Alkane,Alkene and Alkynes

Course: B.Sc. I

Subject: Chemistry I

Unit: III(A)

Organic Chemistry - Introduction

- Organic chemistry is the study of carbon compounds.

- Animals, plants, and other forms of life consist of organic compounds.

Bonding in Organic Compounds

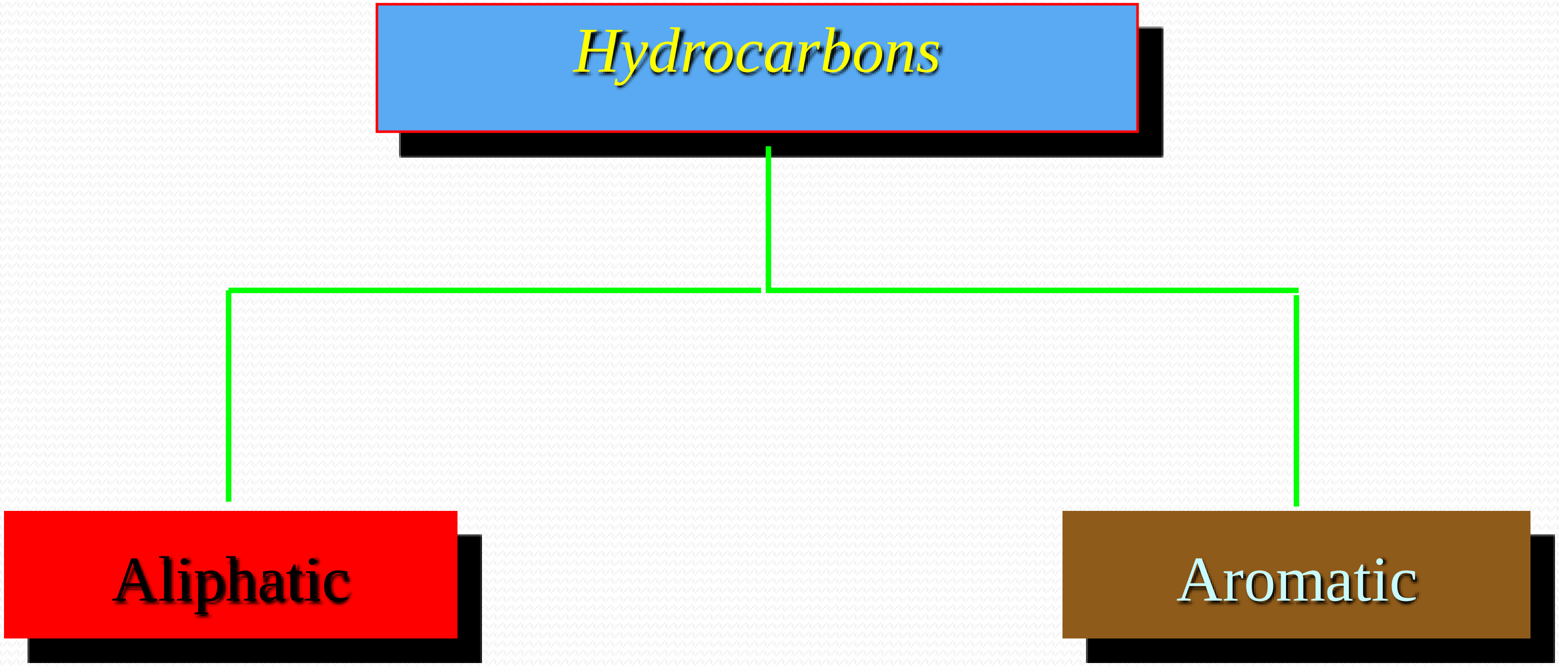
- Besides carbon, the most common elements in organic compounds are hydrogen, oxygen, nitrogen, sulfur, and the halogens.

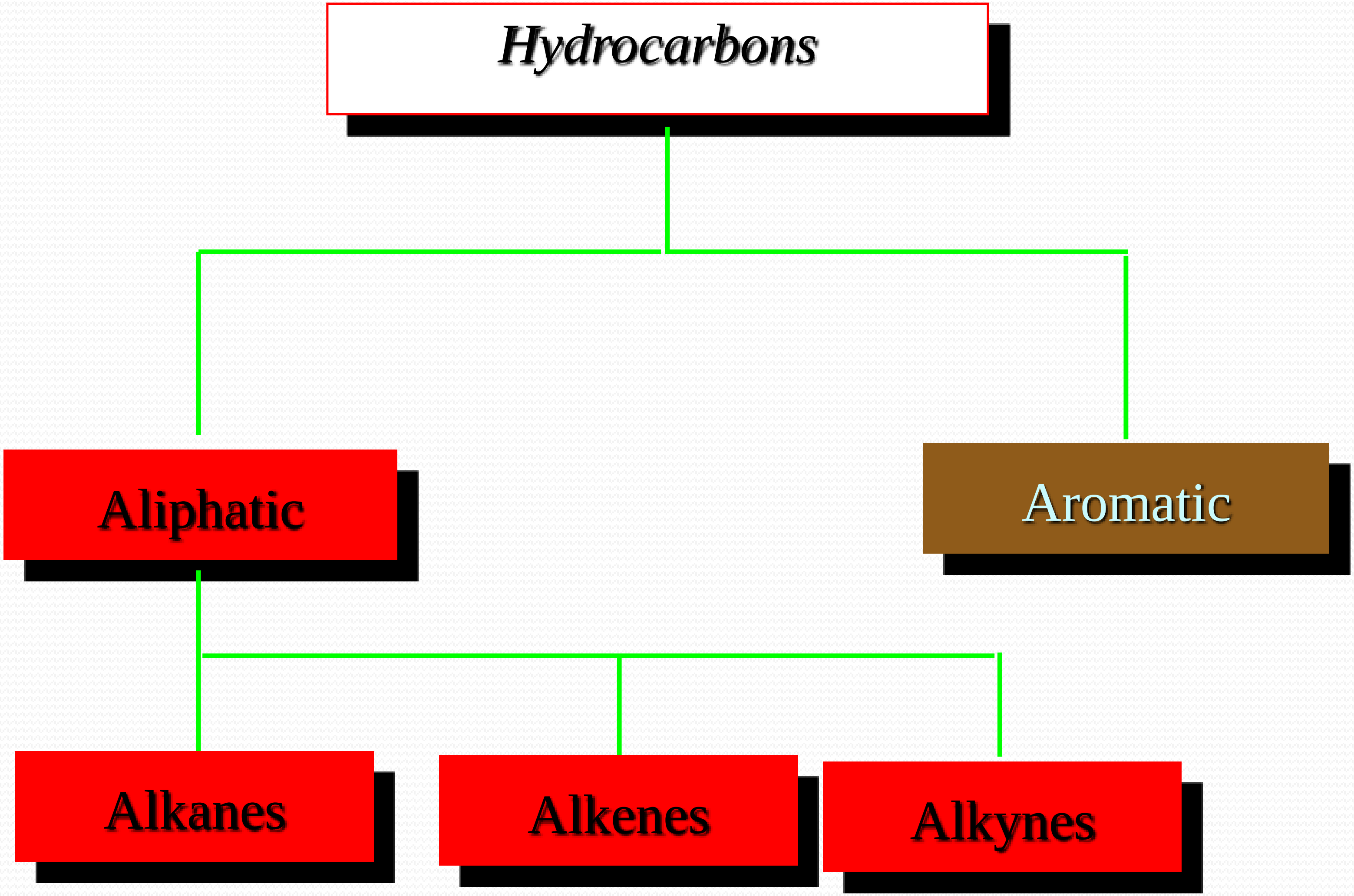
- organic compounds have covalent bonding.

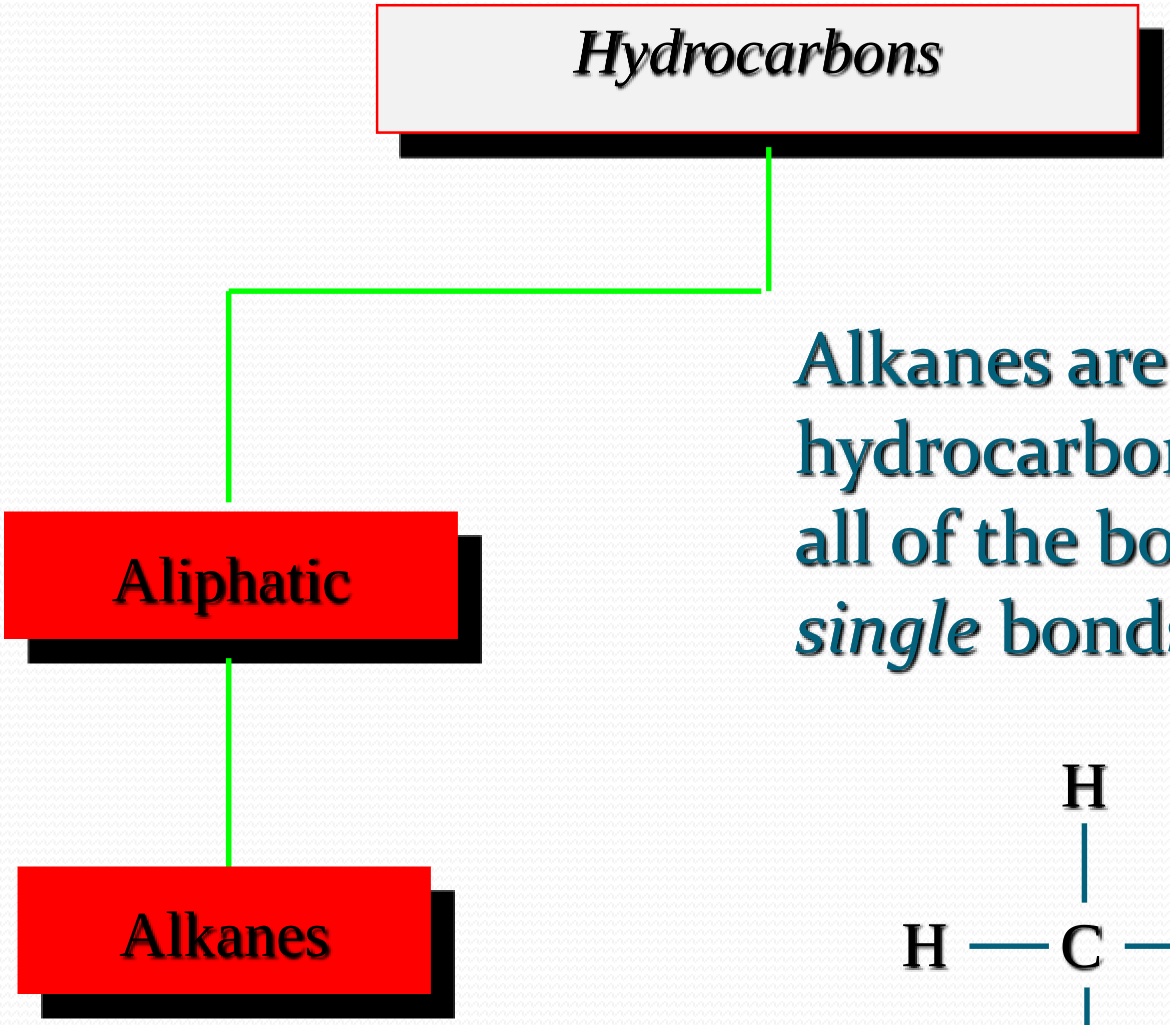
Hydrocarbons

- Hydrocarbons are the most simple organic compounds.
- Hydrocarbons contain only carbon (C) and hydrogen (H).
- For classification purposes, all other organic compounds are considered derivatives of hydrocarbons.

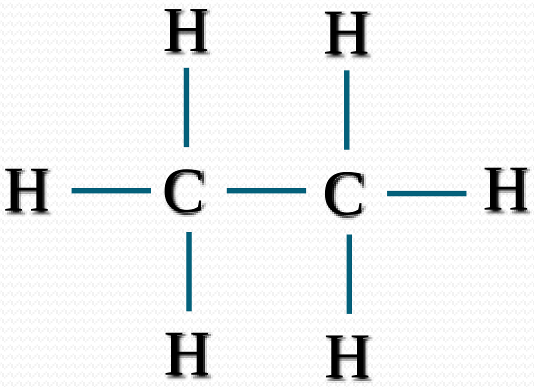
- Hydrocarbons can be divided into aromatic and aliphatic hydrocarbons.

