

Lecture 1.  
Biomedical and Bioorganic  
Chemistry

Lecturer  
Yanovska Anna Olexandrivna

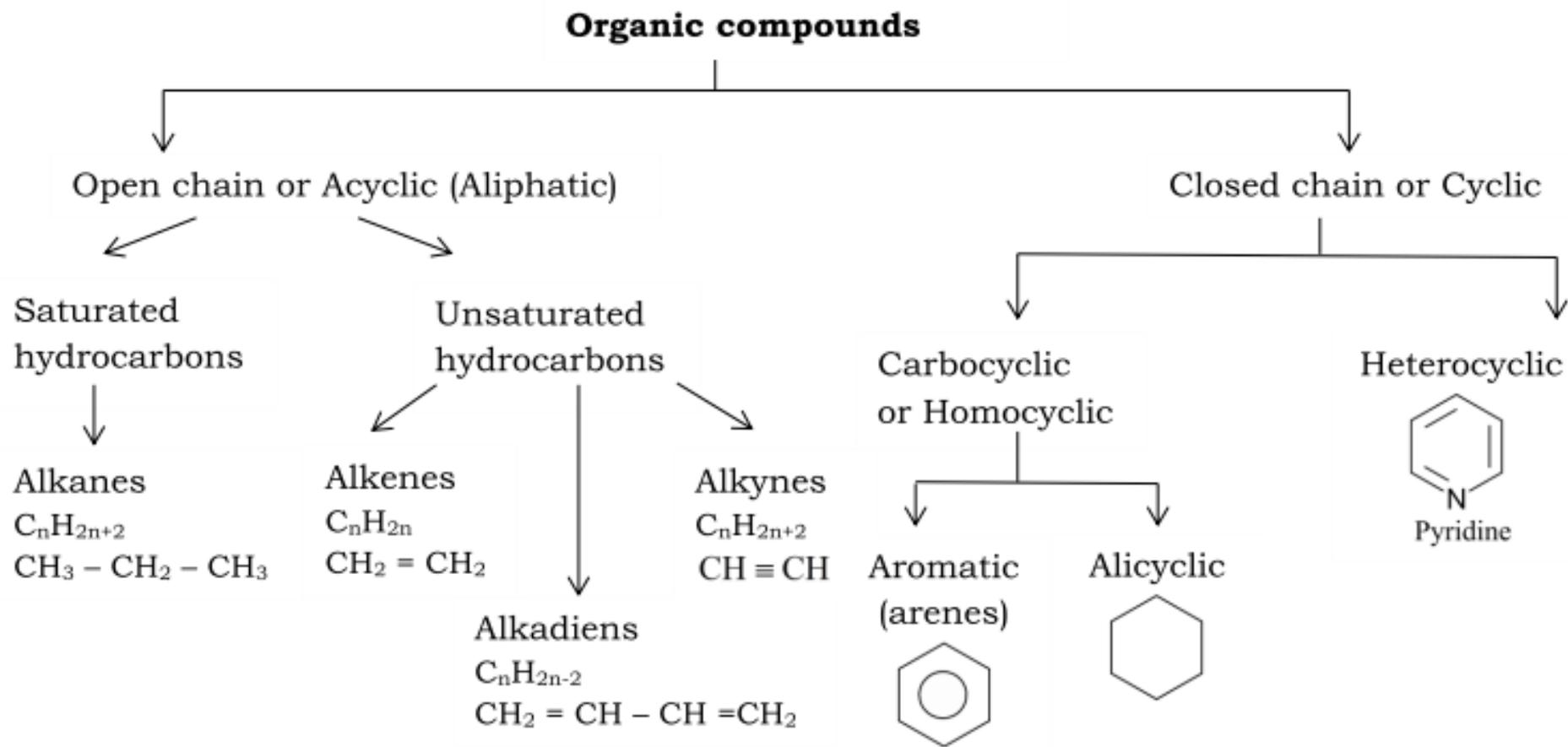
# Calculate grade:

- Total (200)
- General module (80 total)
- Tests (Nomenclature - 10 points, Heterofunctional compounds – 14 points, Lipids – 14 points, Aminoacids, Peptides – 14 points).
- Individual homework (30 possible)
- 20 points (laboratory works)
- 18 points work in class
- Grades:
- 170-200 - excellent
- 169 – 140 - good
- 139 – 120 – satisfied
- Less than 120 - unsatisfied

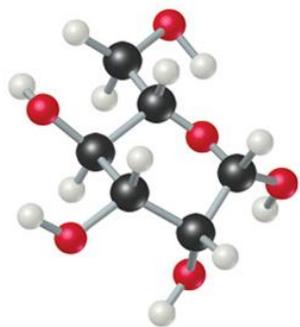
**Organic chemistry** is the chemistry of compounds of carbon.

**Bioorganic chemistry** is the part of organic chemistry that studies the carbon compounds, which are present in the living organism – the so-called biomolecules. The major biomolecules are carbohydrates, proteins, lipids, and nucleic acids. It also studies drugs and their derivatives.

By carbon chain organic compounds are classified in following way:

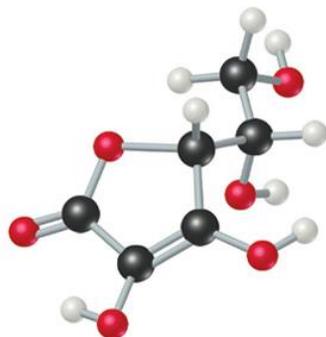


# Organic Chemistry

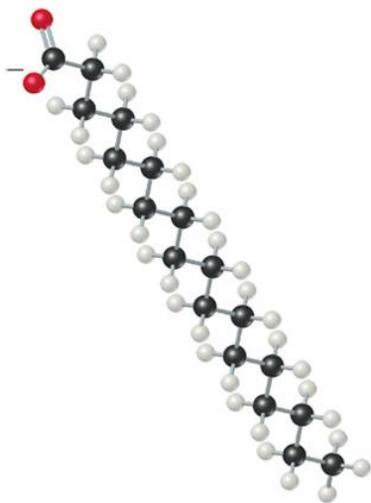


Glucose ( $C_6H_{12}O_6$ )

- The chemistry of carbon compounds.
- What's special about carbon?
  - tetravalent ( $sp^3$  hybridization)
  - wide choice in oxidation states
    - $CO_2$  C, +4
    - $CH_4$  C, -4
  - bonds well to O, N, halides, itself, etc.
  - Covalent bonds are very strong

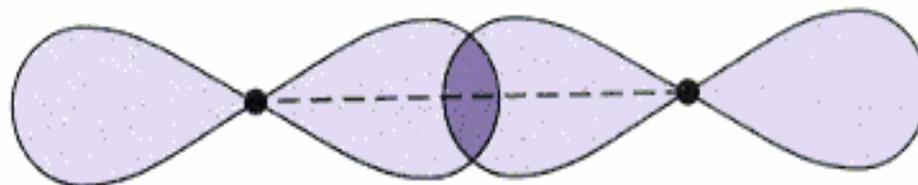
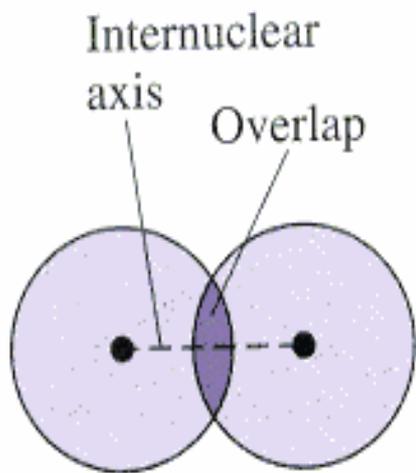


Ascorbic acid ( $HC_6H_7O_6$ )

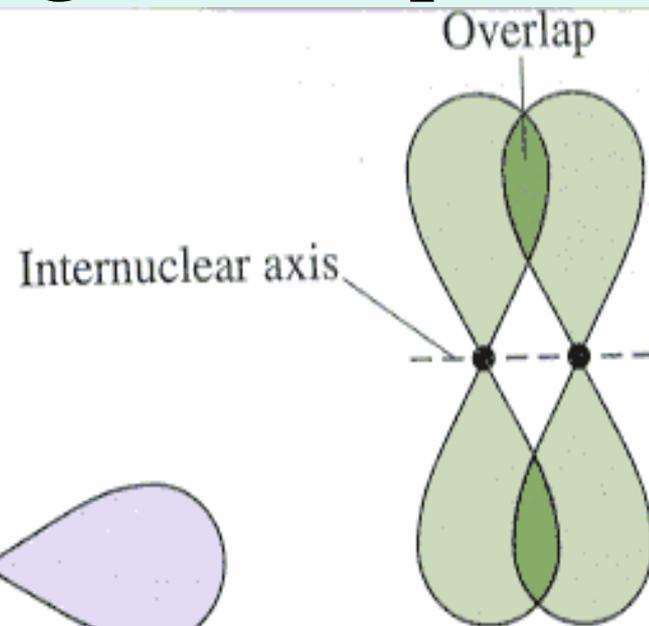


Surfactant ( $C_{17}H_{35}COO^-$ )

