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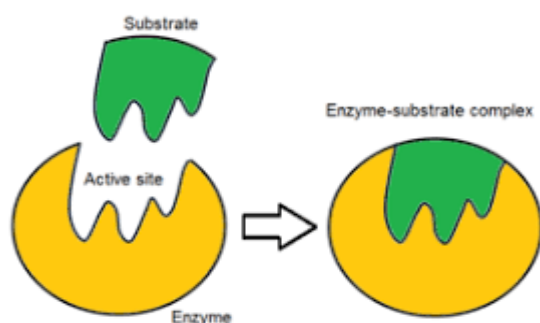
NAAC ACCREDITED 'A' GRADE



Topic : Enzyme Catalysis
Course Title : Enzymes
Paper : CC4
Unit : 1
Semester : 2
Name of the Teacher : Dr. Kakali Roy
Name of the Department : Biochemistry

Concept of Active site

Enzyme molecules contain a special pocket or cleft called the active site. The active site contains amino acid side chains that create a three-dimensional surface complementary to the substrate. The active site binds the substrate, forming an enzyme-substrate (ES) complex. ES is converted to enzyme-product (EP), which subsequently dissociates to enzyme and product.



Catalytic Power

Catalytic power is also called as the catalytic efficiency of enzyme. It is ultimately derived from the free energy released in forming the multiple weak bonds and interactions that occur between an enzyme and its substrate. This binding energy provides specificity as well as catalysis.

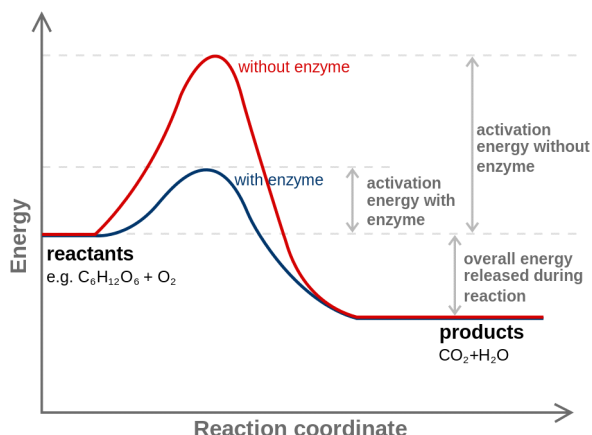
Binding Energy

The interaction between substrate and enzyme in the ES complex is mediated by the forces that stabilize enzyme protein structures including Hydrogen bonds, hydrophobic or ionic interaction. Formation of such weak interaction in the ES complex is accompanied by release of a small amount of free energy that provides a degree of stability to the interaction and this energy derived from enzyme substrate interaction is called binding energy, ΔG_B . Binding energy is a major source of free energy used by enzymes to lower the activation energies of reaction.

Standard free Energy change

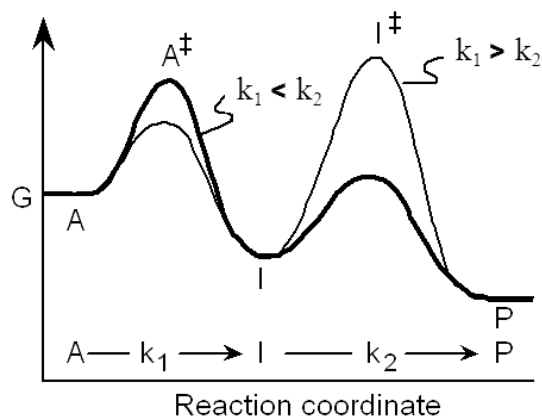
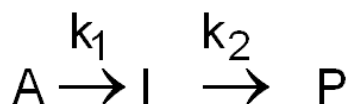
Standard free energy is the change in free energy that follows the formation of a mole of a substance from its constituent elements in their standard state (temperature 298 K, partial pressure of each gas 1 atm and concentration of each solute 1M).

Energy of Activation



Rate determining step

For a reaction that involves several steps, each step will have a corresponding transition state.



