

Fundamentals of Organic Chemistry CHEM 108

Credit hrs.: (3+1)

King Saud University

College of Science, Chemistry Department

CHEM 108

CHAPTER 1. INTRODUCTION

Learning Outcomes



At the end of this chapter, students will be able to:

- □ Recognize the definition and importance of organic chemistry.
- □ Arrange the electrons in atoms.
- Differentiate between ionic and covalent bonds in chemical compounds.
- Identify the hybridization of carbon atom.
- □ Know dipole moment & inductive effect in chemical compounds.
- □ Classify the organic compounds according to functional groups.
- □ Define the types of organic reactions.

Importance of Organic Chemistry in every day life



- Organic chemistry touches our daily lives. We are made of and surrounded by organic compounds.
- □ Almost all of the reactions in living matter involve **organic** compounds.
- The major constituents of living matter e.g. proteins, carbohydrates, fats, nucleic acid (DNA and RNA), enzymes and hormones are organic.
- Other organic materials include the gasoline, oil, tires, clothing we wear, wood for our furniture, the paper for our books, the medicines we take and plastic containers, camera film, perfume, carpeting and fabrics.
- In short, organic chemistry is more than just a branch of science for the professional chemist or for student preparing to become a physician, dentist, pharmacist, nurse or agriculturist. It is part of our technological culture.

Organic Chemistry: Definition



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- The word Organic can be a biological or chemical term, in biology it means anything that is living or has lived. The opposite is Non-Organic.
- Organic Chemistry is unique in that it deals with vast numbers of substances, both natural and synthetic.
 - The clothes, the petroleum products, the paper, rubber, wood, plastics, paint, cosmetics, insecticides, and drugs
- But, from the chemical makeup of organic compounds, it was recognized that one constituent common to all was the element carbon.
- Organic chemistry is defined as the study of carbon/hydrogen-containing compounds and their derivatives.

The Uniqueness of Carbon



- What is unique about the element carbon?
- $\circ~$ Why does it form so many compounds?
 - The answers lie in
 - \succ The structure of the carbon atom.
 - \succ The position of carbon in the periodic table.
- \circ These factors enable it to form strong bonds with
 - > other carbon atoms
 - \succ and with other elements (hydrogen, oxygen, nitrogen, halogens,...etc).
- Each organic compound has its own characteristic set of physical and chemical properties which depend on the *structure of the molecule*.

IA								Zero
н	IIA		IIIA	IVA	VA	VIA	VIIA	He
Li	Be		В	С	N	0	F	Ne
Na	Mg		Ai	Si	Ρ	S	С	Ar
ĸ	Са	Transition Elements	Ga	Ge	As	Se	Br	Kr
Rb	Sr		In	Sn	Sb	Те	Ι	Xe
Cs	Ва		TI	Pb	Bi	Po	At	Rn
Fr	Ra							

Atomic Structure



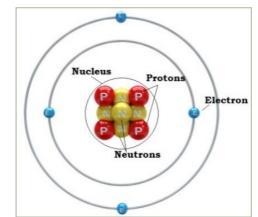
- 6
- Atoms consist of three main particles: neutrons (have no charge), protons (positively charged) and electrons (negatively charged).
 - > Neutrons and protons are found in the nucleus.
 - > Electrons are found outside the nucleus.

Electrons are distributed around the nucleus in successive shells (principal energy levels).