# Bond formation in molecules of organic compounds

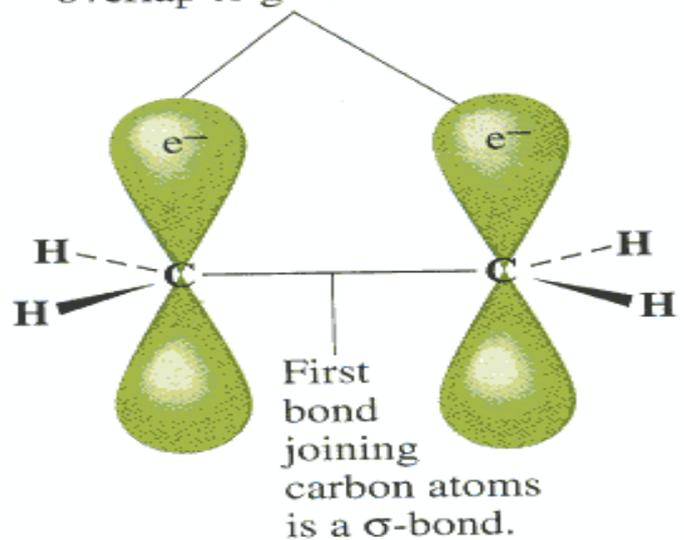


(a)  $\sigma$ -bonds

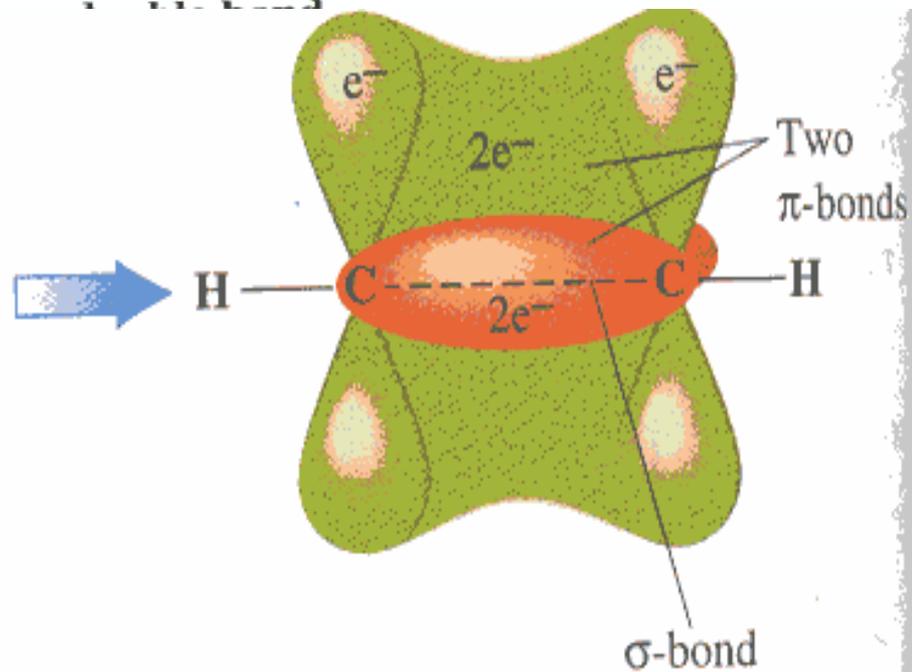
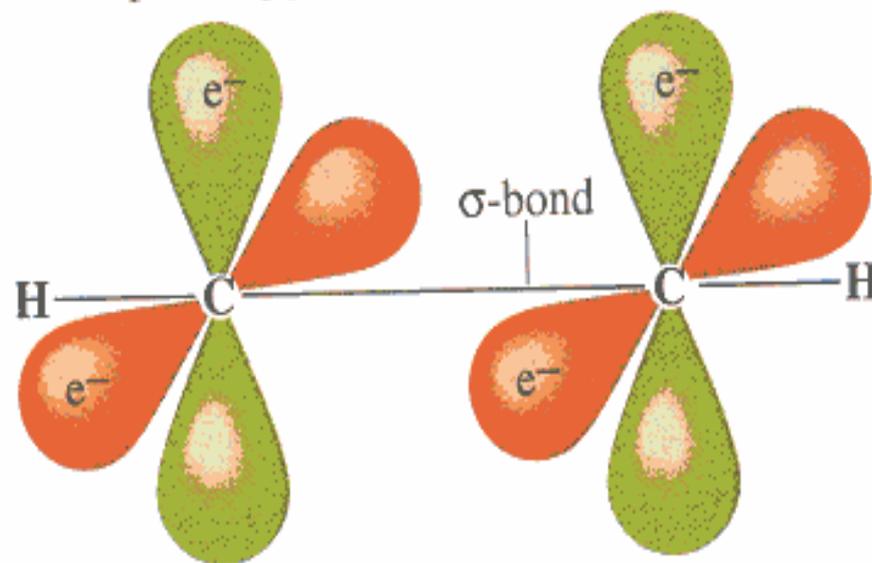
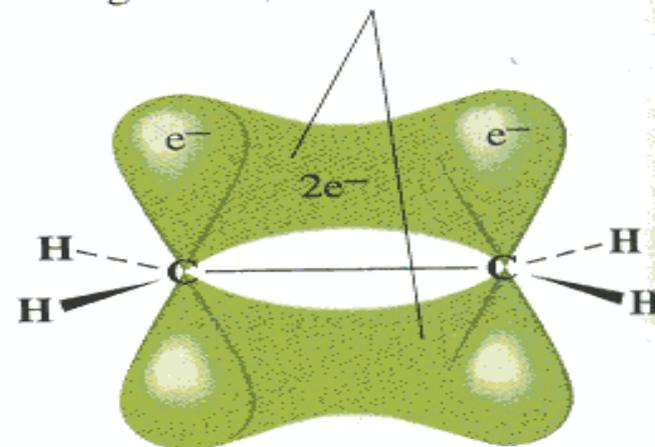


(b)  $\pi$  bond

Two  $p$  orbitals, each with one  $e^-$ , overlap to give a  $\pi$ -bond.



The two overlap regions together constitute one  $\pi$ -bond.



Functional Group	Type of Compound	Suffix or Prefix	Example	Systematic Name (common name)
	Alkene	-ene		Ethene (Ethylene)
$\text{—C}\equiv\text{C—}$	Alkyne	-yne	$\text{H—C}\equiv\text{C—H}$	Ethyne (Acetylene)
	Alcohol	-ol		Methanol (Methyl alcohol)
	Ether	ether		Dimethyl ether
 (X = halogen)	Haloalkane	halo-		Chloromethane (Methyl chloride)
	Amine	-amine		Ethylamine
	Aldehyde	-al		Ethanal (Acetaldehyde)
	Ketone	-one		Propanone (Acetone)
	Carboxylic acid	-oic acid		Ethanoic acid (Acetic acid)
	Ester	-oate		Methyl ethanoate (Methyl acetate)
	Amide	-amide		Ethanamide (Acetamide)

# Functional Groups

Term used to refer to parts of organic molecules where reactions tend to occur.

**By amount of functional groups and their type** organic compounds are classified onto

- ***Monofunctional*** (one functional group):  
alcohol  $C_2H_5-OH$ , carboxylic acid  $CH_3COOH$
- ***Polyfunctional*** – has two or more same  
functional groups:  $HO-CH_2-CH_2-OH$
- ***Heterofunctional*** – has two or more different  
functional groups:  $HO-CH_2-CH_2-NH_2$

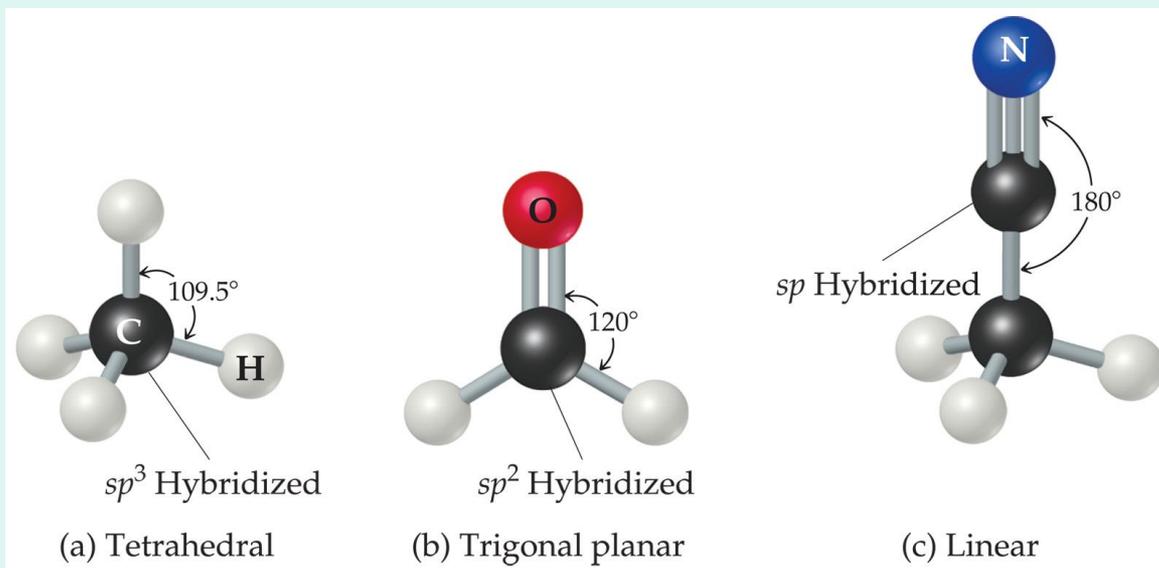
**Functional Group** is a part of an organic compound, by which it belongs to class of organic compounds and has specific properties.

NAME OF CLASS	GENERAL FORMULA	FUNCTIONAL GROUP		IUPAC	
		FORMULA	NAME	PREFIX	SUFFIX
Carboxylic acids	RCOOH	$-(C)OOH^*$	Carboxyl	-----	-oic acid
		-COOH		Carboxy-	
Sulfonic acids	R-SO <sub>3</sub> H	-SO <sub>3</sub> H	Sulfonate	Sulfo-	- sulfo acid
Esters	R-COO-R	$-(C)OOR^*$	Carbalkoxy	-----	-oate
Amides	R-CONH <sub>2</sub>	-CONH <sub>2</sub>	Amide	Carbamyl-	-amide
Nitriles	R-C≡N	$-(C)≡N^*$	Nitrile	-----	-nitrile
		-CN		Cyano-	-----
Aldehydes	$R-\overset{\text{O}}{\parallel}{C}-H$	$-(C)\overset{\text{O}}{\parallel}{C}-H$	Carbonyl	Formyl-	-al
Ketones	R-CO-R	$\diagup C=O$		Oxo or keto-	-one

<i>Alcohols</i>	<i>R-OH</i>	<i>-OH</i>	<i>Hydroxyl</i>	<i>Hydroxy-</i>	<i>-ol</i>
<i>Thioalcohols</i>	<i>R-SH</i>	<i>-SH</i>	<i>Thiol</i>	<i>Mercapto-</i>	<i>-thiol</i>
<i>Amines</i>	<i>R-NH<sub>2</sub></i>	<i>-NH<sub>2</sub></i>	<i>Amino</i>	<i>Amino-</i>	<i>-amine</i>
<i>Nitro compound</i>	<i>R-NO<sub>2</sub></i>	<i>-NO<sub>2</sub></i>	<i>Nitro</i>	<i>Nitro-</i>	<i>-----</i>
<i>Ethers</i>	<i>R-O-R</i>	<i>-OR</i>	<i>Alkoxy</i>	<i>Alkoxy-</i>	<i>-----</i>
<i>Halogen derivatives</i>	<i>R-Hal</i>	<i>-Hal(-F, -Cl, -Br, -I)</i>	<i>Halogens</i>	<i>Fluoro-, chloro-, bromo-, iodo-</i>	<i>-----</i>

# Structure of Carbon Compounds

- There are three hybridization states and geometries found in organic compounds:
  - $sp^3$  Tetrahedral
  - $sp^2$  Trigonal planar
  - $sp$  Linear



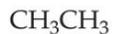
# Hydrocarbons

(contain only H and C)

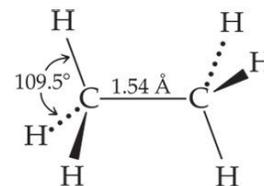
- Four types:

– Alkanes

ALKANE  
Ethane

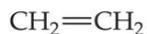


(a)

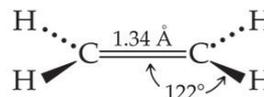


– Alkenes

ALKENE  
Ethylene



(b)

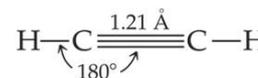


– Alkynes

ALKYNE  
Acetylene

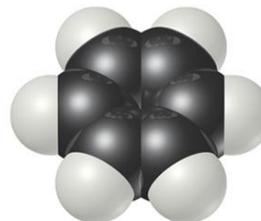


(c)

