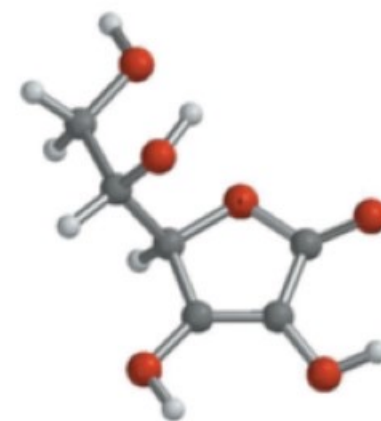

CHEM 240

PRINCIPLES OF ORGANIC CHEMISTRY I

FOR CHEMISTRY' STUDENTS, COLLEGE OF SCIENCE

PRE-REQUISITES COURSE; CHEM 101

CREDIT HOURS; 2 (2+0)



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TOPICS TO BE COVERED

- **Introduction**

(Lectures; 4)

Introduction (Carbon Compounds, Chemical Bonds (ionic, Covalent), Atomic and Molecular orbitals, Hybridization, Polarity and Inductive effect).

- **Alkanes and Cycloalkanes**

(Lectures; 4)

(Alkyl groups, IUPAC nomenclature, Physical properties, Sources of, Synthesis. Reactions (Combustion, Halogenation, Ring opening). Configuration, cyclohexanes.

- **Stereochemistry**

(Lectures; 4)

(Structural isomers and Stereoisomerism, Enantiomers, Diastereomers and Chirality, D and L, The R-S system, Resolution, Molecules with more than one chiral carbon, Reactions of chiral molecules: Inversion, Racemization).

- 1st Midterm Exam**

(Lectures; 1)

TOPICS TO BE COVERED

○ Alkenes and Alkynes

(Lectures 7)

(IUPAC nomenclature, Physical properties, Synthesis (Dehydrohalogenation, from vicinal dihalides, Dehydration of alcohols). Reactions (Acidity of terminal alkynes, Addition reactions (Reduction, Halogenation, Addition of HX - Markovnikov rule, Carbonium ions and their stability, Reaction mechanism), Addition in the presence of peroxides, Hydration, Halohydrin formation), Oxidation of Alkenes (KMnO₄, Peroxides and Ozonolysis).

○ Conjugated Dienes

(Lectures 3)

(Allyl radical and stability, Allyl cation, 1,3-Butadiene - electron delocalization, Resonance and the Stability of conjugated dienes, 1,4-Addition and 1,4-Cycloaddition reactions of diene).

○ Aromatic Compound

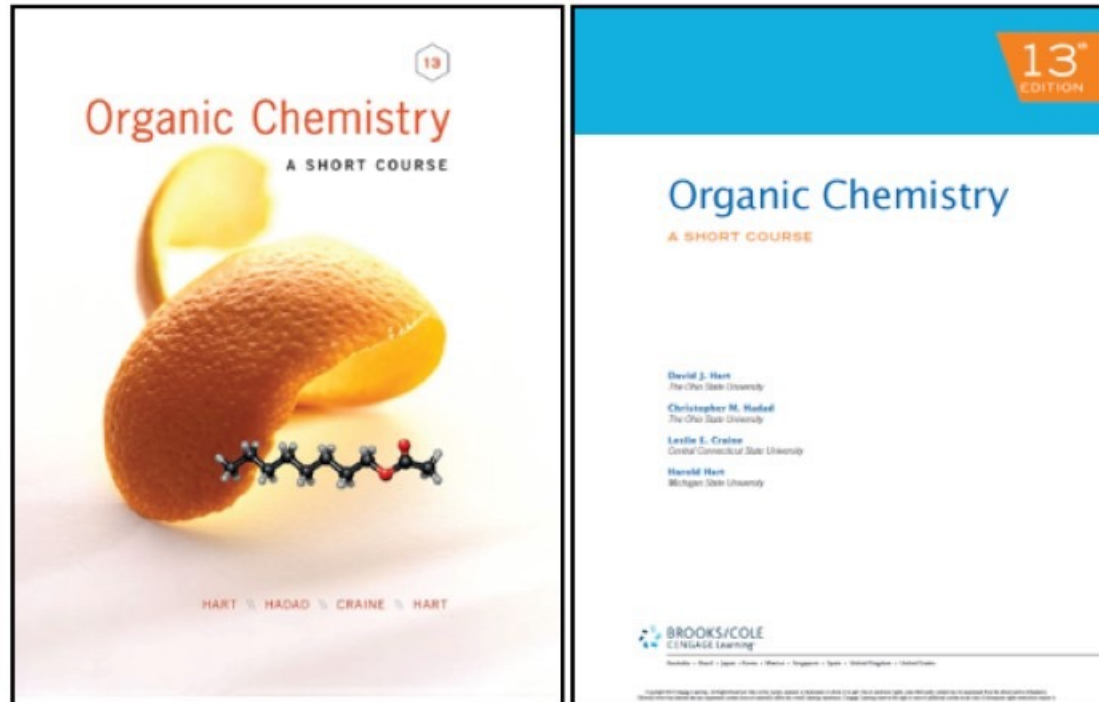
(Lectures 6)

(Aromatic character, Hukel rule, Nomenclature, Electrophilic substitution reactions (Alkylation, Acylation, Halogenation, Sulphonation, Nitration; reaction mechanism), Side chain halogenation and oxidation, Reactivity and Orientation in substituted benzene, Polynuclear aromatics).

REFERENCES

- ❑ **Organic chemistry: A short course by I Harold Hart, David J. Hart and Leslie E. Craine, Houghton Mifflin Company, USA, 2012.**
- ❑ **Elements of Organic Chemistry (second edition) is written by Isaak Zimmerman and Henry Zimmerman and published by Macmillan Publishing Co., Inc. New York in 1983.**

❑ أسس الكيمياء العضوية - أ.د./ سالم بن سليم الذياب - الناشر: مؤسسة نافثة



SCHEDULE OF ASSESSMENT TASKS DURING THE SEMESTER

Assessment task	Week Due	Proportion of Total Assessment
1. Home work & Projects	All weeks	10 %
2. Quizzes	5, 10	10 %
4. 1 st Midterm exam	7	20 %
5. 2 nd Midterm exam	13	20 %
6. Final exam	16	40 %

COURSE OBJECTIVES

Upon successful completion of this course, the student will be able to:

- **Name** organic compounds using IUPAC naming system, their occurrence in nature, physical properties.
- **Identify, classify and understand** physical and chemical properties of the major functional groups.
- **Understand** the basic organic reaction for preparation of common functional groups.
- **Understand** the reaction of functional groups and families of organic compounds.
- The practical uses of organic compounds as drugs, food additives, pesticides, plastics, and other products, as well as their occurrence in nature

COURSE LEARNING OUTCOMES

1. Knowledge

- 1.1 To recognize structures of organic compounds.
- 1.2 To memorize naming, constitutional isomer, physical properties and reactions.

2.0 Skills

- 2.1 To differentiate between ionic and covalent bonds in chemical compounds.
- 2.2 To recognize the IUPAC nomenclature of organic chemical compounds.
- 2.3 To differentiate between aromatic and non-aromatic compounds according to Hukel's rule.
- 2.4 To predict the type of nucleophilic or electrophilic substitutions in organic reactions.

3.0 Competence

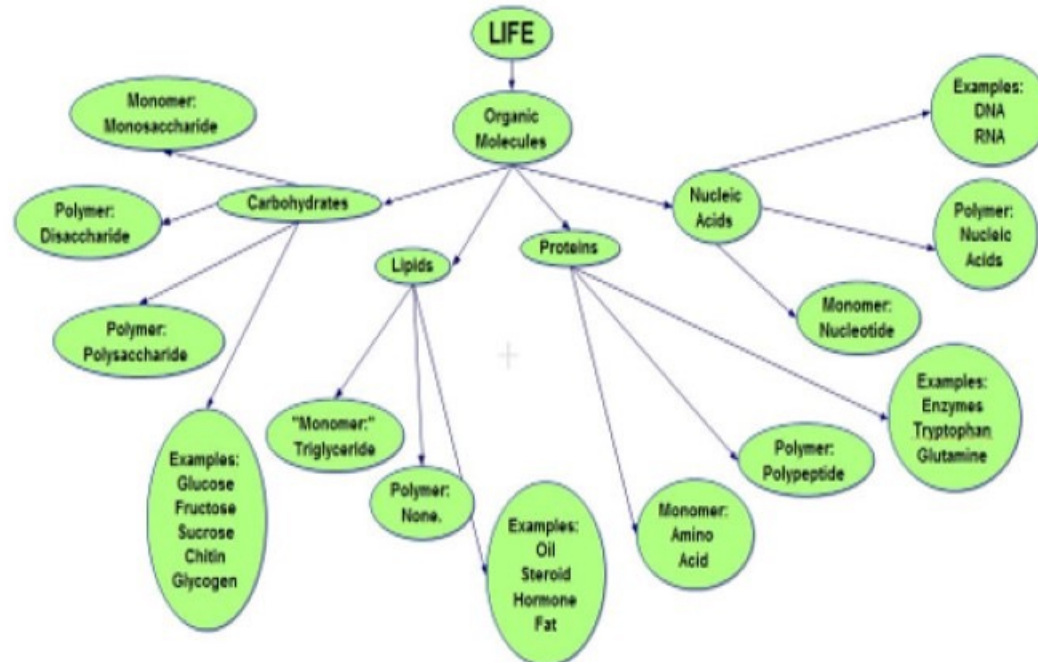
- 3.1 Work independently and as a part of a team during class session.
- 4.1 Utilizing university electronic resources of learning.

CHAPTER 1

INTRODUCTION

ORGANIC CHEMISTRY: DEFINITION

- The term **organic** suggests that this branch of chemistry has something to do with *organisms*, or living things.
- Originally, organic chemistry did deal only with substances obtained from living matter.
- In particular, most compounds in living matter are made up of the same few elements: **carbon, hydrogen, oxygen, nitrogen, and sometimes sulfur, phosphorus**, and a few others.



ORGANIC CHEMISTRY: DEFINITION

What Is Organic Chemistry?



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

*This definition broadens the scope of the subject to include **not only compounds from nature but also synthetic compounds** - compounds invented by organic chemists and prepared in their laboratories.*

