

### lec. 3

• **ACID** is a substance that can release hydrogen ions [protons  $H^+$ ].

• **BASE** is a substance that can accept hydrogen ions.

• **pH** is the concentration of hydrogen ions it determines the acidity of the solution. + why we use the pH not the [H+] concentration? because the pH is easier to remember and easier to calculate and work with.

• The pH of a solution is the negative base 10 logarithm of its hydrogen ion concentration.

$$\sim pH = -\log_{10}[H^+] \sim [H^+] = 10^{-pH}$$

1	2	3	4	5	6	7	8	9	10	11	12	13	14	pH
$10^{-1}$	$10^{-2}$	$10^{-3}$	$10^{-4}$	$10^{-5}$	$10^{-6}$	$10^{-7}$	$10^{-8}$	$10^{-9}$	$10^{-10}$	$10^{-11}$	$10^{-12}$	$10^{-13}$	$10^{-14}$	$[H^+]$ (mol/L)

← Increasing acidity — Neutral — Increasing alkalinity →

(pH) Inverse relationship with  $[H^+]$ .

~ How to calculate the pH of acidic and basic solutions ?!

Ex: What is the pH of a solution whose hydrogen ion concentration is  $3.2 \times 10^{-4}$  mol / L ?!

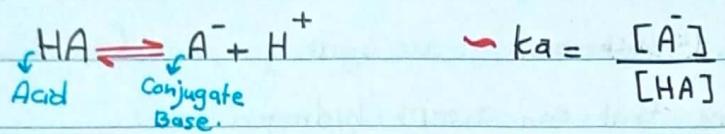
$$\begin{aligned} \sim pH &= -\log [H^+] \sim \\ &= -\log (3.2 \times 10^{-4}) \\ &= -\log (3.2) - \log (10^{-4}) \\ &= -0.5 + 4 \end{aligned}$$

$$pH = 3.5$$

#### • Dissociation Constants ( $K_a$ )

✓ The tendency of any acid (HA) to lose a proton and form its conjugate base ( $A^-$ ) is called [dissociation constants ( $K_a$ )].

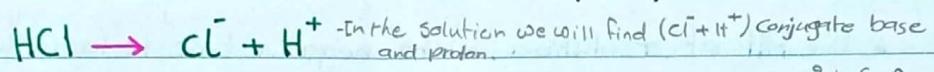
✓ when an acid loses a proton, its conjugate base is formed.



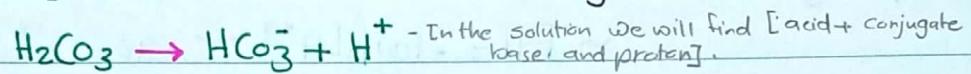
$$K_a = \frac{[\text{A}^-]}{[\text{HA}]}$$

\* The stronger the acid, the greater its tendency to lose its proton.

\* Strong acids are acids that dissociate completely in solution.



\* Weak acids are acids that dissociate only to a limited extent.



\* The weak acid  $\hookrightarrow$  proton donor  $\rightsquigarrow$  dissociates into a hydrogen ion ( $\text{H}^+$ ) and an anionic component ( $\text{A}^-$ ), called the  $\hookrightarrow$  conjugate base (or salt).

### - $\text{pK}_a$ -

.  $\text{pK}_a = -\log K_a$       p the acid dissociate to base so half of the acid dissociate to base and half remain as acid.

.  $\text{pK}_a$  is the pH at which 50% dissociation occurs.

.  $\text{pK}_a$  value is easier to work with and remember than  $K_a$  value.

$$\text{pK}_a \uparrow \text{K}_a \downarrow$$

. The stronger the tendency of an acid to dissociate the higher is the  $K_a$  and the lower is its  $\text{pK}_a$ .