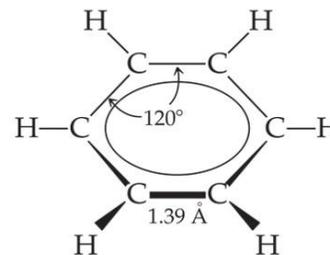


– Aromatic hydrocarbons

AROMATIC  
Benzene

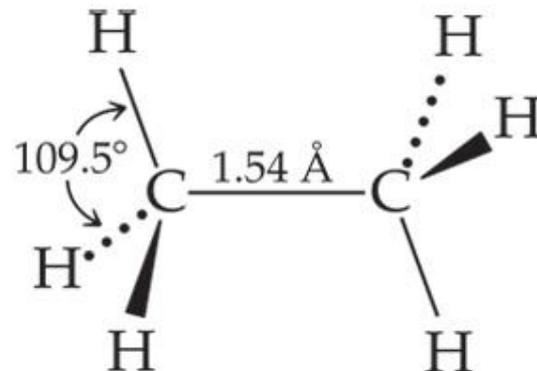


(d)



# Alkanes

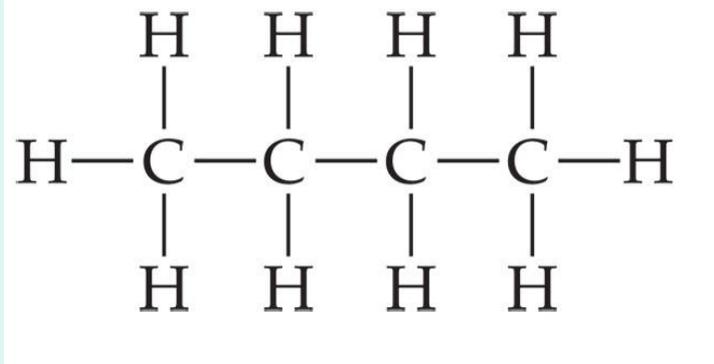
ALKANE  
Ethane



- Only single bonds.
- Saturated hydrocarbons.
  - “Saturated” with hydrogens.

# Formulas

- Lewis structures of alkanes look like this.
- Also called **structural formulas**.
- Often not convenient, though, more often condensed formulas are used



or

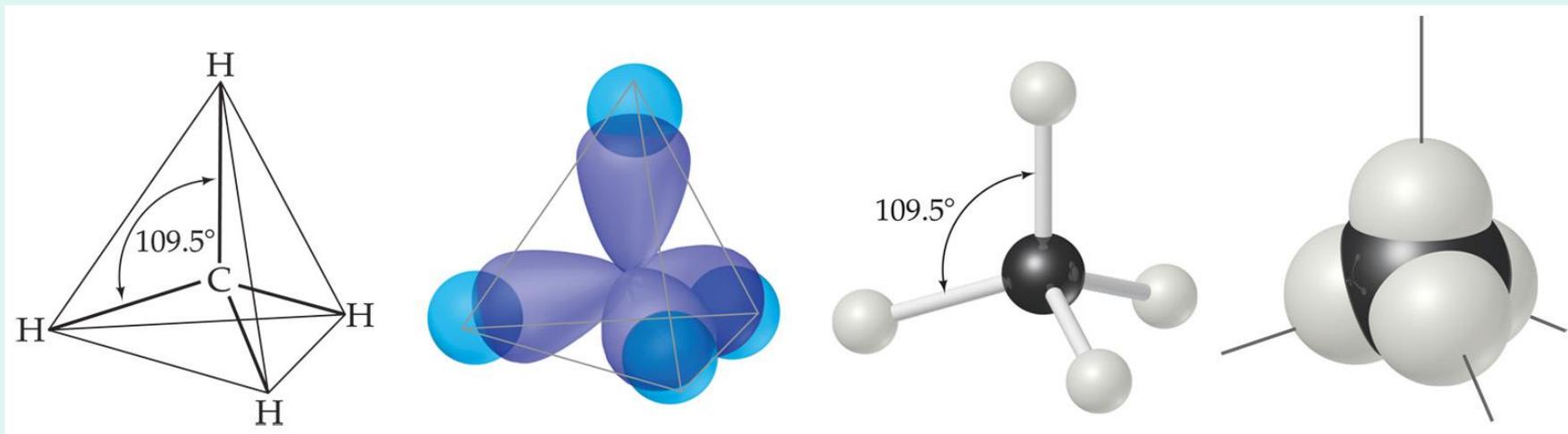


# Properties of Alkanes

Molecular Formula	Condensed Structural Formula	Name	Boiling Point (°C)
CH <sub>4</sub>	CH <sub>4</sub>	Methane	-161
C <sub>2</sub> H <sub>6</sub>	CH <sub>3</sub> CH <sub>3</sub>	Ethane	-89
C <sub>3</sub> H <sub>8</sub>	CH <sub>3</sub> CH <sub>2</sub> CH <sub>3</sub>	Propane	-44
C <sub>4</sub> H <sub>10</sub>	CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub>	Butane	-0.5
C <sub>5</sub> H <sub>12</sub>	CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub>	Pentane	36
C <sub>6</sub> H <sub>14</sub>	CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub>	Hexane	68
C <sub>7</sub> H <sub>16</sub>	CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub>	Heptane	98
C <sub>8</sub> H <sub>18</sub>	CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub>	Octane	125
C <sub>9</sub> H <sub>20</sub>	CH <sub>3</sub> CH <sub>2</sub> CH <sub>3</sub>	Nonane	151
C <sub>10</sub> H <sub>22</sub>	CH <sub>3</sub> CH <sub>2</sub> CH <sub>3</sub>	Decane	174

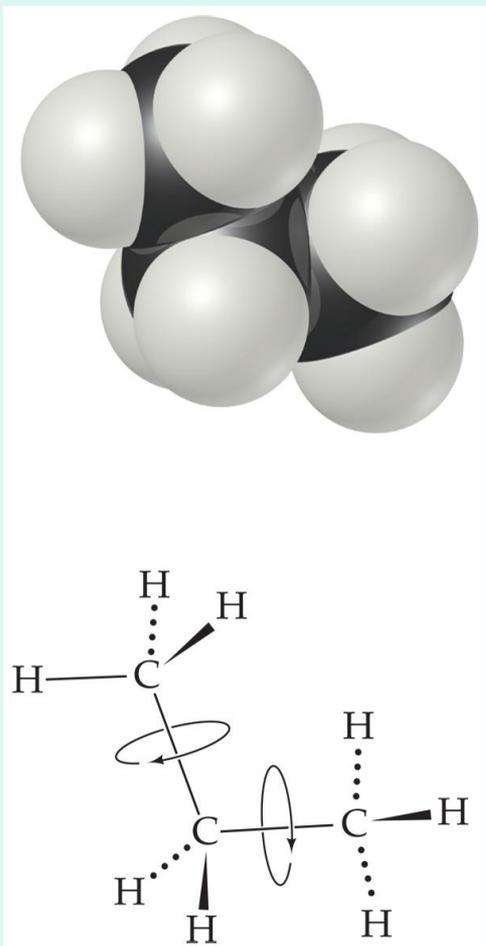
- Only van der Waals force: London force.
- Boiling point increases with length of chain.

# Structure of Alkanes



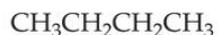
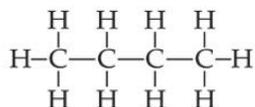
- Carbons in alkanes  $sp^3$  hybrids.
- Tetrahedral geometry.
- $109.5^\circ$  bond angles.

# Structure of Alkanes



- Only  $\sigma$ -bonds in alkanes
- Free rotation about C—C bonds.

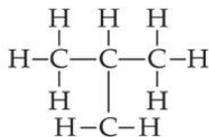
# Structural Isomers



Butane

mp  $-135^\circ\text{C}$

bp  $-0.5^\circ\text{C}$

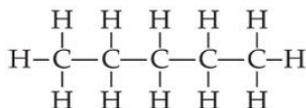


Isobutane

(2-methylpropane)

mp  $-145^\circ\text{C}$

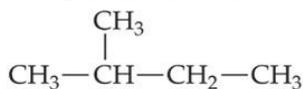
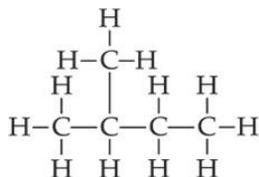
bp  $-10^\circ\text{C}$



Pentane

mp  $-130^\circ\text{C}$

bp  $+36^\circ\text{C}$

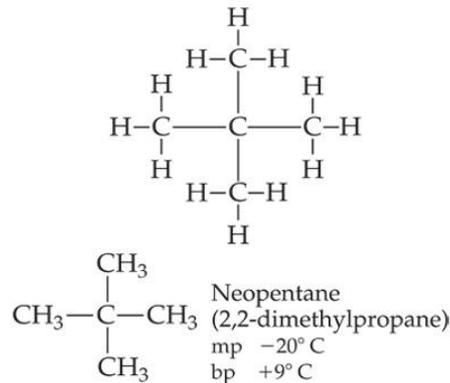
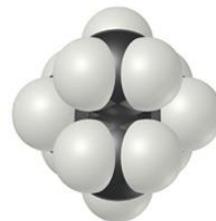


Isopentane

(2-methylbutane)

mp  $-160^\circ\text{C}$

bp  $+28^\circ\text{C}$



Have same molecular formulas, but atoms are bonded in different order.

# NOMENCLATURE

- Common (trivial)
- International. In order to systematize the nomenclature of organic compounds, IUPAC (**International Union of Pure and Applied Chemistry**) system of nomenclature was first introduced in 1947.

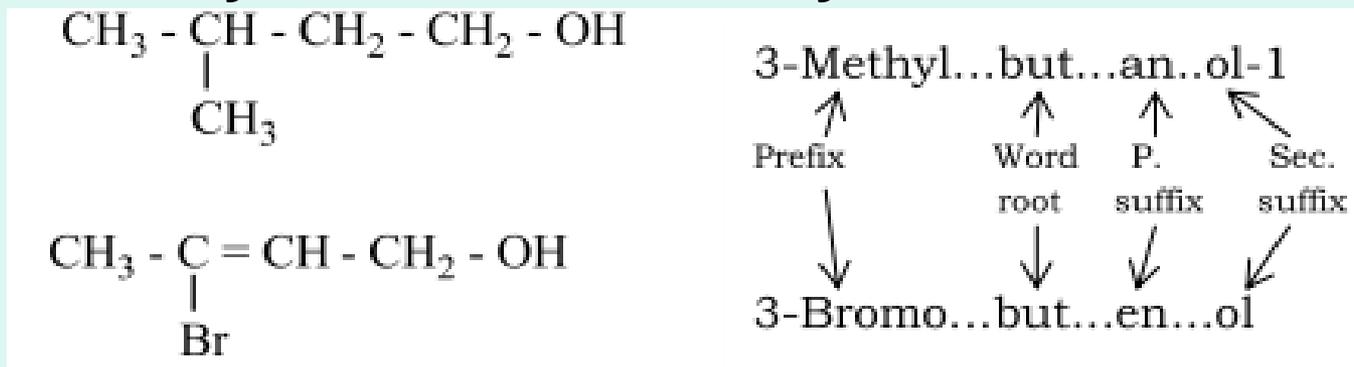
# General rules for IUPAC nomenclature:

The **IUPAC** name of any organic compound essentially consists of three parts:

1. word root;
2. suffix;
3. prefix.

