10.2 : Collision Theory & Transition State Theory

Objectives:

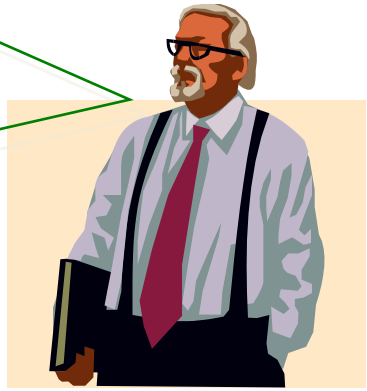
- Explain the requirements for an effective collision
- State the conditions for a reaction to occur
- Draw and label the Energy Profile Diagram
- Define activation energy and activated complex
- State the characteristics of an activated complex

QUESTION?

Does every collision result in a reaction?

ANSWER!

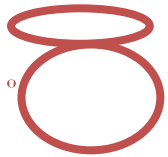
Only a small fraction of collisions results in a reaction. (~1 in every 10^{13} collisions!)



QUESTION?

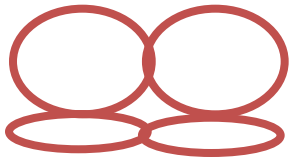
Why doesn't every molecular collision result in a reaction?

Illustration 1:



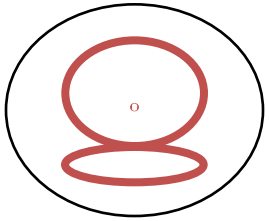
$2AB \longrightarrow A_2 + B_2$

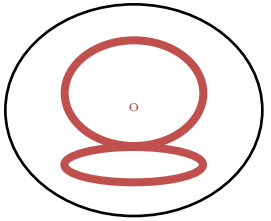
A - A



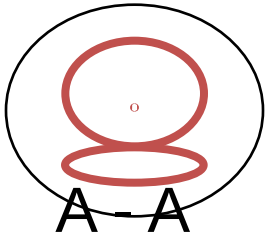
B - B

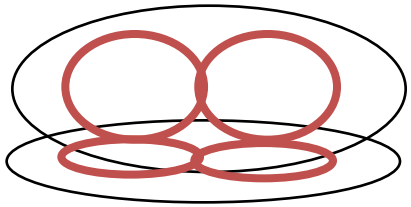
Illustration 2:

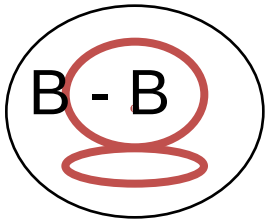




- If molecules are moving too slowly, they collide with insufficient energy (unable to overcome the repulsion between electron clouds), and just bounce off each other instead of reacting.







- If the reacting species are colliding with sufficient kinetic energy--activation energy--(to stretch, bend and break the present bonds), this leads to the formation of products.

Collision Theory

For a chemical reaction to occur

Reacting species must ;

- Collide to react
- Possess a certain minimum kinetics energy, called the activation energy, Ea to initiate the chemical energy
- Collide in the right orientation (steric factor)

$$\text{Rate} \propto \frac{\text{Number of effective collisions}}{\text{Time}}$$

Transition State Theory

- Describes what happens to the reacting species prior to their change into products.
- An intermediate species (activated complex) is formed in the transition state.