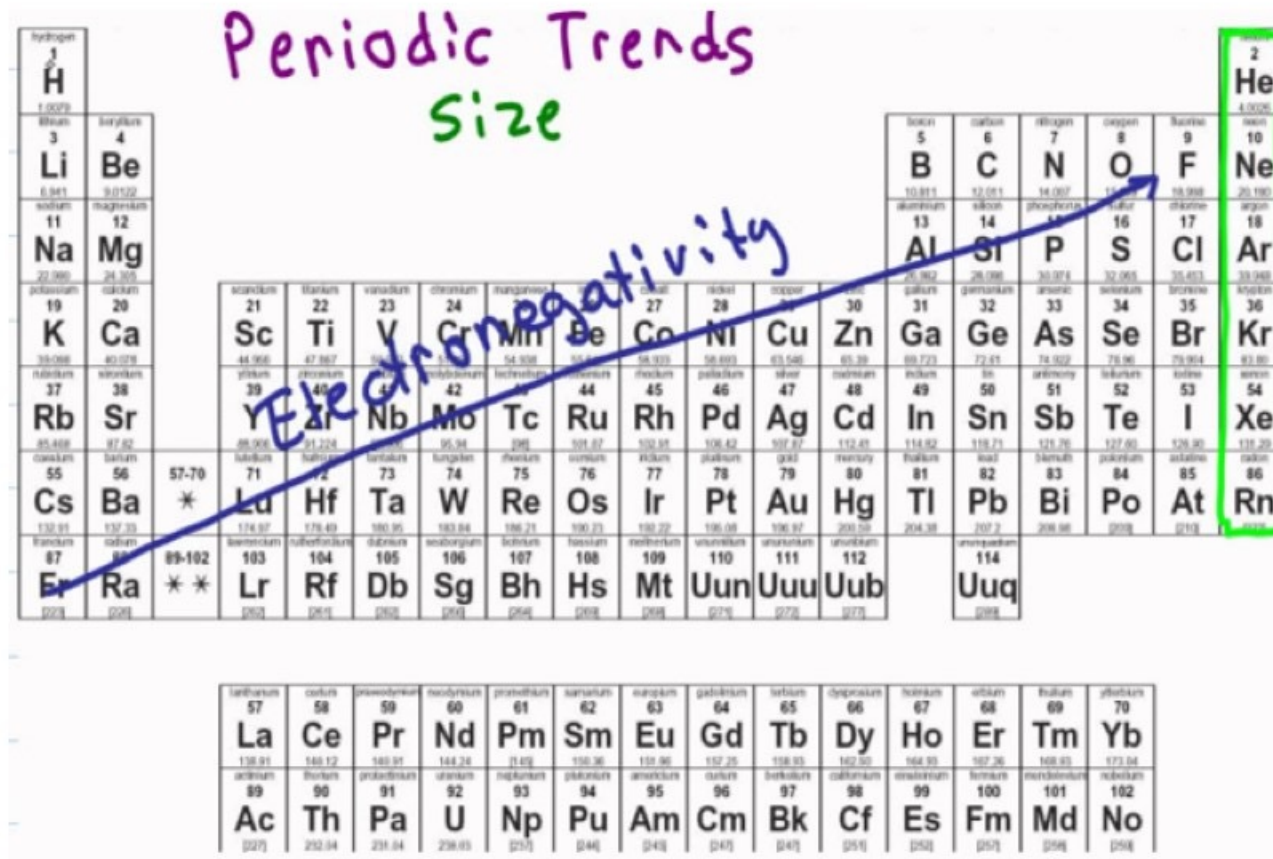
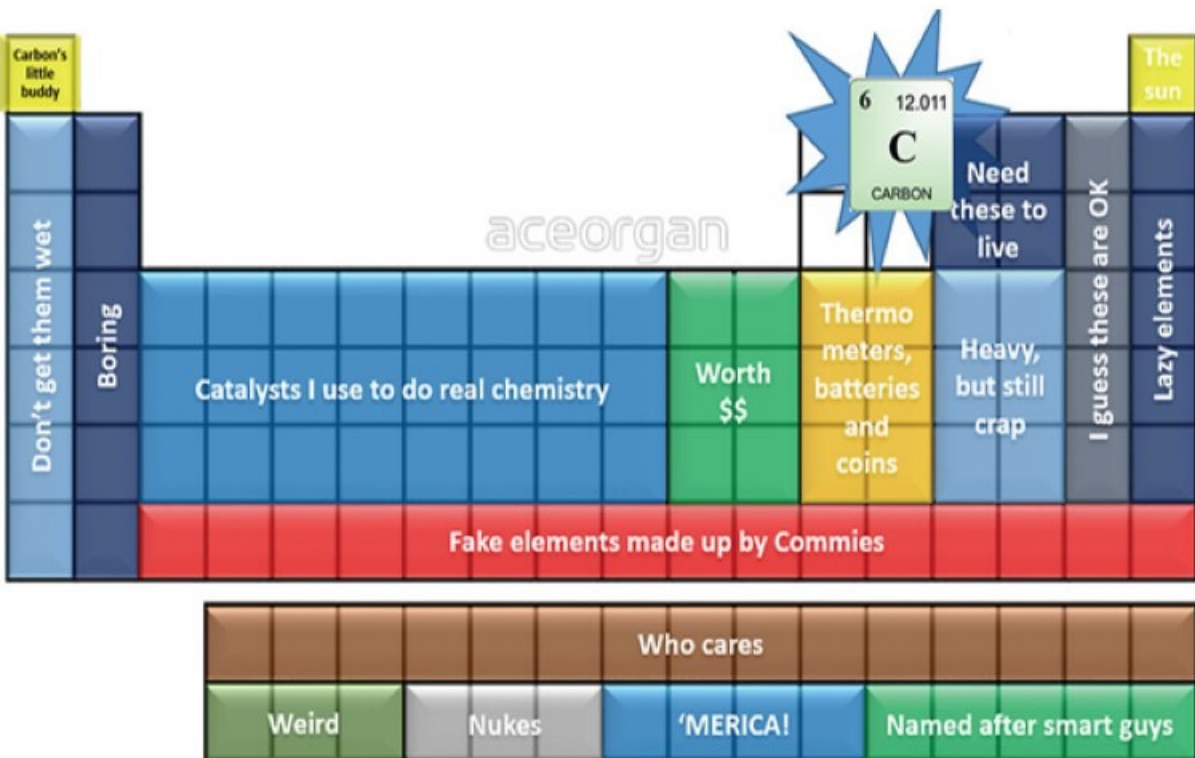
Examples:

The clothes, the petroleum products, the paper, rubber, wood, plastics, paint, cosmetics, insecticides and drugs.

ORGANIC CHEMISTRY: DEFINITION

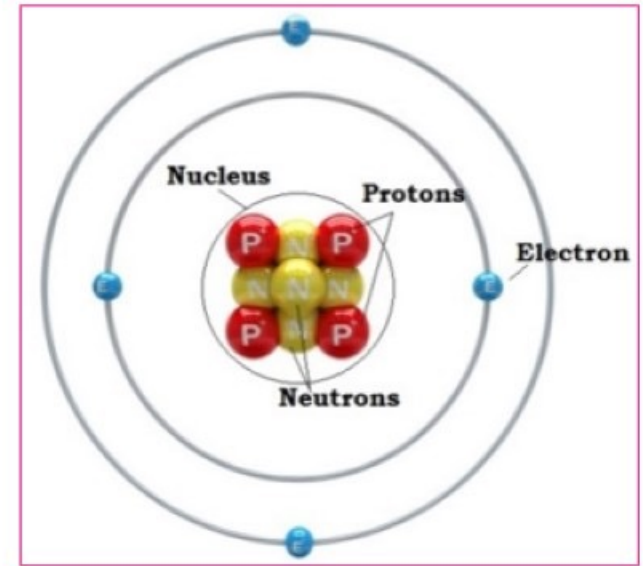
The Periodic Table:

As seen by an organic chemist



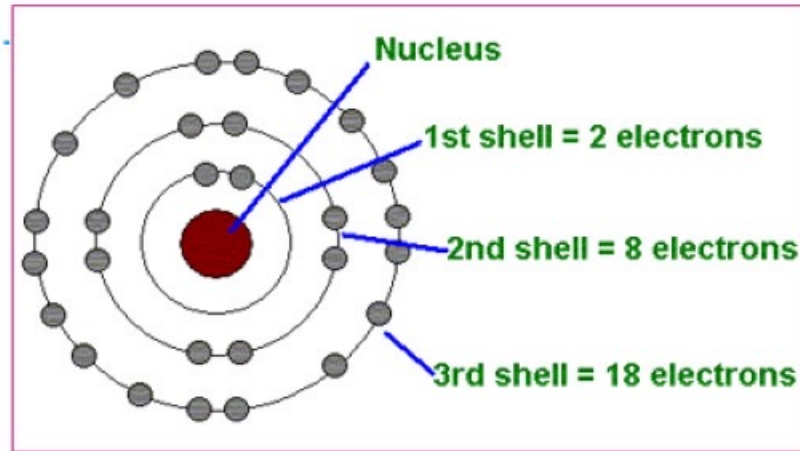
ATOMIC STRUCTURE

- **Atoms** consist of three main particles: neutrons (have no charge), protons (positively charged) and electrons (negatively charged).
 - **Neutrons** and **protons** are found in the nucleus.
 - **Electrons** are distributed around the nucleus in successive *shells* (*principal energy levels*).
- The **atomic number** of an element is equal to *the number of protons in its nucleus* (and to *the number of electrons around the nucleus in a neutral atom*).
- The **atomic weight** is approximately equal to the *sum of the number of protons and the number of neutrons in the nucleus*.

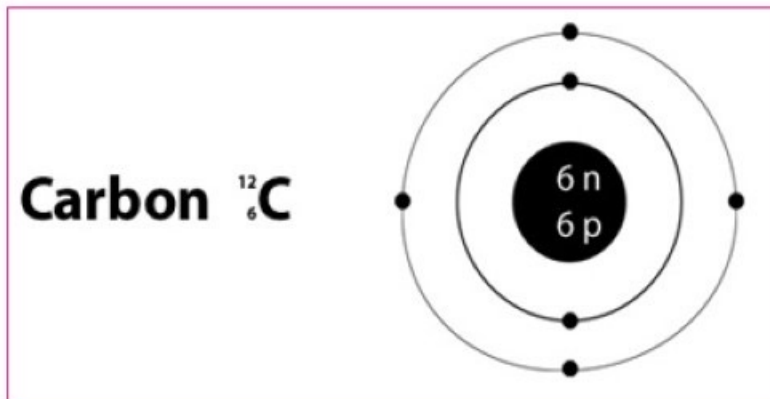
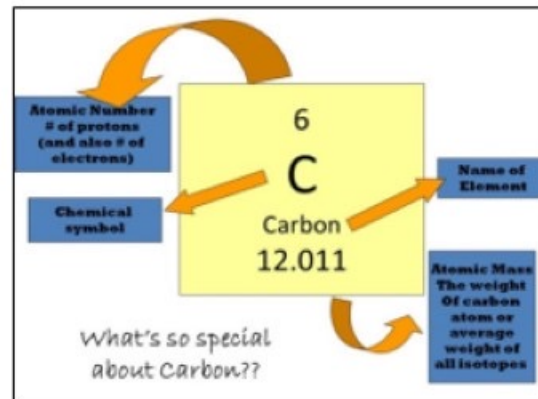


ATOMIC STRUCTURE

- **The energy levels** are designated by capital letters (K, L, M, N, ..).
- The maximum capacity of a shell = $2n^2$ electrons.
 n = number of the energy level.



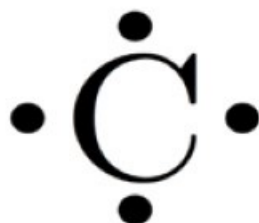
- **Example**, the element **carbon** (atomic number 6)



ATOMIC STRUCTURE

○ Electron-dot structures

- The symbol of the element represents the core of the atom and the **valance electrons** are shown as dots around the symbol.



- **Valance Electrons** are those electrons located in the outermost energy level (the valance shell).

Valences of Common Elements						
Element	H·	·C·	·N:	·O:	:F:	:Cl:
Valence	1	4	3	2	1	1

TYPES OF CHEMICAL BONDS

- **In 1916 G.N. Lewis** pointed out that:

The noble gases were stable elements and he ascribed their lack of reactivity to their having their valence shells filled with electrons.

- 2 electrons in case of helium.
- 8 electrons for the other noble gases.

- **Types of Chemical Bonds**

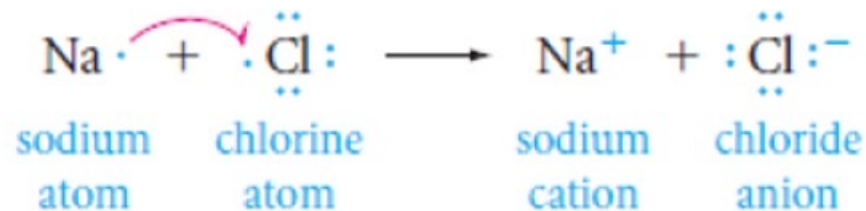
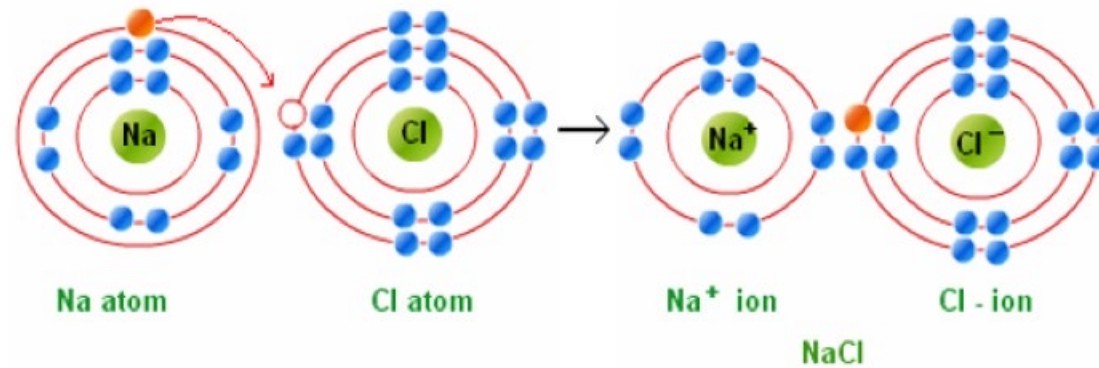
A) Ionic Bonding

B) Covalent Bonding

TYPES OF CHEMICAL BONDS

A) IONIC BOND

- **Ionic bonds** are formed by the transfer of one or more valence electrons from one atom to another.
 - The atom that **gives up electrons** becomes positively charged, a **cation**.
 - The atom that **receives electrons** becomes negatively charged, an **anion**.



Ionic Bond is the electrostatic force of attraction between oppositely charged ions.

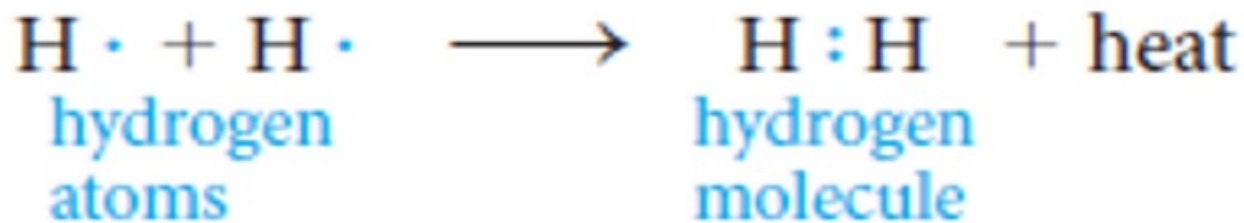
- The majority of ionic compounds are **inorganic substances**.