So, a complete IUPAC name of an organic compound consists of the following parts:

- **Secondary prefix + Primary prefix + Word root + Primary suffix + Secondary suffix**

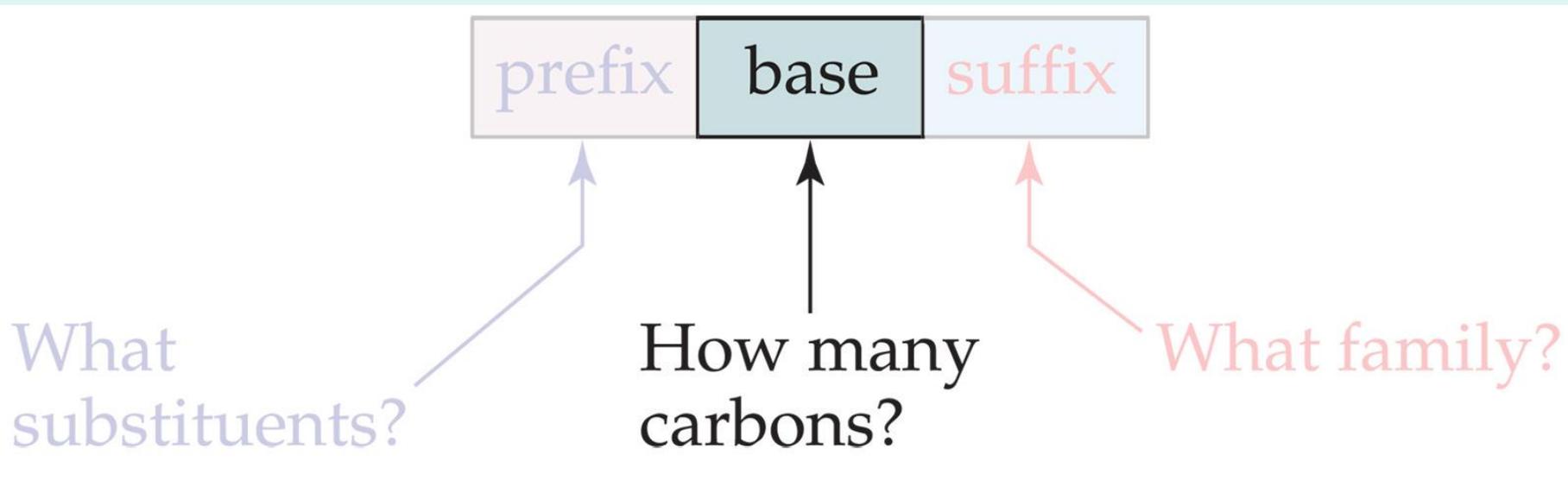


The prefixes, word root and suffixes are arranged as follows while writing the name.

Prefix(es) + Word root + p. suffix + sec. suffix

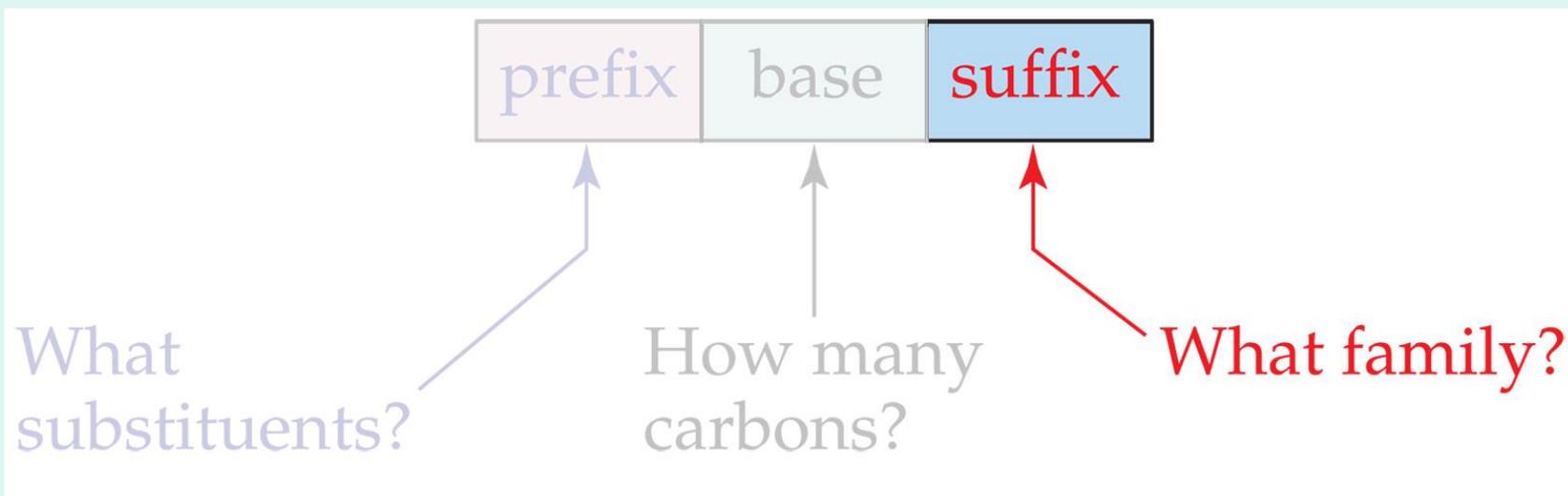
# Organic Nomenclature

- Three parts to a compound name:
  - *Base*: Tells how many carbons are in the longest continuous chain.



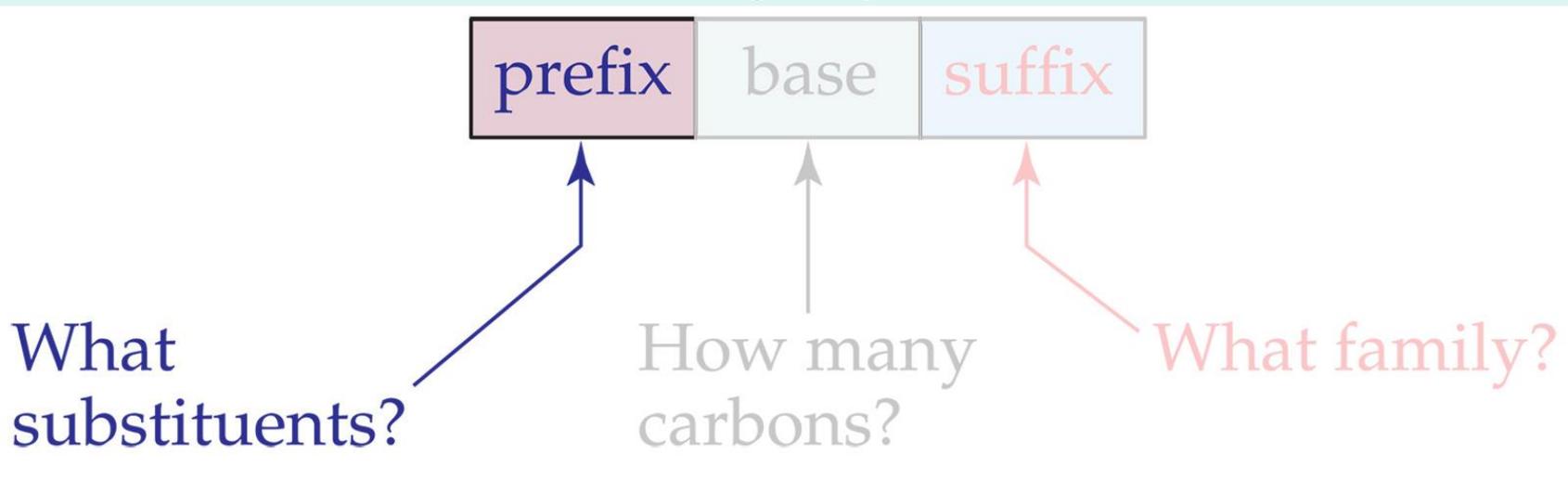
# Organic Nomenclature

- Three parts to a compound name:
  - Base: Tells how many carbons are in the longest continuous chain.
  - Suffix: Tells what type of compound it is.



# Organic Nomenclature

- Three parts to a compound name:
  - Base: Tells how many carbons are in the longest continuous chain.
  - Suffix: Tells what type of compound it is.
  - Prefix: Tells what groups are attached to chain.



# ***PREFIX***

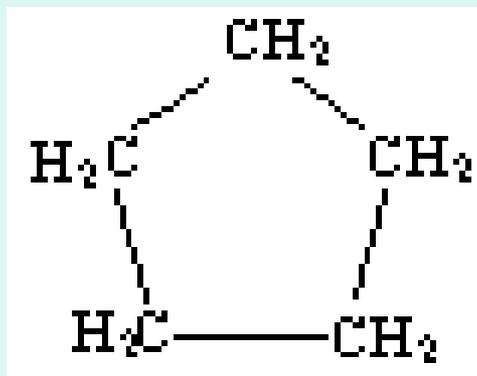
There are two types of prefixes:

**Primary prefix.** A primary prefix is used simply to distinguish cyclic from acyclic compounds.

For example, in case of carbocyclic compounds, a primary prefix, cyclo is used immediately before the word root.

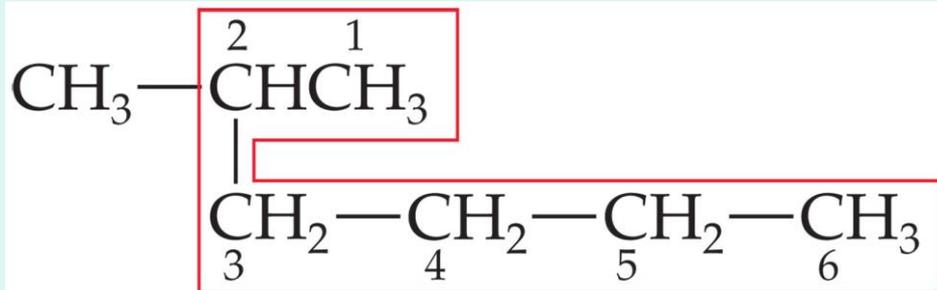
Thus:

- Cyclopentane



**Secondary prefix.** In IUPAC system of nomenclature, certain groups are not considered as functional groups but instead are treated as substituents. These are called secondary prefixes.

