃ – CH ₂ – CH ₃ | Prop + ane | = | Propane |
|  | But + ane | = | Butane |
|  | Pent + ane | = | Pentane |
|  | hex + ane | = | Hexane |
| CH ₃ (CH ₂) ₉ CH ₃ | Undec + ane | = | Undecane |
| CH ₃ (CH ₂) ₂₈ CH ₃ | Triacont + ane | = | Triacontane |

Branched Chain Hydrocarbons

In branched chain hydrocarbons, there are smaller chains of carbon atoms attached to the main carbon chain. These smaller chains are called alkyl groups and are added at the beginning of the name of the main alkane. Alkyl groups come from alkanes by taking away one hydrogen atom, so their general formula is C_nH_{2n+1}, and they are represented by the letter R. To name an alkyl group, you replace the 'ane' in the alkane name with 'yl'.

Ex:

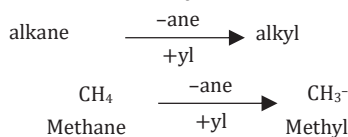


Table: Some Alkyl Groups

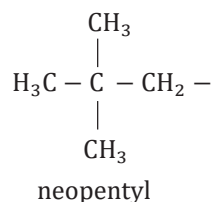
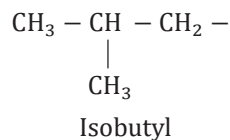
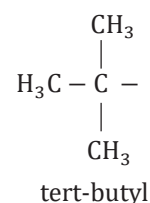
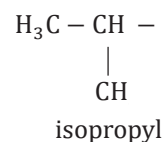
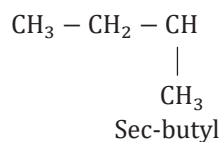
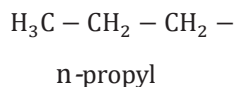
| Alkane | | Alkyl group | |
|---------------------------------|----------------|------------------------------------------------------------------|---------------------|
| Molecular formula | Name of alkane | Structural formula | Name of alkyl group |
| CH ₄ | Methane | –CH ₃ | Methyl |
| C ₂ H ₆ | Ethane | –CH ₂ CH ₃ | Ethyl |
| C ₃ H ₈ | Propane | –CH ₂ CH ₂ CH ₃ | Propyl |
| C ₄ H ₁₀ | Butane | –CH ₂ CH ₂ CH ₂ CH ₃ | Butyl |
| C ₁₀ H ₂₂ | Decane | –CH ₂ (CH ₂) ₈ CH ₃ | Decyl |

Sometimes, we use abbreviations for alkyl groups.

For example, methyl becomes Me, ethyl becomes Et, propyl becomes Pr, and butyl becomes Bu.

Alkyl groups don't always have to be straight; they can be branched too. When they are branched, we add certain prefixes like iso, sec, tert, neo, etc.

Here are some examples of branched alkyl groups:



To name hydrocarbons with branches, you need a secondary prefix, a word root, and a primary suffix.

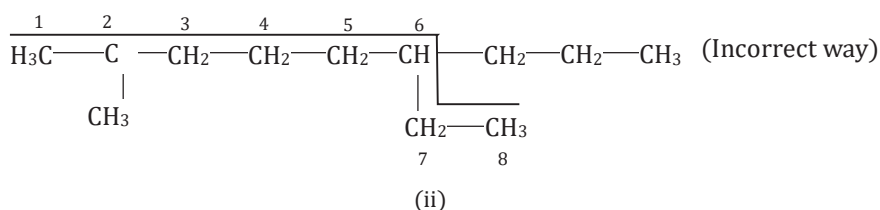
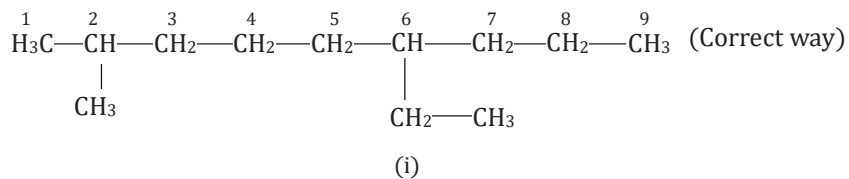
Secondary prefix + Word root + Primary suffix

Nomenclature of Branched Chain Alkanes

Naming branched chain hydrocarbons becomes easy by following certain rules:

(i) Longest Chain Rule

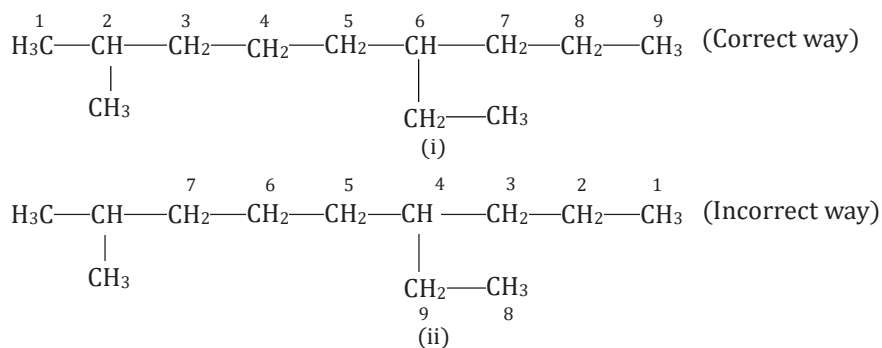
The first step in naming is to find the longest chain of carbon atoms, which is called the parent chain.