B) COVALENT BOND

- A **covalent bond** is formed when two atoms share one or more electron pairs.

Elements that are neither strongly electronegative nor strongly electropositive, or that have similar electronegativities, tend to form bonds by sharing electron pairs rather than completely transferring electrons.

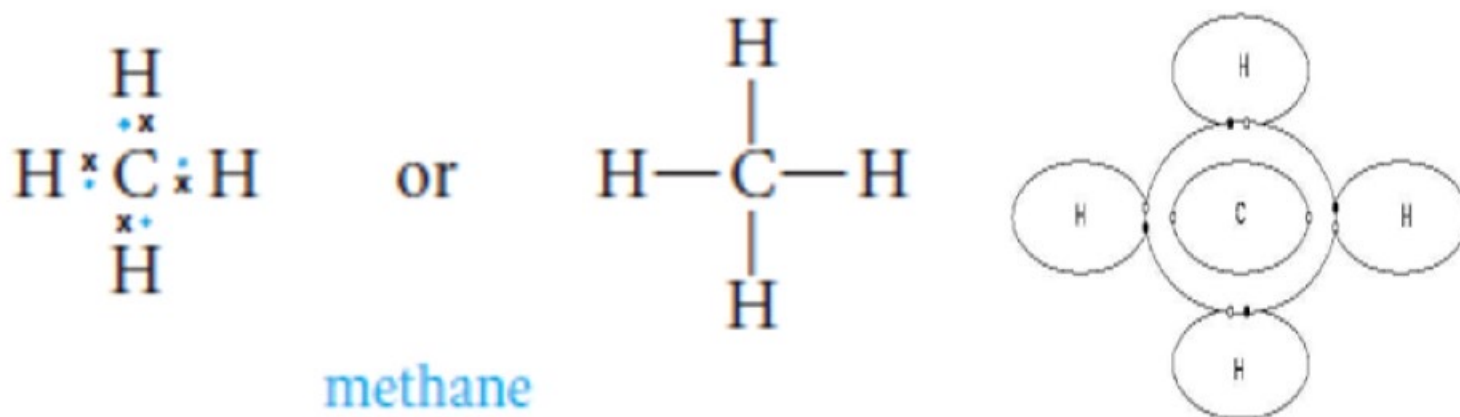
- A **molecule** consists of two or more atoms joined by covalent bonds.
 - When the **two atoms are identical or have equal electronegativities**, the electron pairs are shared **equally**.



TYPES OF CHEMICAL BONDS

B) COVALENT BOND

- **For example**, carbon combines with four hydrogen atoms (each of which supplies one valence electron) by sharing four electron pairs. The substance formed is known as **methane**.

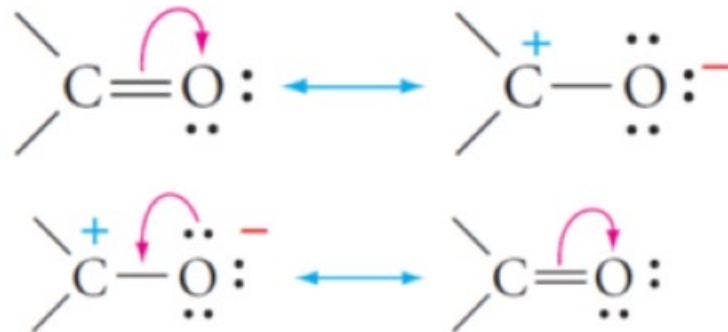
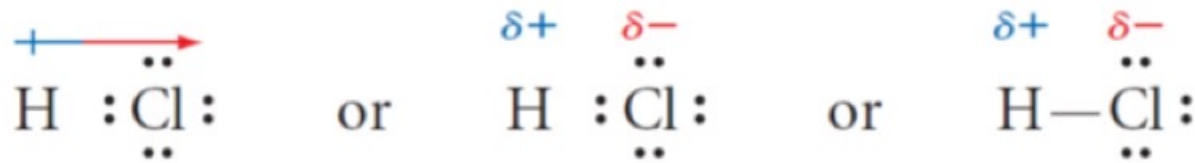


B) COVALENT BOND

1) POLAR COVALENT BONDS

- A **polar covalent bond** is a covalent bond in which the electron pair is not shared equally between the two atoms.

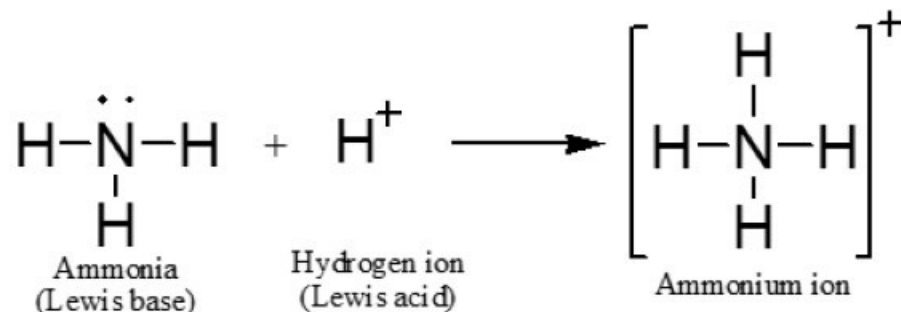
The more electronegative atom assumes a partial negative charge and the less electronegative atom assumes a partial positive charge.



B) COVALENT BOND

2) COORDINATE COVALENT BONDS

- There are molecules in which one atom supplies both electrons to another atom in the formation of a covalent bond.
- For example;

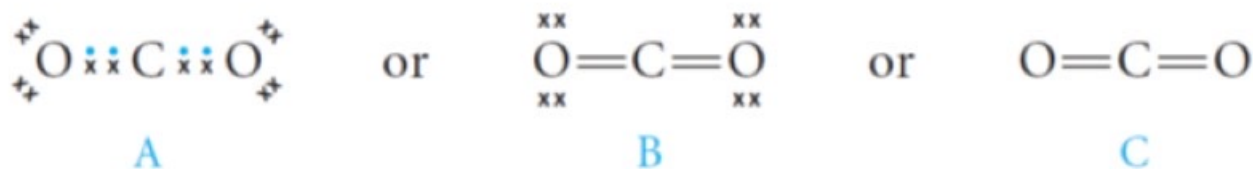


- **Lewis base;** *The species that furnishes the electron pair to form a coordinate covalent bond.*
- **Lewis acid;** *The species that accepts the electron pair to complete its valance shell.*

MULTIPLE COVALENT BONDS

- In a **double bond**, two electron pairs are shared between two atoms.

Example; Carbon dioxide, CO₂

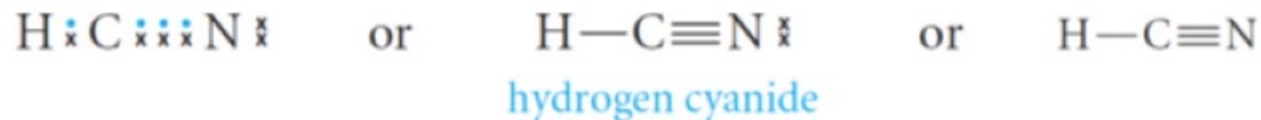


Structure A, the **dots** represent the electrons from carbon, and the **x's** are the electrons from the oxygens.

Structure B shows the **bonds'** and oxygens' **unshared electrons** (nonbonding electrons).

Structure C shows only the covalent **bonds**.

- In a **triple bond**, three electron pairs are shared between two atoms.



QUIZZES

PROBLEM 1.1 Write an equation for the reaction of sodium atoms (Na) with chlorine atoms (Cl).

PROBLEM 1.2 Write an equation for the formation of a fluorine molecule from two fluorine atoms.

PROBLEM 1.3 Draw the structures for dichloromethane (also called methylene chloride), CH_2Cl_2 , and trichloromethane (chloroform), CHCl_3 .

PROBLEM 1.4 Draw the structure of the refrigerant dichlorodifluoromethane, CCl_2F_2 (CFC-12), and indicate the polarity of the bonds. (The C atom is the central atom.)

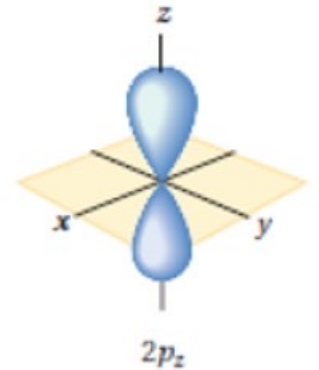
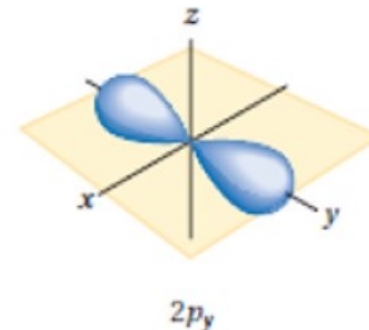
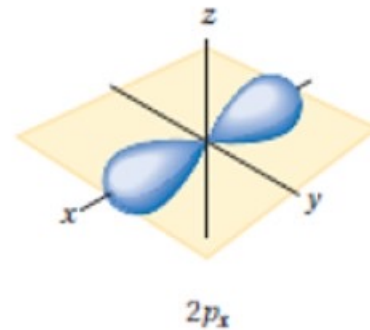
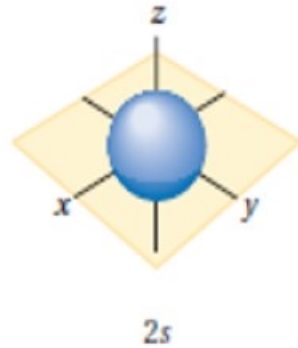
PROBLEM 1.5 Draw the formula for methanol, CH_3OH , and (where appropriate) indicate the bond polarity with an arrow, $\text{+} \longrightarrow \text{-}$. (The C atom is bonded to three H atoms and the O atom.)

PROBLEM 1.6 Draw an electron-dot structure for carbon monoxide, CO.

PROBLEM 1.7 Draw three different structures that have the formula C_4H_8 and have one carbon-carbon double bond.

ATOMIC ORBITALS

- An **atomic orbital** represents a specific region in space in which an electron is most likely to be found.
- **Atomic orbitals** are designated in the order in which they are filled by the letters **s**, **p**, **d**, and **f**.
 - An **s orbital** is **spherically shaped** electron cloud with the atom's nucleus and its center.
 - A **p orbital** is a **dumbbell-shaped** electron cloud with the nucleus between the two lobes.



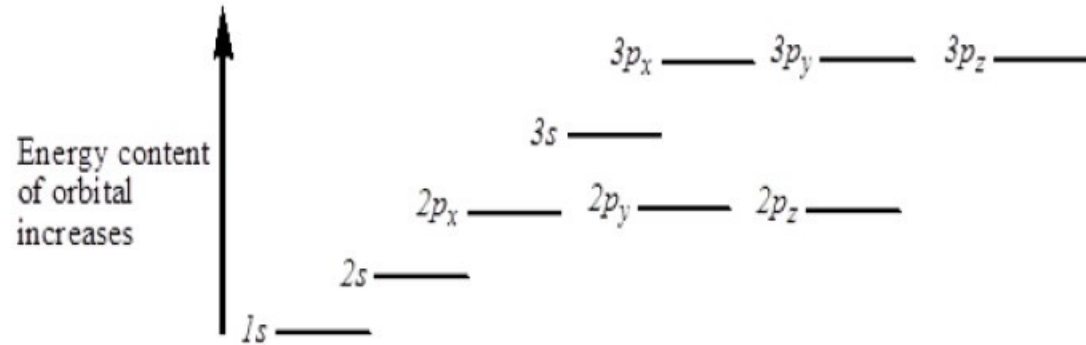
- **Examples:**

K shell has only **one 1s** orbital.

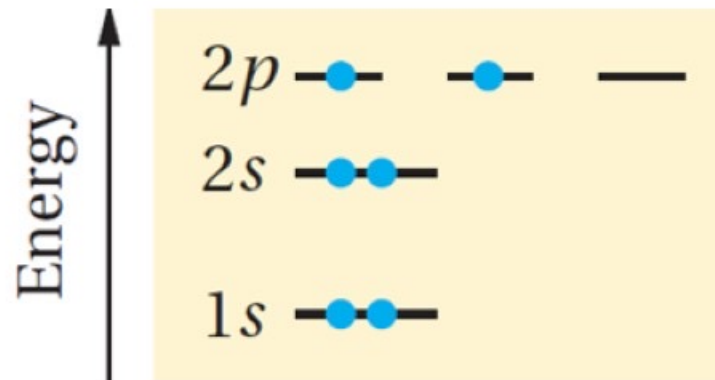
L shell has **one 2s** and **three 2p** (**2p_x**, **2p_y** and **2p_z**).