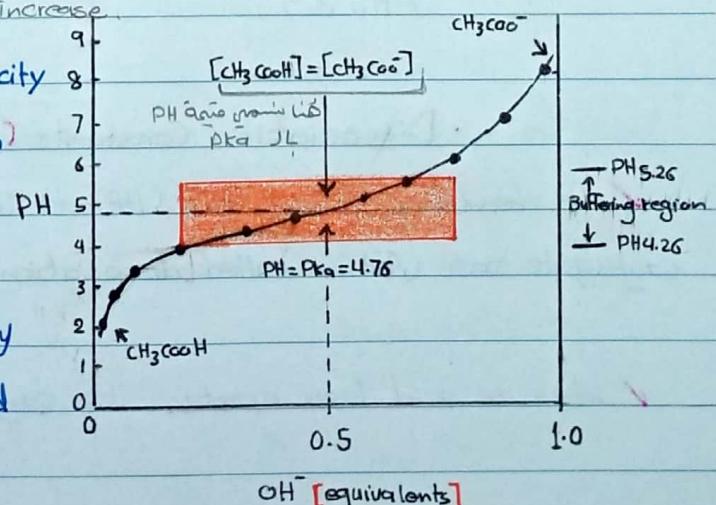
$$\text{pK}_a \downarrow \text{K}_a \uparrow \rightarrow \text{less dissociation, more acid}$$

- pH increase, the dissociation of acid increases (thus the concentration of the acid decreases and the  $\uparrow$  conjugate base increases).

. The maximum buffering capacity exists when the pH of the solution

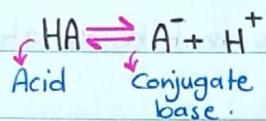
equals the  $\text{pK}_a$  of the buffer,

$[\text{conjugate base}] = [\text{acid}]$ , the buffer can then respond equally to both added acid and added base.



## [Buffers]

- A buffer is a solution that resists pH changes when acids or bases are added to the solution.
- Buffer solutions consist of a weak acid [undissociated acid] and its conjugate base (the form of the acid having lost its proton).



- A buffer works because added acids ( $\text{H}^+$ ) are neutralized by the conjugate base ( $\text{A}^-$ ) which is converted to the acid (HA).
- Added bases are neutralized by the acid (HA), which is converted to the conjugate base ( $\text{A}^-$ ).

- Two factors determine the effectiveness of a buffer

- 1- its  $\text{pKa}$  relative to the  $\text{pH}$  of the solution.
- 2- its concentration.

### - Henderson - Hasselbalch Equation -

- adjusted equation shown below describe the relationship between the acid and its conjugate base with pH and pKa.

$$(\text{pH} = \text{pKa} + \log \frac{\text{[A}^-]}{\text{[HA]}}) \rightarrow (\text{pH} = \text{pKa} + \log_{10} \frac{\text{[Conjugate Base]}}{\text{[Acid]}})$$

- The most effective buffers is when  $\text{pH} = \text{pKa}$  means it has equal concentrations of acid [HA] and its conjugate base  $\text{A}^-$  (50% of both forms  $\text{AH}$  &  $\text{A}^-$  present in solution).

$$\begin{aligned} & [\text{A}^-] = [\text{HA}] = 1 \\ & \text{pH} = \text{pKa} + \log \frac{1}{1} \\ & \boxed{\text{pH} = \text{pKa}} \end{aligned}$$

- At ( $\text{pH} = \text{pK}_a \pm 1$ ) the buffer capacity falls to 33% of the maximum value. Therefore the buffer is effective one point up or down the pH  $\text{pK}_a$  value.
- if pH less than  $\text{pK}_a$ , the concentration of acid higher than concentration of base

