Nomenclature of Organic Compound

Nomenclature of Alkanes

Definition and Basic Concept:

- Alkanes are saturated hydrocarbons — compounds consisting only of carbon (C) and hydrogen (H) atoms, where all carbon-carbon bonds are single bonds.
- These compounds follow the general formula:

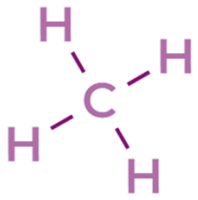
$$C_nH_{2n+2}$$

- They are also known as paraffins. The IUPAC system provides a systematic way to name these compounds based on the number of carbon atoms, type and position of substituents, and branching in the carbon chain.

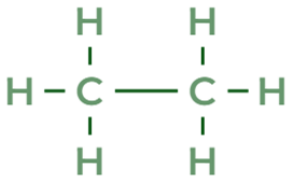
IUPAC Nomenclature Rules for Alkanes:

1. Identify the Longest Continuous Carbon Chain:

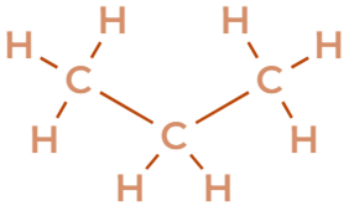
- This is known as the **parent chain** or **root chain**.
- This chain determines the **parent name** (e.g., methane, ethane, propane, etc.).
  - 1 carbon: Methane **(CH_4)**



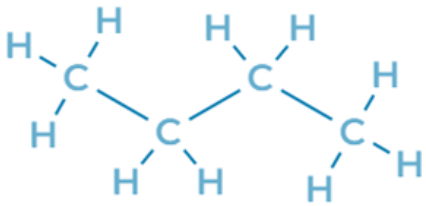
  - 2 carbons: Ethane **(C_2H_6)**



  - 3 carbons: Propane **(C_3H_8)**



  - 4 carbons: Butane **(C_4H_{10})**..and so on.



- It must contain the maximum number of carbon atoms.
- If two chains are of equal length, the one with more substituents (branches) is chosen.

2. Number the Carbon Atoms in the Parent Chain:

- Start from the end nearer to the first substituent group.
- The goal is to assign lowest possible numbers to the substituents.

3. Identify and Name the Substituents:

- Substituents are alkyl groups (like $-CH_3$, $-C_2H_5$).
- Use prefixes like methyl-, ethyl-, propyl-, butyl-, etc.

4. Assign Numbers to Substituents:

- Based on the position where the branch appears in the main chain.
- **Use lowest locant rule:** The sum of the numbers should be as low as possible.

5. Multiple Substituents of the Same Type:

- Use prefixes: di-, tri-, tetra-, penta-, etc.
- Each substituent must have its own position number, even if they are of the same type.

6. Arrange Substituents Alphabetically:

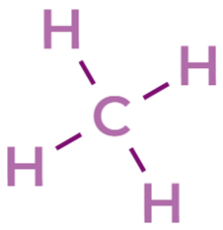
- Prefixes like di-, tri-, etc. are not considered in alphabetizing.
- Only the alkyl name is considered.

7. Combine the Name:

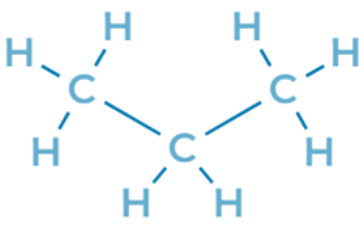
- Positions + substituents (in alphabetical order) + base name of the parent chain.

Examples:

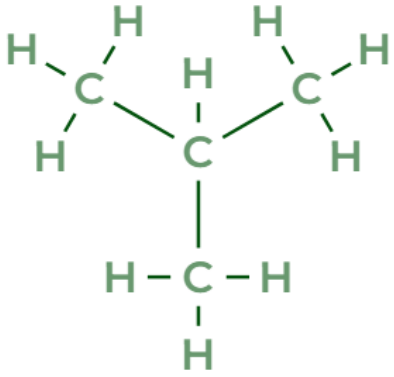
- **CH_4**: Methane
  - (Only one carbon, no branches)



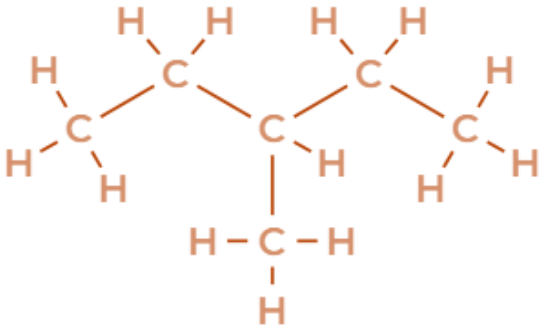
- **$CH_3CH_2CH_3$**: Propane
  - (Straight chain of 3 carbon atoms)