ATOMIC ORBITALS

- An **energy level diagram** of atomic orbitals.

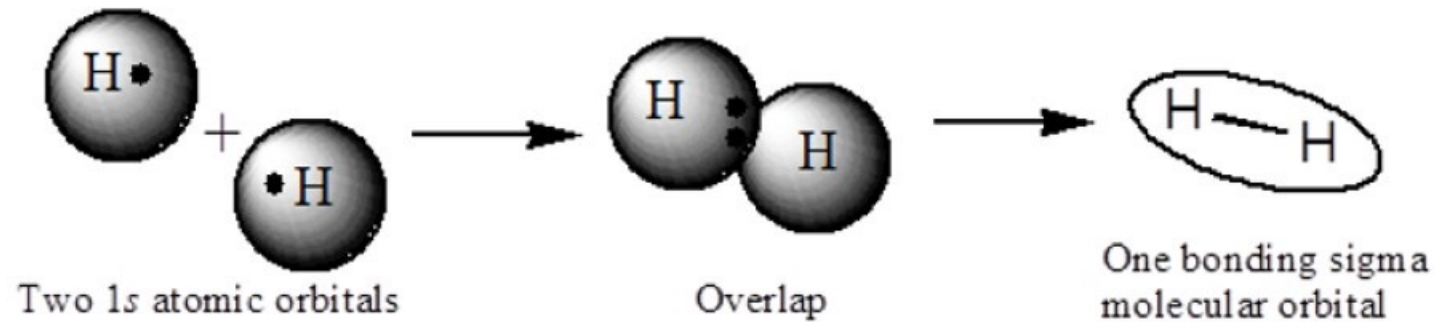


- The electronic configuration of **carbon (atomic number 6)** can be represented as



MOLECULAR ORBITALS

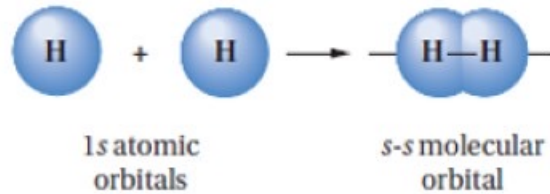
- A covalent bond consists of the overlap between two atomic orbitals to form a **molecular orbital**.
- **Example:** Molecular orbital of H_2



SIGMA (σ) AND pi (π) BONDS

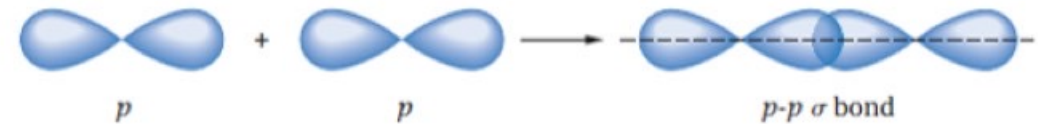
○ **Sigma bonds (σ bonds)** can be formed from

- The overlap of **two s** atomic orbitals.



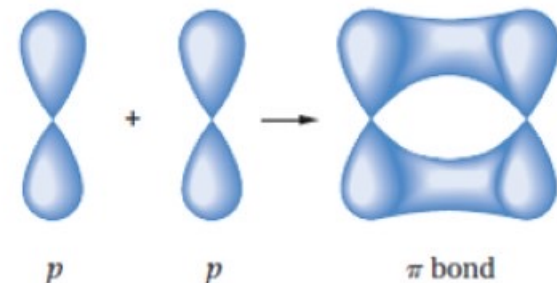
- The **end-on overlap** of **two p** atomic orbitals.

- The overlap of two an **s** atomic orbital with a **p** atomic orbital.



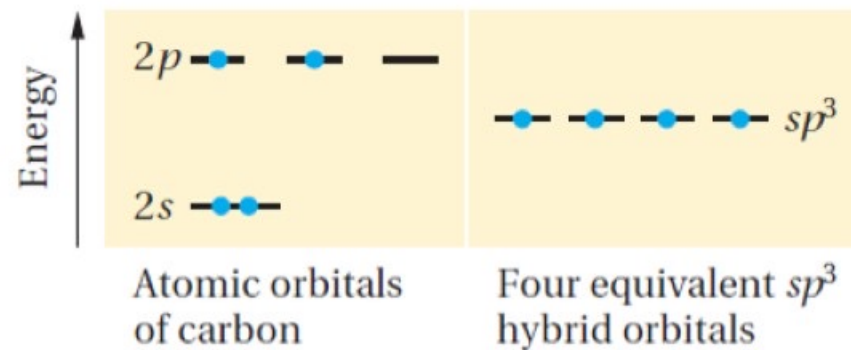
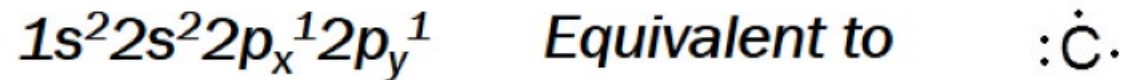
○ **pi bonds (π bonds)** can be formed from

- The **side-side overlap** between two p atomic orbitals.



CARBON sp^3 HYBRID ORBITALS

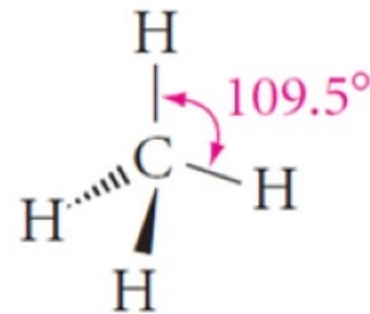
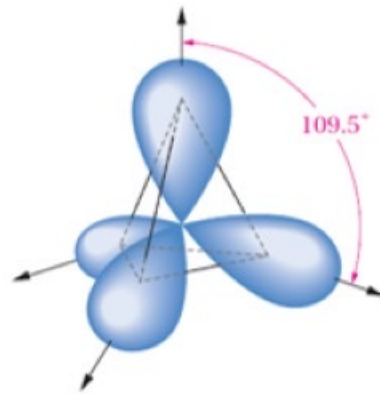
- The electronic configuration of the isolated or ground-state carbon



- Mix or combine the four atomic orbitals of the valence shell to form four identical hybrid orbitals, each containing one valence electron. In this model, the hybrid orbitals are called **sp^3 hybrid orbitals** because each one has one part s character and three parts p character
- Each sp^3 orbital has the same energy: less than that of the 2p orbitals but greater than that of the 2s orbital.

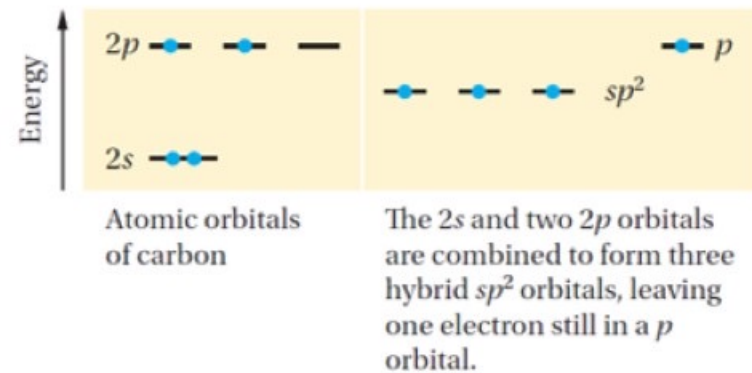
CARBON sp^3 HYBRID ORBITALS

- The angle between any two of the four bonds formed from sp^3 orbitals is approximately 109.5° .
- Regular tetrahedral geometry
- The tetrahedral is a pyramid-like structure with the carbon atom at the center and the four attached atoms located at a corner.

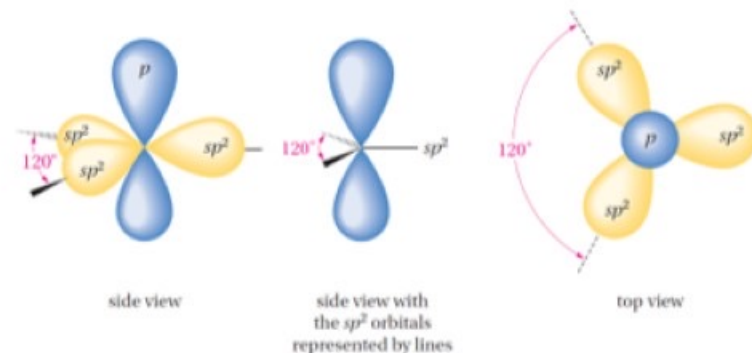


CARBON sp^2 HYBRID ORBITALS

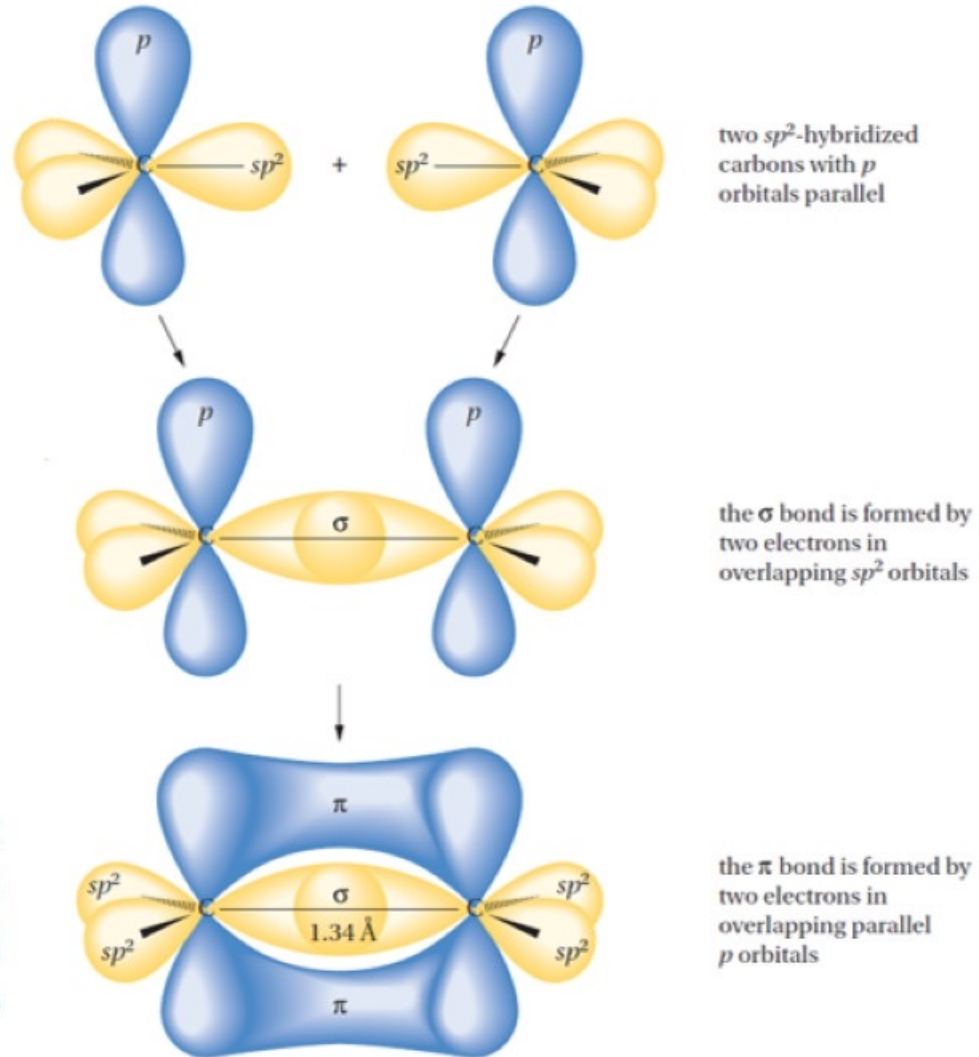
- Combine only three of the orbitals, to make three equivalent sp^2 -hybridized orbitals (called sp^2 because they are formed by combining one s and two p orbitals)



- Three valence electrons are placed in the three sp^2 orbitals. The fourth valence electron is placed in the remaining 2p orbital, whose axis is perpendicular to the plane formed by the three sp^2 hybrid orbitals
- The angle between them is 120° .
- A trigonal carbon



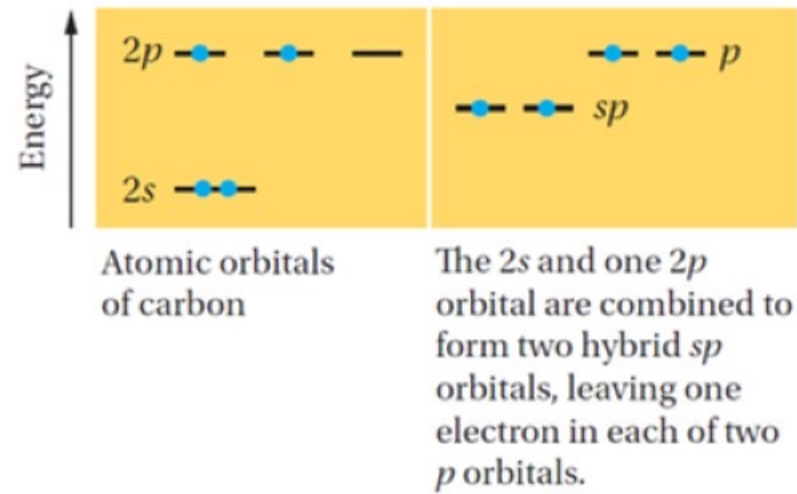
CARBON sp^2 HYBRID ORBITALS



Schematic formation of a carbon-carbon double bond. Two sp^2 carbons form a sigma (σ) bond (end-on overlap of two sp^2 orbitals) and a pi (π) bond (lateral overlap of two properly aligned p orbitals).