• Atom is electrically neutral.

i.e. Number of electrons = Number of protons

- Atomic number of an element is the number of protons.
- The atomic weight is approximately equal to the sum of the number of protons and the number of neutrons in the nucleus



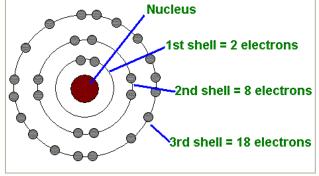
Atomic Structure

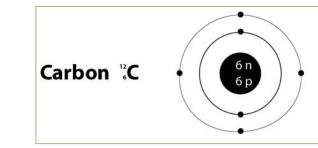


- The energy levels are designated by capital letters (K, L, M, N, ..) or whole numbers (n).
- The maximum capacity of a shell = $2n^2$ electrons. n = number of the energy level.
- For example, the element carbon (atomic number 6)

6 electrons are distributed about the nucleus as







Atomic Structure

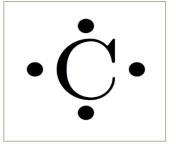


- Valance Electrons are those electrons located in the outermost energy level (the valance shell).
- Electron-dot structures
 - \succ The symbol of the element represents the core of the atom.
 - \succ The valance electrons are shown as dots around the symbol.

	Valences	of Comm	on Elments	i	
Element H·	٠ċ٠	• N ÷	· ö :	÷Ë÷	: çi :
Valence 1	4	3	2	1	1

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







Chemical Bonding



• In 1916 G.N. Lewis pointed out that:

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

 \geq 2 electrons in case of helium.

 \geq 8 electrons for the other noble gases.

• According to Lewis,

in interacting with one another atoms can achieve a greater degree of stability

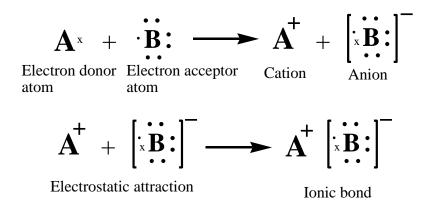
by rearrangement of the valence electrons

to acquire the outer-shell structure of the closest noble gas in the periodic table.



- Elements at the left of the periodic table give up their valance electrons and become +ve charged ions (cations).
- Elements at the right of the periodic table gain the electrons and become -ve charged ions (anions).
- \circ lonic bond

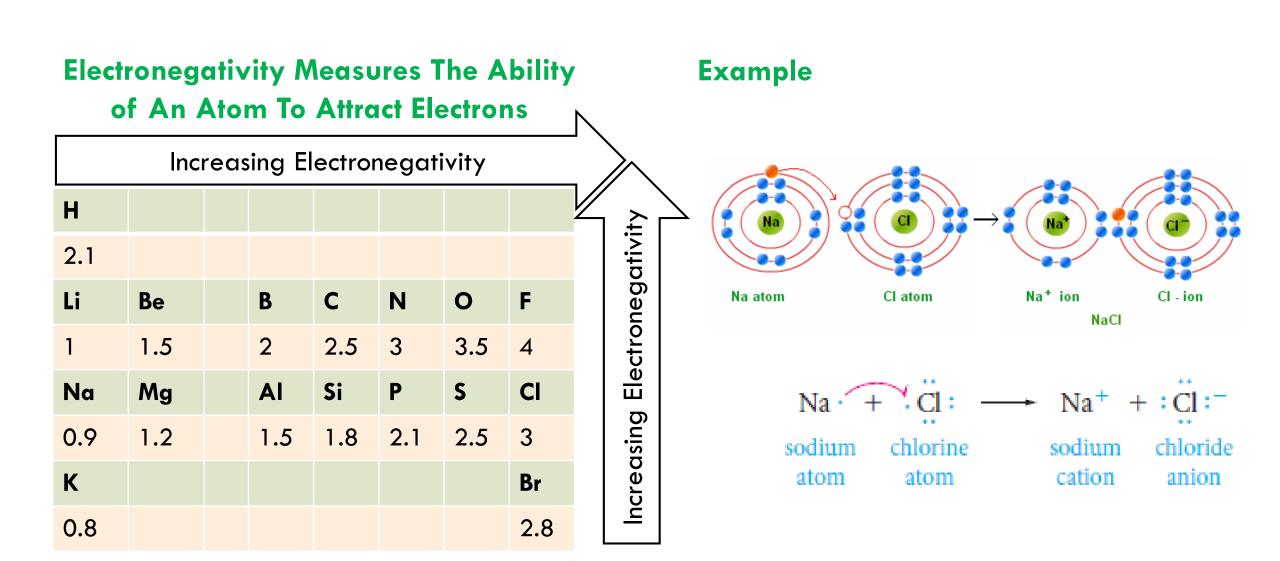
The electrostatic force of attraction between oppositely charged ions.



