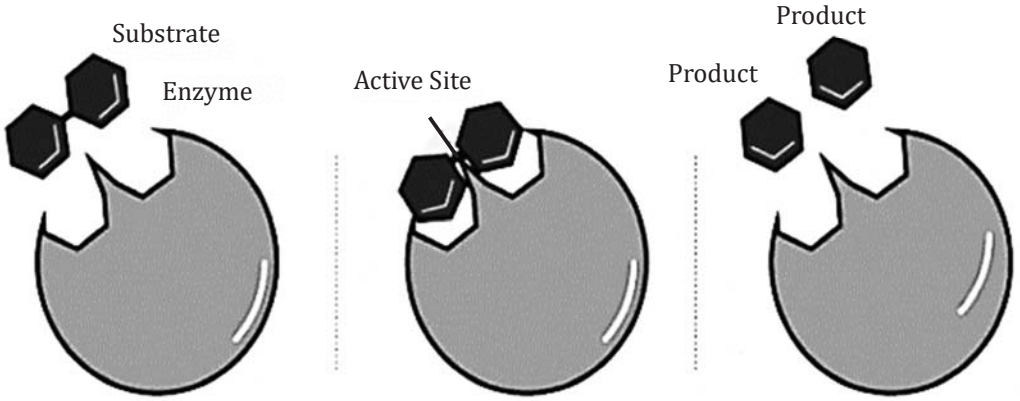
CATALYSIS

Catalyst and Catalysis and some other terms

Catalysis involves the acceleration of chemical reactions by the addition of substances known as catalysts. Importantly, catalysts are not consumed in the reaction and remain unchanged afterward, typically requiring only a minute quantity. The concept of selectivity and the activity of a catalyst plays a crucial role. The catalytic surface is generally inert, but when a reactant is adsorbed on this surface, it activates the catalyst, initiating the subsequent reaction process. Catalysts exhibit high specificity, meaning a substance that acts as a catalyst for one reaction might act as an inhibitor for another. Additionally, the same set of reactants with different catalysts can yield distinct products.



1. Enzyme + Substrate 2. Enzyme – Substrate complex 3. Enzyme + Product

Some basic properties of catalyst are explained below

Activity of Catalyst

A catalyst possesses the capability to enhance the rate of a reaction, a property referred to as the catalyst's activity. This activity is contingent upon the adsorption of reactants onto the catalyst's surface, with chemisorption being the primary determinant of catalytic activity. The bond formed during adsorption must strike a balance, being sufficiently strong to activate the catalyst but not so robust that it immobilizes reactant molecules on the catalytic surface, preventing the adsorption of new reactants. Generally, for hydrogenation reactions, the catalytic activity increases from Group 5 to Group 11 metals. Notably, the highest catalytic activity is observed for elements belonging to Groups 7-9 in the periodic table.

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

Selectivity of Catalyst

Catalysts are characterized by their high specificity, possessing the ability to guide a reaction toward the production of a specific product. When the same set of reactants is subjected to different catalysts, the outcomes may vary, illustrating the selectivity of the catalyst. Catalysts exhibit a remarkable degree of selectivity, enabling them to enhance a particular reaction while impeding another. Therefore, a specific catalyst is tailored to catalyze a particular reaction exclusively and may not be effective in catalyzing other reactions of the same type.

For instance, the reaction between hydrogen and carbon monoxide can result in methane with nickel as a catalyst, methanol with a mixture of zinc oxide and chromium oxide, and methanal when only copper is utilized as the catalyst.

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

$$CO(g) + 2H_2(g) \xrightarrow[Cu/ZnO-C_2O_3]{} CH_3OH(g)$$

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

Types of catalysts

A catalyst is a chemical compound that expedites a reaction by lowering the activation energy barrier without being consumed during the process.

(i) Homogeneous Catalyst

Homogeneous catalysts typically consist of soluble metal salts or compounds dissolved in an effective organic solvent, serving as the reaction medium. In this scenario, the catalyst and the reactants exist in the same phase.

(ii) Heterogeneous Catalyst

A heterogeneous catalyst is a functional material that, under reaction conditions, consistently generates active sites with its reactants. In this case, the catalyst and the reactants are in different phases.