Secondary functional group	Prefix	Secondary functional group	Prefix
- X(F, Cl, Br, I)	Halo	- CN	Cyano
- OH	Hydroxy	R - CH = CH -	Alkenyl
- OR	Alkoxy	R - C $\equiv$ C -	Alkynyl
- SH	Mercapto (thio)	- CHO	Formyl or Alkanoyl
- SR	Alkythio	> C = O	Oxo or Keto
- NH <sub>2</sub>	Amino	- COOH	Carboxy
- NHR	Alkylamino	- COOR	Alkoxy carbonyl or carbalkoxy
- NR <sub>2</sub>	Dialkylamino	- COCl	Halocarbonyl or haloalkanoyl



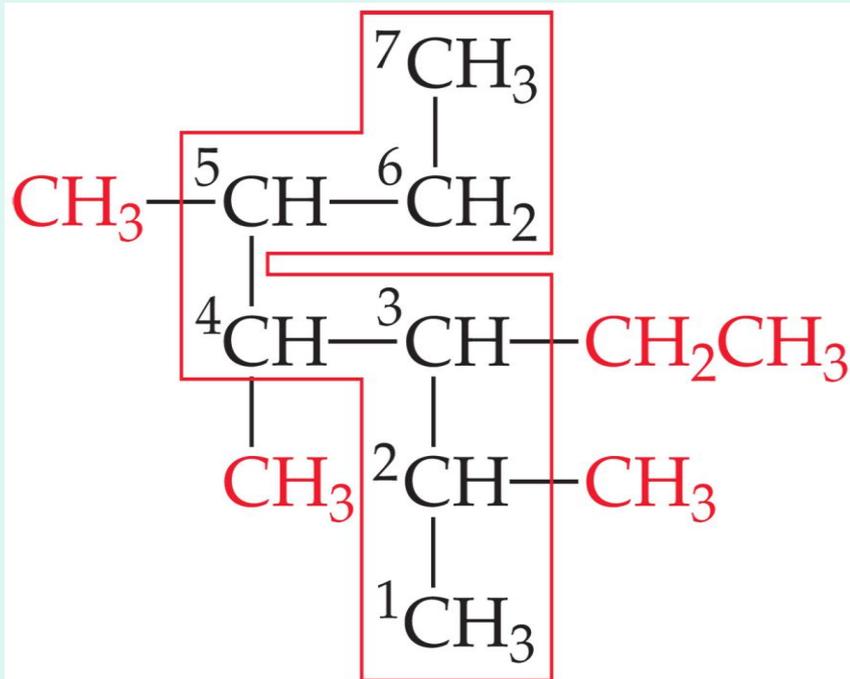
2-Methylhexane

Group	Name
CH <sub>3</sub> —	Methyl
CH <sub>3</sub> CH <sub>2</sub> —	Ethyl
CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> —	Propyl
CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> —	Butyl
$  \begin{array}{c}  \text{CH}_3 \\    \\  \text{HC} - \\    \\  \text{CH}_3  \end{array}  $	Isopropyl
$  \begin{array}{c}  \text{CH}_3 \\    \\  \text{CH}_3 - \text{C} - \\    \\  \text{CH}_3  \end{array}  $	<i>tert</i> -Butyl

# To Name a Compound...

1. Find the longest chain in the molecule.
2. Number the chain from the end nearest the first substituent encountered.
3. List the substituents as a prefix along with the number(s) of the carbon(s) to which they are attached.

# To Name a Compound...



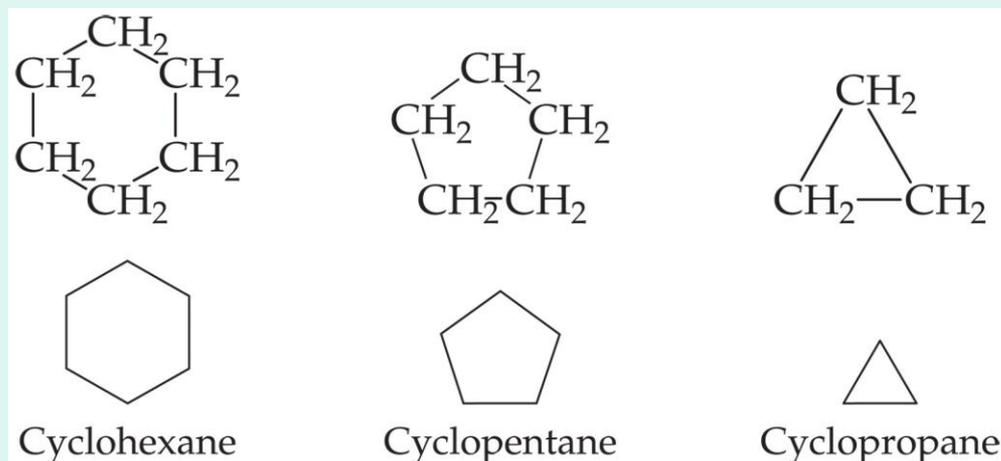
3-Ethyl-2,4,5-trimethylheptane

If there is more than one type of substituent in the molecule, list them alphabetically.

If there is more than one way to make the longest chain, pick the one with the most substituents.

# Cycloalkanes

- Carbon can also form ringed structures.
- Five- and six-membered rings are most stable.
  - Can take on conformation in which angles are very close to tetrahedral angle.
  - Smaller rings are quite strained.

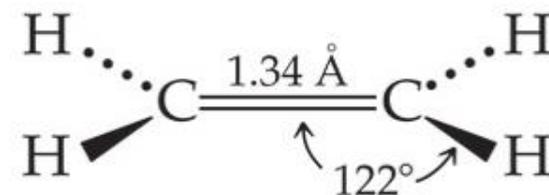
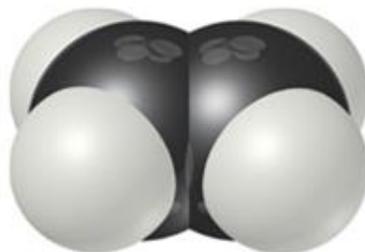
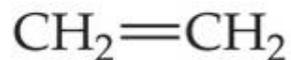


# Reactions of Alkanes

- Rather unreactive due to presence of only C—C and C—H  $\sigma$ -bonds.
- Therefore, great nonpolar solvents.
- General rule of organic chemistry;
- reactivity comes from the functional groups, ie. the part of the molecule that is not a straight alkane.
- different functional groups give rise to different kinds of activity.

# Alkenes

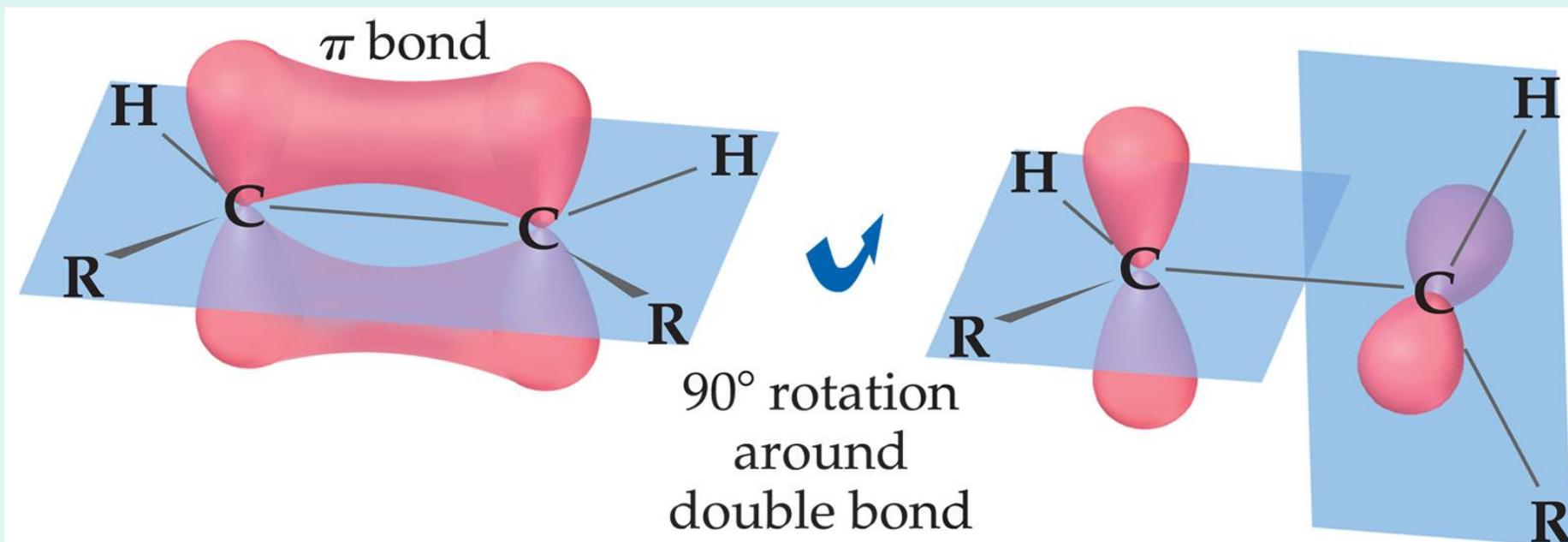
ALKENE  
Ethylene



- Contain at least one carbon–carbon double bond.
- Unsaturated.
- General formula  $\text{C}_n\text{H}_{2n}$ 
  - Have fewer than maximum number of hydrogens.

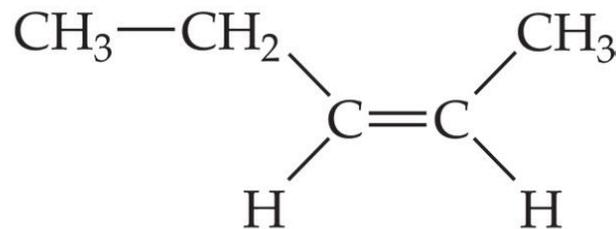
# Structure of Alkenes

- Unlike alkanes, alkenes cannot rotate freely about the double bond.
  - **Side-to-side overlap makes this impossible without breaking  $\pi$ -bond.**

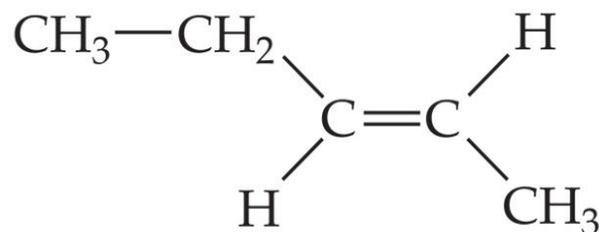


# Structure of Alkenes

This creates **geometric isomers**, which differ from each other in the spatial arrangement of groups about the double bond.