### - Chemical bonds -

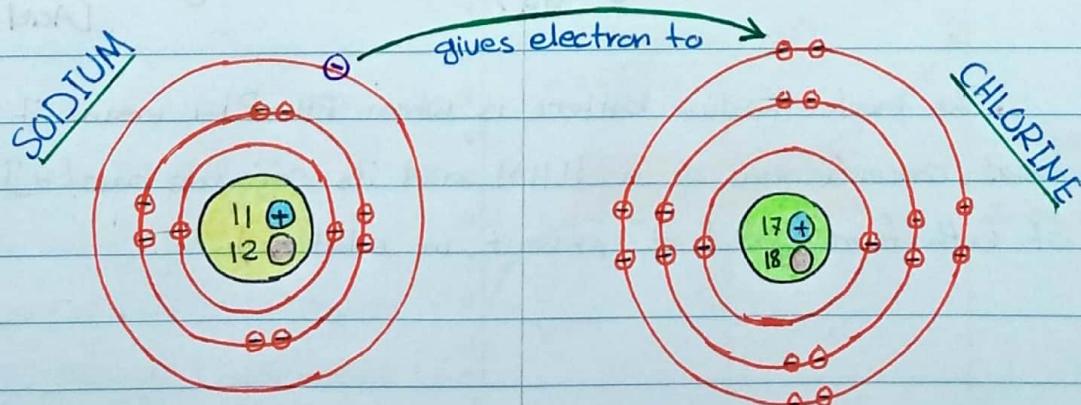
- Refers to the attractive forces that hold atoms together in compounds.
- chemically, bonding occurs when an atom give up electrons, accept electrons, or share electrons with another atom.
- A stable compound occurs when the total energy of the combination has lower energy than the separated atoms.

#### [Major Bonds in Biological Molecules]

- (1) Ionic bonding    (2) Covalent bonding    (3) Hydrogen bond    (4) Hydrophobic Interactions.

##### (1) Ionic bonding

- electrons are completely transferred from one atom to another.
- The oppositely charged ions are attracted to each other by electrostatic forces, which are the basis of the ionic bond.



- loses  $e^-$   $\rightarrow$  positively charged

- gain  $9e^-$   $\rightarrow$  negatively charged.  
or accept

- Ionic compounds common features :

1- form between metals and non-metals.

2- In naming simple ionic compounds, the metal is always first, the non-metal second ~ Ex: (Sodium Chloride)

3- dissolve easily in Water and other polar solvents.

4- In solution, ionic compounds easily conduct electricity.

5- Tend to form crystalline solids with high melting temperatures

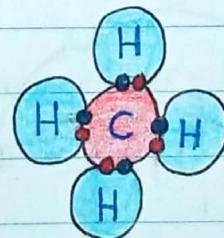
## (2) Covalent bonding

- results from sharing one or more electron pairs between two atoms.

- occurs because the atoms in the compound have a similar tendency for electrons (generally to gain electrons).

- The elements involved will share electrons in an effort to fill their valence shells.

- Covalent bonding in carbon -



- Electron from hydrogen.
- Electron from carbon.

- Covalent Bond -

1- Polar covalent bonds.

2- NonPolar covalent bonds.

1- Polar covalent bonds result when electrons are unequally shared between atoms [formed between atoms with different electronegativity].