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



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- Elements that are close to each other in the periodic table attain the stable noble gas configuration by sharing valence electrons between them.
- A shared electron pair between two atoms or single covalent bond, will be represented by a dash (-).
- A covalent bond involves the mutual sharing of one or more electron pairs between atoms.
 - When the two atoms are <u>identical or have equal electronegativities</u>, the electron pairs are shared equally

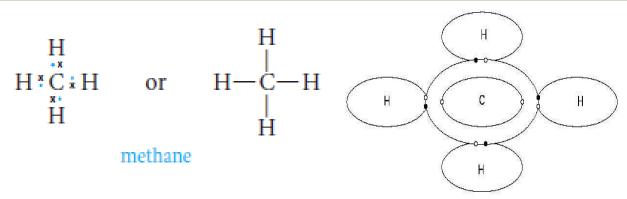
$$H_2$$
 $H_{\bullet} + \bullet H \longrightarrow H_{\bullet}^{\bullet} H$ or $H_{\bullet}^{\bullet} H$

each H shares two electrons (He configuration)



B) Covalent Bonds

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When two unlike atoms;

the bonding electrons are no longer shared equally (shared unequally).

1) A Polar Covalent Bond

A bond, in which an electron pair is shared unequally.

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

$$\leftarrow C \longrightarrow O$$
 or $C \longrightarrow O$



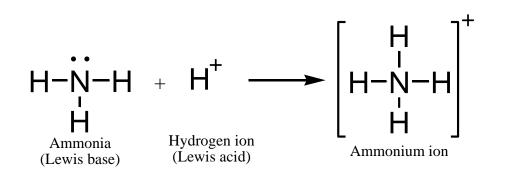
$\circ~$ Lewis base

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.

• For example;





How Many Bonds to an Atom? Covalence Number

The number of covalent bonds that an atom can form with other atoms.

i.e. the covalence number is equal to the number of electrons needed to fill its valance shell.

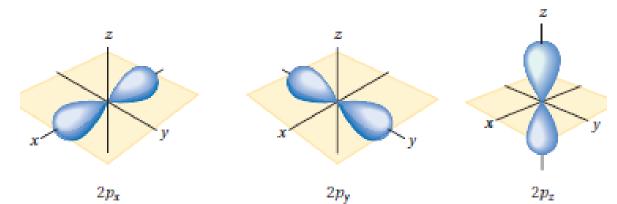
Element	Number of	Number of Number of electrons	
	valence electrons	in filled valence shell	number
н	1	2	1
С	4	8	4
Ν	5	8	3
0	6	8	2
F, CI, Br, I	7	8	1

Atomic Orbitals

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 - 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.
 - Examples: K shell has only one 1s orbital.
 L shell has one 2s and three 2p (2p_x, 2p_y and 2p_z).
 - An <u>s orbital</u> is spherically shaped electron cloud with the atom's nucleus and its center.
 - x y

2s

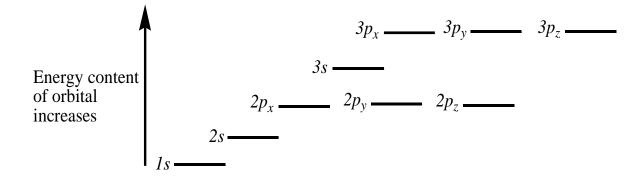
A <u>p orbital</u> is a dumbbell-shaped electron cloud with the nucleus between the two lobes.



Atomic Orbitals

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> An energy level diagram of atomic orbitals.