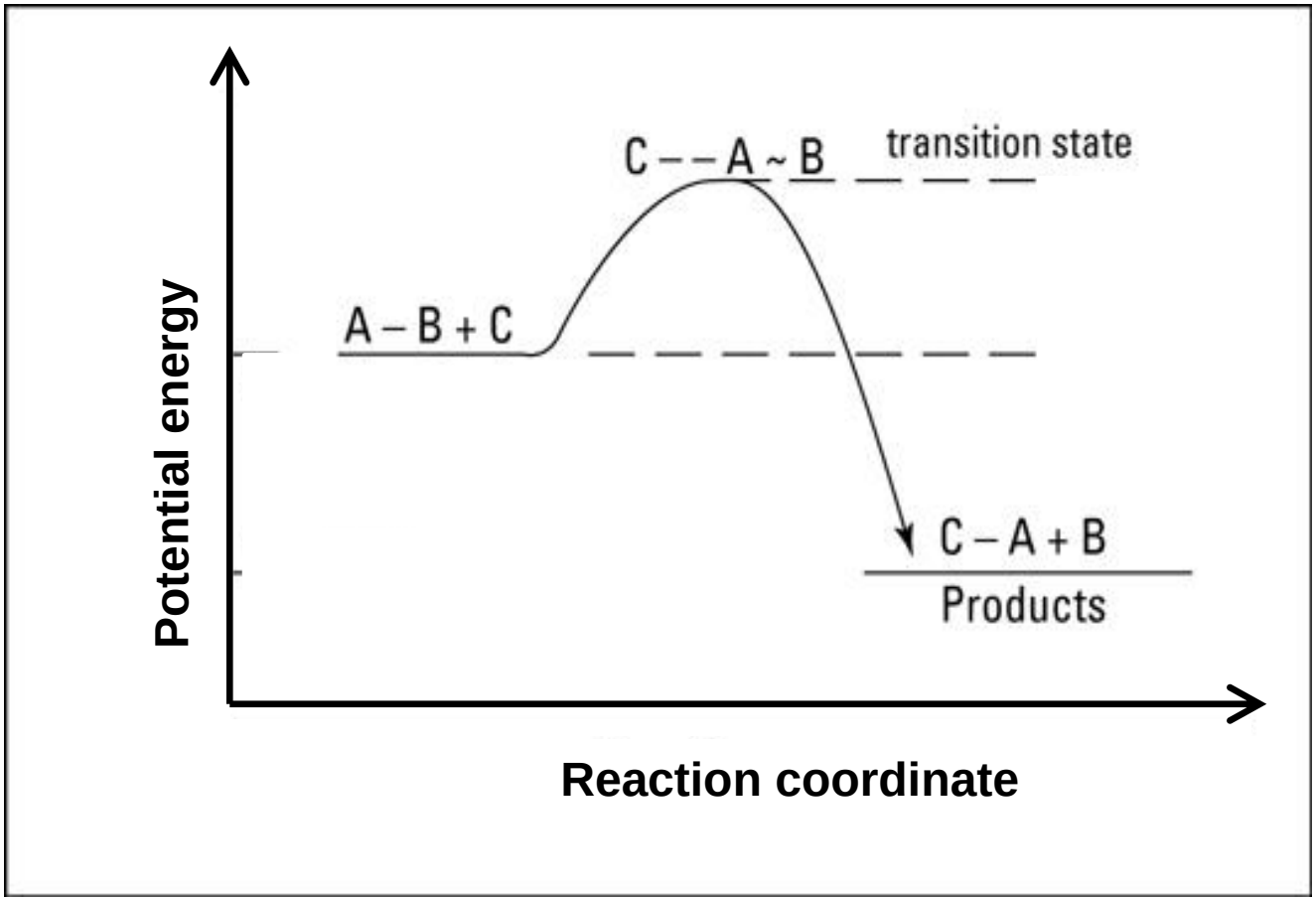
Transition State Theory

Characteristics of Activated Complex:

- **Very unstable** i.e. It has a short half-life.
- Its **potential energy is greater** than reactants or products.
- The activated complex and the reactants are in chemical equilibrium.
- It decomposes to form products or reactants.

Energy profile diagram for an exothermic reaction

$$A - B + C \longrightarrow C \text{ --- } A - B \longrightarrow C - A + B$$



E_{a1}: activation energy for forward reaction (diff in energy between the reactant & the activated complex)

E_{a2}: activation energy for reverse reaction (diff in energy between the activated complex & the product)