CARBON sp HYBRID ORBITALS

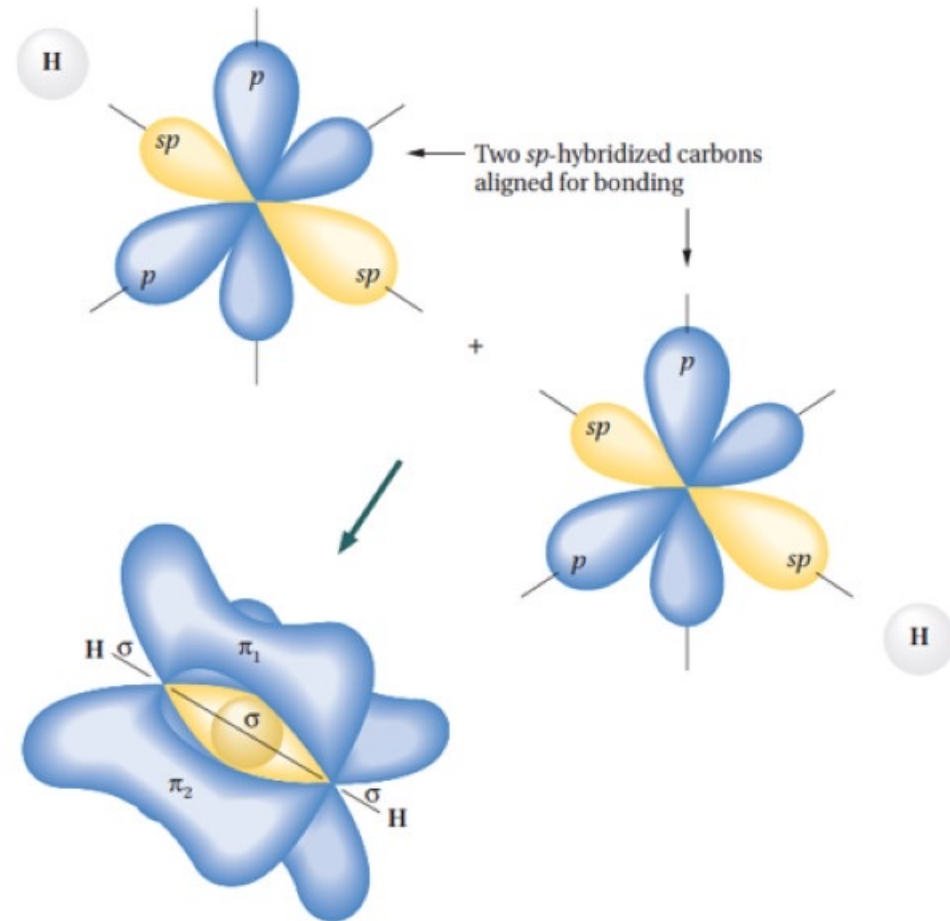
- The carbon atom of an acetylene is connected to only two other atoms. Therefore, we combine the 2s orbital with only one 2p orbital to make two sp -hybrid orbitals



- The angle between the two hybrid orbitals is 180°
- Linear



CARBON sp HYBRID ORBITALS

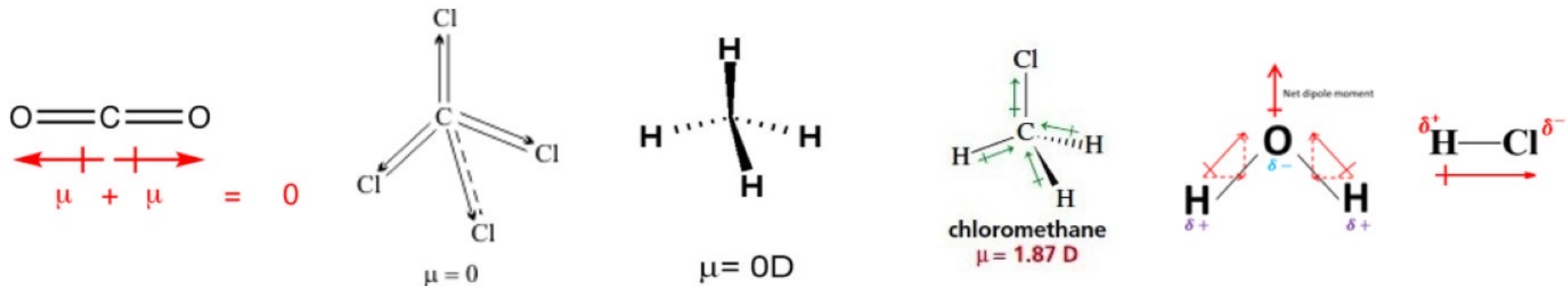


A triple bond consists of the end-on overlap of two sp -hybrid orbitals to form a σ bond and the lateral overlap of two sets of parallel-oriented p orbitals to form two mutually perpendicular π bonds.

The resulting carbon-carbon triple bond, with a hydrogen atom attached to each remaining sp bond. (The orbitals involved in the C—H bonds are omitted for clarity.)

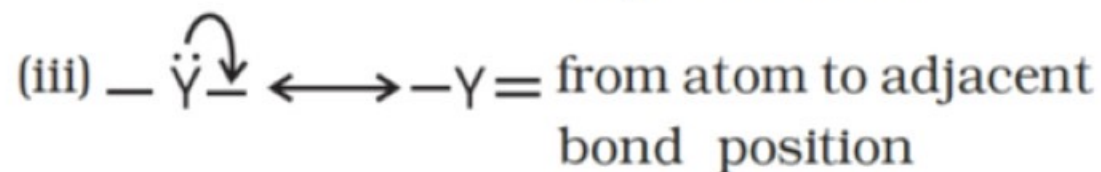
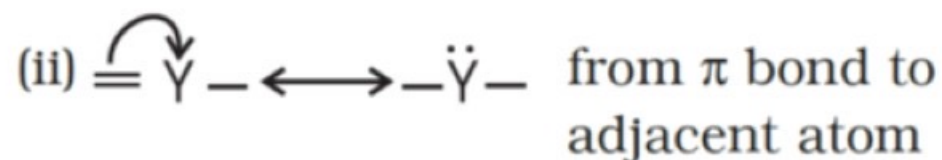
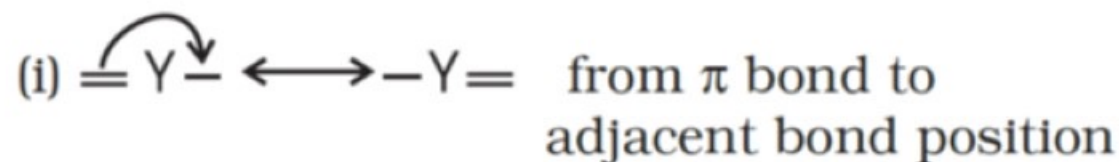
BOND POLARITY AND DIPOLE MOMENT (μ)

- A **polar bond** is a covalent bond between two atoms where the electrons forming the bond are **unequally** distributed.
- A **nonpolar bond** is a covalent bond between two atoms where the electrons forming the bond are **equally** distributed.
- A **dipole moment** is a measurement of the separation of two oppositely charged.
- Dipole moments are a **vector** quantity.
- The **magnitude** is equal to the charge multiplied by the distance between the charges and the direction is from negative charge to positive charge.



ELECTRON MOVEMENT IN ORGANIC REACTIONS

- The movement of electrons in organic reactions can be shown by **curved-arrow notation**.



- Movement of single electron is indicated by a single barbed 'fish hooks' (i.e. *half headed curved arrow*).



ELECTRON DISPLACEMENT EFFECTS IN COVALENT BONDS

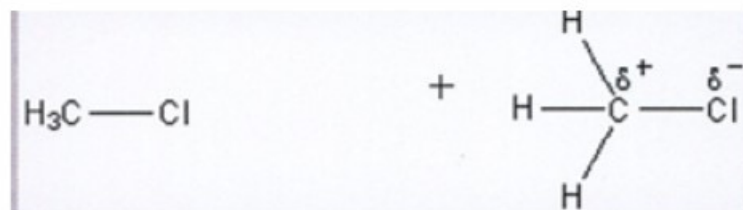
- The electron displacement in an organic molecule may take place either in
 - The ground state under the influence of an atom or a substituent group cause permanent polarization of the bond (*Inductive effect and resonance effects*).

Or

- in the presence of an appropriate attacking reagent.
- Temporary electron displacement effects (*electromeric effect or polarizability effect*).

INDUCTIVE EFFECT

- An **inductive effect** is an electronic effect due to the polarization of σ bonds within a molecule or ion.
- This is typically due to an electronegativity difference between the atoms at either end of the bond.
 - This is the electron-withdrawing inductive effect, also known as the **-I effect**
 - This is electron releasing character and is indicated by the **+I effect**

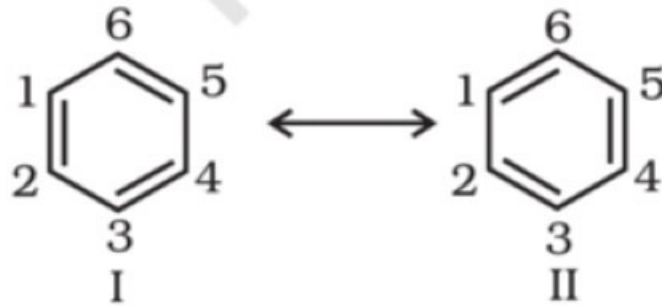


-CH₃, -C₂H₅, -NH₂, -OH, -OCH₃,..... (+ I) electron-donating substituent

-NO₂, -CN, -SO₃H, , (- I) electron-withdrawing substituent

RESONANCE STRUCTURE

- The resonance structures are hypothetical and individually do not represent any real molecule.
- An example:
Benzene; Its cyclic structure containing alternating C–C single and C=C double bonds



- An example:
Nitromethane (CH_3NO_2); It is therefore a resonance hybrid of the two canonical forms I and II.



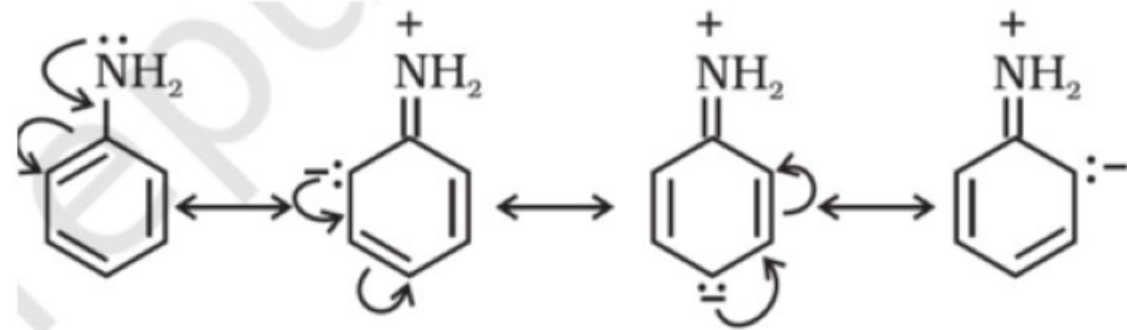
RESONANCE OR MESOMERIC EFFECT

- The resonance effect is defined as 'the polarity produced in the molecule by the interaction of two π -bonds or between a π -bond and lone pair of electrons present on an adjacent atom'.

(i) Positive Resonance Effect (+R effect):

The transfer of electrons is away from an atom or substituent group attached to the conjugated system.

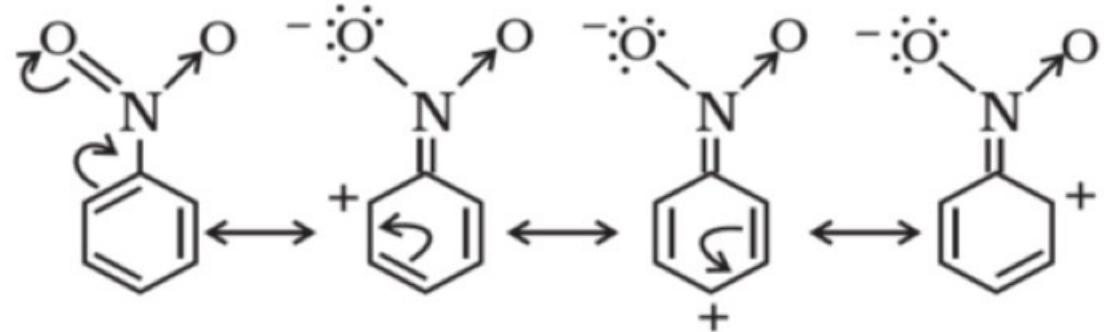
Examples; - halogen, -OH, -OR, -OCOR, -NH₂,
-NHR, -NR₂, -NHCOR,



(ii) Negative Resonance Effect (- R effect):

The transfer of electrons is towards the atom or substituent group attached to the conjugated system.