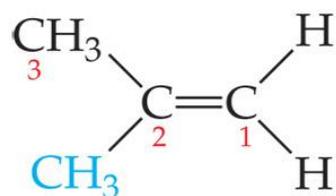


*cis*-2-Pentene

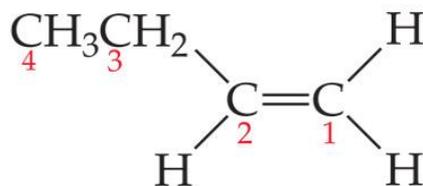


*trans*-2-Pentene

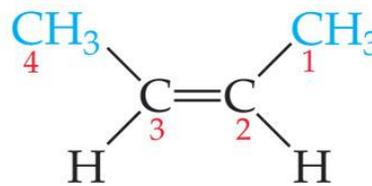
# Properties of Alkenes



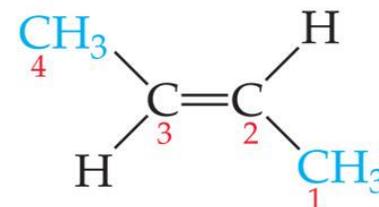
Methylpropene  
bp  $-7^{\circ}\text{C}$



1-Butene  
bp  $-6^{\circ}\text{C}$



*cis*-2-Butene  
bp  $+4^{\circ}\text{C}$



*trans*-2-Butene  
bp  $+1^{\circ}\text{C}$

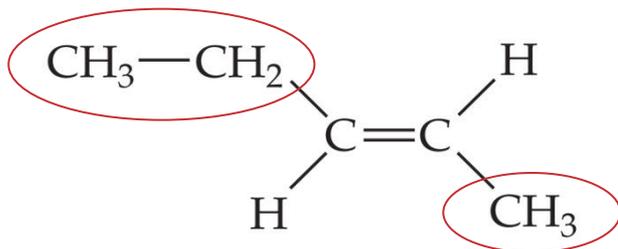
Structure also affects physical properties of alkenes.

# Nomenclature of Alkenes

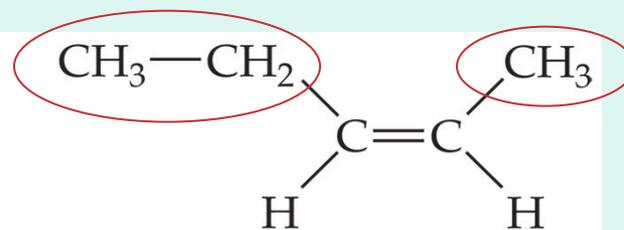
- Chain numbered so double bond gets smallest possible number.
- *cis*- alkenes have carbons in chain on same side of molecule.
- *trans*- alkenes have carbons in chain on opposite side of molecule.



1-Pentene

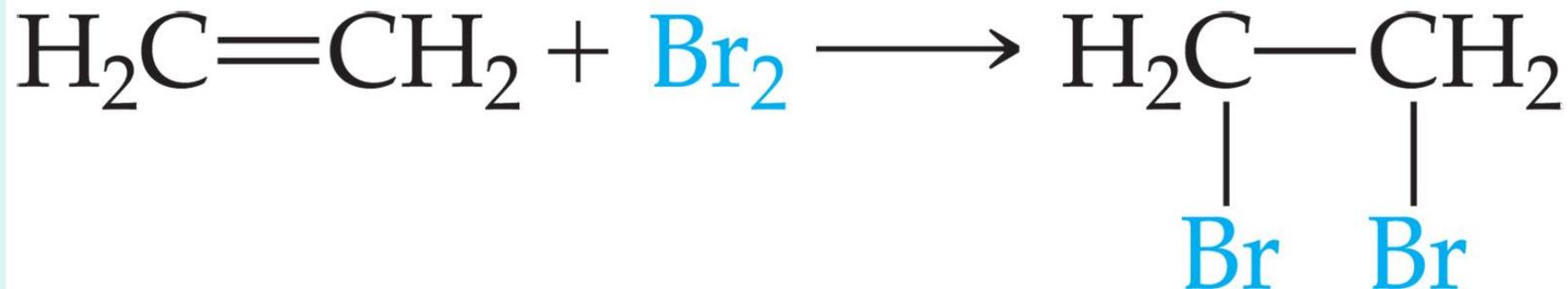


*trans*-2-Pentene



*cis*-2-Pentene

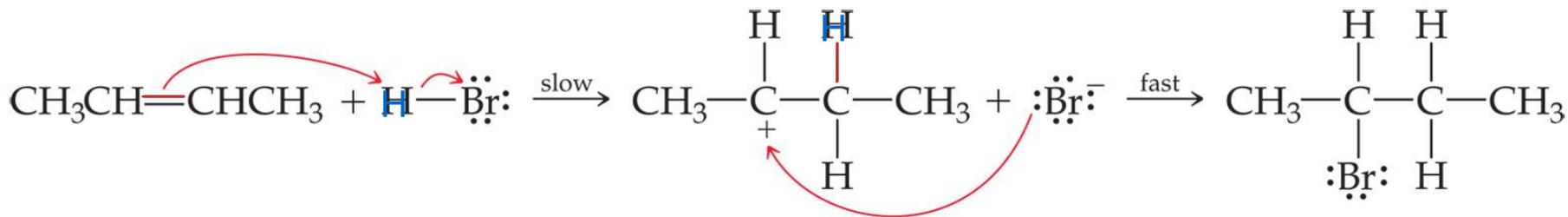
# Reactions of Alkenes



- Addition Reactions

- Two atoms (e.g., bromine) add across the double bond.
- One  $\pi$ -bond and one  $\sigma$ -bond are replaced by two  $\sigma$ -bonds; therefore,  $\Delta H$  is negative.

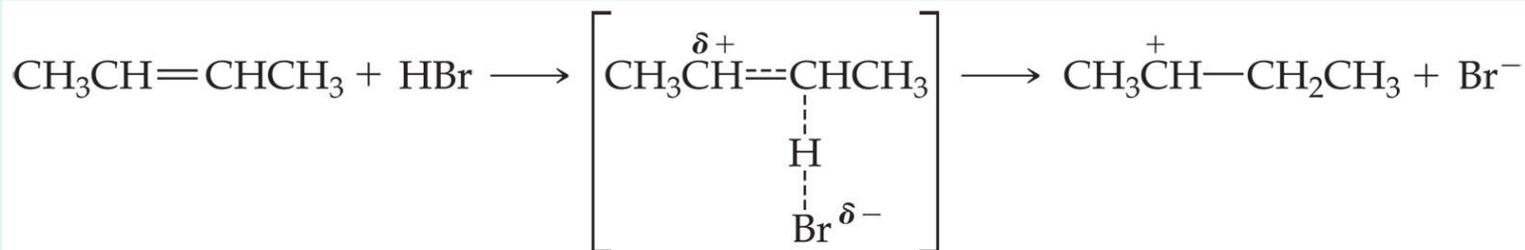
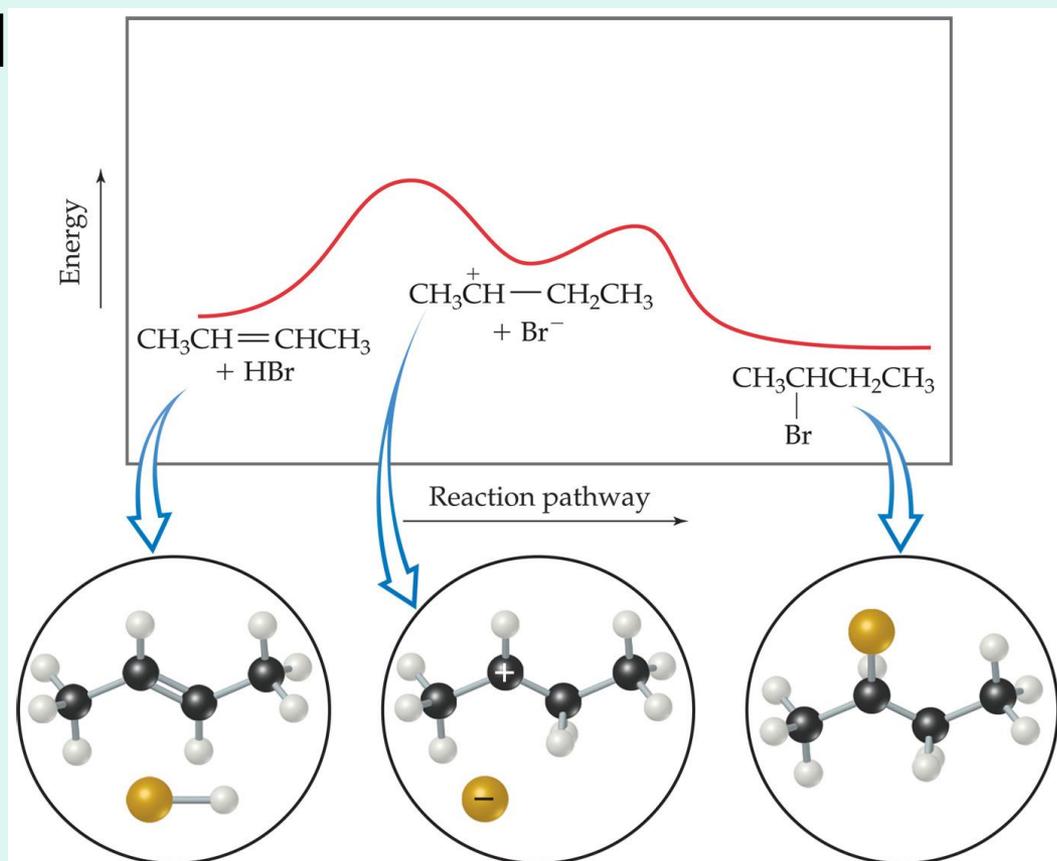
# Mechanism of Addition Reactions



- **The basics of arrow pushing:**
  - Arrow goes from where electrons come from to where they are going.
- **Alkene addition two-step mechanism:**
  - First step is slow, rate-determining step.
  - Second step is fast.

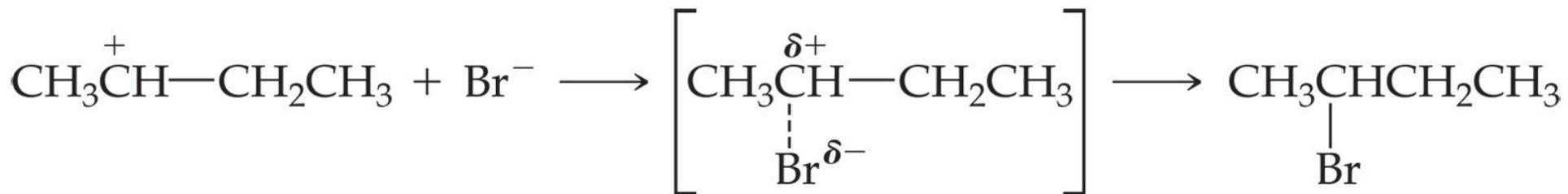
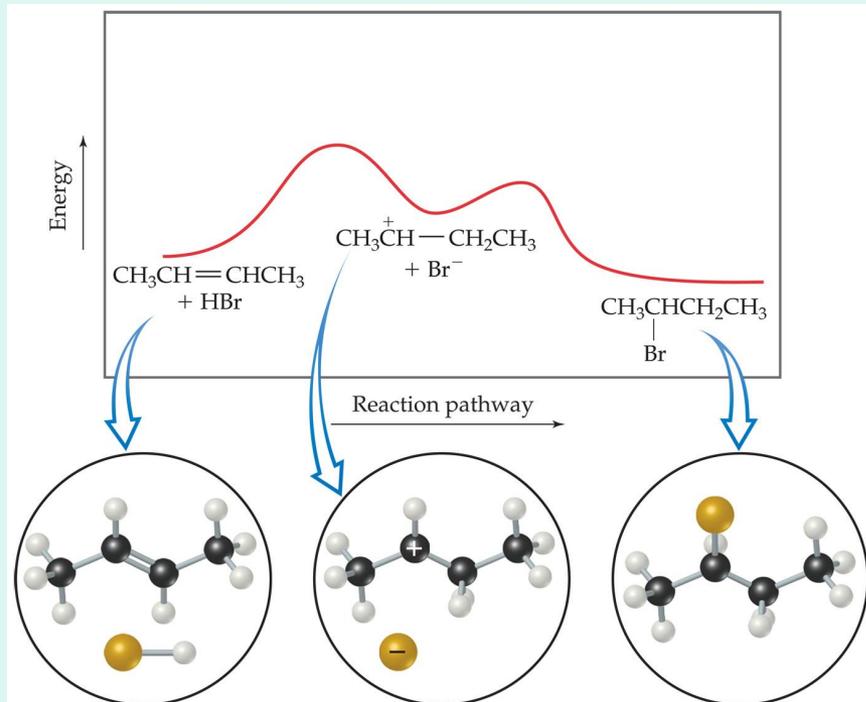
# Mechanism of Addition Reactions

In first step,  $\pi$ -bond breaks and new C—H bond and cation form.



