BRAC UNIVERSITY

Inspiring Excellence

Department of Mathematics and Natural Sciences

CHE 101: Introduction to Chemistry

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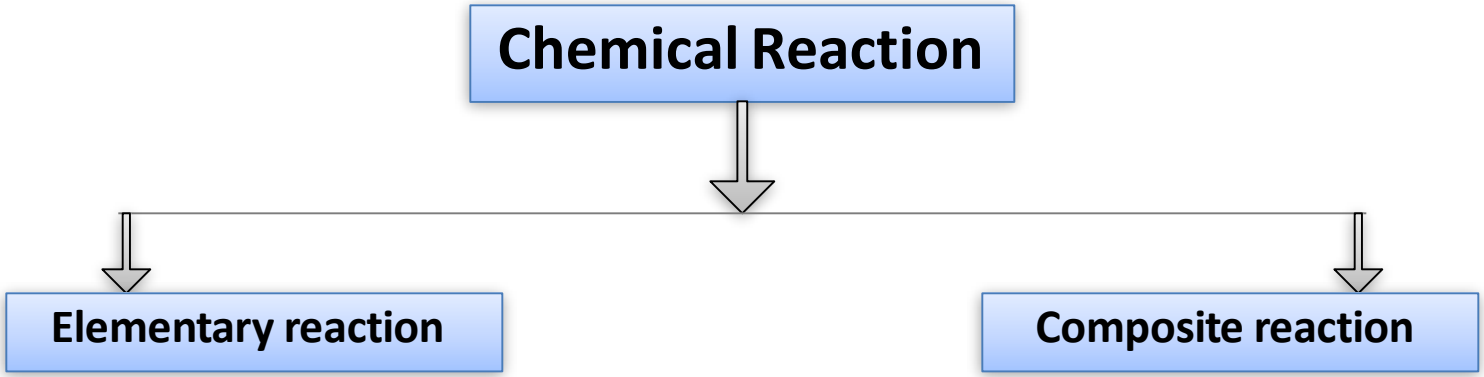
Lecture 4

Content: Molecular events, elementary & composite reaction, potential energy diagram, reaction mechanism



An **elementary reaction** is a simple reaction which occurs in a single step.

Example: A $\longrightarrow$ product

$Br_2 \longrightarrow 2Br$

A **composite or complex reaction** is that which occurs in two or more steps.

Molecularity of an elementary reaction

The **molecularity** of an elementary reaction is defined as the number of reactant molecules involved in a reaction.

The elementary reactions having molecularity 1,2 and 3 are called **unimolecular, bimolecular and termolecular reaction** respectively.

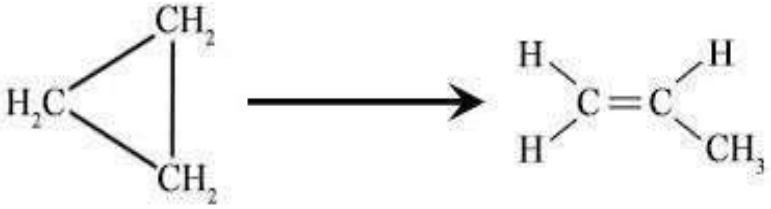
(a) Unimolecular reactions:

Molecularity = 1

A $\longrightarrow$ product

$Br_2 \longrightarrow 2Br$

Example:



Cyclopropane propene

(b) Bimolecular reactions:

Molecularity = 2

A + B $\longrightarrow$ products

A + A $\longrightarrow$ products

$PCl_5 \rightarrow PCl_3 + Cl_2$	unimolecular
$2HI \rightarrow H_2 + I_2$	bimolecular
$NO + O_3 \rightarrow NO_2 + O_2$	bimolecular
$2CO + O_2 \rightarrow 2CO_2$	trimolecular
$2FeCl_3 + SnCl_2 \rightarrow SnnCl_4 + 2FeCl_2$	trimolecular

Example: (i) $2HI \longrightarrow H_2 + I_2$

(ii) $CH_3COOC_2H_5 + H_2O \longrightarrow CH_3COOH + C_2H_5OH$

Ethyl acetate acetic acid ethanol

(c) Termolecular reactions:

Molecularity = 3

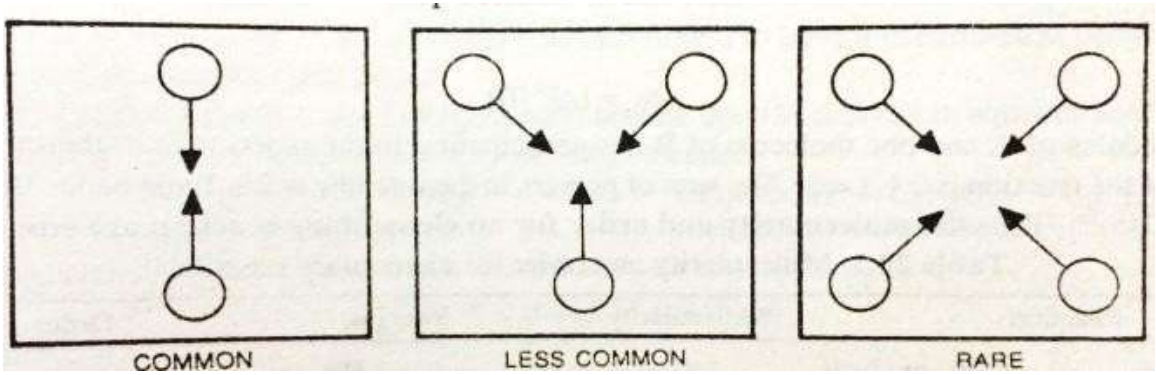
A + B + C $\longrightarrow$ products

Example: (i) $2NO + O_2 \longrightarrow 2NO_2$

(ii) $2NO + Cl_2 \longrightarrow 2NOCl$

Why high molecularity reactions are rare?