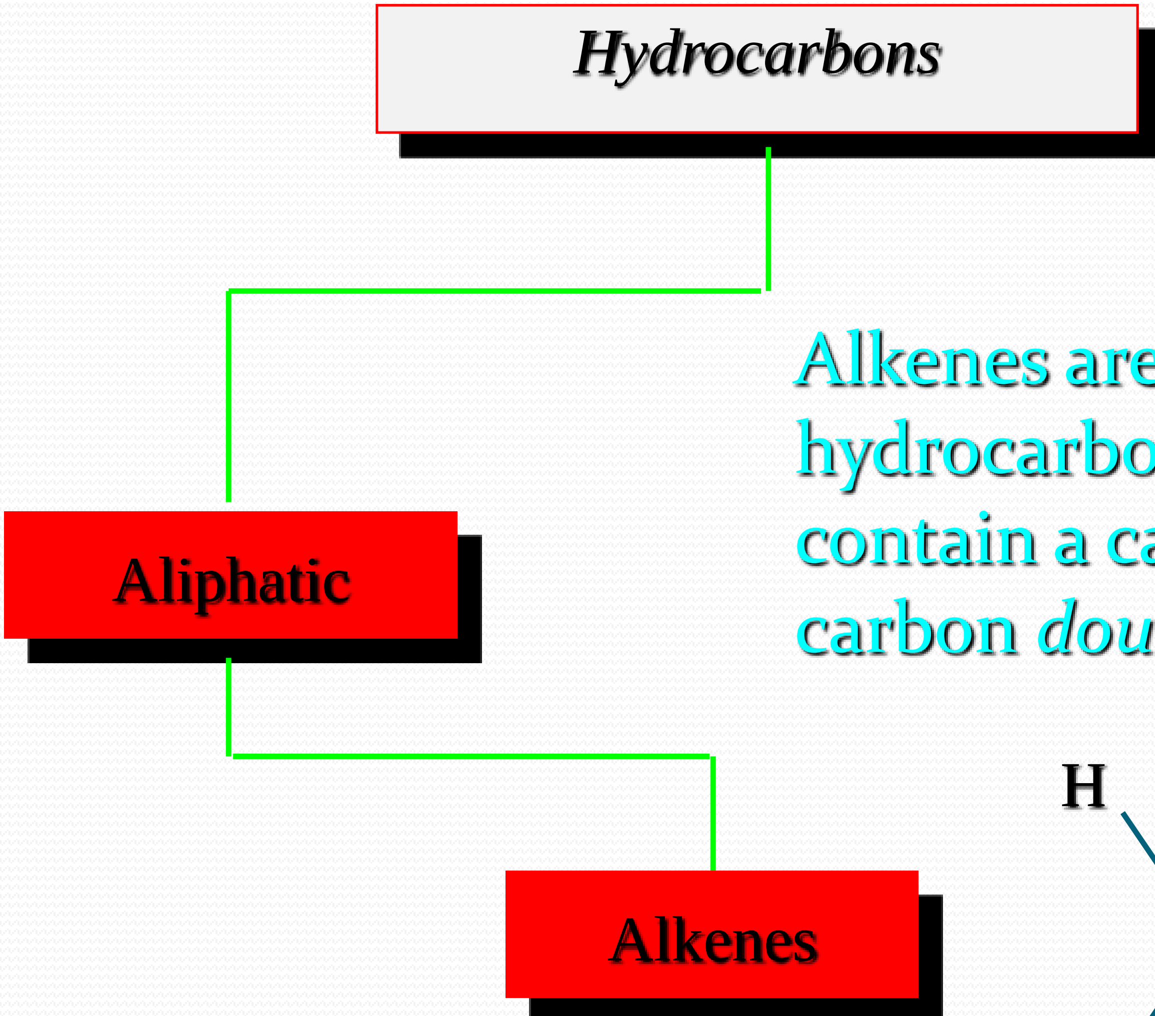

Hydrocarbons
Aliphatic
Aromatic


Hydrocarbons
Aliphatic
Aromatic
Alkanes
Alkenes
Alkynes

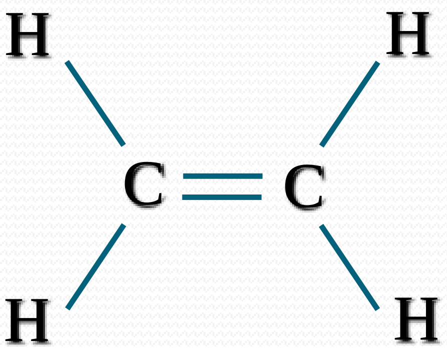


Alkanes are hydrocarbons in which all of the bonds are *single* bonds.





Alkenes are hydrocarbons that contain a carbon-carbon *double* bond.



Hydrocarbons

Aliphatic

Alkynes are hydrocarbons that contain a carbon-carbon *triple* bond.

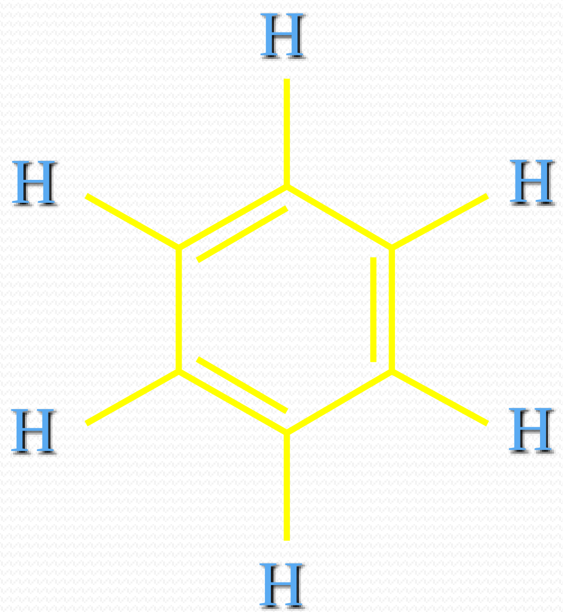
Alkynes

$HC \equiv CH$

Hydrocarbons

Aromatic

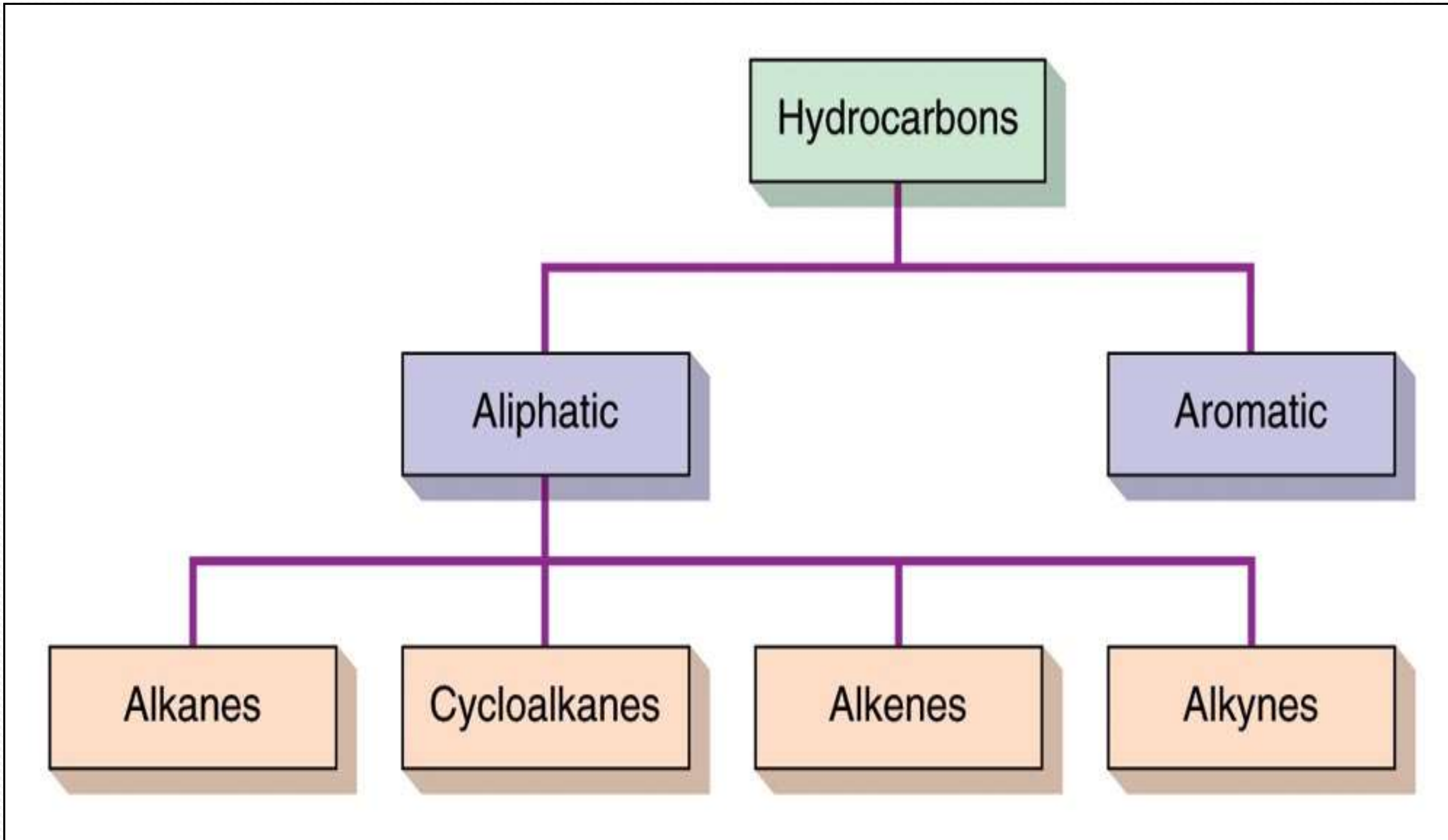
The most common aromatic hydrocarbons are those that contain a benzene ring.



Aliphatic Hydrocarbons

- Aliphatic hydrocarbons are hydrocarbons having no benzene rings.
- Aliphatic hydrocarbons can be divided into four major divisions:
  - *Alkanes*
  - *Cycloalkanes*
  - *Alkenes*
  - *Alkynes*

Classification of Hydrocarbons



Alkanes

- Alkanes are hydrocarbons that contain only single bonds.
- Alkanes are said to be saturated hydrocarbons
  - *Because their hydrogen content is at a maximum.*

- Alkane general formula → C_nH_{2n+2}

- The names of alkanes all end in "-ane."
- Methane → butane are gases
- Pentane → $C_{17}H_{36}$ are liquids
- $C_{18}H_{38}$ and higher are solids

Physical Properties

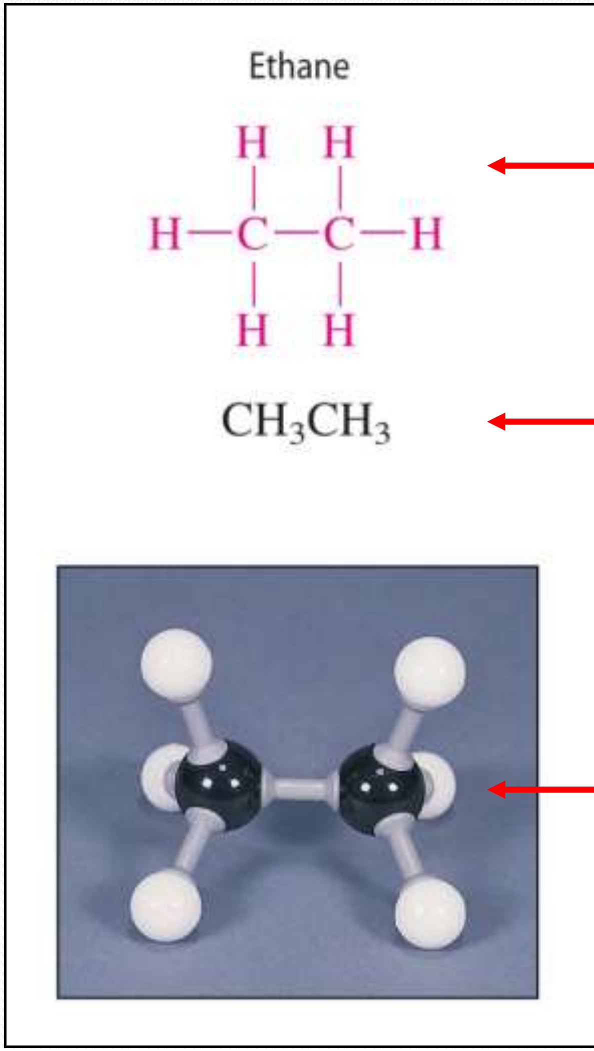
- No color & odour
- Lower alkane: gases
- Middle alkane: liquids
- Higher alkane: solid
- Higher boiling point : higher molecular wt.
- Branched chain: decrease surface area
- Long chain : higher surface area.
- Even no. of carbon : higher M.P
- Odd no. of carbon : lower M.P
- Higher density: higher mol. Wt
- Non polar : soluble in organic solvent
- Higher mol. Wt : decrease solubility

The First Eight Members of the Alkane Series

All satisfy the general formula C_nH_{2n+2}

Name	Molecular Formula	Condensed Structural Formula
Methane	CH_4	CH_4
Ethane	C_2H_6	CH_3CH_3
Propane	C_3H_8	$CH_3CH_2CH_3$
Butane	C_4H_{10}	$CH_3(CH_2)_2CH_3$
Pentane	C_5H_{12}	$CH_3(CH_2)_3CH_3$
Hexane	C_6H_{14}	$CH_3(CH_2)_4CH_3$
Heptane	C_7H_{16}	$CH_3(CH_2)_5CH_3$
Octane	C_8H_{18}	$CH_3(CH_2)_6CH_3$