# Mechanism of Addition Reactions

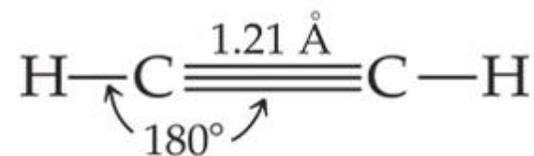
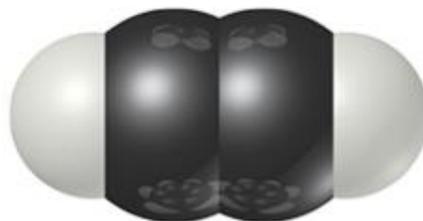
In second step, new bond forms between negative bromide ion and positive carbon.



# Alkynes

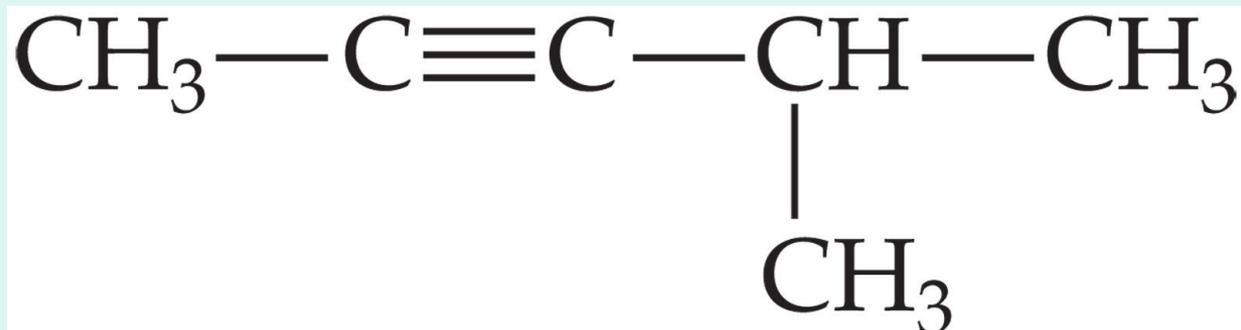
ALKYNE

Acetylene  $\text{CH}\equiv\text{CH}$



- Contain at least one carbon–carbon triple bond.
- Carbons in triple bond *sp*-hybridized and have linear geometry.
- Also unsaturated.

# Nomenclature of Alkynes

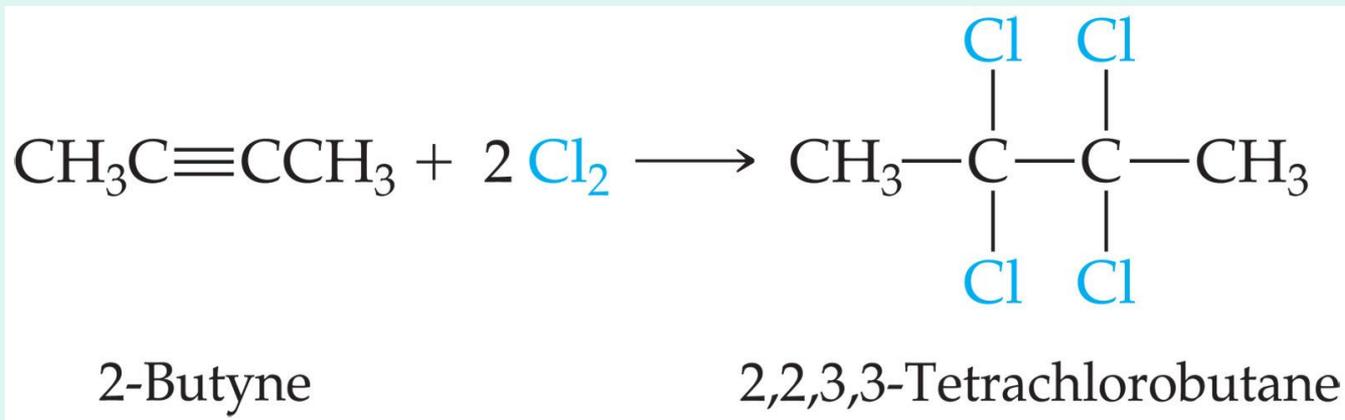


4-methyl-2-pentyne

- Analogous to naming of alkenes.
- Suffix is *-yne* rather than *-ene*.

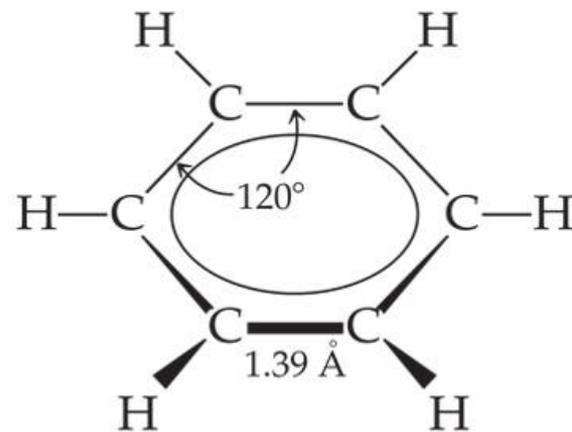
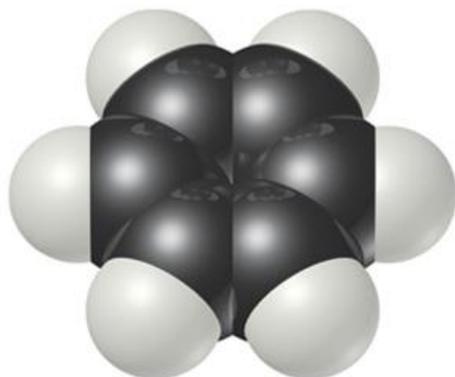
# Reactions of Alkynes

- Undergo many of the same reactions alkenes do.
- As with alkenes, impetus for reaction is replacement of  $\pi$ -bonds with  $\sigma$ -bonds.



# Aromatic Hydrocarbons

AROMATIC  
Benzene  $C_6H_6$



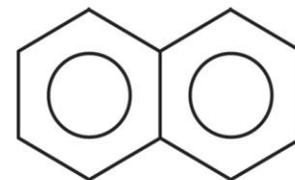
- Cyclic hydrocarbons.
- *p*-Orbital on each atom.
  - Molecule is planar.
- Odd number of electron pairs in  $\pi$ -system.

# Aromatic Nomenclature

Many aromatic hydrocarbons are known by their common names.