Examples; - COOH, -CHO, >C=O, - CN, -NO₂

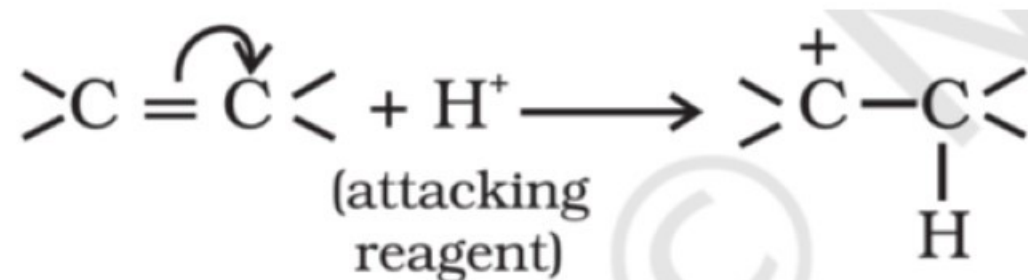


ELECTROMERIC EFFECT (E EFFECT)

- The organic compounds having a multiple bond (a double or triple bond) show this effect in the presence of an attacking reagent only.
- The complete transfer of a shared pair of π -electrons to one of the atoms joined by a multiple bond on the demand of an attacking reagent.

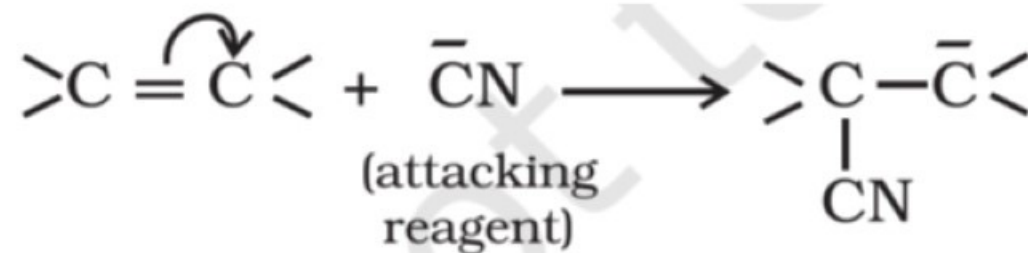
(i) Positive Electromeric Effect (+E effect):

the π -electrons of the multiple bond are transferred to that atom to which the reagent gets attached.



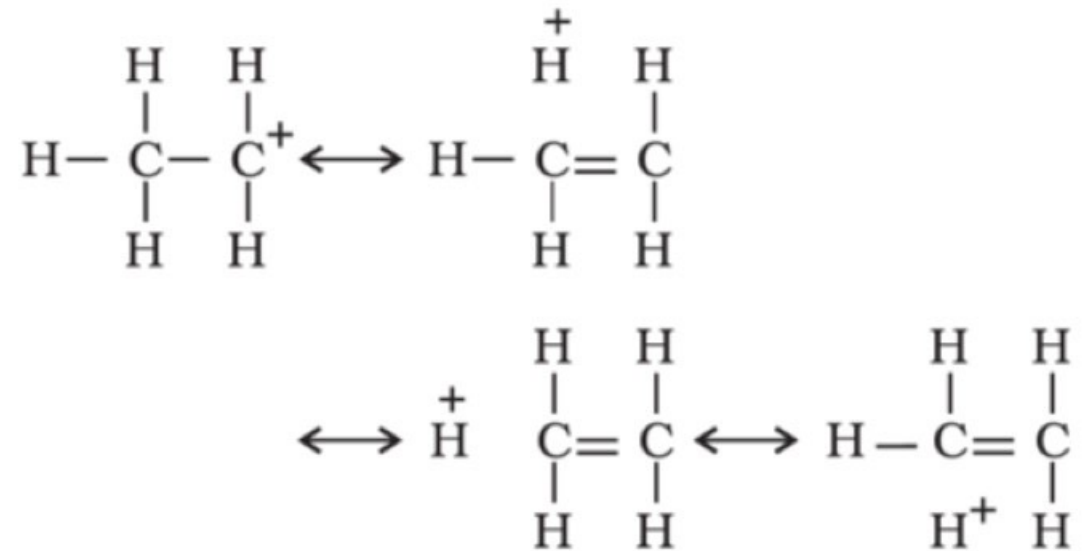
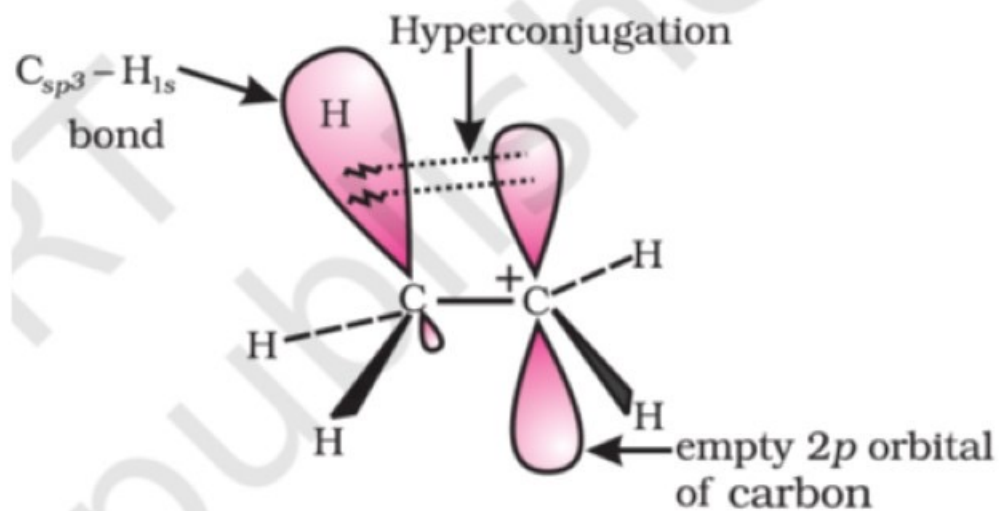
(ii) Negative Electromeric Effect (-E effect):

the π - electrons of the multiple bond are transferred to that atom to which the attacking reagent does not get attached.



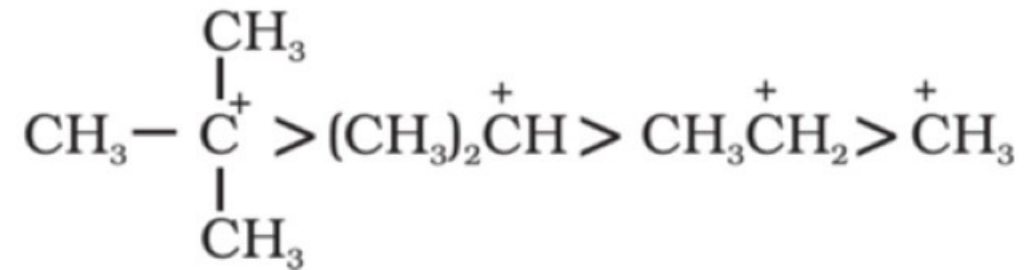
HYPERCONJUGATION

- It involves delocalization of σ electrons of C–H bond of an alkyl group directly attached to an atom of unsaturated system or to an atom with an unshared p orbital.
- CH_3CH_2^+ (ethyl cation); the positively charged carbon atom has an empty p orbital. One of the C–H bonds of the methyl group can align in the plane of this empty p orbital and the electrons constituting the C–H bond in plane with this p orbital can then be delocalized into the empty p orbital.

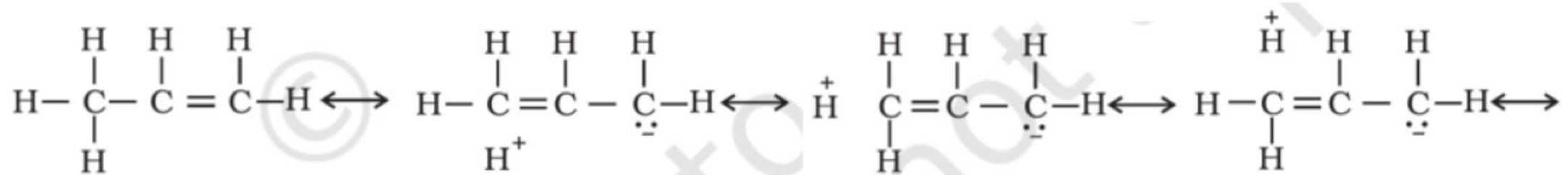


HYPERCONJUGATION

- This type of overlap stabilizes the carbocation because electron density from the adjacent σ bond helps in dispersing the positive charge.
- In general, greater the number of alkyl groups attached to a positively charged carbon atom, the greater is the hyperconjugation interaction and stabilization of the cation.



- Hyperconjugation is also possible in alkenes and alkylarenes.



ACID-BASE CONCEPT

- In the Brønsted–Lowry definitions (1923),

An acid is a species that donates a proton, and a base is a species that accepts a proton (or any compound possessing a lone pair).

- Example:

Hydrogen chloride (HCl) meets the Brønsted–Lowry definition of an acid because it donates a proton to water.

Water (H₂O) meets the definition of a base because it accepts a proton from HCl.



Acid-Base reactions are often called proton-transfer reactions.

In the reverse reaction, H₃O⁺ is an acid because it donates a proton to Cl⁻, and Cl⁻ is a base because it accepts a proton from H₃O⁺.

ACID-BASE CONCEPT

- When a compound loses a proton, the resulting species is called its conjugate base.

Thus, Cl^- is the conjugate base of HCl , and H_2O is the conjugate base of H_3O^+

Thus, HCl is the conjugate acid of Cl^- and H_3O^+ is the conjugate acid of H_2O

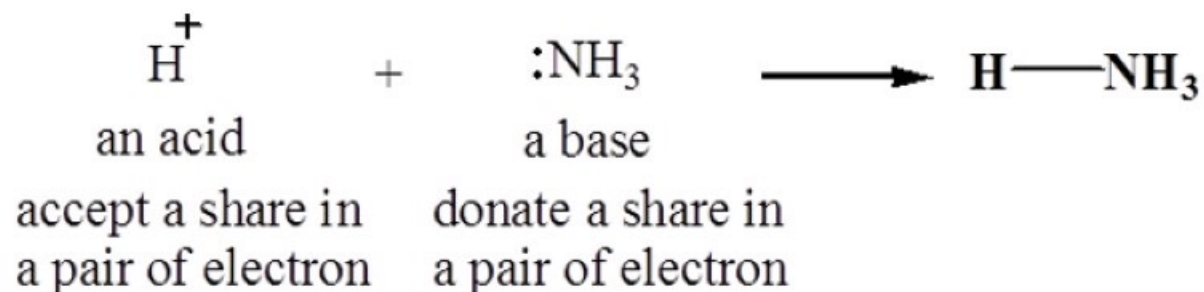
- **Acidity** is a measure of the tendency of a compound to give up a proton.
- **Basicity** is a measure of a compound's affinity for a proton.

ACID-BASE CONCEPT

- In 1923, G. N. Lewis offered new definitions for the terms “acid” and “base.”

An acid as a species that accepts a share in an electron pair.

A base as a species that donates a share in an electron pair.



- **Lewis acid** such as aluminum chloride (AlCl₃) boron trifluoride (BF₃) and borane (BH₃).

The term “acid” is used to mean a proton-donating acid, and the term “Lewis acid” is used to refer to non-proton-donating acids such as AlCl₃ or BF₃.

- All bases are **Lewis bases** because they have a pair of electrons that they can share, either with an atom such as aluminum or boron or with a proton.