Among two ways of selecting the parent chain, the correct method (way I) is chosen. This is because the parent chain in way I has nine carbon atoms, while in way II, it only has eight.

(ii) Lowest Number Rule

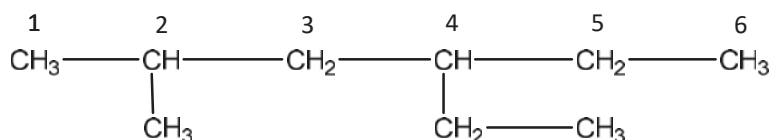
The parent chain is numbered in a way that the substituents attached to it get the lowest possible position.



Between the two options, way I is the right choice. In way I, the substituents have the lowest positions at 2 and 6, while in way II, the positions for the substituents are 4 and 8.

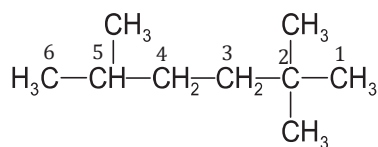
(iii) Alphabetical Order of the Side Chain

The side chain is named by putting the alkyl group names in alphabetical order before the parent chain's name. We mark the position of the alkyl group by numbering the parent chain. Additionally, when there are different alkyl groups as substituents, we make sure to list them in alphabetical order.

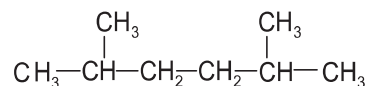


4-Ethyl-2-methylhexane

- (iv) In the IUPAC name of an organic compound, we use commas to separate numbers, put a dash (-) between a number and a letter, and combine successive words into one word. When a branched hydrocarbon has more than one alkyl group, we don't repeat their names. Instead, we indicate how many of the same alkyl substituents are present using prefixes like "di" for two, "tri" for three, "tetra" for four, "penta" for five, "hexa" for six, and so on. This rule is illustrated in the following examples:

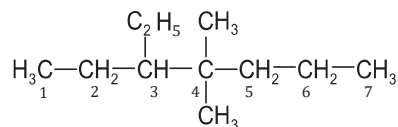


2, 2, 5-Trimethylhexane



2,4-Dimethylpentane

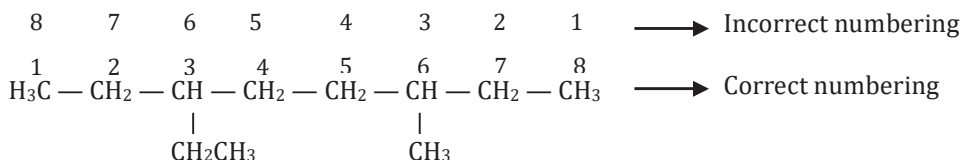
- (v) If an organic compound has multiple alkyl groups, we write their names in alphabetical order. However, when it comes to prefixes like di, tri, etc., they don't affect the alphabetical order. So, the right name for the given compound is 3-Ethyl-4,4-dimethylheptane.



3-Ethyl-4,4-dimethylheptane

(vi) Numbering of Different Alkyl Groups at Equivalent Positions

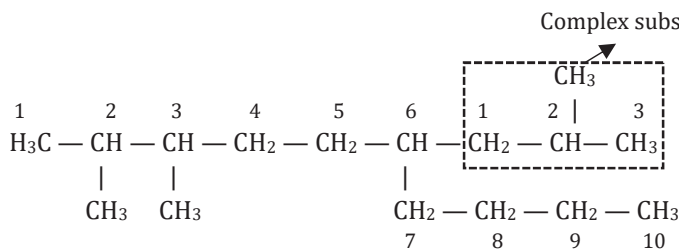
When there are two different alkyl groups at equivalent positions, we number the parent chain in a way that gives the lower number to the alkyl group that appears first in alphabetical order.



3-Ethyl-6-methyloctane

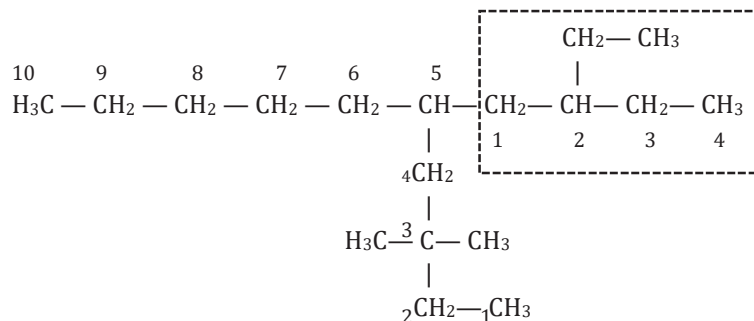
(vii) Naming the Hydrocarbon with Complex Substituent

- a) If the substituent on the main chain is complicated, meaning it has a branched structure, we name it as a substituted alkyl group. We do this by numbering the carbon atom of this alkyl group attached to the main chain as 1. When naming the compound, the name of this branched chain alkyl group is enclosed in parentheses.