Visualization of an Alkane's Structure



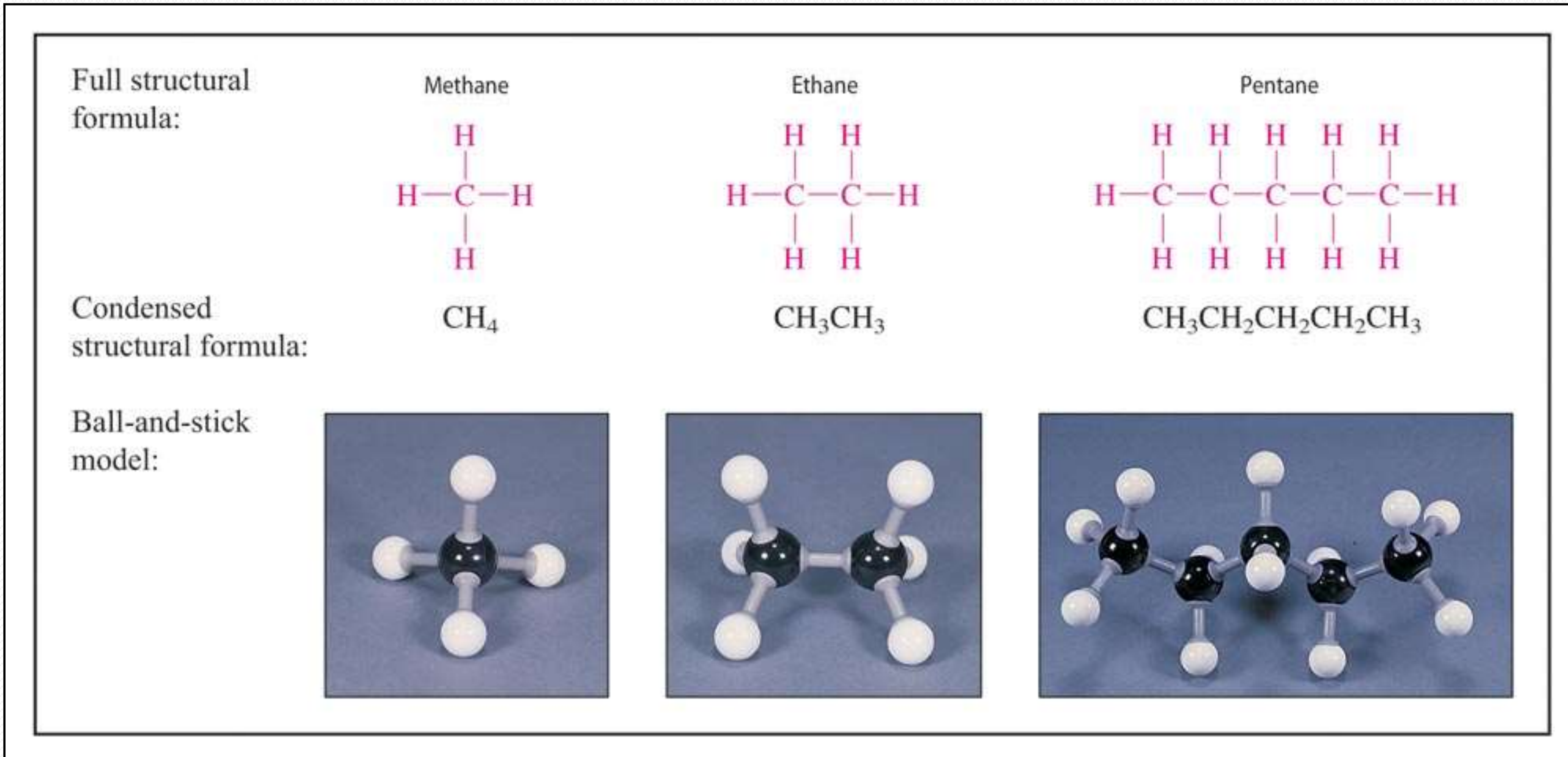
<u>Structural formula</u> – a graphical representation of the way atoms are connected

<u>Condensed structural formula</u> – save time/space and are convenient

<u>Ball-and-Stick models</u> – 3D models that can be built by students

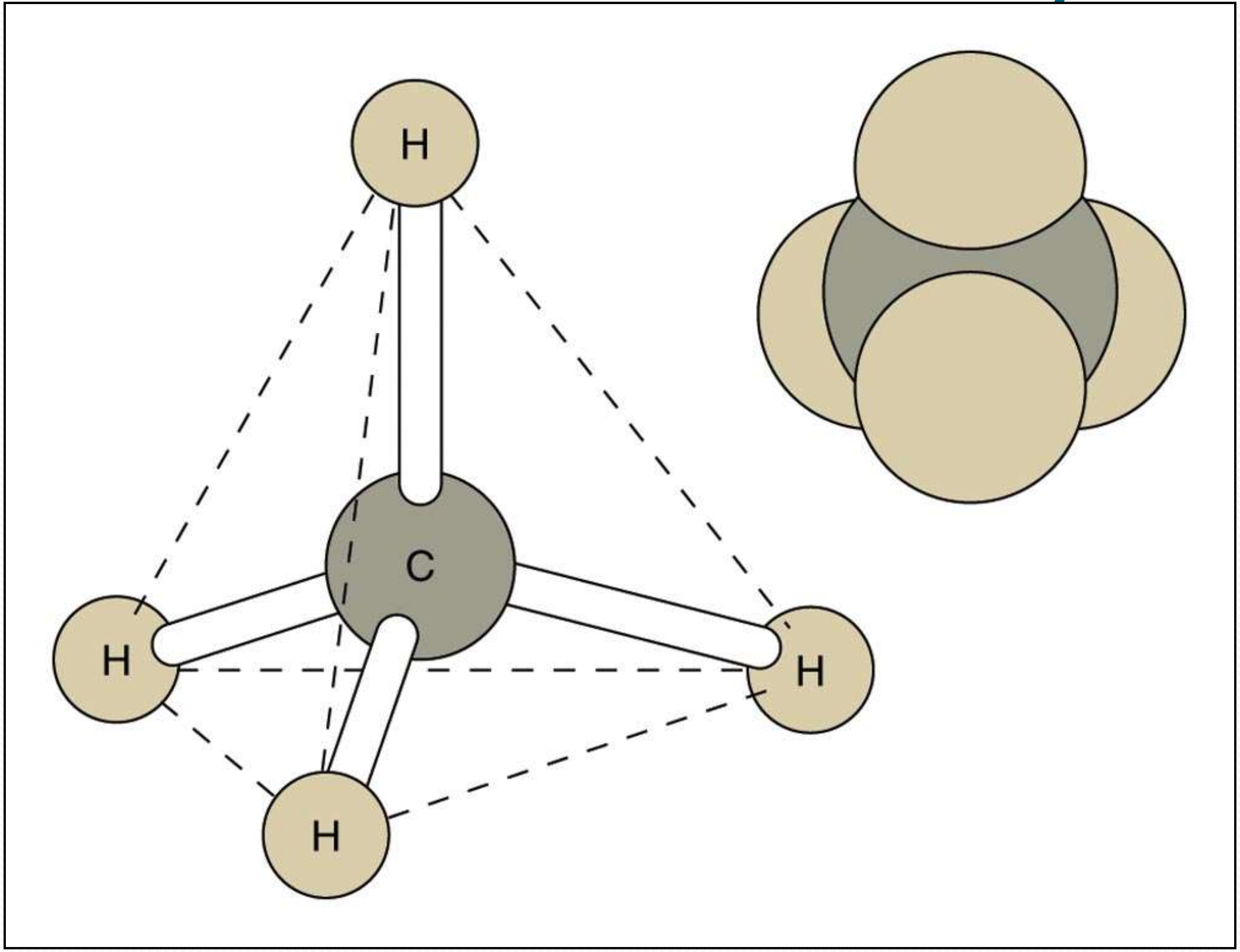
Models of Three Alkanes

- *Names, Structural Formulas, Condensed Structural Formulas, and Ball-and-Stick Models*



Methane – Tetrahedral Geometry

Ball-and-Stick & Space-Filling Models Carbon's four single bonds form angles of 109.5°



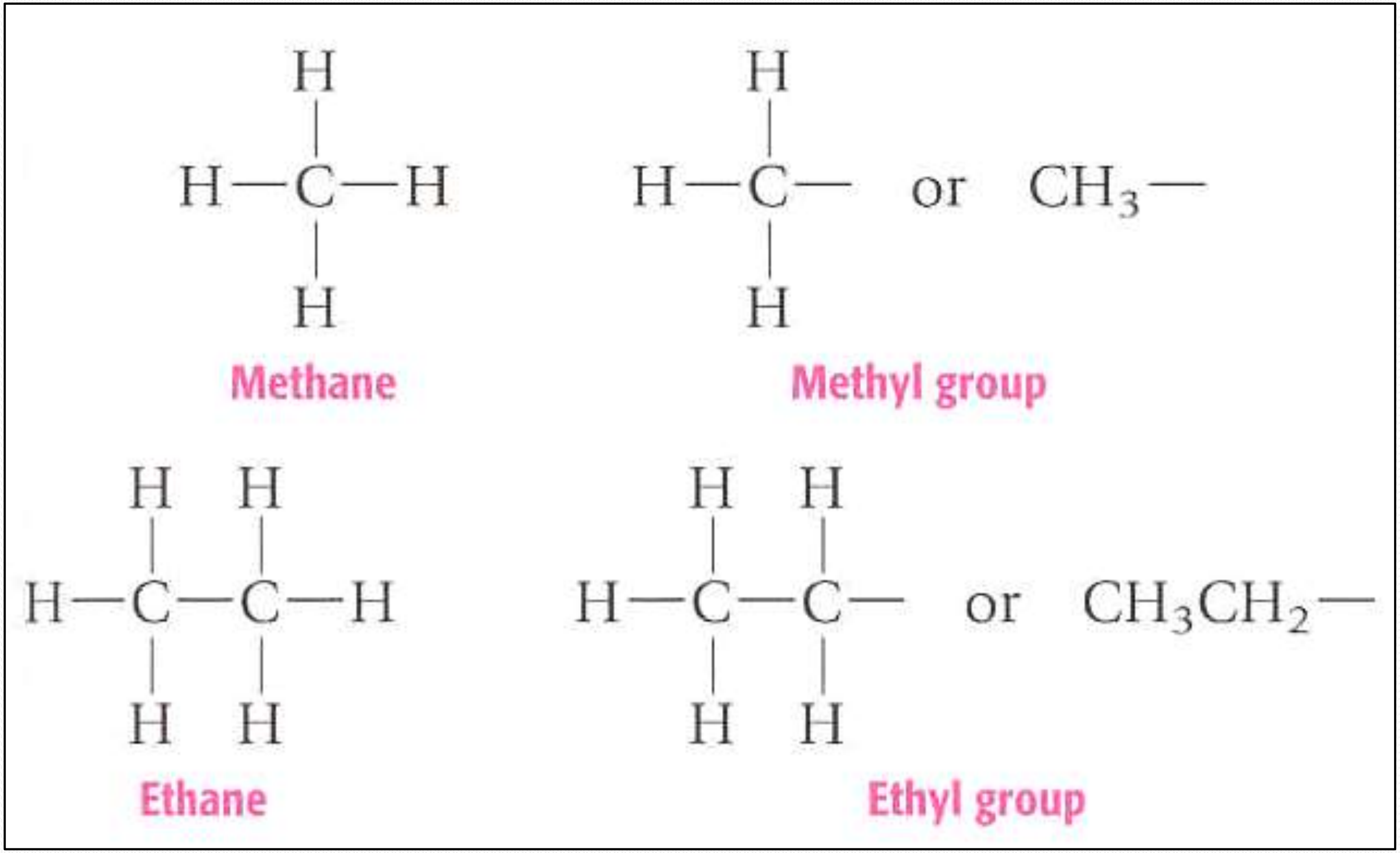
Alkyl Group

- Alkyl group contains one less hydrogen than the corresponding alkane.
- General abbreviation "R" (for Radical, an incomplete species or the "rest" of the molecule)

- In naming this group the "-ane" is dropped and "-yl" is added.
  - CH_3 is "methyl" (from methane)
  - CH_2CH_3 is "ethyl" from ethane

Alkyl Group

This group does not exist independently but occurs bonded to another atom or molecule.