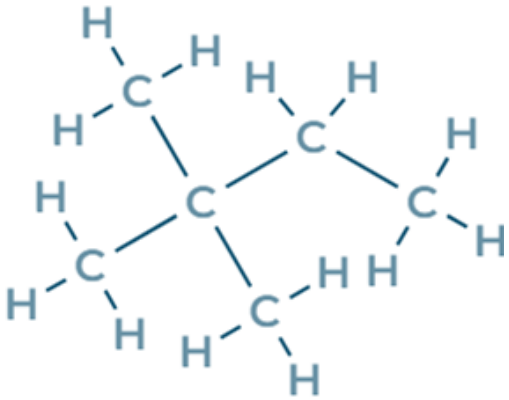
- **$CH_3CH(CH_3)CH_3$**: 2-Methylpropane
  - (Longest chain is 3 carbons, with a methyl group on second carbon)

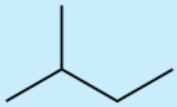


- **$CH_3CH_2CH(CH_3)CH_2CH_3$**: 3-Methylpentane
  - (Parent chain: pentane, methyl at position 3)



- **$(CH_3)_3CCH_2CH_3$**: 2,2-Dimethylbutane
  - (Two methyl groups on second carbon of a four-carbon chain)



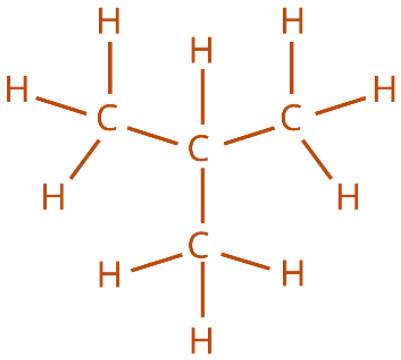
Comparison of nomenclatures for three isomers of C_5H_{12}			
Common name	*n*-pentane	isopentane	neopentane
IUPAC name	pentane	2-methylbutane	2,2-dimethylpropane
Structure			

Branched and Complex Substituents:

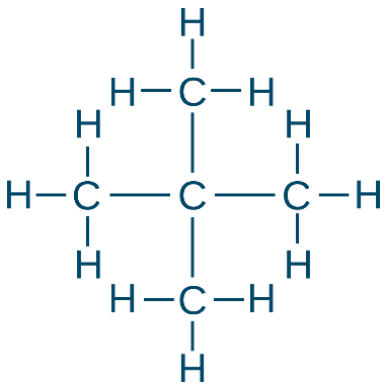
- If a substituent itself is branched, treat it as a mini-alkyl chain.
- Use parentheses to enclose the name of the complex substituent.
- Number within the substituent starting from the carbon attached to the main chain.
- Example:
  - $CH_3CH_2CH(CH_2CH_3)CH_3$ → 3-Ethylpentane

Common vs IUPAC Names:

- Some alkanes have trivial (common) names like:
  - Isobutane → IUPAC: 2-Methylpropane



  - Neopentane → IUPAC: 2,2-Dimethylpropane



- These are acceptable in informal contexts, but IUPAC naming is required in formal chemistry.

Nomenclature of Alkenes

Definition and Basic Concept:

- Alkenes are **unsaturated hydrocarbons** containing at least one **carbon-carbon double bond (C=C)**.
- The general formula is:

$$C_nH_{2n}$$

- Due to the presence of the double bond, **position and geometry (cis/trans or E/Z)** must be considered in naming.

IUPAC Nomenclature Rules for Alkenes:

1. Select the Longest Chain Containing the Double Bond:

- The chain must include the double bond, even if another longer chain is present.

2. Number the Chain from the End Nearest the Double Bond:

- The double bond should get the **lowest number** possible.

3. Indicate the Position of the Double Bond:

- Number the carbon at the **start** of the double bond.
- If multiple double bonds are present, use **di-, tri-** prefixes (e.g., diene, triene).

4. Name Substituents and Position Them:

- Follow same rules as alkanes for branches.

5. Add Stereochemistry (cis/trans or E/Z):

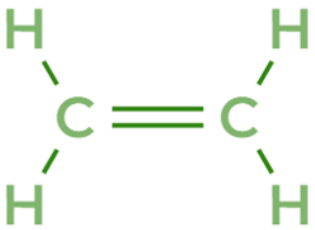
- **Cis**: Same side of double bond
- **Trans**: Opposite side
- For complex molecules, use **E/Z** system based on atomic numbers of attached atoms.

6. Combine Name:

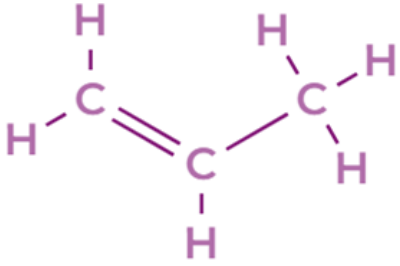
- Positions + substituents + location of double bond + base name + suffix **–ene**

Examples:

- **CH_2=CH_2**: Ethene
  - (2 carbons, one double bond)



- **CH_3CH=CH_2**: Propene



- **CH_3CH=$CHCH_3$**: But-2-ene
  - If both methyl groups are on the same side: **cis-but-2-ene**
  - On opposite sides: **trans-but-2-ene**

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