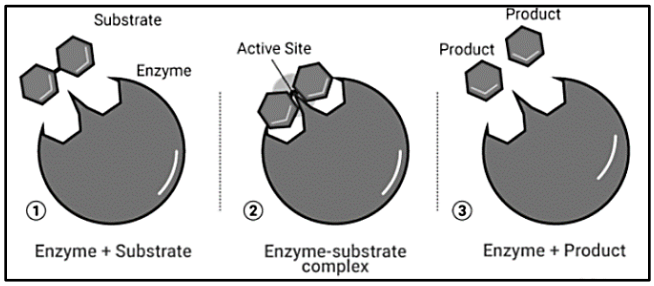
SURFACE CHEMISTRY

CATALYSIS

Catalyst and catalysis and some other terms: -

Catalysis is the process of increasing the speed of chemical reactions by adding substances called catalysts. The catalyst is not consumed during the reaction and remains unchanged after the reaction. Usually only a very small amount of catalyst is required.

Selectivity of catalyst and its activity is an important concept. Catalytic surface is generally inactive in nature. When a reactant is adsorbed on the catalyst surface, it makes the catalyst active. This incites the further process of reaction. Catalysts are highly specific in nature, that is, what may be a catalyst for one can be an inhibitor for another. Some catalysts with the same set of reactants give different products in comparison to other catalysts.



Some basic properties of catalyst are explained below:

Activity of Catalyst

Catalyst has an ability to increase the rate of reaction. This ability of catalyst is known as the activity of catalyst. It depends upon adsorption of reactants on the surface of catalyst. Chemisorption is the main factor governing the activity of catalysts. The bond formed during adsorption between the catalytic surface and the reactants must not be too strong or too weak.

It must be strong enough to make the catalyst active whereas, not so strong that the reactant molecules get immobilized on the catalytic surface leaving no further space for the new reactants to get adsorbed. Generally for the hydrogenation reaction, from Group 5 to Group 11 metals, the catalytic activity increases. The catalytic activity is found to be highest for group 7-9 elements of the periodic table.

$$2H_2(g) + O_2(g) \xrightarrow{Pt} 2H_2O(l)$$

Selectivity of Catalyst

Catalysts are highly specific compounds. They have an ability to direct the reaction to yield a particular product. The reaction with same reactants but different catalyst may yield different products. This is termed as the selectivity of catalyst. Catalysts are highly selective in nature. They can accelerate a particular reaction while inhibit another reaction. Hence, we can say a particular catalyst can catalyse one particular reaction only. It may fail to catalyse another reaction of the same type. For example: reaction of hydrogen and carbon monoxide yields methane when nickel is used as catalyst, methanol when a mixture of zinc oxide and chromium oxide is used as catalyst and methanal when only copper is used as catalyst.

$$CO(g) + 3H_2(g) \xrightarrow{Ni} CH_4(g) + H_2O(g)$$

$$CO(g) + 2H_2(g) \underset{Cu/ZnO-Cr_2O_3}{\longrightarrow} CH_3OH(g)$$

$$CO(g) + H_2(g) \xrightarrow{Cu} HCHO(g)$$

Types of catalysts

A catalyst is a chemical compound which makes the reaction occur more quickly by reducing the reaction's activation energy barrier. During the reaction it isn't eaten.

- **Homogeneous catalyst –**

  Homogeneous catalysts are usually soluble metal salts or compounds that are dissolved in an effective organic solvent that is used as the medium for reaction. (here catalyst and the reactants are on the same phase)

- **Heterogeneous catalyst –**

  A heterogeneous catalyst is a functional material which under conditions of reaction continually creates active sites with its reactants. (here catalyst and reactants are on different phase)

Catalysis

Catalysis definition or catalysis meaning can be given as the increase in the rate of a chemical reaction because of the participation of an additional substance, which is known as a catalyst. Catalyst is not consumed in the catalyzed reaction, but it can continue to act repeatedly. Even a small amount of catalyst is usually sufficient to bring about this effect. In contrast with the catalyzed mechanisms,

usually, the catalyst reacts to generate a temporary intermediate, which then regenerates the original catalyst with the help of a cyclic process.