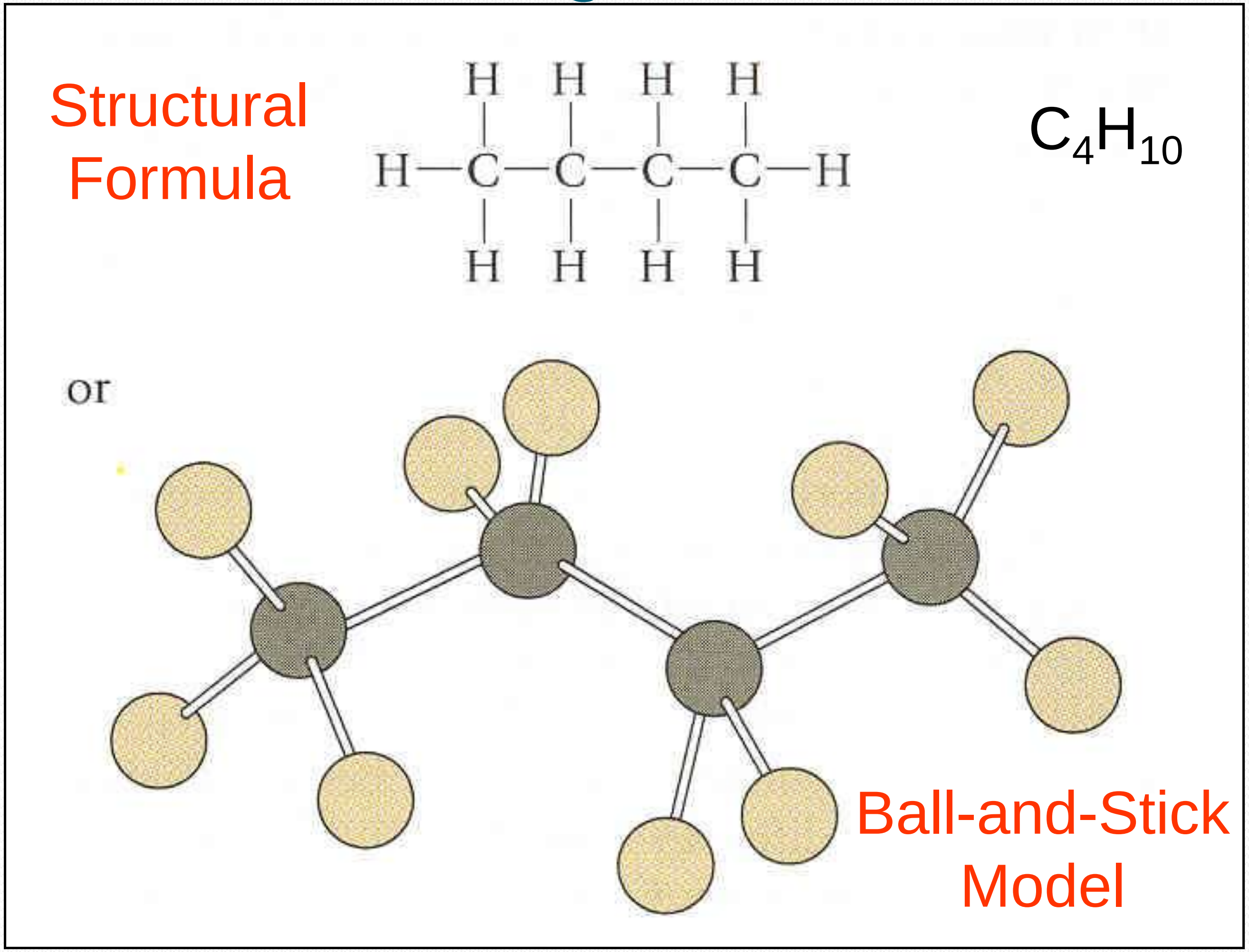


Types of Alkyl groups

- Classified by the connection site
  - a carbon at the end of a chain (primary alkyl group)
  - a carbon in the middle of a chain (secondary alkyl group)
  - a carbon with three carbons attached to it (tertiary alkyl group)

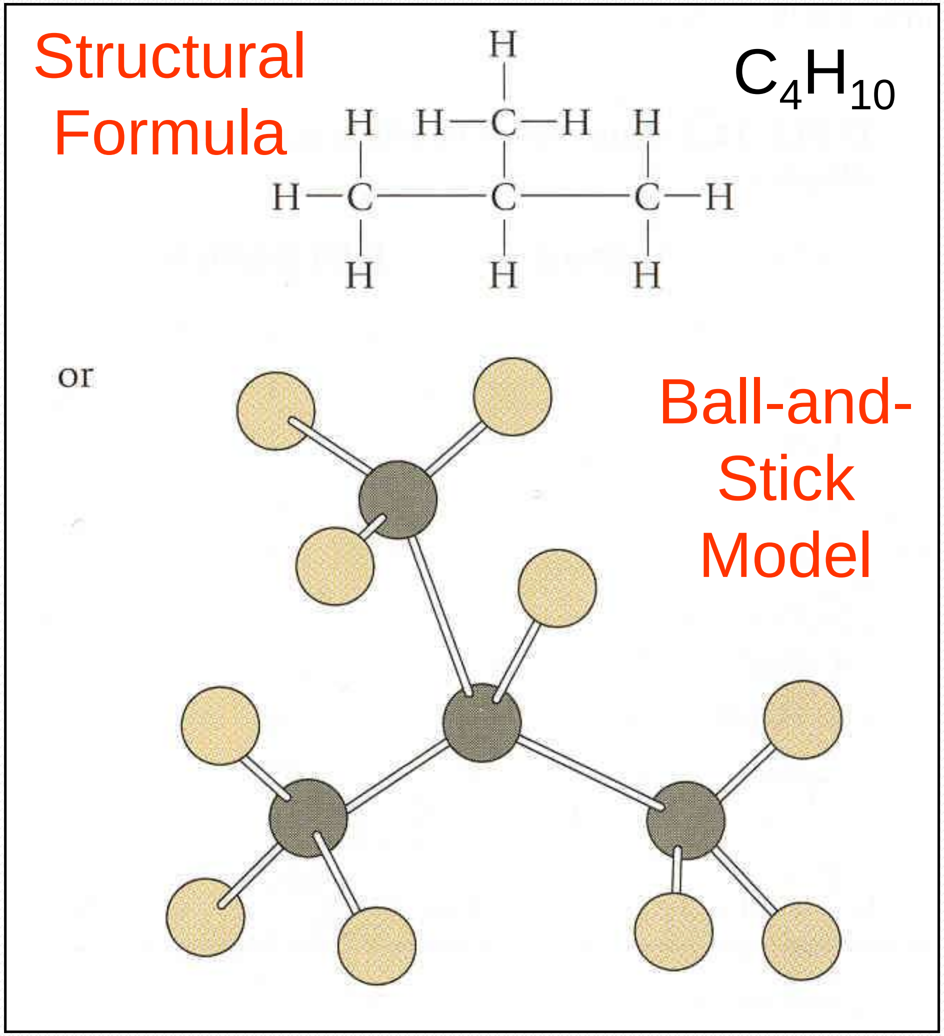
Butane

Continuous-Chain or Straight-Chain Structure



Isobutane (2-methylpropane)

Branched-chain Structure



Organic Compound Nomenclature

- Due to the large number, variety, and complexity of organic compounds, a consistent method of nomenclature has been developed.

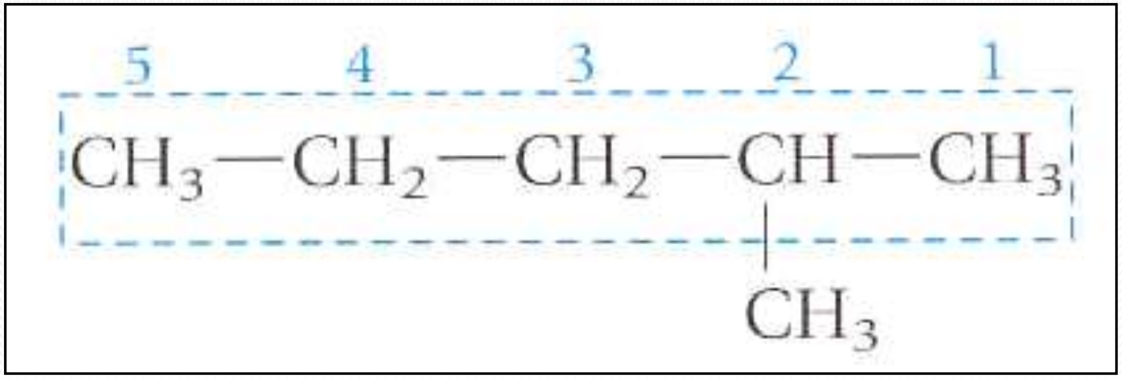
IUPAC System of Nomenclature

For Alkanes

- Identify the longest chain -- parent
- number from the end closest to first branch
- Name the groups attached to the chain, using the carbon number as the locator.
- Alphabetize substituents.
- Use di-, tri-, etc., for multiples of same substituent
- combine number and name of substituent with parent name, separating with hyphen

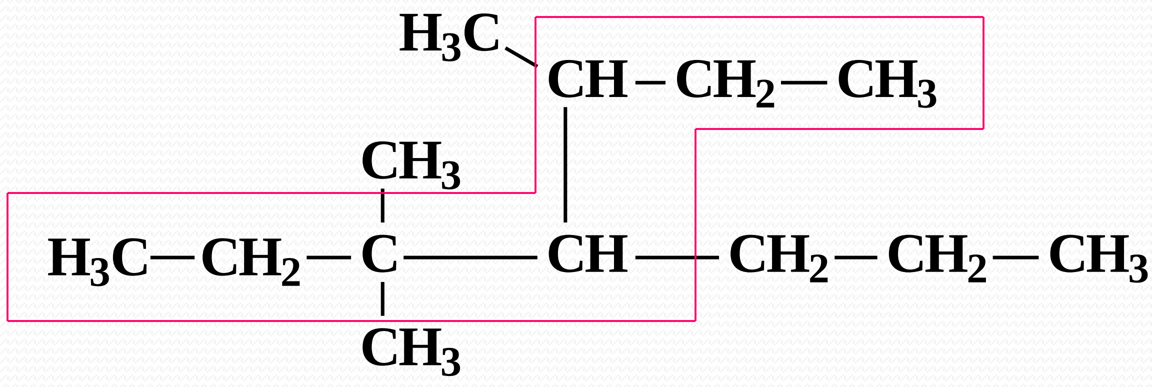
An Example to Consider

- The longest continuous chain of C atoms is five
- Therefore this compound is a pentane derivative with an attached methyl group
  - *Start numbering from end nearest the substituent*
  - The methyl group is in the #2 position
- The compound's name is <u>2-methylpentane</u>.

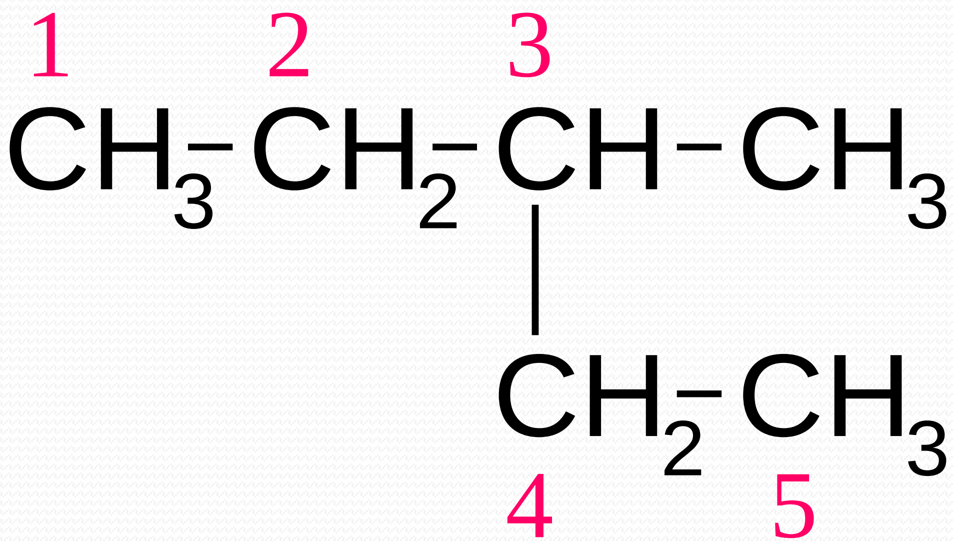


Longest Chain

- The number of carbons in the longest chain determines the base name: ethane, hexane.
- If there are two possible chains with the same number of carbons, use the chain with the most substituents.

