Activated Complex Theory:

Activated complex theory is also called as transition state theory. Theory of chemical reaction that relates the rate of reaction to an equilibrium between the reactants and an activated complex or transition state, which is a maximum energy configuration of the reactants as they proceed along the reaction coordinate.

The collision theory was inadequate to explain the mechanism of most of reactions. Therefore a more modern theory, known as transition state theory was given by Eyring and Polany in 1935 It is also known as theory of absolute reaction rates or activated complex theory.

Postulates of Transition State Theory:

These are as follows:

(1) As the recent molecule approach eachother, there is continuous series of changes in bond distance. These changes are accompained by energy changes.

(2) The reactant molecules are transformed into an energy rich intermediate called activated complex or transition state.

(3) The activated complex may be formed by some loose association or binding of reactant molecules with necessary rearrangement of valance bonds and energy. Or if it be a unimolecular reaction, the reactant molecule may produce the activated complex by rearrangement of atoms and redistribution of energy.

(4) The activated complex, though unstable, has transient existance. It is treated formally as a definite molecule with an independent entity. The activated complex is in equilibrium with the reactants. The potential energy of activated complex is maximum.

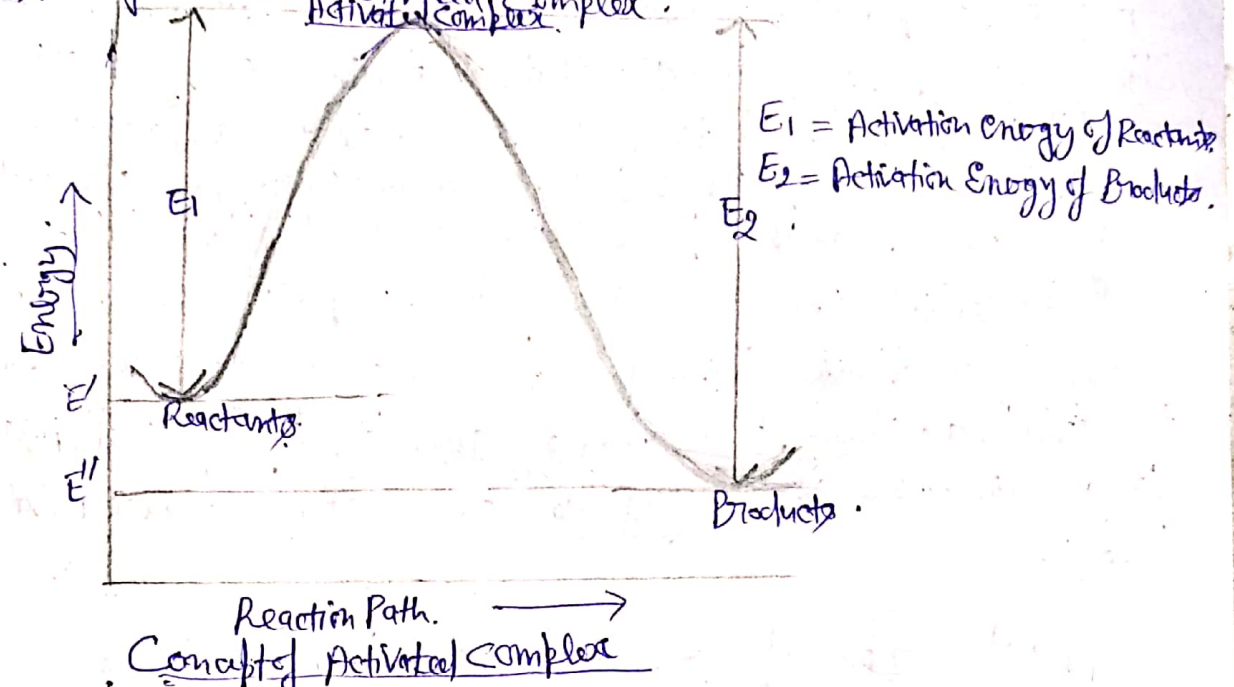
Reactants $\rightleftharpoons$ Activated complex.

(5) The activated complex decomposes into products as.

Reactants $\rightleftharpoons$ Activated complex $\longrightarrow$ Products

Contd.

⑥ The activation energy of reaction, in the light of transition state theory, is defined as the additional energy which the reacting molecules must aquire to form the activated complex.



Concept of Activated complex

Mathematical OR Thermodynamic Treatment of Transition State Theory.

Consider a bimolecular reaction between reactants A and B. Then according to transition state theory.

$$A + B \rightleftharpoons X^{\neq} \longrightarrow \text{Products}$$

Reactants. Activated complex

The equilibrium constant (K^*) for the formation of activated complexes.

$$K^* = \frac{X^*}{[A][B]} \quad \text{---(1)}$$

or

$$[X^*] = K^*[A][B] \quad \text{---(2)}$$

According to transition state theory, the rate of reaction is the number of activated complexes, which pass over the potential barrier in a unit time. This in turn, is equal to the concentration of activated complex multiplied by the frequency at which the complex would decompose into products. Mathematically,

$$\frac{dx}{dt} = [X^*] : \text{Rate (or frequency) of dissociation of activated complex} \quad \text{---(3)}$$

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