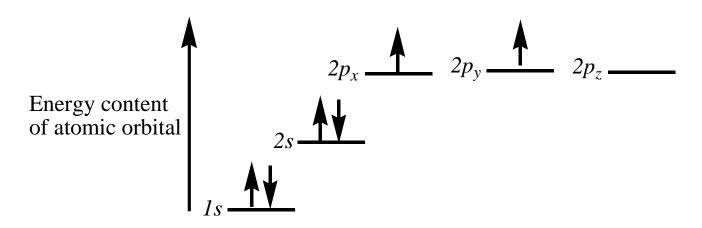


- \circ When filling the atomic orbitals, keep in mind that
 - (1) An atomic orbital contain no more 2 electrons.
 - (2) Electrons fill orbitals of lower energy first.
 - (3) No sub-orbital is filled by 2 electrons until all the sub-orbitals of equal energy have at least one electron.

Atomic Orbitals

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

 $1s^{2}2s^{2}sp_{x}^{1}2p_{y}^{1}$ or $1s^{2}2s^{2}2p^{2}$

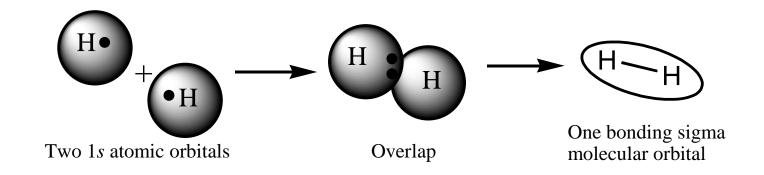


Energy level diagram for carbon.

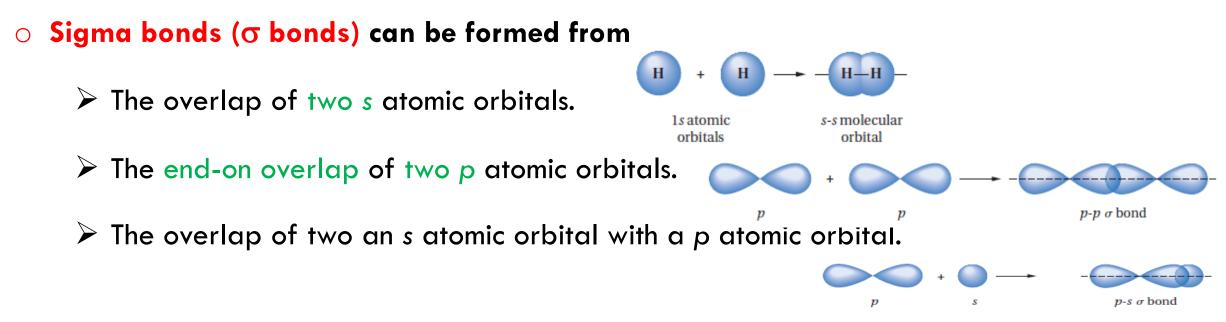
Molecular Orbitals

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

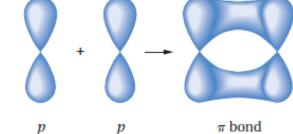
Molecular orbital of H₂



Molecular Orbitals



• **pi bonds (\pi bonds)** can be formed from the side-side overlap between two p atomic orbitals.



Bond Energy and Bond Length

 $\circ~$ A molecule is more stable than the isolated constituent atoms.

This stability is apparent in the release of energy during the formation of the molecular bond.

• Heat of formation (bond energy)

The amount of energy released when a bond is formed.

Bond dissociation energy

The amount of energy that must be absorbed to break a bond.