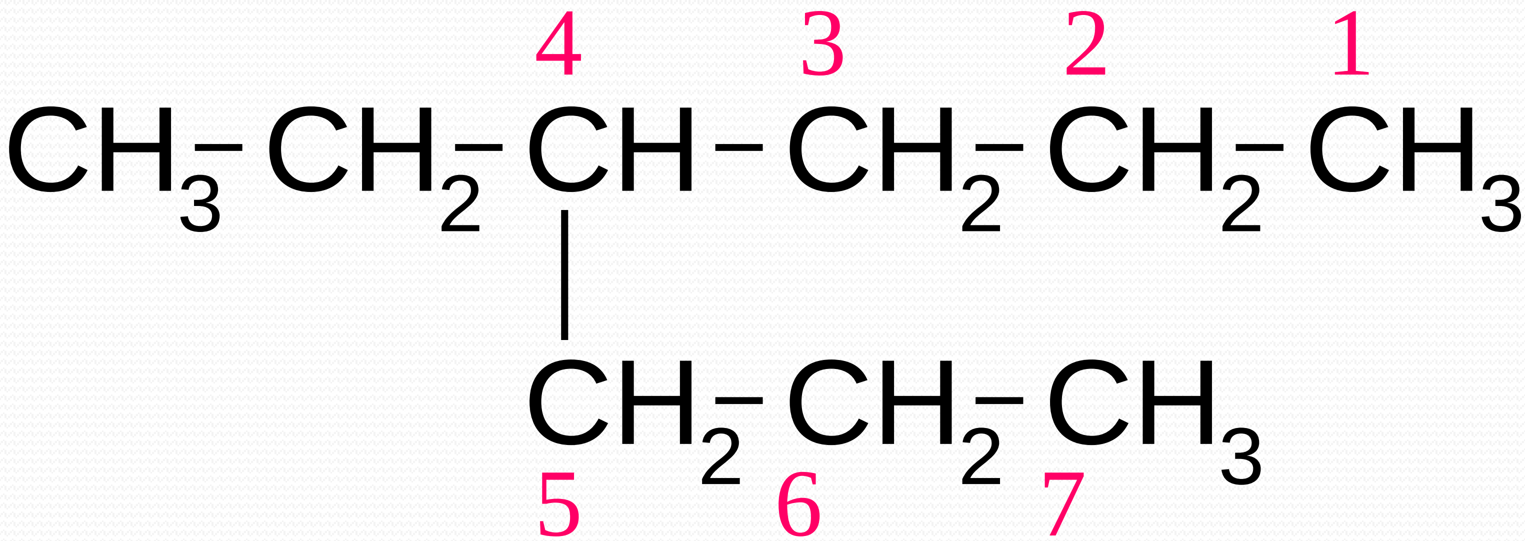


Find the longest continuous carbon chain



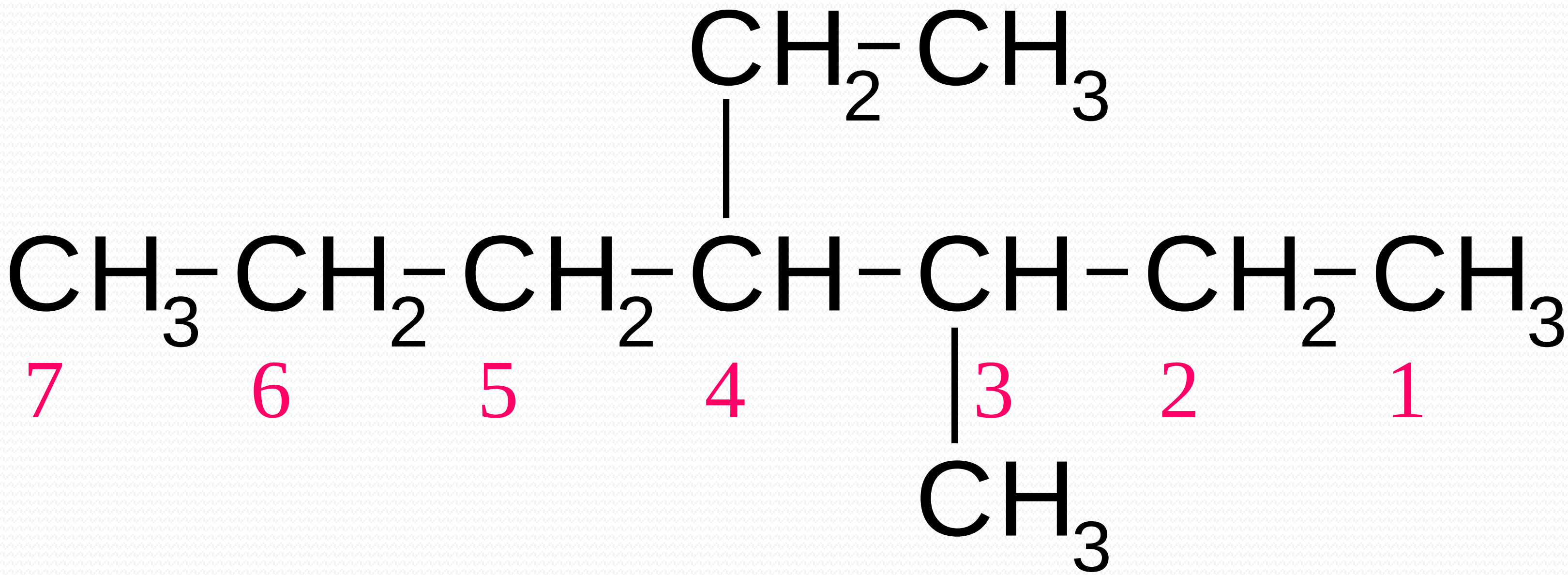
3-methylpentane

You must choose the longest continuous carbon chain



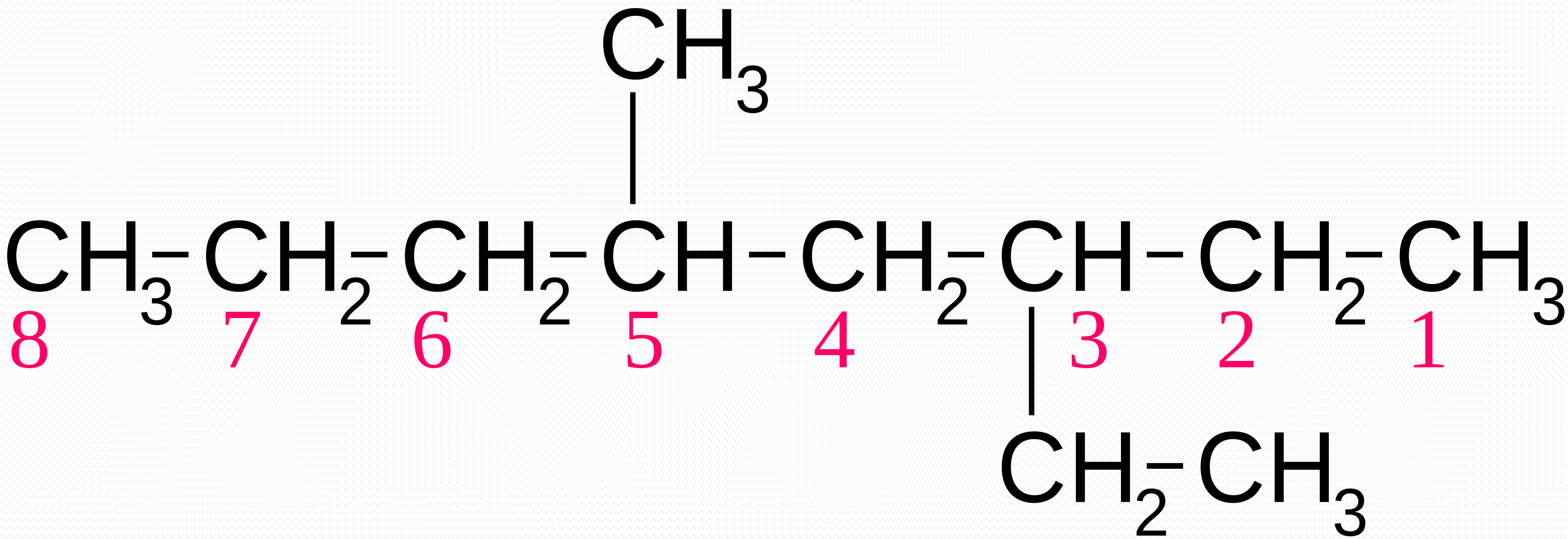
4-ethylheptane

Number from the end nearest the first substituent



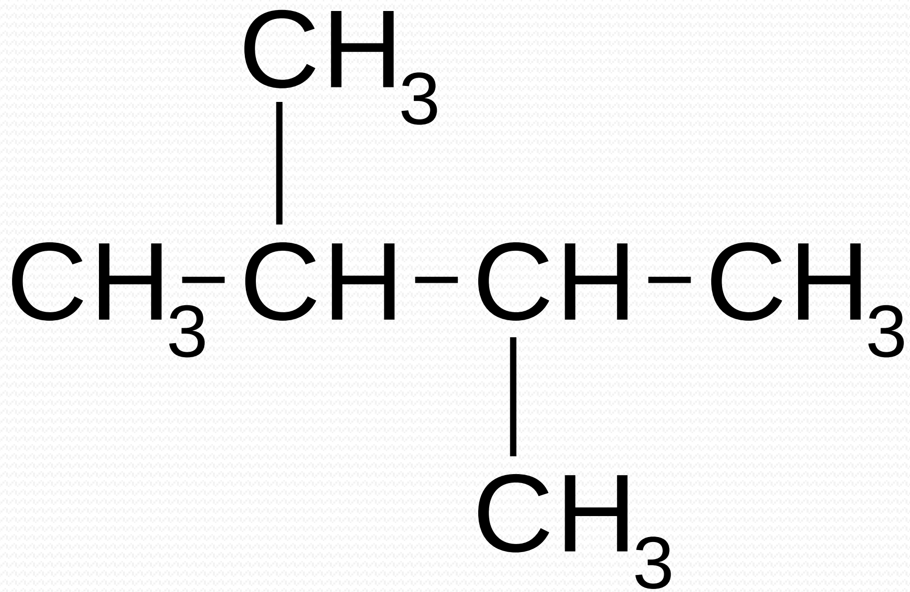
4-ethyl-3-methylheptane

Number from the end nearest the first substituent



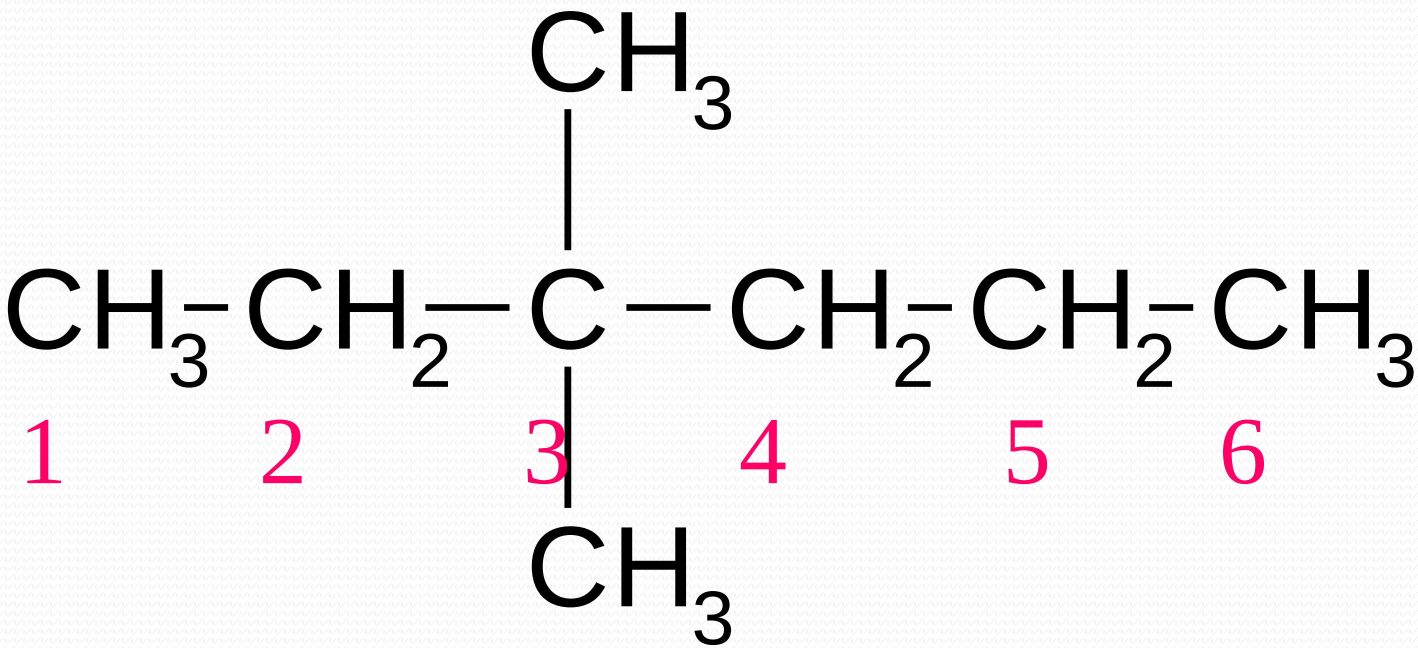
3-ethyl-5-methyloctane

Use “di-” with two substituents



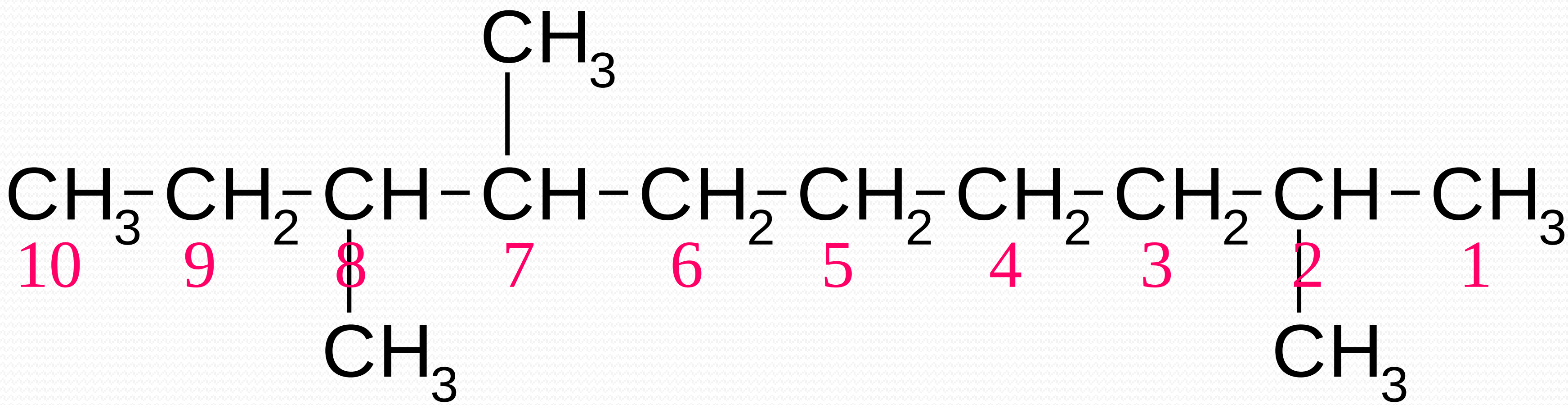
2,3-dimethylbutane

Every substituent must get a number



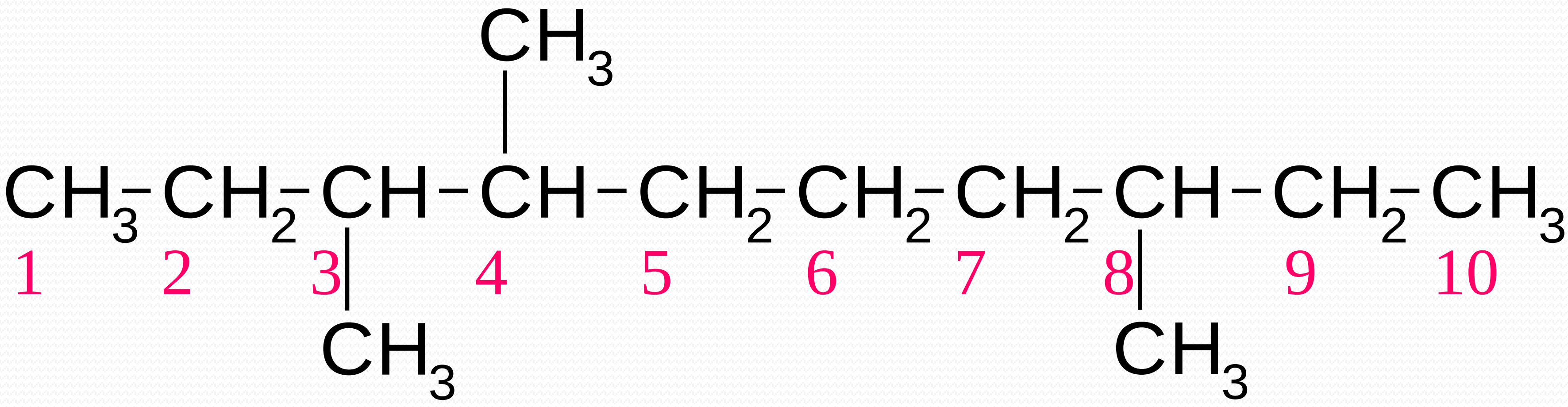
3,3-dimethylhexane

Number from the end nearest first substituent



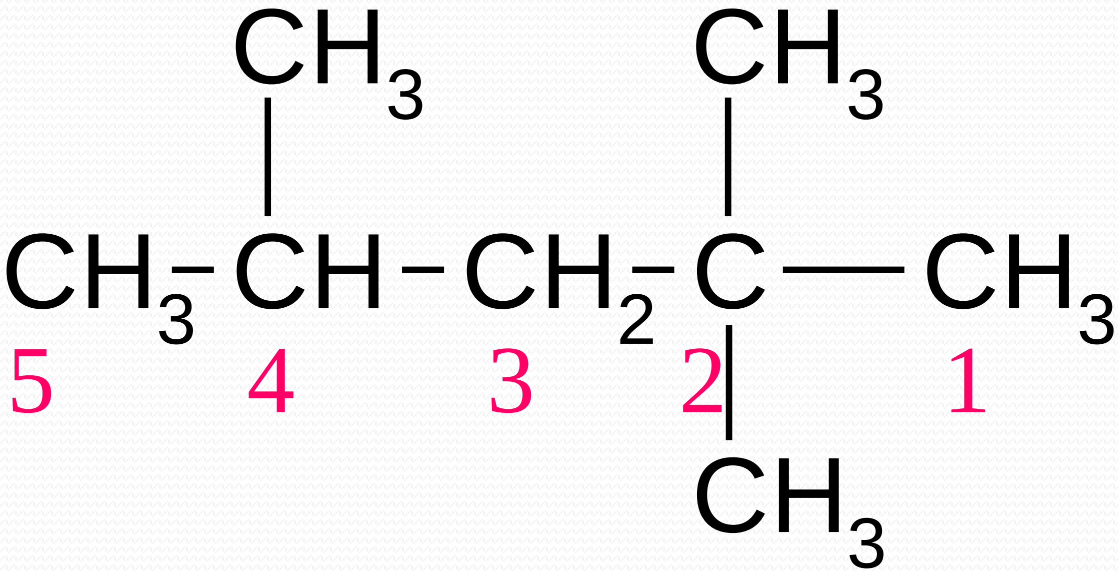
2,7,8-trimethyldecane

Number from the end which has the “first difference”



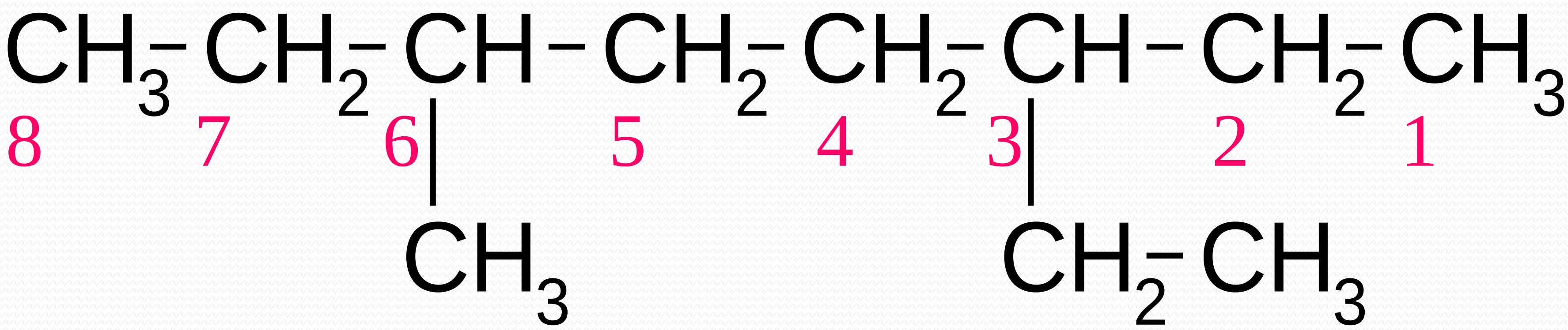
3,4,8-trimethyldecane

A More-Highly-Substituted Carbon Takes Precedence



2,2,4-Trimethylpentane

Which end do we number from?



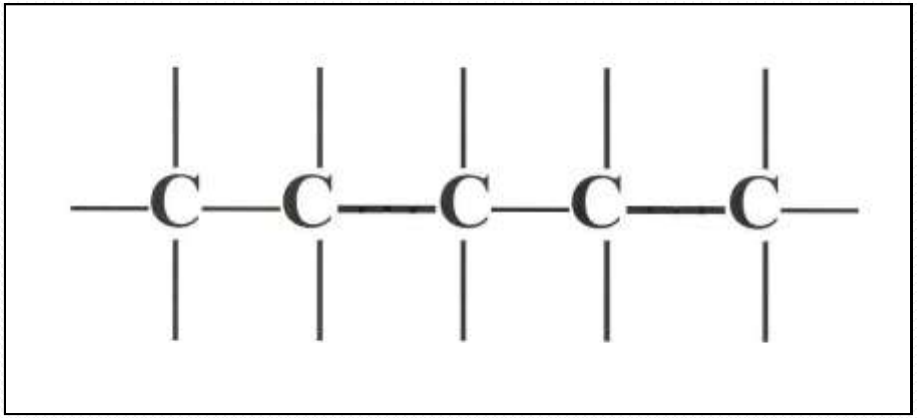
