

Lecture 3 - 4

Chemical Reactions and Chemical Equations

- A **chemical reaction** is a process that always results in the interconversion of chemical substances.
- The substance or substances initially involved in a chemical reaction are called reactants.
- Chemical reactions are usually characterized by a chemical change, and they yield one or more products, which are in general different from the reactants .



- Classically, chemical reactions encompass changes that strictly involve the [motion of electrons](#) in the forming and breaking of [chemical bonds](#) .
- Different chemical reactions are used in combinations in [chemical synthesis](#) in order to get a desired product.
- In [biochemistry](#), series of chemical reactions [catalyzed](#) by [enzymes](#) form [metabolic pathways](#), by which syntheses and decompositions ordinarily impossible in conditions within a cell are performed.

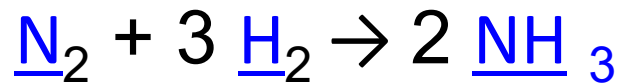


- **A chemical equation** describes what happens in a chemical reaction.
- The equation identifies the reactants (starting materials) and products (resulting substance), the formulas of the participants, the phases of the participants (solid, liquid, gas), and the amount of each substance.
- **Balancing a chemical equation** refers to establishing the mathematical relationship between the quantity of reactants and products (**Stoichiometry**).
- The quantities are expressed as grams or moles.



Reaction types

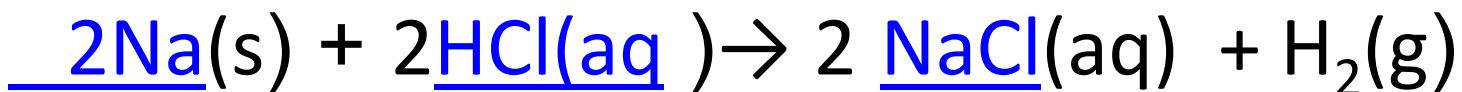
- **Isomerisation** ,
in which a chemical compound undergoes a structural rearrangement without any change in its net atomic composition; see stereoisomerism
- **Direct combination** or **synthesis**, in which 2 or more chemical elements or compounds unite to form a more complex product :



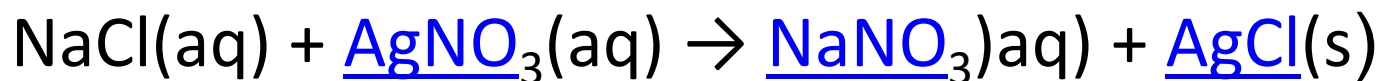
- **Chemical decomposition** or **analysis**, in which a compound is decomposed into smaller compounds or elements:
$$2 \underline{\text{H}}_2\underline{\text{O}} \rightarrow 2 \text{H}_2 + \underline{\text{O}}_2$$



- **Single displacement or substitution**, characterized by an element being displaced out of a compound by a more reactive element :



Metathesis or Double displacement reaction, in which two compounds exchange ions or bonds to form different compounds :

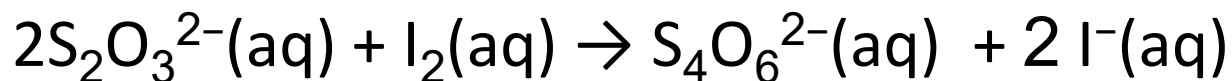


- **Acid-base reactions**, broadly characterized as reactions between an acid and a base, can have different definitions depending on the acid-base concept employed. Some of the most common are :
- Arrhenius definition: Acids dissociate in water releasing H_3O^+ ions; bases dissociate in water releasing OH^- ions .
- Brønsted-Lowry definition: Acids are proton (H^+) donors; bases are proton acceptors. Includes the Arrhenius definition .
- Lewis definition: Acids are electron-pair acceptors; bases are electron-pair donors. Includes the Brønsted-Lowry definition .



- **Redox reactions** ,
- in which changes in **oxidation numbers** of atoms in involved species occur. Those reactions can often be interpreted **as transferences of electrons** between different molecular sites or species.