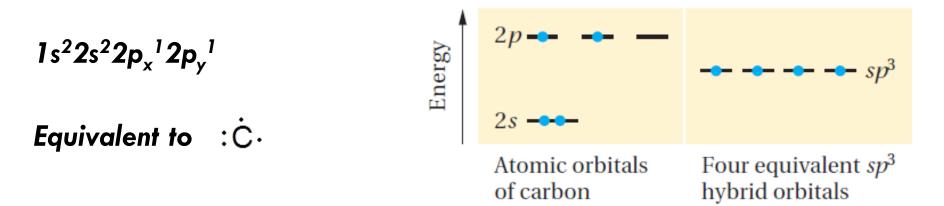
Bond length

The distance between nuclei in the molecular structure.



Hybridization (Alkanes sp³)

 $\,\circ\,$ The electronic configuration of the isolated or ground-state carbon

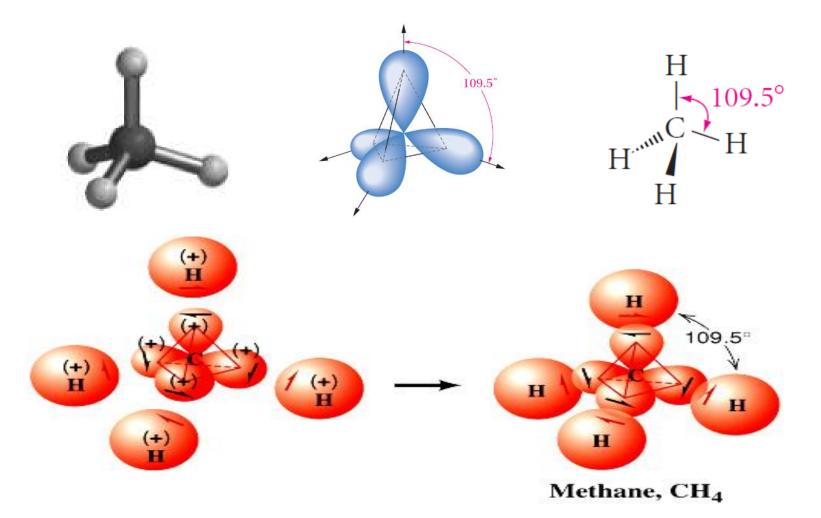


- Mix or combine the four atomic orbitals of the valence shell to form four identical hybrid orbitals, each containing one valence electron.
- In this model, the hybrid orbitals are called sp³ hybrid orbitals because each one has one part s character and three parts p character
- Each sp³ orbital has the same energy: less than that of the 2p orbitals but greater than that of the 2s orbital.

Hybridization (Saturated Hydrocarbons: Alkanes sp³)

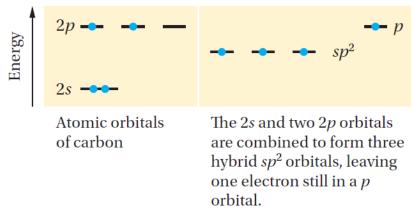
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• Regular tetrahedron with all H-C-H bond angles of 109.5°.

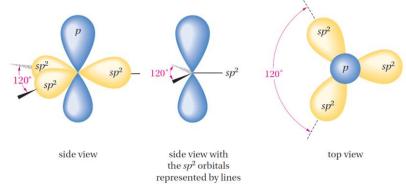


Hybridization (Unsaturated Hydrocarbons: Alkenes sp²)

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- Combine only three of the orbitals, to make three equivalent sp²-hybridized orbitals (called sp² because they are formed by combining one s and two p orbitals)