3-ethyl-6-methyloctane

Substituents in Organic Compounds

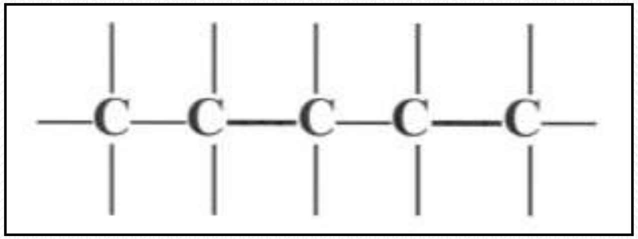
Formula of Substituent	Name of Substituent
Br—	Bromo
Cl—	Chloro
F—	Fluoro
I—	Iodo
CH_3—	Methyl
CH_3CH_2—	Ethyl

Drawing a Structure from a Name

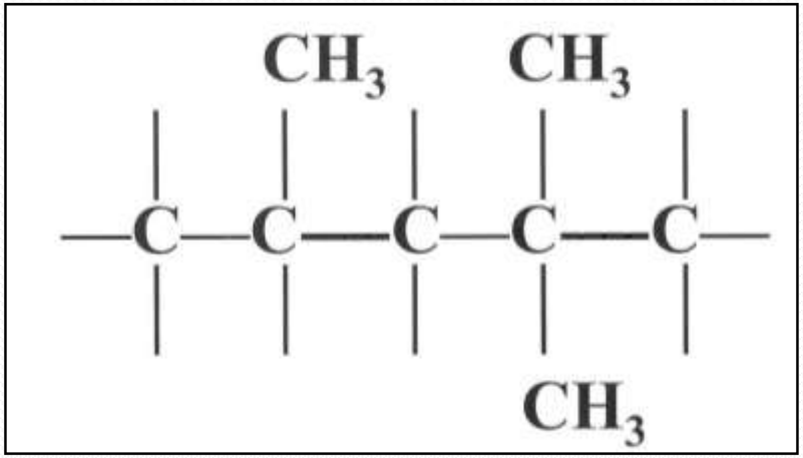
- *Draw the structural formula for 2,2,4trimethylpentane.*
- Note that the end name is *pentane* .
- Draw a continuous chain of five carbon (C) atoms, with four bonds around each.



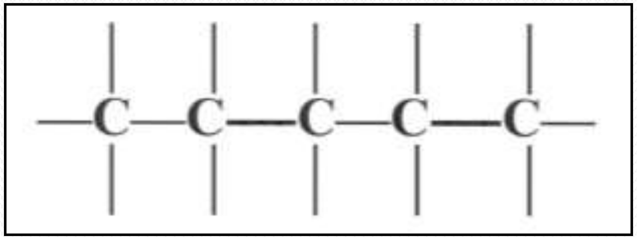
Drawing a Structure from a Name



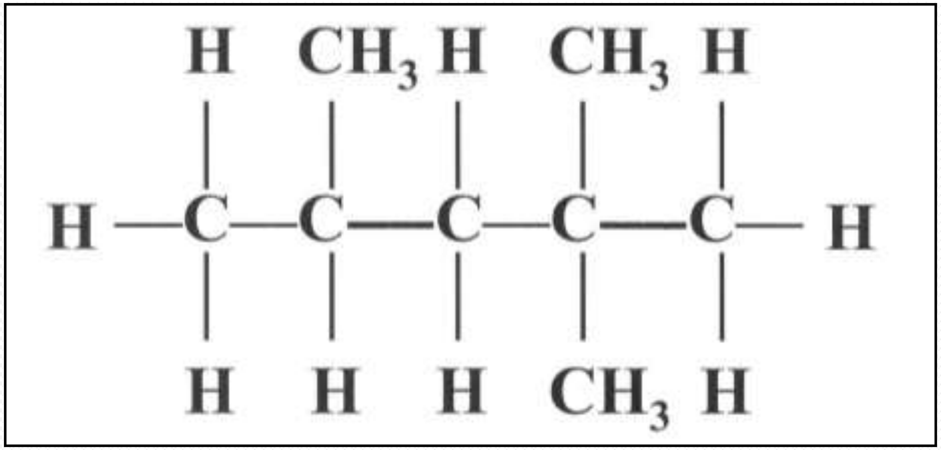
- Number the C atoms from right to left.
- Attach two methyl groups (CH_3--) to carbon number 2 and one to number 4.



Drawing a Structure from a Name



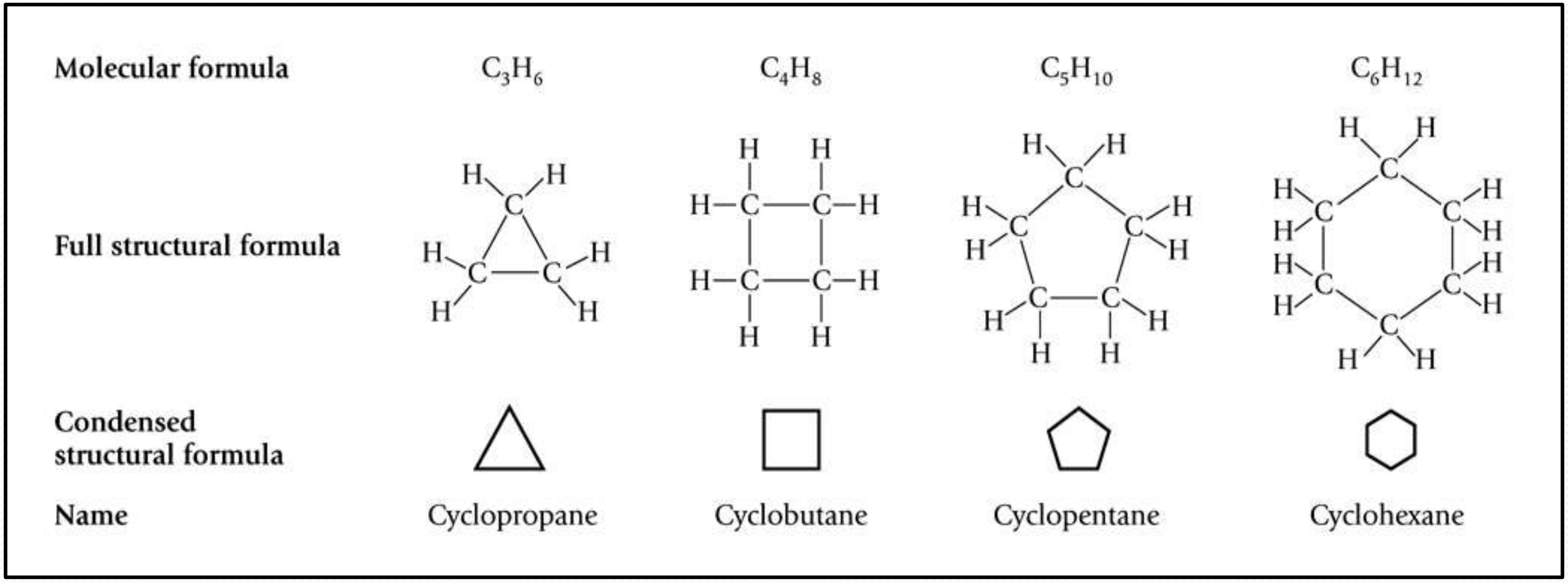
- Add necessary H atoms.
- 2,2,4-trimethylpentane



Cycloalkanes

- Members of the cycloalkane group possess rings of carbon atoms.
- They have the general formula C_nH_{2n}.
- Each carbon atom is bonded to a total of four carbon or hydrogen atoms.
- The smallest possible ring consists of cyclopropane, C_3H_6.