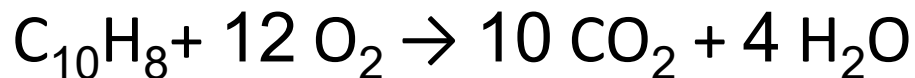
A typical example of redox reaction is :



In which I_2 (iodine) is reduced to I^{-} (iodide) and $\text{S}_2\text{O}_3^{2-}$ (**thiosulfate** anion) is oxidized to $\text{S}_4\text{O}_6^{2-}$ (tetrionate)

Combustion ,

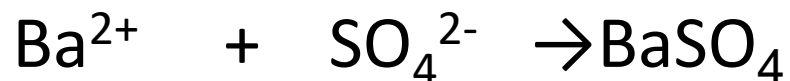
- a kind of redox reaction in which any combustible substance combines with an oxidizing element, usually oxygen, to generate heat and form oxidized products .



- **Precipitation reactions**

The formation of a solid product from a reaction in solution

A – by simple ionic interaction e.g.

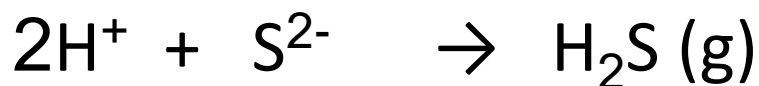
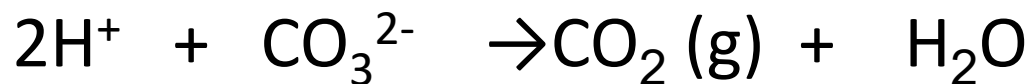


B – by reaction with organic reagent

e.g. $\text{Ni}^{2+} + \text{Dimethylglyoxim} \rightarrow \text{red ppt}$

- **Volatilization reactions**

In these reactions formation of gas or vapor occur by simple ionic reaction e.g.

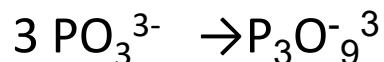
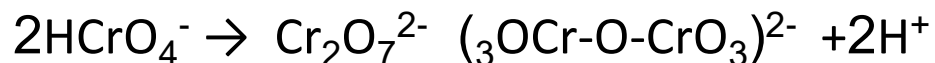
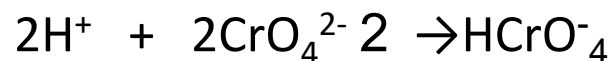


- Complex-forming reactions



- Polymerization reactions

many chemical species are capable of reacting with like species to form chain or ring e.g.



III. Chemical Reactions in Aqueous Solution

- Reactions occur rapidly when the reactants are dissolved in a solvent, usually water is the solvent used.
- Solution terminology:
- Solution - two or more substances in a single phase. It is made up of a solvent (the dissolver) and the solute (the dissolved). Although we think of solutions as liquids, they can also be gases or solids. 18-karat gold is a solid solution .
- Suspension - although these may look like solutions, the particles in it are large enough that they may condense. Muddy water is an example of this .
- Colloid - somewhere in the middle, this is neither a solution nor a suspension. Jello and mayonnaise are examples. Colloids can be distinguished from solutions with a flashlight - colloids will look cloudy under bright light .



- The **solvent** is generally taken to be the substance present in the solution in largest proportion , all other substance present in solution are considered to be **solute** .
- **Concentrated solution** : has a relatively large proportion of solute to solvent.
- **dilute solution** : has a relatively smaller proportion of solute to solvent.



- **Saturated solution** contains the maximum amount of a solute that will dissolve in a given solvent at a specific temperature.
- **Unsaturated solution** contains less solute than it has the capacity to dissolve.
- **Supersaturated solution** contains more solute than is present in a saturated solution.
- **Solutes and the conducting of electricity** - some substances break up into ions and conduct electricity when dissolved. These are called **electrolytes** .All ionic compounds are electrolytes **Nonelectrolytes** , on the other hand, do not conduct electricity when dissolved. Electrolytes are the reason that tap water conducts electricity .