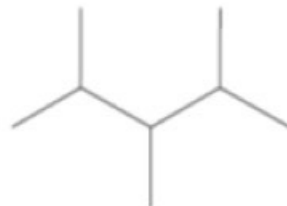
CLASSIFICATION ACCORDING TO MOLECULAR FRAMEWORK

a) Acyclic Compounds

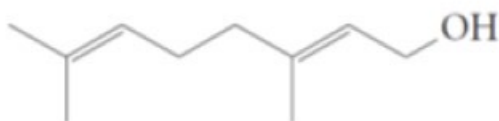
Acyclic organic molecules have chains of carbon atoms but no rings.



unbranched chain of
eight carbon atoms



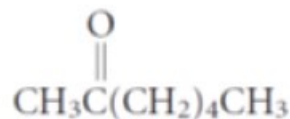
branched chain of
eight carbon atoms



geraniol
(oil of roses)
bp 229–230°C



heptane
(petroleum)
bp 98.4°C



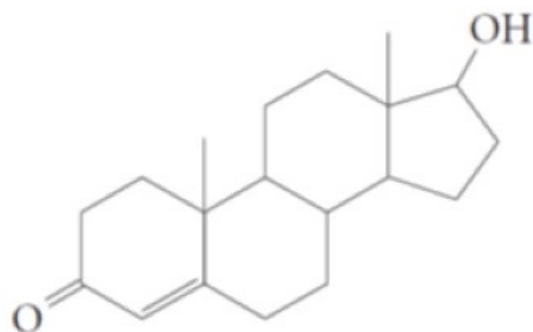
2-heptanone
(oil of cloves)
bp 151.5°C

CLASSIFICATION ACCORDING TO MOLECULAR FRAMEWORK

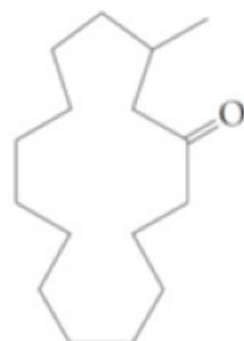
b) Carbocyclic Compounds

Carbocyclic compounds contain rings of carbon atoms.

- The **smallest** possible carbocyclic ring has **three carbon atoms**.
- **Five- and six-membered rings** are most common, but smaller and larger rings are also found.
- Many compounds with more than one carbocyclic ring are known.



testosterone
(testes)
mp 155°C



muscone
(musk deer)
bp 327–330°C



limonene
(citrus fruit oils)
bp 178°C

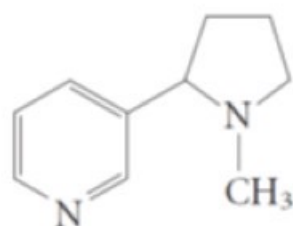


benzene
(petroleum)
mp 5.5°C, bp 80.1°C

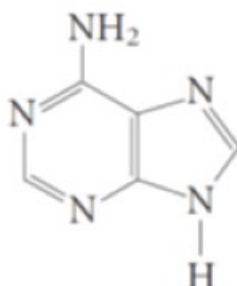
CLASSIFICATION ACCORDING TO MOLECULAR FRAMEWORK

c) Heterocyclic Compounds

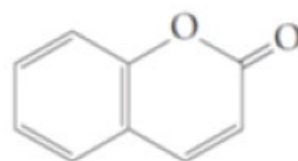
- **Heterocyclic compounds** make up the third and largest class of molecular frameworks for organic compounds.
- In **heterocyclic compounds**, at least one atom in the ring must be a heteroatom, an atom that is not carbon.
- The most common heteroatoms are **oxygen**, **nitrogen**, and **sulfur**, but heterocyclics with other elements are also known.



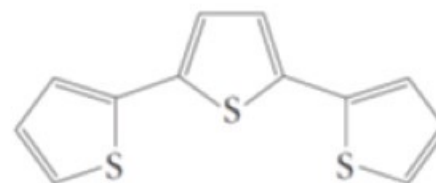
nicotine
bp 246°C



adenine
mp 360–365°C
(decomposes)



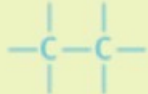
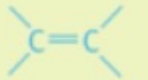



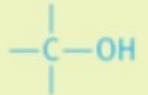
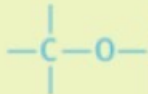
coumarin
mp 71°C



α -terthienyl
mp 92–93°C

CLASSIFICATION ACCORDING TO FUNCTIONAL GROUP

The Main Functional Groups

	Structure	Class of compound	Specific example	Common name of the specific example
<i>A. Functional groups that are a part of the molecular framework</i>		alkane	$\text{CH}_3\text{—CH}_3$	ethane, a component of natural gas
		alkene	$\text{CH}_2\text{=CH}_2$	ethylene, used to make polyethylene
		alkyne	$\text{HC}\equiv\text{CH}$	acetylene, used in welding
		arene		benzene, raw material for polystyrene and phenol
<i>B. Functional groups containing oxygen</i>				
	<i>1. With carbon–oxygen single bonds</i>			
		alcohol	$\text{CH}_3\text{CH}_2\text{OH}$	ethyl alcohol, found in beer, wines, and liquors
		ether	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_3$	diethyl ether, once a common anesthetic

CLASSIFICATION ACCORDING TO FUNCTIONAL GROUP

continued

	Structure	Class of compound	Specific example	Common name of the specific example
2. With carbon-oxygen double bonds*	$\begin{array}{c} \text{O} \\ \parallel \\ -\text{C}-\text{H} \end{array}$	aldehyde	$\text{CH}_2=\text{O}$	formaldehyde, used to preserve biological specimens
	$\begin{array}{c} \text{O} \\ \parallel \\ -\text{C}-\text{C}-\text{C}- \\ \quad \quad \end{array}$	ketone	$\begin{array}{c} \text{O} \\ \parallel \\ \text{CH}_3\text{CCH}_3 \end{array}$	acetone, a solvent for varnish and rubber cement
3. With single and double carbon-oxygen bonds	$\begin{array}{c} \text{O} \\ \parallel \\ -\text{C}-\text{OH} \end{array}$	carboxylic acid	$\begin{array}{c} \text{O} \\ \parallel \\ \text{CH}_3\text{C}-\text{OH} \end{array}$	acetic acid, a component of vinegar
	$\begin{array}{c} \text{O} \\ \parallel \\ -\text{C}-\text{O}-\text{C}- \\ \quad \end{array}$	ester	$\begin{array}{c} \text{O} \\ \parallel \\ \text{CH}_3\text{C}-\text{OCH}_2\text{CH}_3 \end{array}$	ethyl acetate, a solvent for nail polish and model airplane glue
C. Functional groups containing nitrogen**	$\begin{array}{c} \\ -\text{C}-\text{NH}_2 \\ \end{array}$	primary amine	$\text{CH}_3\text{CH}_2\text{NH}_2$	ethylamine, smells like ammonia
	$-\text{C}\equiv\text{N}$	nitrile	$\text{CH}_2=\text{CH}-\text{C}\equiv\text{N}$	acrylonitrile, raw material for making Orlon

CLASSIFICATION ACCORDING TO FUNCTIONAL GROUP

continued

	Structure	Class of compound	Specific example	Common name of the specific example
D. Functional group with oxygen and nitrogen	$\begin{array}{c} \text{O} \\ \\ -\text{C}-\text{NH}_2 \end{array}$	primary amide	$\begin{array}{c} \text{O} \\ \\ \text{H}-\text{C}-\text{NH}_2 \end{array}$	formamide, a softener for paper
E. Functional group with halogen	$-\text{X}$	alkyl or aryl halide	CH_3Cl	methyl chloride, refrigerant and local anesthetic
F. Functional groups containing sulfur [†]	$\begin{array}{c} \\ -\text{C}-\text{SH} \\ \end{array}$	thiol (also called mercaptan)	CH_3SH	methanethiol, has the odor of rotten cabbage
	$\begin{array}{c} \quad \\ -\text{C}-\text{S}-\text{C}- \\ \quad \end{array}$	thioether (also called sulfide)	$(\text{CH}_2=\text{CHCH}_2)_2\text{S}$	diallyl sulfide, has the odor of garlic

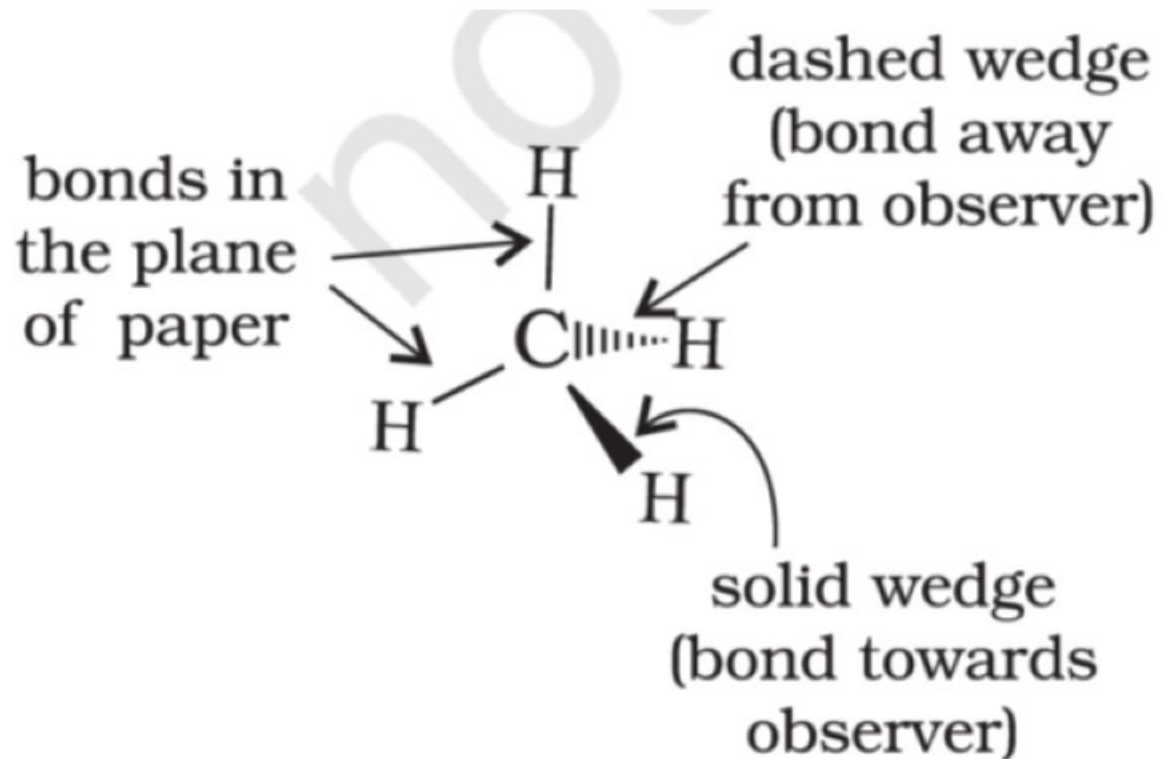
*The $\begin{array}{c} \diagup \\ \text{C}=\text{O} \\ \diagdown \end{array}$ group, present in several functional groups, is called a **carbonyl group**. The $\begin{array}{c} \text{O} \\ || \\ -\text{C}-\text{OH} \end{array}$ group of acids is called a **carboxyl group** (a contraction of *carbonyl* and *hydroxyl*).

The $-\text{NH}_2$ group is called an **amino group.

[†]Thiols and thioethers are the sulfur analogs of alcohols and ethers.

THREE-DIMENSIONAL REPRESENTATION OF ORGANIC MOLECULES

- Wedge-and-dash representation of CH_4

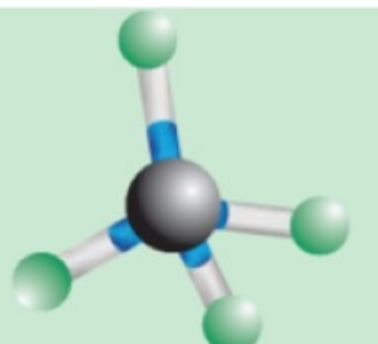


MOLECULAR MODELS

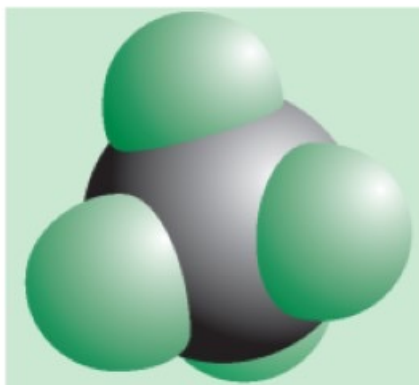
- Molecular models are physical devices that are used for a better visualization and perception of three-dimensional shapes of organic molecules. These are made of wood, plastic or metal and are commercially available.
- Commonly three types of molecular models are used:
 - (1) Framework model; only the bonds connecting the atoms of a molecule and not the atoms themselves are shown
 - (2) Ball-and-stick model; both the atoms and the bonds are shown
 - (3) Space filling model; emphasizes the relative size of each atom based on its van der Waals radius and bonds are not shown in this model.



Framework model



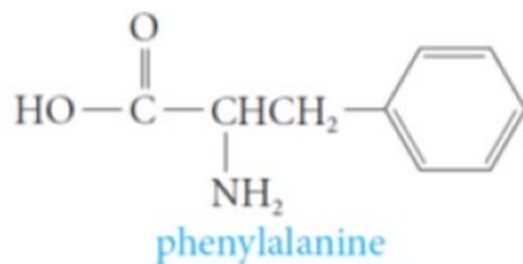
Ball and stick model



Space filling model

QUIZZES

PROBLEM 1.1 Many organic compounds contain more than one functional group. An example is phenylalanine (shown below),



- What functional groups are present in phenylalanine?
- Redraw the structure, adding all unshared electron pairs.
- What is the molecular formula of phenylalanine?