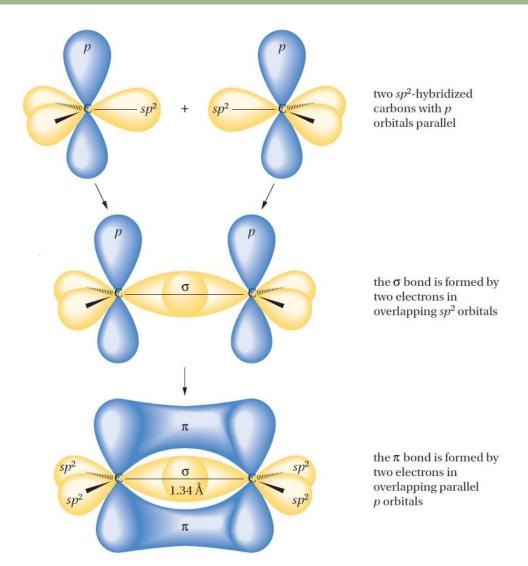
- Three valence electrons are placed in the three sp^2 orbitals. The fourth valence electron is placed in the remaining 2p orbital, whose axis is perpendicular to the plane formed by the three sp^2 hybrid orbitals
- $\circ\,$ A trigonal carbon with bond angles of 120°.





Hybridization (Alkenes sp²)

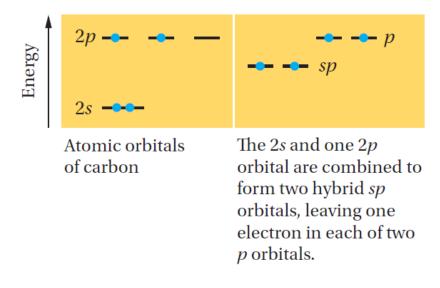
Schematic formation of a carbon–carbon double bond. Two sp^2 carbons form a sigma (s) bond (end-on overlap of two sp^2 orbitals) and a pi (p) bond (lateral overlap of two properly aligned p orbitals).



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Hybridization (Unsaturated Hydrocarbons: Alkynes sp)

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- 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

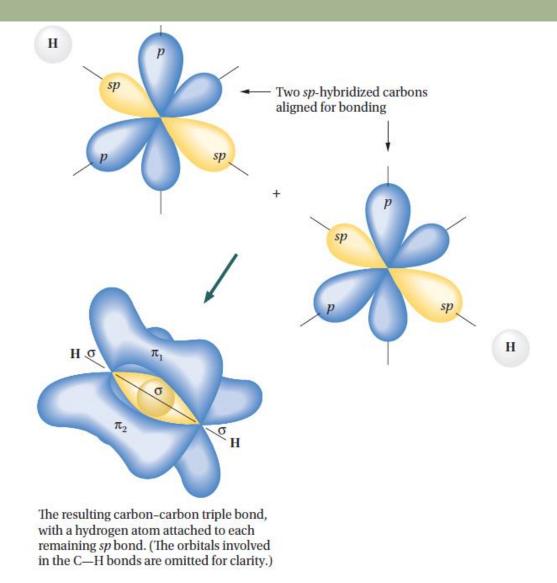


- \circ The angle between the two hybrid orbitals is 180°
- Linear $H^{180^{\circ}}_{H^{-}C \equiv C-H}$



Hybridization (Alkynes sp)

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 paralleloriented *p* orbitals to form two mutually perpendicular π bonds.





 $^{\delta^{+}}$ H—Cl $^{\delta^{-}}$

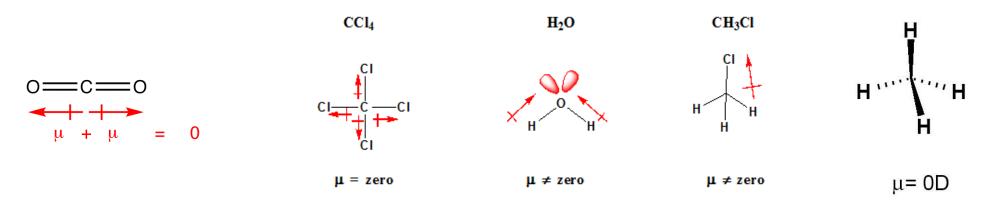
- Inductive effect can be defined as the permanent displacement of electrons forming a covalent bond (sigma σ bonds) towards the more electronegative element or group.
- The inductive effect is represented by the symbol, the arrow pointing towards the more electronegative element or group of elements.