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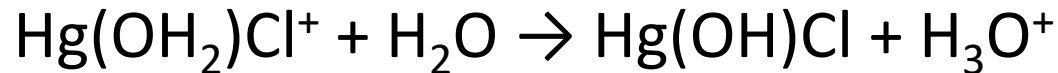
- **Weak electrolytes**

Incomplete dissociation in solution and ion-pair formation

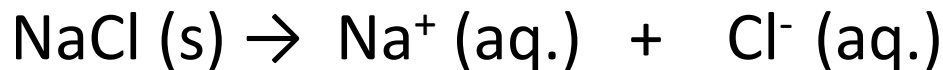
This happens with weak acids and bases



There are also many salts, such as HgCl_2



- **Strong electrolytes** Highly ionic salts such as NaCl which are essentially totally dissociated in solution.



Molecular substance can also be strong electrolyte e.g.

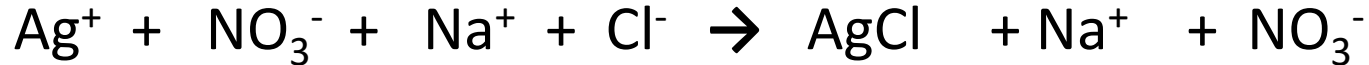


Reaction between ions

Molecular equation



Ionic equation



Net ionic equation



- **Acids and Bases**

acid. ([Lat. *acidus*, sour])

1. a compound which releases hydrogen ions (H^+) in solution (*Arrhenius*).
2. a compound containing detachable hydrogen ions (*Bronsted-Lowry*).
3. a compound that can accept a pair of electrons from a base (*Lewis*)..



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- **Acid conjugate base (anion)**

- HCl Cl⁻ (chloride)

- HCN CN⁻ (cyanide)

- H₂S S²⁻ (sulphide)

- **Oxoacids**

- HNO₃ , H₂SO₄ , H₃PO₄

- Monoprotic acid: are able to furnish one H⁺ (HCl, HNO₃)

- Dioprotic acid: are able to furnish 2 H⁺ (H₂SO₄)

- trioprotic acid: are able to furnish 3 H⁺ (H₃PO₄)

- Acidic anhydride: acid without water (CO₂ , SO₂)

- Acid salts: when a base reacts with polyprotic acid, two or more salts may be formed. (NaHSO₄, Na₂SO₄ , Na₂HPO₄, NaH₂PO₄, Na₃PO₄).



base. alkali; alkaline; basic. Compare with acid.

1. a compound that reacts with an acid to form a salt.
2. a compound that produces hydroxide ions in aqueous solution (*Arrhenius*).
3. **a molecule or ion that captures hydrogen ions.**(*Bronsted-Lowry*).
4. a molecule or ion that donates an electron pair to form a chemical bond.(*Lewis*).

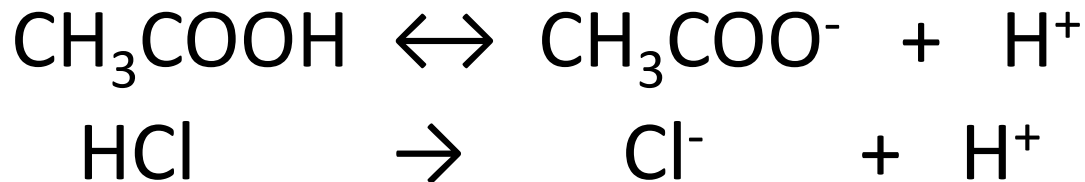
Examples of bases NaOH ,KOH ,NH₃ .