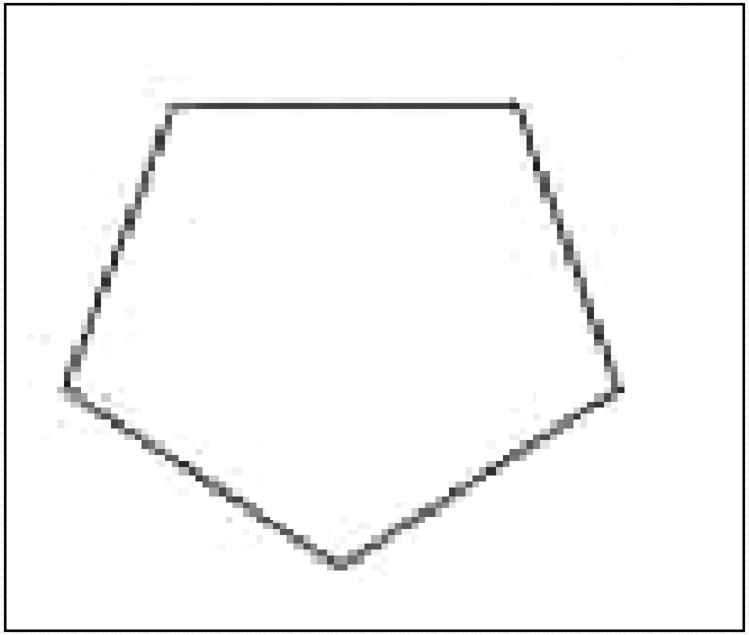
The First Four Cycloalkanes



Note that in the condensed structural formulas, there is a carbon atom at each corner and enough hydrogens are assumed to be attached to give a total of four single bonds.

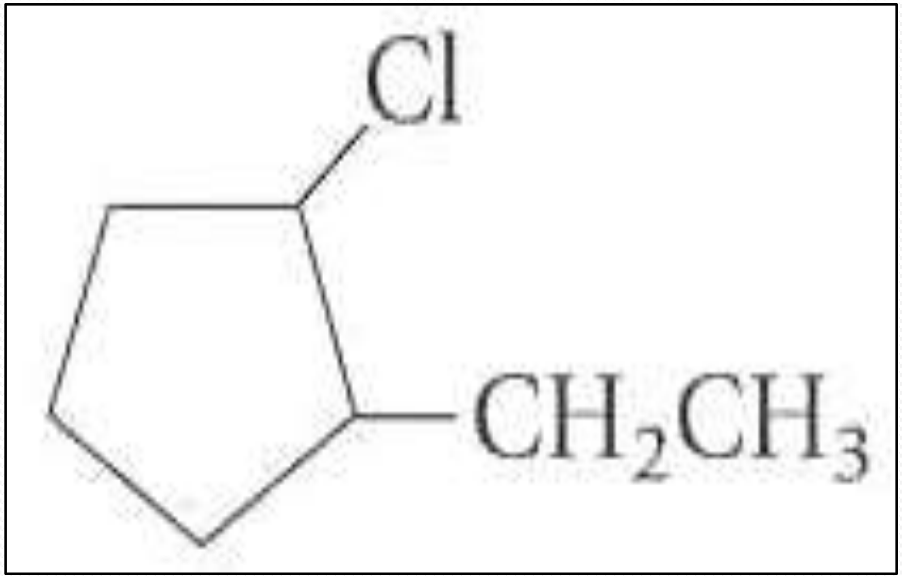
Drawing the Structure of a Cycloalkane

- Draw the geometric figure indicated by the compound's name , "pentane."



Drawing the Structure of a Cycloalkane

- Place each substituent on the ring in the numbered position → "1 chloro-2-ethyl-"
- 1-chloro-2-ethylcyclopentane



Classes of Carbon and Hydrogen atoms

- 1° Carbon - primary carbon is attached to only one other C atoms

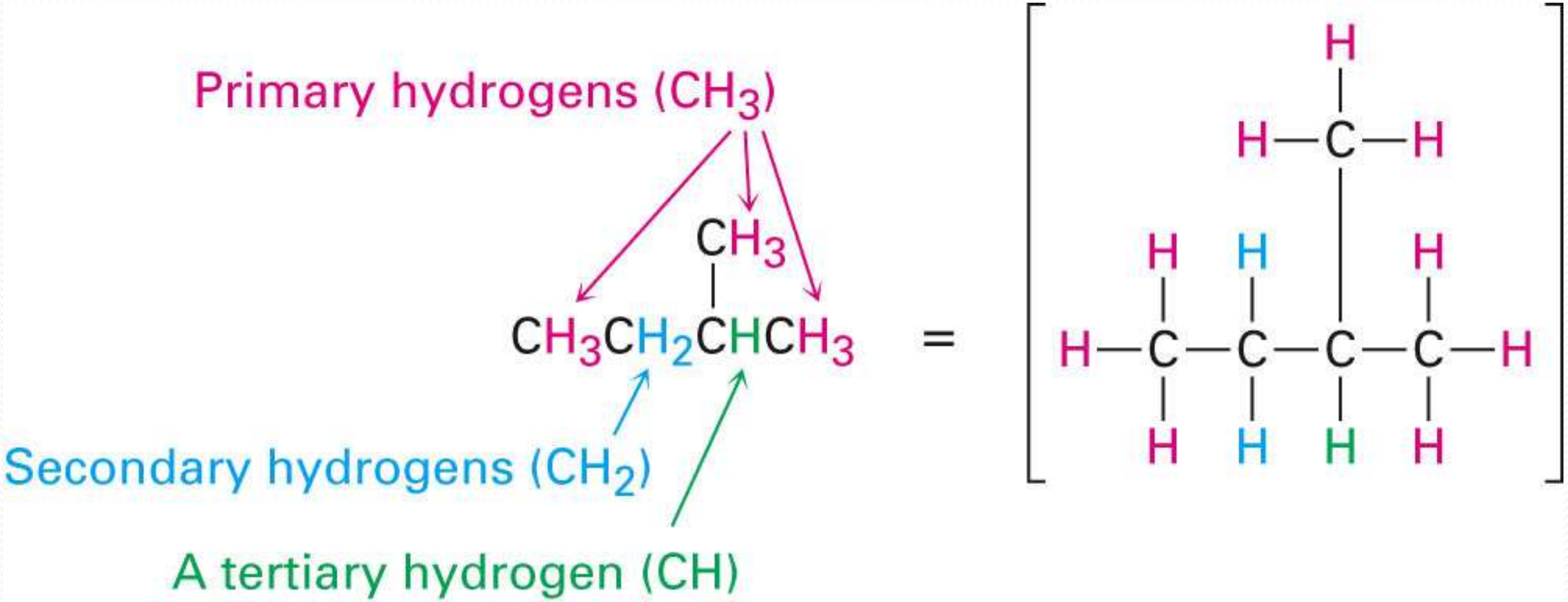
- 2° Carbon - secondary carbon is attached to two other C atoms

- 3° Carbon - tertiary carbon is attached to three other C atoms

$$CH_3CH_2CH_2CH(CH_3)CH_2CH_3$$

1º 2º 2º 3º 1º 2º 1º

Types of Hydrogens

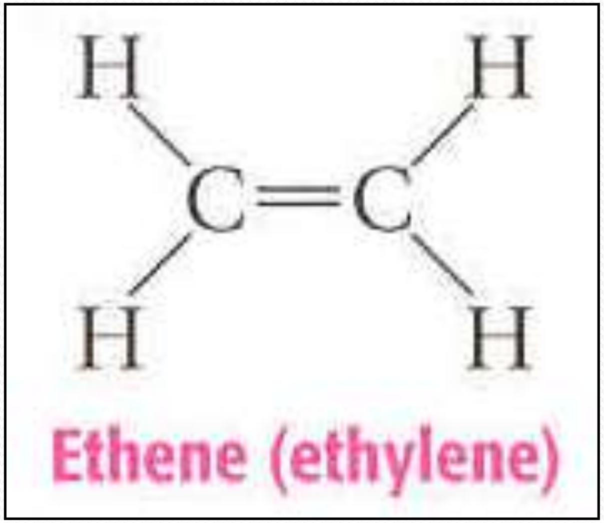


Derivatives of Hydrocarbons

- Organic molecule characteristics depend on the number, arrangement, and type of atoms.
- Functional Group – any atom, group of atoms, or organization of bonds that determine specific properties of a molecule
  - *Generally the functional group is the reactive part of the molecule.*
  - *Due to the functional group's presence, certain predictable properties rise.*

Alkenes

- Members of the alkene group have a double bond between two carbon atoms.
- One hydrogen atom has been removed from two adjacent carbon atoms, thereby allowing the two adjacent carbon atoms to form a double bond.
- General formula is C_nH_{2n}
- Begins with ethene (ethylene)
- C_2H_4



Some Members of the Alkene Series

Name	Molecular Formula	Condensed Structural Formula
Ethene (ethylene)	C_2H_4	$CH_2{=}CH_2$
Propene	C_3H_6	$CH_3CH{=}CH_2$
1-Butene	C_4H_8	$CH_3CH_2CH{=}CH_2$
2-Butene	C_4H_8	$CH_3CH{=}CHCH_3$
1-Pentene	C_5H_{10}	$CH_3(CH_2)_2CH{=}CH_2$

Physical properties:

- Carbon-carbon double bond changes the physicals properties of alkenes.
- At R.T. , alkenes exist in all three phases, solid, liquids, and gases.

- 1. Physical state:
- Ethene, Propene, and Butene exists as colorless gases.
- Members of the 5 or more carbons such as Pentene, Hexene, and Heptene are liquid
- Members of the 15 carbons or more are solids.

- 2. Density: Alkenes are lighter than water

3.Solubility: insoluble in water.

Alkenes are only soluble in nonpolar solvent like benzene, ether, chloroform.

4.Boiling point : depends on more molecular mass (chain length).

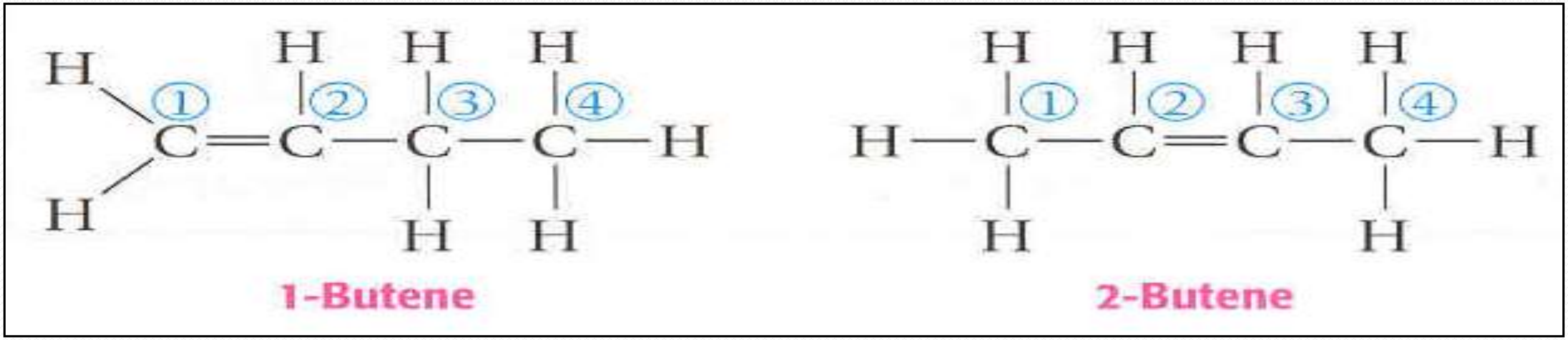
more intermolecular mass is added, the higher the boiling point.