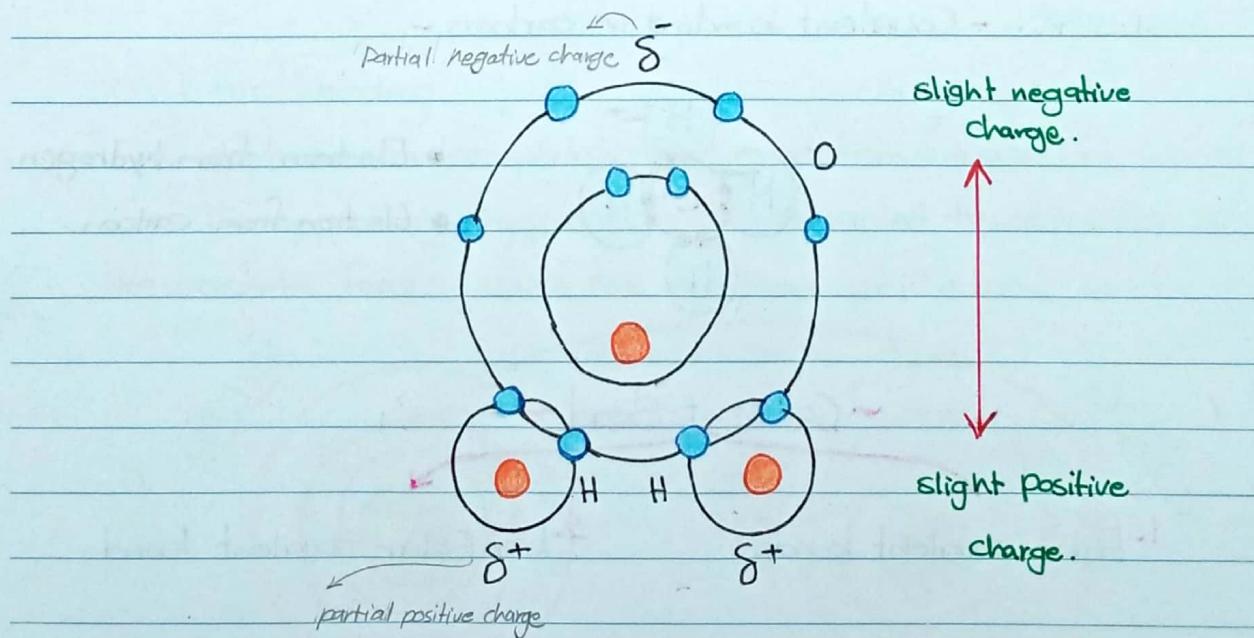
2- Non Polar covalent bonds result when electrons are equally shared between atoms [formed between atoms with the same electronegativity].

- Electronegativity is the ability of an atom to attract electrons towards itself in a covalent bond.

- Polar covalent bonding occurs because one atom has a stronger affinity for electrons (electronegativity) than the other.

- In a Polar covalent bond, the bonding electrons will spend a greater amount of time around the atom that has the stronger affinity for electrons.

- Polar bond in Water molecule. The large oxygen atom has a stronger affinity for electrons than the small hydrogen atoms.



## \* The Electronegativities of Selected Elements.

P	H	C	N	O	F
2.1	2.1	2.5	3.0	3.5	4.0
K 0.8	Na 0.9	Ca 1.0	Mg 1.2	Cl 3.0	

1-  $\boxed{\text{Na-Cl}}$   $3.0 - 0.9 = 2.1$  Ionic.

2-  $\boxed{\text{C-H}}$   $2.5 - 2.1 = 0.4$  non-

3-  $\boxed{\text{H-O}}$   $3.5 - 2.1 = 1.4$  polar

- \* If the electronegativity difference between two atoms is less than about 0.5 it will be essentially [non-Polar] and if the difference is 0.5 and less than 2 it is [Polar] and if the difference is greater than 2.0 it is often considered to be [Ionic].

## 3- Hydrogen bond

- Hydrogen bond is the attractive interaction of a hydrogen atom which covalently bonded to an electronegative atom with another electronegative atom like nitrogen, oxygen or fluorine.

- The Partial positive region of hydrogen is attracted to the Partial negative region of another molecule.
- The hydrogen must be covalently bonded to another electronegative atom to create the bond.
- The hydrogen bond is stronger than a van der waals interaction, but weaker than covalent and ionic bonds.

#### 4- Hydrophobic Interactions

- Nonpolar groups do not form hydrogen bond to water so they are insoluble in water. ex: [oil, wax, fat, lipid]

- Hydrophobic substances are "excluded" from aqueous solution this drives these molecules to cluster together.

- No affinity between nonpolar substances except Van der Waals forces that promote the weak bonding of nonpolar substances.

##### Van der Waals forces.

✓ are weak attractive forces between electrically neutral atoms or molecules.

✓ They are much weaker than the ionic bond or the covalent bond.

✓ These forces may develop because the rapid shifting of electrons within molecules causes some parts of the molecule to become momentarily charged, either positively or negatively.

✓ for this reason, weak, transient forces of attraction can develop between particles that are actually neutral.

The magnitude of the forces is dependent on the distance between neighbouring molecules.