Basic anhydride: metal oxides (Na₂O,CaO)



common-ion effect

- Is brought about by adding to a solution of weak electrolyte a strong electrolyte having an ion in common with the weak electrolyte.
- example :
ionization of a solution of acetic acid will depress by the addition of HCl



- Example : calculate the hydrogen ion concentration in liter of solution containing 0.1 mole of acetic acid and 0.1 mole sod. acetate.



$$K_a = [\text{H}^+] \cdot [\text{Ac}^-] / [\text{AcH}] = 1.8 \times 10^{-5} .$$

Since sod. acetate is a strong electrolyte , it is completely ionized, hence concentration of acetate ion is 0.1 mol.



$$0.1 - x \quad x + 0.1 \quad x$$

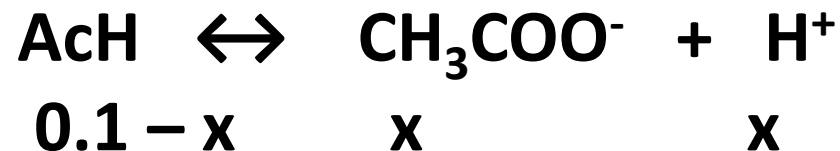
Negligting x (very small) then

$$(x) \cdot (0.1) / 0.1 = 1.8 \times 10^{-5} .$$

$$X = \text{H}^+ = 1.8 \times 10^{-5} .$$

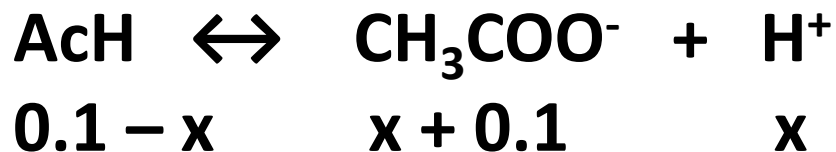


- If pure 0.1 M acetic acid the hydrogen ion concentration is



Negligting x (very small) then

$$(x) \cdot (x) / 0.1 = 1.8 \times 10^{-5} .$$



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$$(x) \cdot (0.1) / 0.1 = 1.8 \times 10^{-5} .$$

$$X^2 = 1.8 \times 10^{-5} .$$

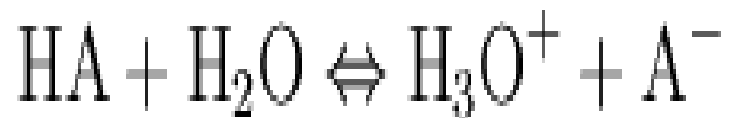
$$X = \text{H}^+ = \sqrt{1.8 \times 10^{-5}} .$$

- $= 1.8 \times 10^{-3} .$



Acids in equilibrium

- Consider an imaginary acid, HA, in water. According to the Brønsted-Lowry acid/base theory, the acid should protonate the water to form hydronium and the *conjugate base*, A⁻. There will be an **equilibrium** between the acid and water, and hydronium and the conjugate base.



- This equilibrium can be used to calculate the concentrations of species in the solution.



Acid Dissociation Constant

- Like all equilibria, an acid/base dissociation will have a particular **equilibrium constant** which will determine the extent of the reaction (whether it lies to the left or right of the equation)

$$K = \frac{[\text{H}_3\text{O}^+][\text{A}^-]}{[\text{H}_2\text{O}][\text{HA}]}$$

- Because the equilibrium is used for calculating the concentrations of weak acids, very little water actually reacts. The concentration of water during the reaction is, therefore, a constant, and can be included in the expression for K. This gives rise to a special equilibrium constant, K_a , known as the **acid dissociation constant**. It is simply K multiplied by the concentration of water.



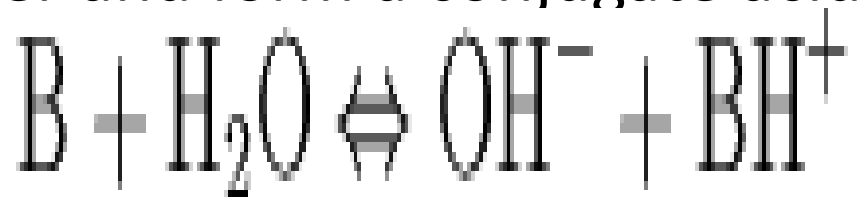
$$K_a = K[\text{H}_2\text{O}] = \frac{[\text{H}_3\text{O}^+][\text{A}^-]}{[\text{HA}]}$$