5. Melting point : depends on the packaging of the molecules.

Alkenes have similar melting points to that of alkanes,

Naming Alkenes

- "*-ane*" suffix for the corresponding alkane is changed to "*-ene*" for alkenes.
- A number preceding the name indicates the C atom on which the double bond starts.
  - *The carbons are numbered such that the double bond has the lowest number.*
- For example, 1-butene and 2-butene

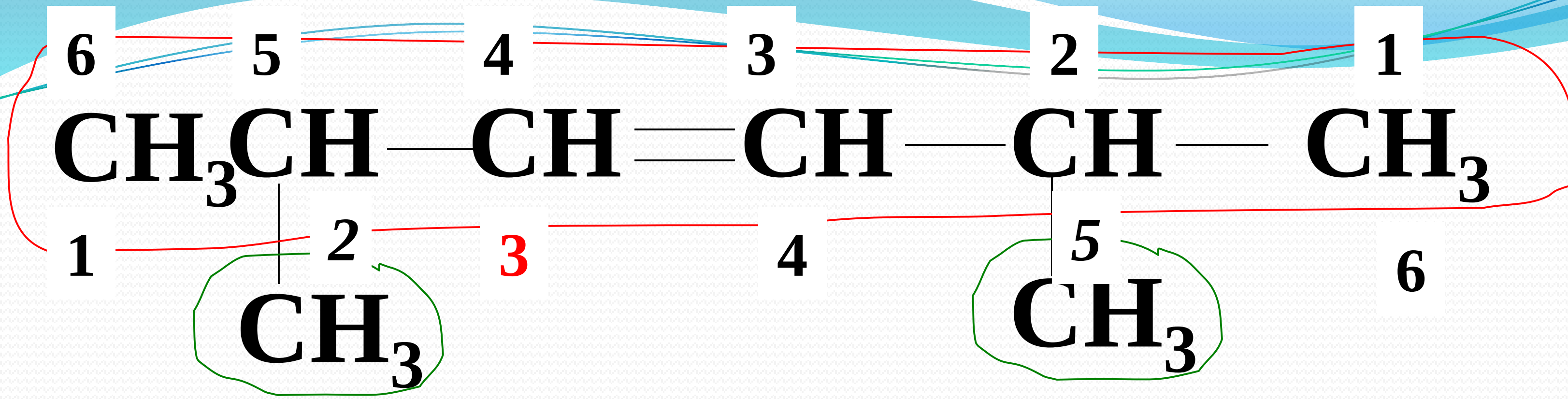


Example

Write the IUPAC name for each of the following:

$$
\begin{array}{l}
\qquad\qquad\quad CH_3 \\
\qquad\qquad\quad | \\
\text{B.}\quad CH_3{-}CH_2{-}C{=}CH{-}CH_3
\end{array}
$$

3 –methyl 2-pentene



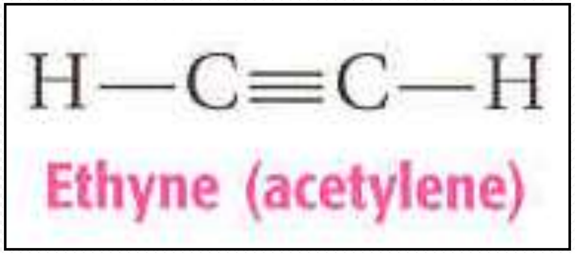
Correct name is : 2,5-dimethyl-3-hexene

Note: Always number so that double bond gets the lowest number

Alkynes

- Members of the alkyne group have a triple bond between two carbon atoms.
- Two hydrogen atoms have been removed from each of two adjacent carbon atoms, thereby allowing the two adjacent carbon atoms to form a triple bond.

- General formula is C_nH_{2n-2}
- Begins with ethyne (acetylene)
- C_2H_2



Some Members of the Alkyne Series

Name	Molecular Formula	Condensed Structural Formula
Ethyne (acetylene)	C_2H_2	$HC{\equiv}CH$
Propyne	C_3H_4	$CH_3C{\equiv}CH$
1-Butyne	C_4H_6	$CH_3CH_2C{\equiv}CH$
2-Butyne	C_4H_6	$CH_3C{\equiv}CCH_3$
1-Pentyne	C_5H_8	$CH_3(CH_2)_2C{\equiv}CH$

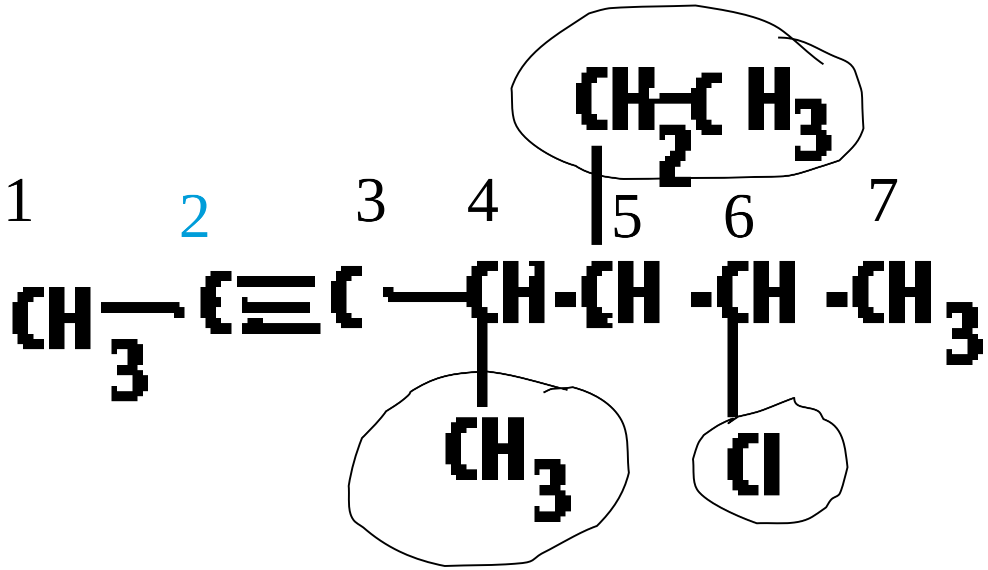
Physical properties

1. Physical properties:

- First 3 members of alkyne : gaseous form

  up to C8 : liquid,

  more than 8 carbons: solid.
- Colorless & except ethyne all are odorless.
- Lighter than water
- Insoluble in polar and soluble in non polar organic solvents.
- Melting point, Boiling point and increase with molecular mass.



Longest chain containing triple bond

2-heptyne

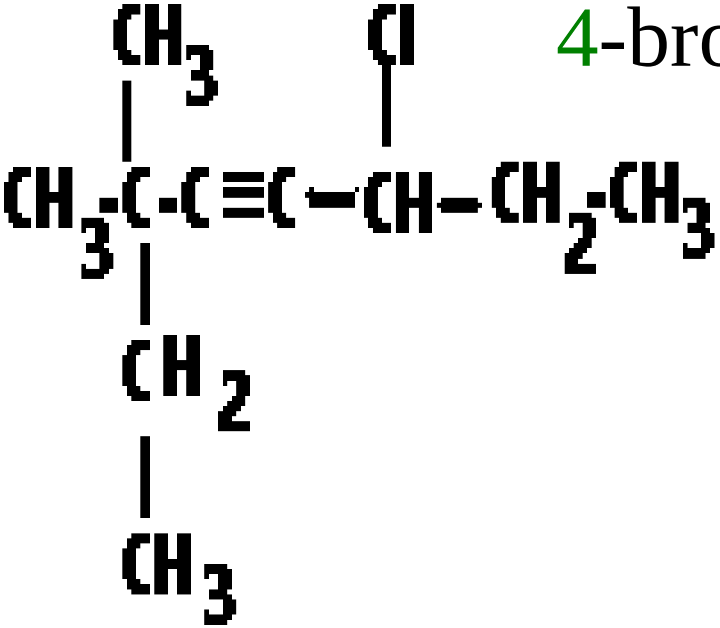
(triple bond)

Location and number of groups?

4-methyl 5-ethyl 6-chloro

Name: 6-chloro-5-ethyl-4-methyl-2-heptyne

4-bromo-5-methyl-2-hexyne



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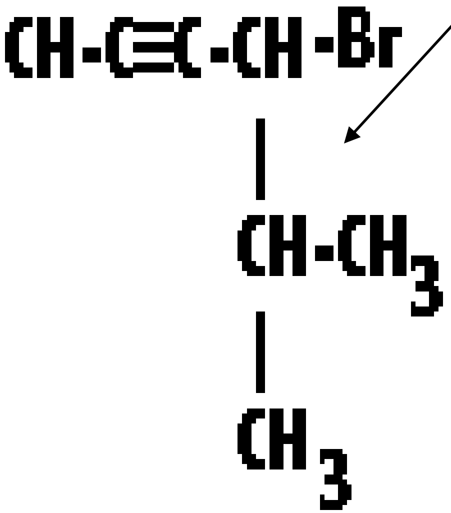
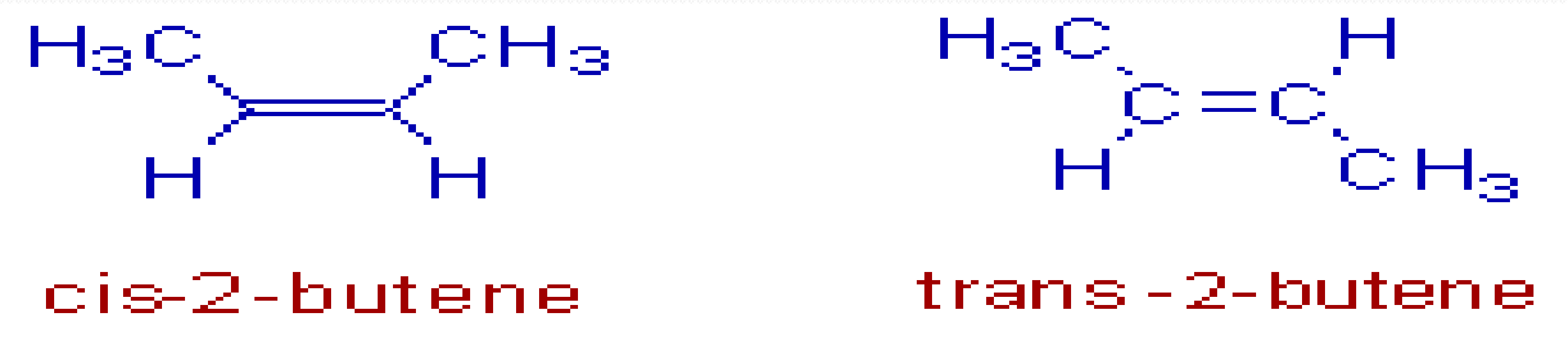


(b)

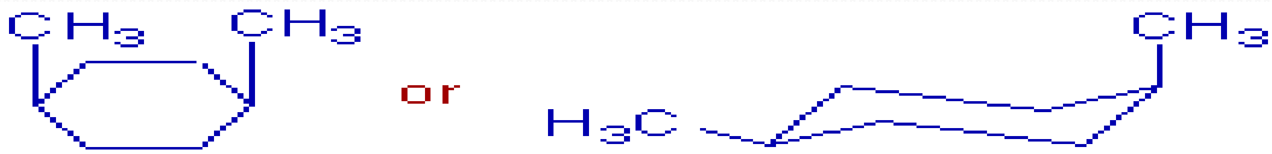
6-chloro-3,3-dimethyl-4-octyne

GEOMETRICAL ISOMERISM

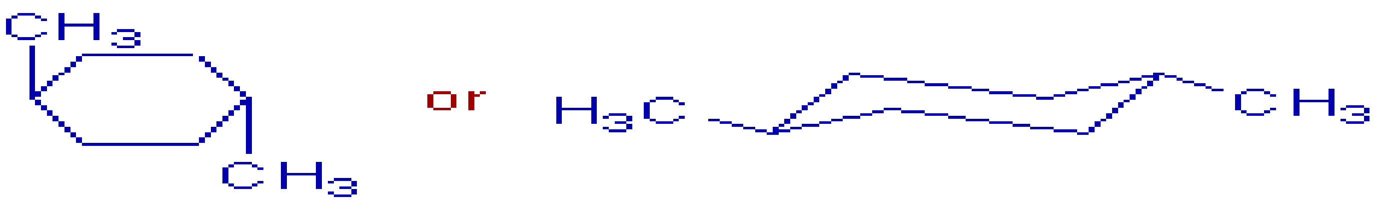
- ***The geometrical isomerism arises when atoms or groups are arranged differently in space due to restricted rotation of a bond or bonds in a molecule.***
- E.g.,
- 1) Two different spatial arrangements of methyl groups about a double bond in 2-butene give rise to the following geometrical isomers.
- i.e., cis-2-butene and trans-2-butene



- Above two forms are not inter convertible due to restricted rotation of double bond.
- In the cis isomer, the two methyl groups are arranged on the same side of a double bond.
- Whereas in the trans isomer, they are on the opposite side.
- 2) There are two geometrical isomers (cis & trans) possible in case of 1,4–dimethylcyclohexane as shown below:
-



cis-1,4-dimethylcyclohexane



trans-1,4-dimethylcyclohexane

- In the above geometrical isomers, the methyl groups are arranged differently about the plane of the cyclohexane ring. These isomers are not inter convertible since it is not possible to rotate the bonds in the cyclohexane ring.

- The geometrical isomers often show different physical and chemical properties. The difference in their physical properties is more significant when there is more difference in their polarity.

- Usually the dipole moment of cis-isomers is greater than that of trans isomers. Hence the cis isomers usually have more solubility in polar solvents.

- In general, the trans isomers are more stable than cis isomers.

References

1.Organic Chemistry by Morrison and Boyd
2.https://www.google.com
3. https://sites.google.com