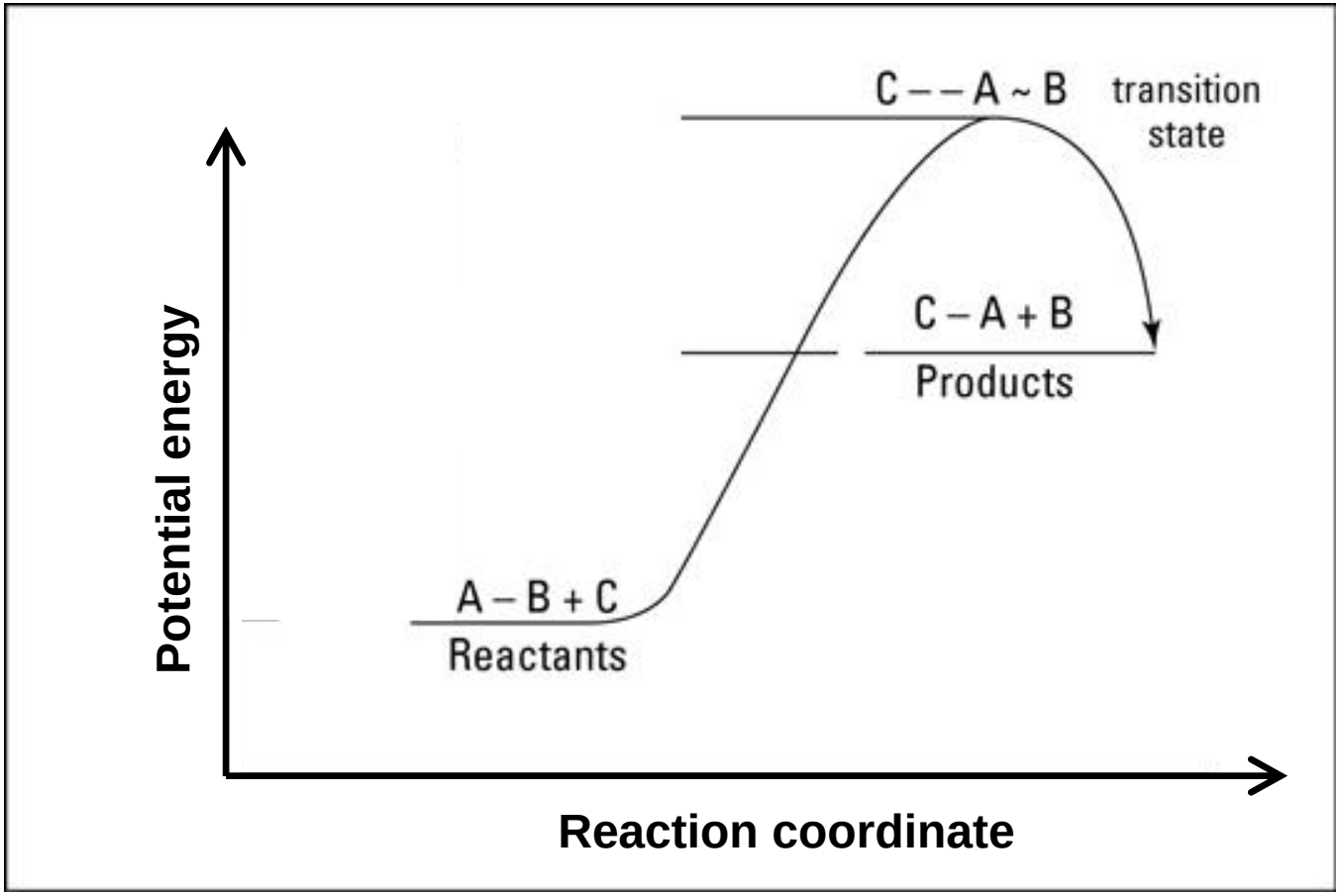
ΔH: enthalpy of reaction

An exothermic chemical reactions

- *Exothermic Reaction* — a reaction in which heat is given off (released) when going from reactants to products.
- The reactants start off at a higher energy state than the products, so energy is released in going from reactants to products.
- The energy diagram shows the collision of C and A-B with the breaking of the A – B bond and the forming of the C – A bond at the top of an activation energy hill.
- This grouping of reactants at the top of the activation energy hill is called the *transition state* of the reaction.
- The difference in the energy level of the reactants and the energy level of the products is the amount of energy (heat) that is released in the reaction.

Energy profile diagram for an endothermic reaction

$$A - B + C \longrightarrow C \text{ --- } A - B \longrightarrow C - A + B$$



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ΔH: enthalpy of reaction

An endothermic chemical reactions

- *Endothermic Reaction* — a reaction in which heat is absorbed in going from reactants to products
- The reactants are at a lower energy state than the products.
- In going from reactants to products, more energy needed to get the reaction started.
- The transition state appears at the top of the activation energy hill.
- The difference is that, in going from reactants to products, energy (heat) must be absorbed in the reaction.

Check Point

1) For the reaction

$$A + B \rightarrow C + D$$

the enthalpy change of the forward reaction is +21 kJ/mol. The activation energy of the forward reaction is 84 kJ/mol.

a) What is activation energy of the reverse reaction?

b) Sketch the reaction profile of this reaction

SUMMARY

- Characteristics of Activated Complex
- Effective collision