The K_a determine how acidic it is, how far its equilibrium lies to the right



Base Dissociation Constant

- A similar equilibrium exists when a weak base is dissolved in water. The base will abstract a proton from water and form a conjugate acid, BH^+



- This equilibrium has its own special constant, K_b , known as the **base dissociation constant**. Like the acid dissociation constant, it is defined as the equilibrium constant multiplied by the concentration of **water**.



$$K_b = K[\text{H}_2\text{O}] = \frac{[\text{BH}^+][\text{OH}^-]}{[\text{B}]}$$

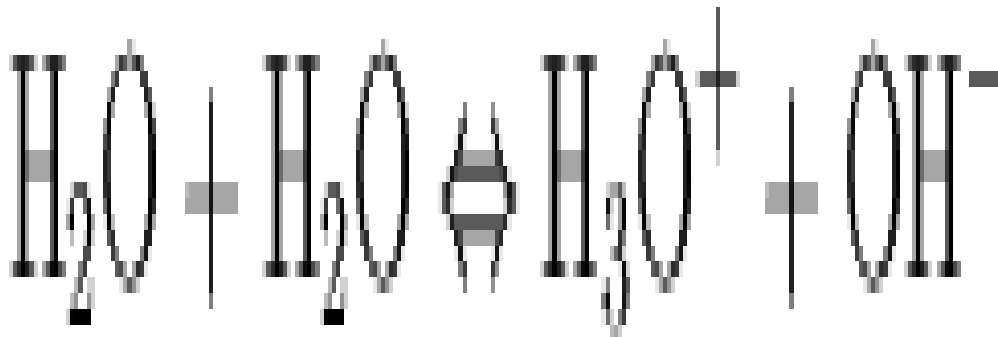


$$\frac{[\text{H}_3\text{O}^+][\text{A}^-]}{[\text{HA}]} \times \frac{[\text{HA}][\text{OH}^-]}{[\text{A}^-]} = [\text{H}_3\text{O}^+][\text{OH}^-]$$
$$K_a \times K_b = K_w$$



Ion Product Constant

- A special equilibrium exists between ordinary water molecules. Occasionally, one water molecule will act as an acid, and donate a proton to another water molecule (which acts as a base). Water can autoionize itself.



- By the Le Chatelier Principle, we can see that if the hydronium ion concentration is increased (say, by adding an acid), the equilibrium will move to the left and there will be a *lower* concentration of hydroxide. Thus, hydronium and hydroxide concentration are inversely related - an increase in one will result in a decrease in the other, and vice versa.

pH & pOH

$$\text{pH} = -\log [\text{H}^+]$$

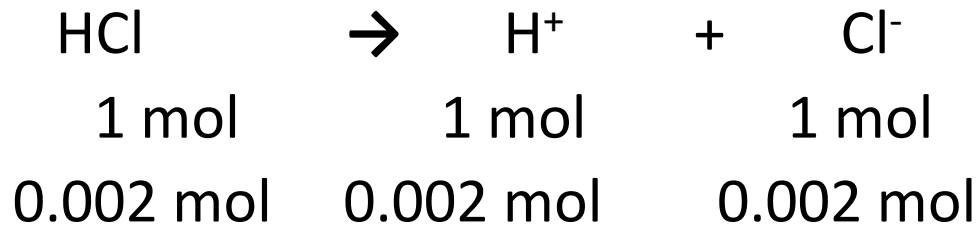
$$\text{pOH} = -\log [\text{OH}^-]$$

$$\text{pH} + \text{pOH} = 14$$

Example:

What is the pH of a solution of 0.002 M HCl?

- HCl is strong acid ,therefore it is completely dissociate in solution .



Therefore $[\text{H}^+] = 0.002 \text{ M}$

$$\text{pH} = -\log [\text{H}^+] = -\log 0.002 = -\log 10^{-3} = 2.7$$



- Example :
- What is the pH of 5×10^{-4} solution of NaOH ?
- $\text{pOH} = -\log [\text{OH}^-]$
 $= -\log 5 \times 10^{-4} = 3.3$
 $\text{pH} = 14 - 3.3 = 10.7$