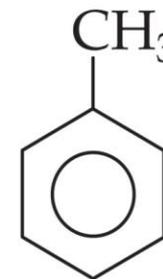
Benzene



Naphthalene

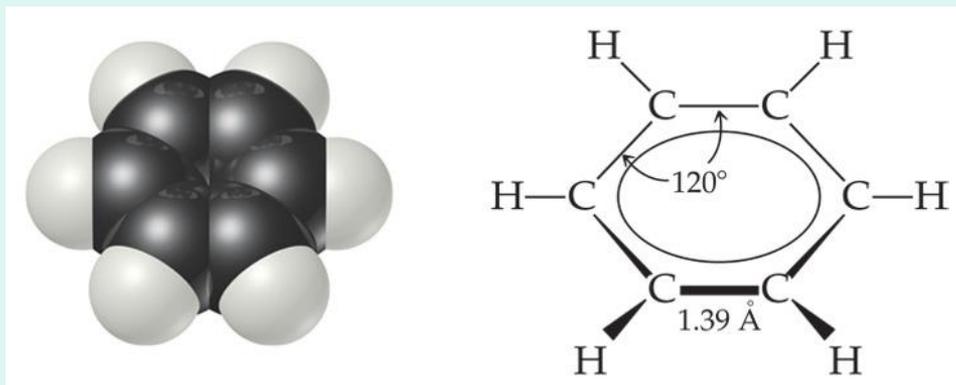


Anthracene



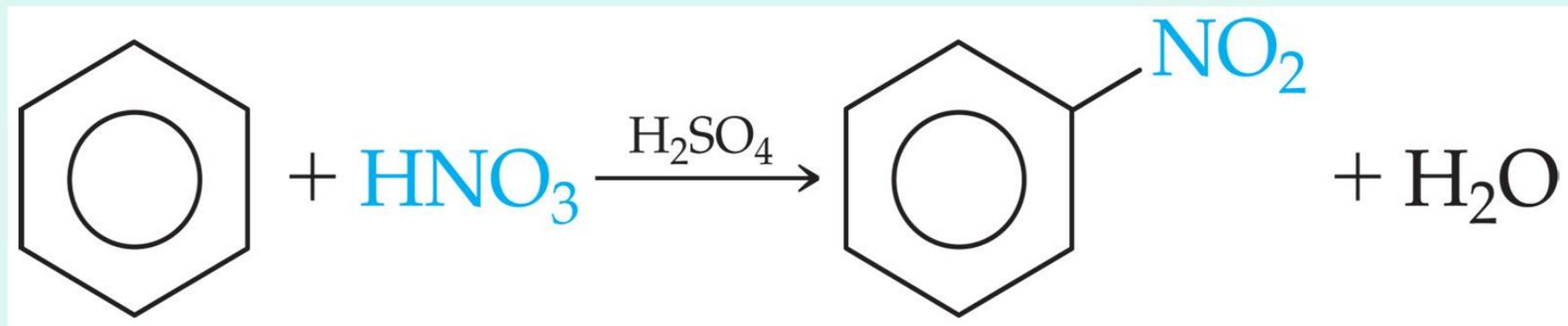
Toluene  
Methylbenzene

# Reactions of Aromatic Compounds



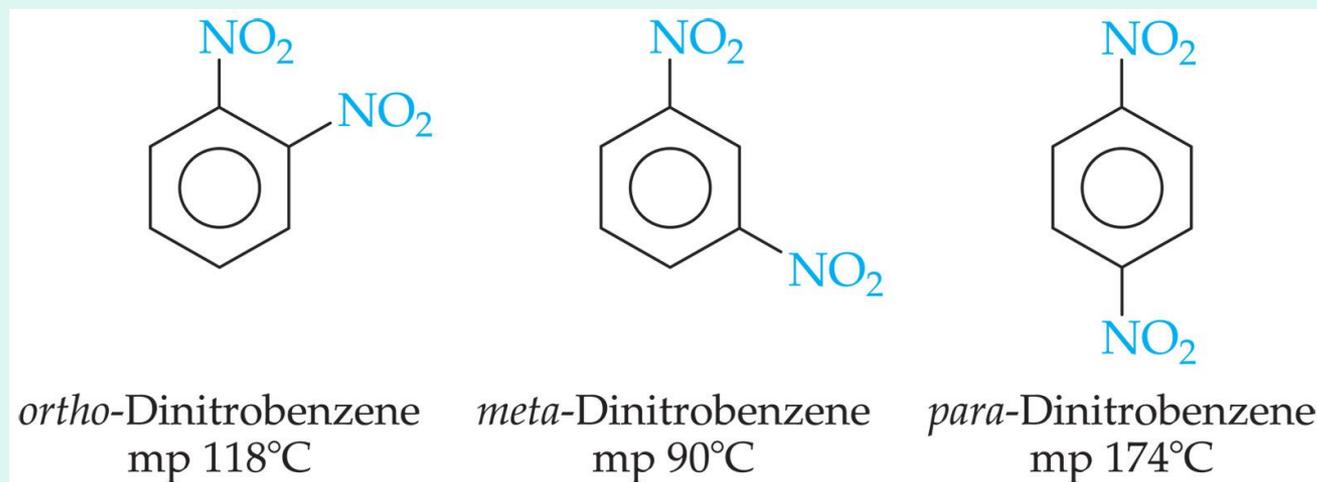
- Unlike in alkenes and alkynes,  $\pi$ -electrons do not sit between two atoms.
- Electrons are delocalized; this stabilizes aromatic compounds.

# Reactions of Aromatic Compounds



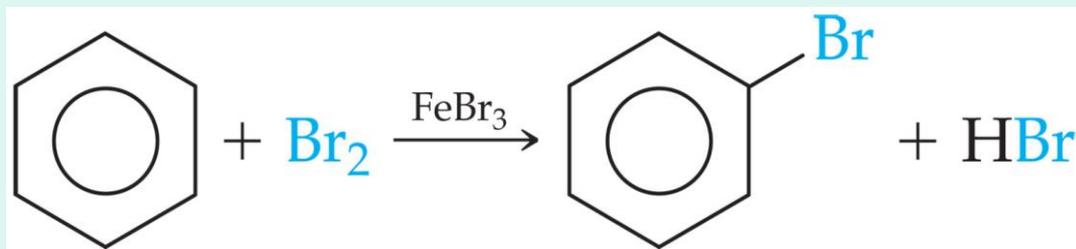
- Due to stabilization, aromatic compounds do not undergo addition reactions; they undergo substitution.
- Hydrogen is replaced by substituent.

# Structure of Aromatic Compounds

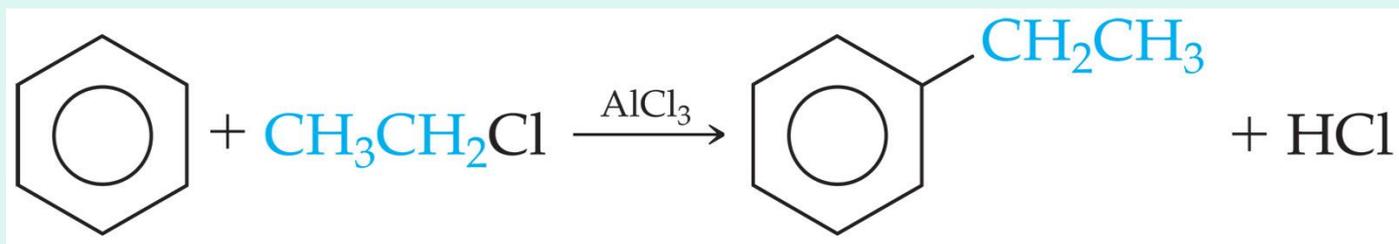


- Two substituents on a benzene ring could have three possible relationships
  - *ortho*-: On adjacent carbons.
  - *meta*-: One carbon between them.
  - *para*-: On opposite sides of ring.

# Reactions of Aromatic Compounds



Halogenation



Friedel-Crafts Reaction

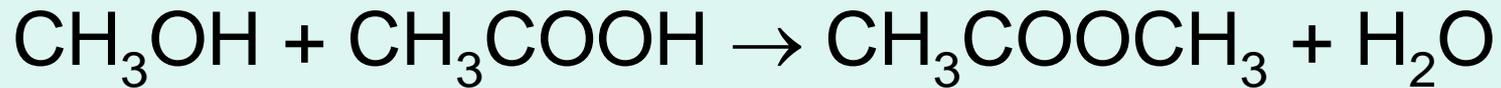
Reactions of aromatic compounds often require a catalyst.

# Types of organic reactions.

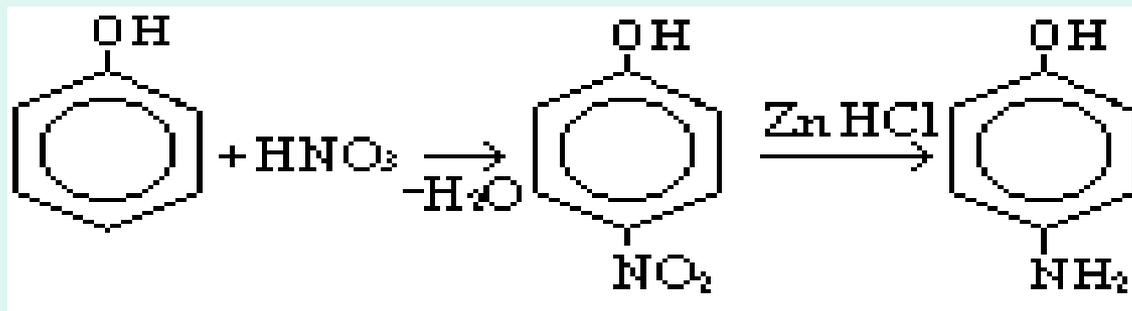
All the organic reactions can be classified into the following types:

- substitution reactions,
- addition reactions,
- elimination reactions,
- rearrangement reactions.

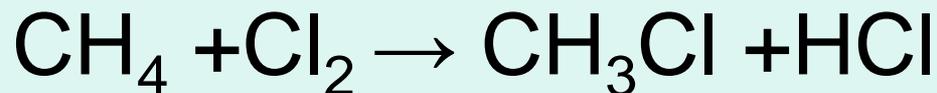
(i) Substitution reactions by nucleophiles are called **nucleophilic substitution reactions**:



(ii) Substitution reactions by electrophiles are called **electrophilic substitution reactions**:



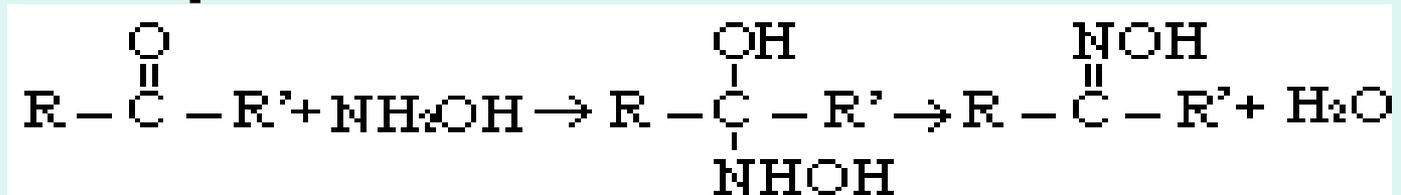
(iii) Substitution reactions by free radicals are called **free radical substitution reactions**:



- Reactions, which involve combination between two reacting molecules to give a single molecule of the product are called addition reactions. Such reactions are typical for compounds containing unsaturated (double or triple) bonds.

**Addition reactions are of the following three types:**

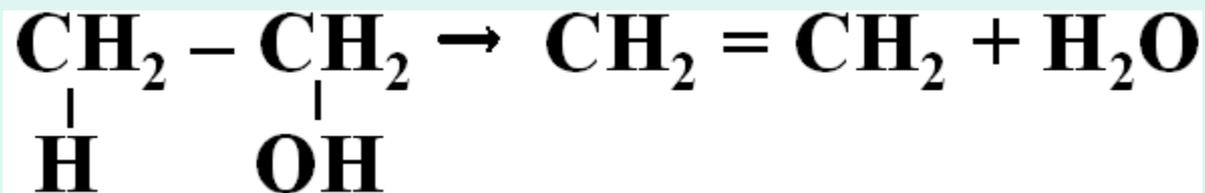
**(i) nucleophilic addition reactions:**



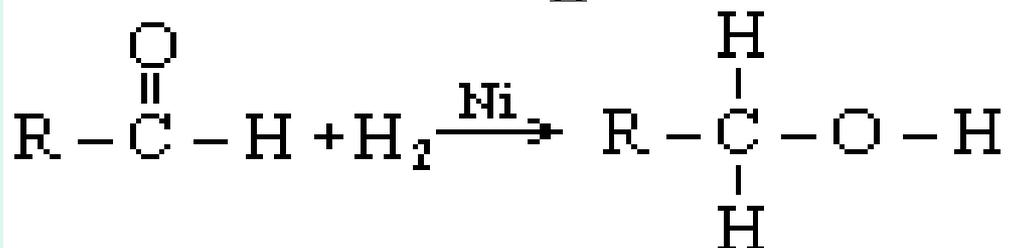
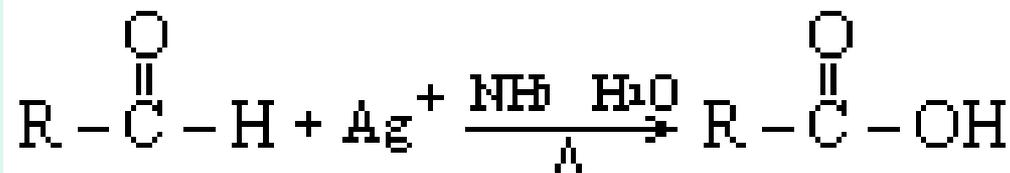
- **electrophilic addition reactions.**

**(i) free radical addition reactions.**

- **Elimination reactions.** An elimination reaction is one that involves the loss of two atoms or groups of atoms leading to the formation of a unsaturated (double or triple) bond:



## Oxidation-reduction reactions



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Thank you for your attention!