FUNDAMENTAL CONCEPTS IN ORGANIC REACTION MECHANISM

- The general reaction is depicted as follows :

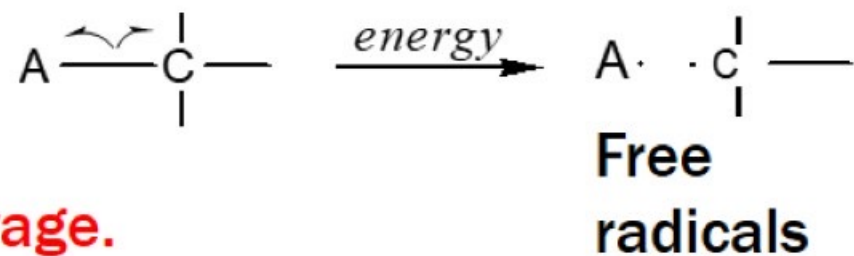


- Substrate; A molecule whose carbon is involved in new bond formation
- and the other one is called reagent.

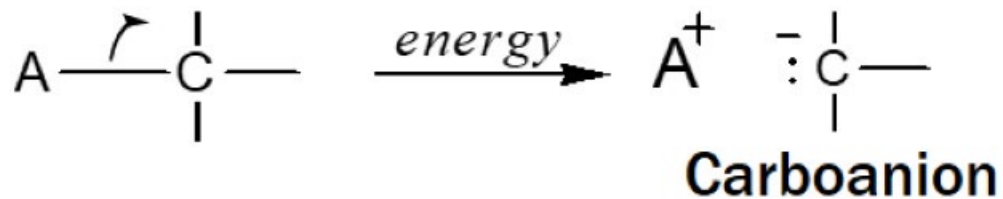
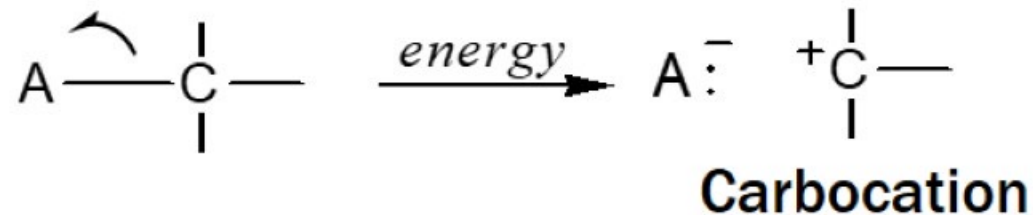
Notations for bond breaking and bond making

- A covalent bond can be broken in either two ways,

- **Homolytic cleavage.**

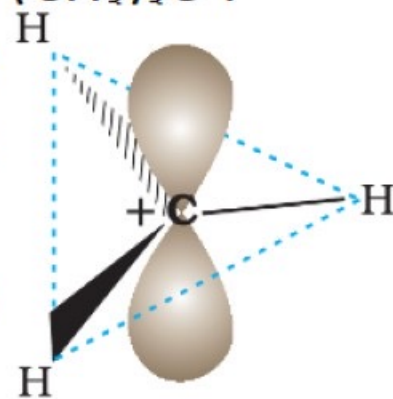


- **Heterolytic cleavage.**



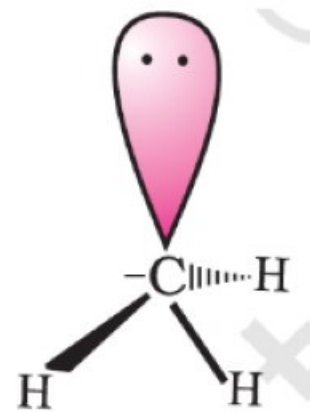
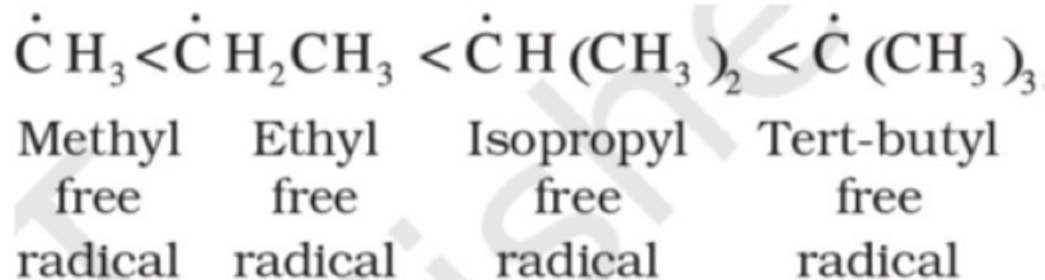
Notations for bond breaking and bond making

- **Carbocations** are classified as *primary*, *secondary* or *tertiary* depending on whether one, two or three carbons are directly attached to the positively charged carbon.
- Some other examples of carbocations are: CH_3CH_2^+ (ethyl cation, a primary carbocation), $(\text{CH}_3)_2\text{CH}^+$ (isopropyl cation, a secondary carbocation), and $(\text{CH}_3)_3\text{C}^+$ (*tert*-butyl cation, a tertiary carbocation).
- Carbocations are highly unstable and reactive species.
- Alkyl groups directly attached to the positively charged carbon stabilize the carbocations due to inductive and hyperconjugation effects.
- The observed order of carbocation stability is: $^+\text{CH}_3 < \text{CH}_3\text{CH}_2^+ < (\text{CH}_3)_2\text{CH}^+ < (\text{CH}_2)_2\text{C}^+$.
- The shape of $^+\text{CH}_3$ may be considered as being derived from the overlap of three equivalent $\text{C}(sp^2)$ hybridized orbitals with $1s$ orbital of each of the three hydrogens.
- Each bond may be represented as $\text{C}(sp^2)\text{--H}(1s)$ sigma bond.
- The remaining carbon orbital is perpendicular to the molecular plane and contains a lone pair of electrons.



Notations for bond breaking and bond making

- Carbon in **carbanion** is generally sp^3 hybridized and its structure is distorted tetrahedron.
- Carbanions are also unstable and reactive species.
- The organic reactions which proceed through heterolytic bond cleavage are called ionic or heteropolar.
- Like carbocations and carbanions, **free radicals** are also very reactive.
- Alkyl radicals are classified as primary, secondary, or tertiary.
- Alkyl radical stability increases as we proceed from primary to tertiary:



- Organic reactions, which proceed by homolytic fission are called free radical or homopolar or nonpolar reactions.

Nucleophiles and Electrophiles

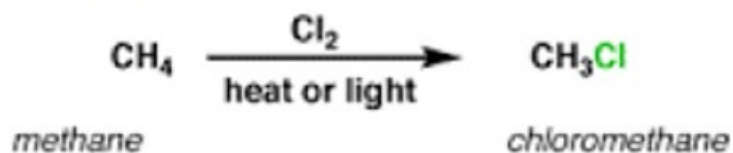
- **Nucleophile (Nu:)**; a reagent that brings an electron pair to the reactive site and the reaction is then called **nucleophilic**.
- **Some examples of nucleophiles** are the negatively charged ions with lone pair of electrons such as hydroxide (HO^-), cyanide (NC^-) ions and carbanions (R_3C^-). Neutral molecules such as $\text{H}_2\ddot{\text{O}}:$, $\text{R}_3\ddot{\text{N}}:$, $\text{R}_2\ddot{\text{N}}\text{H}$ etc., can also act as nucleophiles due to the presence of lone pair of electrons.
- **Electrophile (E^+)**; A reagent that takes away an electron pair from reactive site and the reaction is called **electrophilic**.
- **Examples of electrophiles** include carbocations ($+\text{CH}_3$) and neutral molecules having functional groups like carbonyl group ($>\text{C}=\text{O}$) or alkyl halides ($\text{R}_3\text{C}-\text{X}$, where X is a halogen atom).

SUBSTITUTION REACTIONS

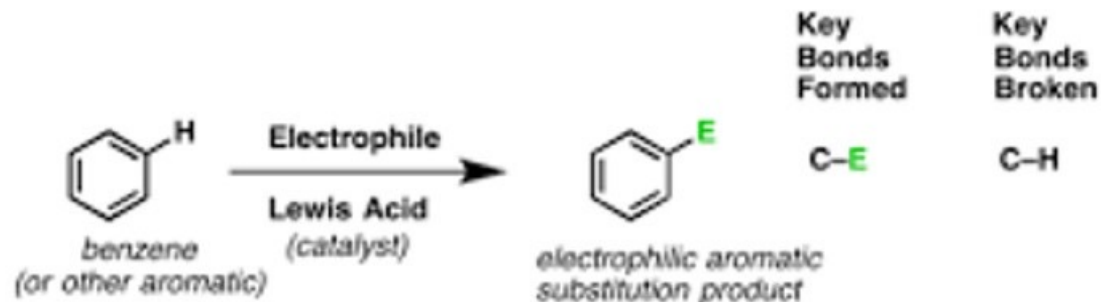
Types of Organic Reactions

Based on the nature of substituents involved

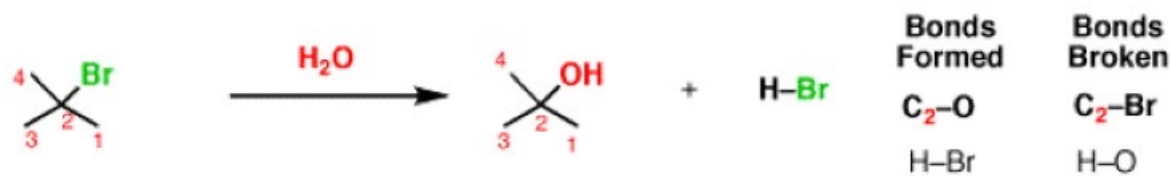
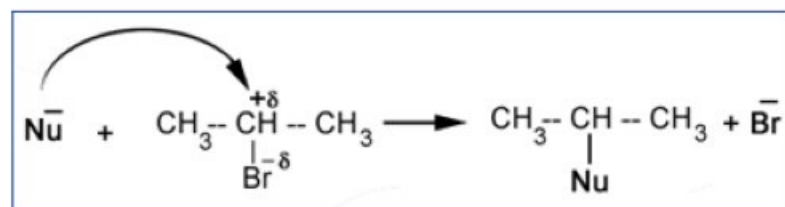
- Free Radical Substitution Reactions



- Electrophilic Substitution Reactions



- Nucleophilic Substitution Reactions

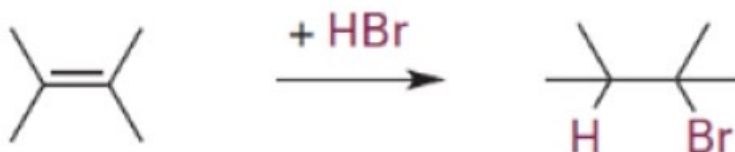


Types of Organic Reactions

Elimination Reactions

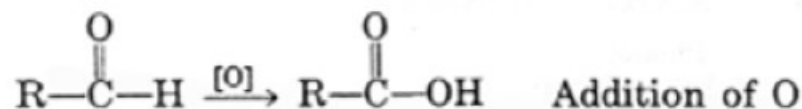
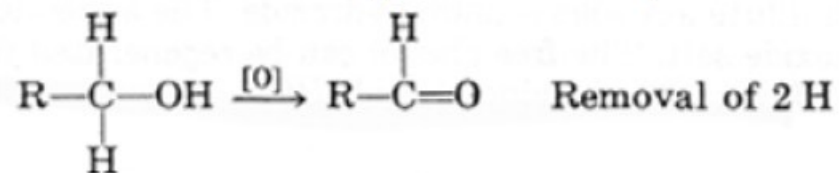


Addition Reactions



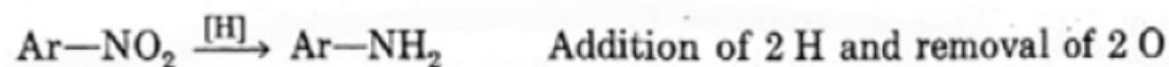
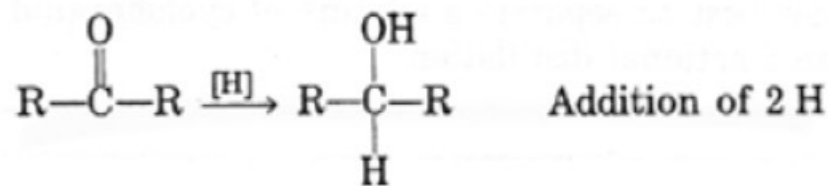
OXIDATION-REDUCTION REACTIONS

- Oxidation** is the **removal of H** from a compound and/or the **addition of O** to a compound.



An oxidizing agent is the chemical reagent that does the oxidation.

- Reduction** is the **addition of H** to a compound and/or the **removal of O** from a compound.



A reducing agent is a substance that does the reduction.