Mechanism of Catalysis

- There requires less free energy to reach the transition state in the presence of a catalyst, but there will be no change in the total free energy from reactants to products. A catalyst can participate in various chemical transformations. Also, the effect of a catalyst may vary because of the presence of other substances such as promoters (which increases the activity and affect the temperature of the reaction as well) or inhibitors (which reduces the catalytic activity).

- Catalyzed reactions carry lower activation energy (the rate-limiting free energy of activation) to that of the identical uncatalyzed reaction, resulting in a higher reaction rate for the same reactant concentration, at the same temperature. As in the case of other chemical reactions, the reaction rate completely depends upon the contact frequency of the reactants in the rate-determining step.

- In this slowest step, the catalyst participates usually, and the reaction rate depends upon the amount of catalyst. Although catalysts are not consumed by the self reaction, they may be deactivated, inhibited, or destroyed by using the secondary processes.

Types of Catalysts

- Based on whether the catalyst exists in the same phase as the substrate, catalysts are classified into Homogeneous and Heterogeneous catalysis. Biocatalysts (also called enzymes) are often seen as a separate group.

Heterogeneous Catalysts

- These types of catalysts act in a different phase compared to the reactants. Most heterogeneous catalysts are solids that act either on the substrates of liquid or gaseous reaction mixture. At the same time, diverse mechanisms for the reactions on the surface are known, based on how the adsorption occurs.

- The total surface area of a solid has a major effect on the reaction rate. The smaller the size of the catalyst particle, the larger the area of surface for a given mass of particles. A heterogeneous catalyst has active sites, which are called crystal faces or atoms where the reaction actually occurs. Most of the catalyst surface is catalytically inactive.

Electrocatalysts

- In the electrochemistry context, specifically in fuel cell engineering, multiple metal-containing catalysts are used to enhance the half-reaction rates that comprise the fuel cell. A common type of fuel cell, named electrocatalyst is based upon the nanoparticles of platinum that are supported on the carbon particles, which are slightly larger. But, when in contact with one of the fuel cell electrodes, this platinum increases the oxygen reduction rate either to hydroxide or to water or hydrogen peroxide.

Homogeneous Catalysts

- These function in the same phase as the reactants, but the mechanistic principles that are involved in the heterogeneous catalysis are generally applicable. Typically, the homogeneous catalysts are dissolved in a substrate solvent. An example of homogeneous catalysis can be the influence of H+ on the carboxylic acids' esterification, like the formation of methyl acetate from methanol and acetic acid.

Photocatalysts

- Photocatalysis is the process where the catalyst can receive light (like visible light), be promoted to an excited state, and then undergoes an intersystem crossing with the starting material, and then, returning to the ground state without being consumed. After that, the excited state of the starting material will undergo the reactions ordinarily. It could not be directly illuminated. For example, usually, the singlet oxygen is produced by photocatalysis. Photocatalysts are also considered as the primary ingredient in the dye-sensitized solar cells.

Enzymes and Biocatalysts

- The enzymes and other biocatalysts are often treated as a third category. In comparison, the same mechanistic principles apply to homogeneous, heterogeneous, and biocatalysis.

Catalysis

- In biology, enzymes are the protein-based compounds that catalyze metabolism and other biochemical reactions as well. Though enzymes are the most commonly called biocatalysts, certain non-protein-based biomolecules classes also exhibit the catalytic properties. These include ribozymes and synthetic deoxyribosymes and as well.

- Biocatalysts are recognized to be an intermediate between the heterogeneous and homogeneous catalysts; soluble enzymes are considered to be homogeneous catalysts, whereas the membrane-bound enzymes can be kept under the heterogeneous enzymes category.

- The catalysis impact factor or various factors affect the activity of enzymes (and other catalysts as well). A few of these include pH, temperature, the concentration of enzyme, products, and substrate. Water is an important reagent that acts as a catalyst. It acts in multiple bond-forming and bond-breaking reactions as well.