Catalysis

Catalysis, defined as the acceleration of a chemical reaction through the involvement of an additional substance known as a catalyst, is characterized by the catalyst's ability to enhance reaction rates without being consumed. Even minute amounts of catalyst can repeatedly induce this effect. In contrast to uncatalyzed mechanisms, catalysts typically engage in a temporary intermediate reaction, subsequently regenerating the original catalyst through a cyclic process.

Mechanism of Catalysis

- The presence of a catalyst lowers the free energy required to reach the transition state, although the total free energy from reactants to products remains unchanged. Catalysts can participate in various chemical transformations, and their impact may be influenced by the presence of other substances like promoters (enhancing activity and affecting reaction temperature) or inhibitors (reducing catalytic activity).
- Catalyzed reactions exhibit lower activation energy, resulting in a higher reaction rate compared to identical uncatalyzed reactions at the same temperature and reactant concentration. The rate of the reaction is primarily determined by the contact frequency of the reactants in the rate-determining step. The catalyst usually participates in this slowest step, and the reaction rate is contingent on the catalyst's quantity. While catalysts are not consumed in self-reactions, they may undergo deactivation, inhibition, or destruction through secondary processes.

Types of Catalysts

Catalysts are categorized into Homogeneous and Heterogeneous catalysis based on their phase relationship with the substrate. Additionally, Biocatalysts, commonly referred to as enzymes, constitute a distinct group.

Heterogeneous Catalysts

- Heterogeneous catalysts operate in a phase distinct from the reactants. Primarily solids, these catalysts interact with liquid or gaseous substrates, showcasing diverse mechanisms on the surface based on the adsorption process.
- The total surface area of a solid profoundly influences the reaction rate. Smaller catalyst particle sizes result in larger surface areas for a given mass of particles. Heterogeneous catalysts feature

active sites, often crystal faces or atoms, where the actual reaction occurs, with a significant portion of the catalyst surface remaining catalytically inactive.

Electrocatalysts

In Fuel Cell Engineering

In the context of electrochemistry, particularly in fuel cell engineering, various metal-containing catalysts enhance half-reaction rates crucial to fuel cell functioning. A prevalent electrocatalyst type involves platinum nanoparticles supported on slightly larger carbon particles. When in contact with a fuel cell electrode, this platinum augments the oxygen reduction rate, leading to the production of hydroxide, water, or hydrogen peroxide.

Homogeneous Catalysts

These function in the same phase as the reactants, employing mechanistic principles akin to heterogeneous catalysis. Typically, these catalysts are dissolved in a substrate solvent. For instance, H+ influence on carboxylic acids' esterification demonstrates homogeneous catalysis, leading to the formation of methyl acetate from methanol and acetic acid.

Photocatalysts

Photocatalysis Process

Photocatalysis involves a catalyst that absorbs light, enters an excited state, undergoes intersystem crossing with the starting material, and then returns to the ground state without being consumed. Subsequently, the excited state of the starting material undergoes reactions typically.

For example, singlet oxygen is often produced through photocatalysis. Photocatalysts are integral components in dye-sensitized solar cells.

Enzymes and Biocatalysts

Intermediate Category

Enzymes and other biocatalysts constitute a distinct category, serving as an intermediate between heterogeneous and homogeneous catalysts. Soluble enzymes are considered homogeneous catalysts, while membrane-bound enzymes are categorized under heterogeneous enzymes.

Catalysis

- **Category:** Enzymes and other biocatalysts constitute a distinct category, serving as an intermediate between heterogeneous and homogeneous catalysts. Soluble enzymes are considered homogeneous catalysts, while membrane-bound enzymes are categorized under heterogeneous enzymes.

- **Catalysis in Biology:** In biology, enzymes, protein-based compounds, catalyze various biochemical reactions, showcasing metabolic activities. Although enzymes are commonly referred to as biocatalysts, certain non-protein-based biomolecules, such as ribozymes and synthetic deoxyribose's, also exhibit catalytic properties.

- **Factors Influencing Catalysis:** The catalysis impact factor and several factors affect enzyme activity, including pH, temperature, enzyme concentration, products, and substrate. Water, acting as a catalyst, plays a crucial role in multiple bond-forming and bond-breaking reactions