(+ I) effect if the substituent electron-donating

(- I) effect if the substituent electron-withdrawing

Electron-donating substituents (+1): $-CH_3$, $-C_2H_5$,.... Electron-withdrawing substituents (-1): $-NO_2$, -CN, $-SO_3H$, COOH, COOR, NH_2 , OH, OCH_3

- **Dipole moment** (depends on the inductive effect).
- A bond with the electrons shared equally between two atoms is called a nonpolar bond like in CI-CI and C-C bond in ethane.
- A bond with the electrons shared unequally between two different elements is called a polar bond.
- \circ The **bond polarity** is measured by its dipole moment (μ).
- **Dipole moment (µ)** defined to be the amount of charge separation ($+\delta$ and $-\delta$) multiplied by the bond length.



Functional Groups



Functional Group is a reactive portion of an organic molecule, an atom, or a group of atoms that confers on the whole molecule its characteristic properties.

Class	General formula	Functional group	Specific	
Alkane	RH	C – C (single bond)	$H_3C - CH_3$	
Alkene	$R - CH = CH_2$	C = C (double bond)	$H_2C = CH_2$	
Alkyne	R−C≡CH	C≡C (triple	НС≡СН	
Alkyl halide	RX	-X (X = F, CI, Br, I)	H ₃ C - Cl	
Alcohol	R – OH	-OH	H ₃ C - OH	
Ether	R – O –R'	- C- O – C -	$H_3C - O - CH_3$	
Aldehyde	O R-Ċ-H	о —с–н	О О H-Č-H, H ₃ C-Č-H	
Ketone	0 R-Č-H 0 R-Č-R	-ç-ç-ç-	$H_{3}C - O - CH_{3}$ O $H - C - H, H_{3}C - C - H$ $H_{3}C - C - CH_{3}$	
Carboxylic acid	О R-Č-OH	' о ' —Ё–ОН	О О Н-Ё-ОН, Н ₃ С-Ё-ОН	
Ester	0 R -Č-OR	O —Ċ-OR	О Н-С-ОСН ₃ О Н ₃ С-С-ОСН ₃	
Amine	R – NH ₂	$-\overset{ }{_{\Gamma}}-\mathrm{NH}_{2}$	H ₃ C – NH ₂	



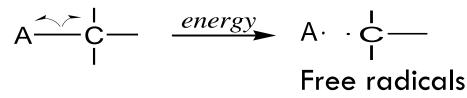
Types of Organic Reactions

Substitution reactions	$CH_3CH_2CH_2CH_2OH + HBr \xrightarrow{120 \circ C} CH_3CH_2CH_2CH_2Br + H_2O$
Addition Reaction	$\begin{array}{cccc} C = C & + & HX & \longrightarrow & \begin{array}{cccc} C - C & (X = CI, Br) \\ H & X & \end{array}$
Elimination Reaction	$\begin{array}{c} \begin{array}{c} \\ C-C \\ / \\ H \end{array} \\ \begin{array}{c} \\ X \end{array} \end{array} \xrightarrow{\text{KOH}} \\ \hline \\ CH_3CH_2OH \end{array} \end{array} \begin{array}{c} C=C \\ \end{array}$
Oxidation	$R^{H} \xrightarrow{(O)} H \xrightarrow{(O)} R^{H} \xrightarrow{(O)} R^{H} \xrightarrow{(O)} R^{H}$
Reduction	$H_{3}C \underbrace{C}_{O} \xrightarrow{[H]} H_{3}C \underbrace{C}_{CH_{2}}^{OH}$
Rearrangement	$\stackrel{R}{\stackrel{\longrightarrow}{\longrightarrow}} \stackrel{\longrightarrow}{\stackrel{\longrightarrow}{\longrightarrow}} \stackrel{\longrightarrow}{\underset{R}{\longrightarrow}}$

Notations for bond breaking and bond making

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

Homolytic cleavage.



Heterolytic cleavage.