If the formation of I, an intermediate, from A is slower than the formation of P from I ($k_1 < k_2$) the activation barrier for the first step must be higher than the activation barrier for the second step (thick line). If k_1 is much slower than k_2 conversion of A to I is the rate-determining step for the reaction. That is, the overall reaction proceeds at a rate that can be no faster than k_1 . Conversely, if formation of P from I is much slower than formation of I from A ($k_2 < k_1$), the activation barrier for the second step is higher (thin line) and formation of P from I is rate-determining.

Collision Theory of reaction rate

Collision theory states that the rate of a chemical reaction is proportional to the number of collisions between reactant molecules. The more often reactant molecules collide, the more often they react with one another, and the faster the reaction rate. In reality, only a small fraction of the collisions are effective collisions. Effective collisions are those that result in a

chemical reaction.

In order to produce an effective collision, reactant particles must possess some minimum amount of energy. This energy, used to initiate the reaction, is called the **activation energy**. For every sample of reactant particles there will be some that possess this amount of energy. The larger the sample, the greater the number of effective collisions, and the faster the rate of reaction. The number of particles possessing enough energy is dependent on the **temperature** of the reactants. If reactant particles do not possess the required activation energy when they collide, they bounce off each other without reacting.

Some chemical reactions also require that the reactant particles be in a **particular orientation** to produce an effective collision. Unless the reactant particles possess this orientation when they collide, the collision will not be an effective one. The reaction of ozone with nitrogen monoxide is an example of how orientation can be important.

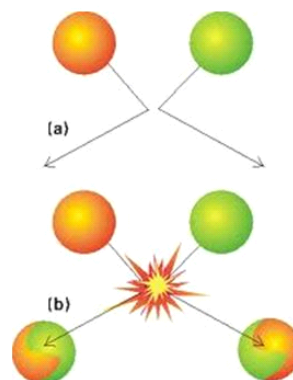
To summarize, the requirements for an effective collision (for a chemical reaction to occur):

1. The reactants must collide with each other.
2. The molecules must have sufficient energy to initiate the reaction (called activation energy).
3. The molecules must have the proper orientation.

Collision Theory

□ **Collision Theory:** A chemical reaction occurs ONLY when an EFFECTIVE COLLISION occurs. This happens under two conditions: WHEN THE REACTANTS COLLIDE WITH ...

1. The same or more energy than the activation energy (hit 'em hard enough)
1. The correct orientation (hit 'em in the right place)



4 Factors that Affect Rates



- **Concentration**
 - Greater concentration of reactants means there will be more collisions and therefore faster rates!
- **Surface Area**
 - Increased surface area means greater chances for collisions, and therefore faster rates!
- **Temperature**
 - Higher temperatures means particles collide with greater kinetic energy, increasing the rate of reaction!
- **Catalysts**
 - Catalysts speed up reactions without being used up. They lower the activation energy, meaning more collisions to be successful!

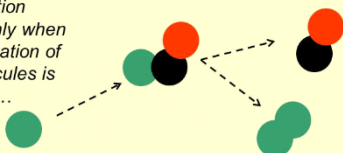
Activation Energy



Orientation factors into the equation

The orientation of a molecule during collision can have a profound effect on whether or not a reaction occurs.

The reaction occurs only when the orientation of the molecules is just right...



When the green atom collides with the green atom on the molecule, a **reactive or effective collision** occurs.

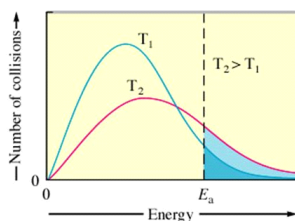
- An **effective(successful)collision** is a collision that occurs with enough energy and with particles aligned correctly
- In an **ineffective(unsuccessful)collision**, the colliding particles remain unchanged

Temperature & Activation Energy



- Collision theory predicts that as temperature increases, reaction rate will increase due to the higher average kinetic energy of the particles involved in the reaction – increasing the frequency of collisions as well as the fraction of collisions with the required activation energy.

Since rate increases with temperature, we expect that the rate constant will increase with temperature also.



References :

1. Voet D, Voet JG (2011), Biochemistry (4th ed.), New York : Wiley
2. www.Bioinfo.org.cn > chapt 08 > bio1
3. www.google.com