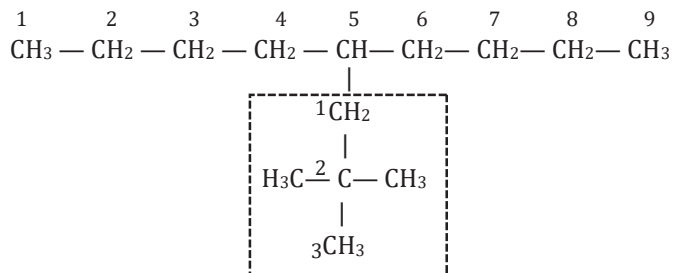
2,3-Dimethyl-6-(2-methylpropyl) decane

- b) If there are two substituted chains of the same length, we choose the one as the parent chain that has more side chains attached to it. Additionally, we number the chain in a manner that gives the substituent the smallest possible number.



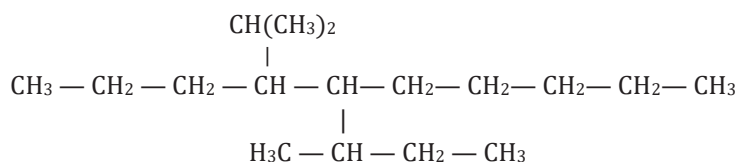
5- (2-Ethylbutyl)-3,3-dimethyldecane (correct)

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



5-(2, 2-Dimethylpropyl) nonane

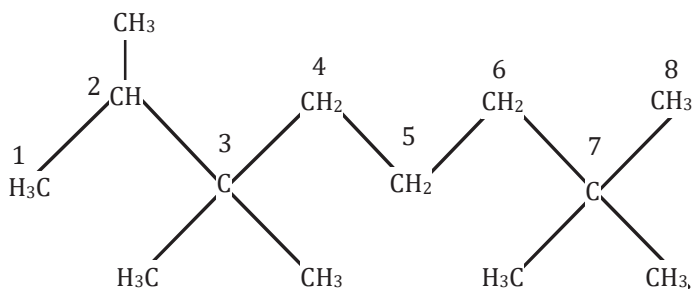
- c) When listing the common names of substituents alphabetically, the prefixes 'iso' and 'neo' are treated as part of the fundamental name of the alkyl group. However, the prefixes 'sec' and 'tert' are not considered part of the fundamental name.



5-Sec-Butyl-4-isopropyldecane

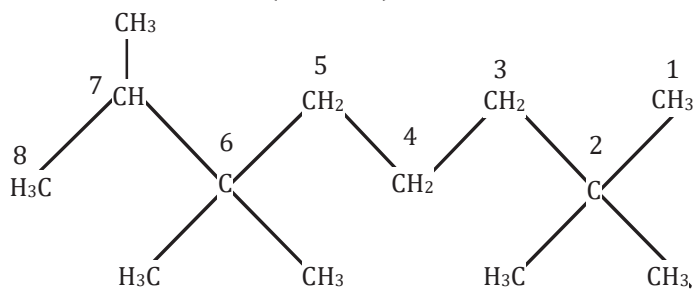
(viii) First Point of Difference Rule

This rule is used when several substituents are at an equal distance from both sides.



(wrong direction)

(Incorrect)



(right direction)

(correct)

2, 2, 6, 6, 7-Pentamethyloctane

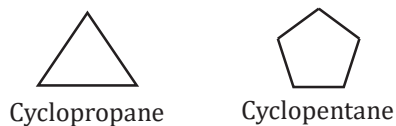
When determining the correct direction, a point of difference arises when one order provides a lower number than another. In this case, although both numbering schemes start with 2 as the first locant, the tie-breaker occurs at the second locant. Following the rule, the preference

goes to 2, 2, 6, 6, 7, where 2 is the second locant, as opposed to 2, 3, 3, 7, 7, where 3 is the second locant. It's important to note that locants are not added together; instead, they are examined one by one.

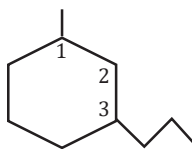
Cyclic Compounds

When naming hydrocarbons with a circular structure, we use the prefix 'cyclo' before the name of the main chain. The other naming rules remain the same as explained before.

Example:

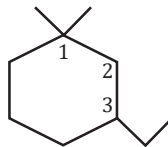


Alphabetical order of Numbering:



1-Methyl-3-propylcyclohexane

More branched carbon gets lower number:



3-Ethyl-1, 1-dimethylcyclohexane (correct)

1-Ethyl-3, 3-dimethylcyclohexane (Incorrect)