Ans: According to kinetic molecular theory, the rate of chemical reaction is proportional to the number of collisions taking place between the reacting molecule. The chances of simultaneous collisions of reacting molecule will decrease with increase in number of reacting molecule. That's why high molecularity reactions are rare



Chances of simultaneous collision between reacting molecules decrease as the molecularity increase

Reaction mechanism

A set of elementary reactions which lead to the overall or net reaction (that convert reactants to products) is called the mechanism of the reaction.

- In any mechanism some of the steps are fast, others are slow.
- The slowest step is the rate-determining step of the reaction.
- Example: Decomposition of N_2O_5

$$2N_2O_5 \longrightarrow 4NO_2 + O_2$$

This is a composite reaction. It occurs by the following steps:

Step 1 :	$2N_2O_5$	$\longrightarrow$ $2NO_2 + 2NO_3$	(slow)
Step 2 :	$NO_2 + NO_3$	$\longrightarrow$ $NO + NO_2 + O_2$	(slow)
Step 3 :	$NO + NO_3$	$\longrightarrow$ $2NO_2$	(fast)
step 1 + step 2 + step 3	$2N_2O_5$	$\longrightarrow$ $4NO_2 + O_2$	

Second step is the rate determining step.

Composite reaction

The reaction which have more than one elementary step is called complex reaction.

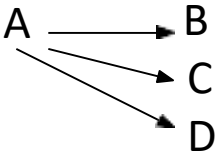
Example:

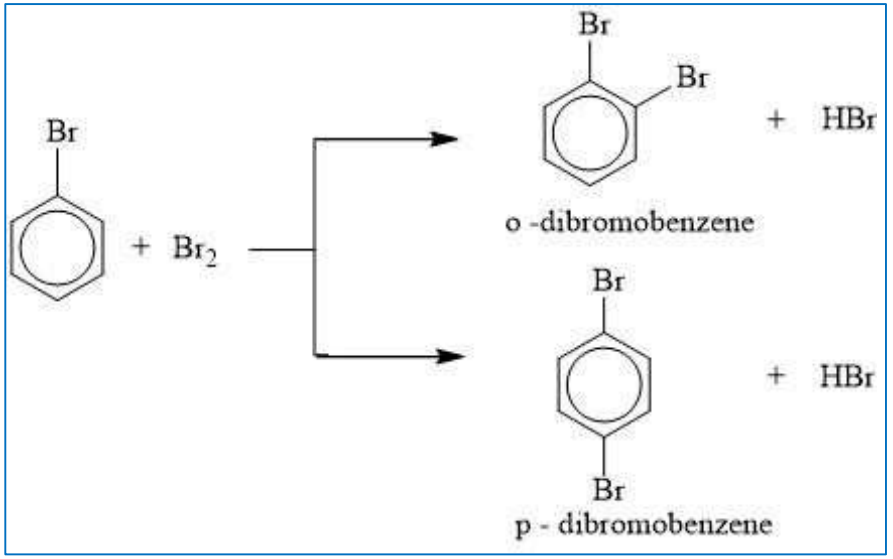
1. ***Side or parallel reaction***
2. ***Reversible or opposing reaction***
3. ***Consecutive reaction***

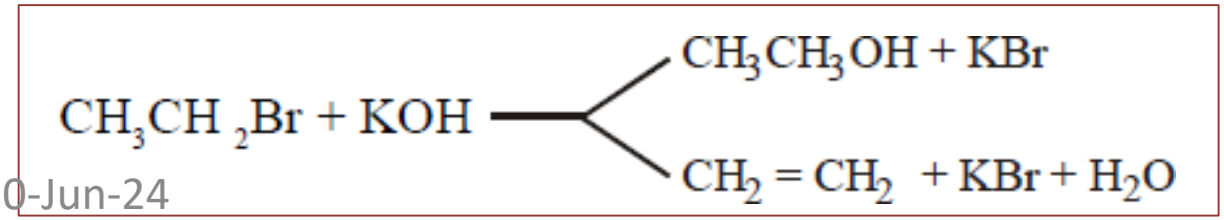
Side or parallel reaction

The reaction in which more than one product formed from the reactant.

Example:







Composite reaction

Reversible or opposing reaction

A reaction is said to be reversible if forward reaction is opposed by backward reaction.

A ⟷ B

Reversible Reaction Examples

$N_2(g)$	+	$O_2(g)$	⇌	$2\,NO(g)$
Nitrogen		Oxygen		Nitrous oxide
$H_2(g)$	+	$I_2(g)$	⇌	$2\,HI(g)$
Hydrogen		Iodine		Hydrogen iodide
$N_2(g)$	+	$3\,H_2(g)$	⇌	$2\,NH_3(g)$
Nitrogen		Hydrogen		Ammonia

Consecutive reaction

The reaction in which the final product is formed through one or more intermediate steps are called consecutive reaction.

A ⟶ B ⟶ C

$$CH_3CH_2OH \xrightarrow[H^+]{K_2Cr_2O_7} CH_3CHO \xrightarrow[H^+]{K_2Cr_2O_7} CH_3COOH$$

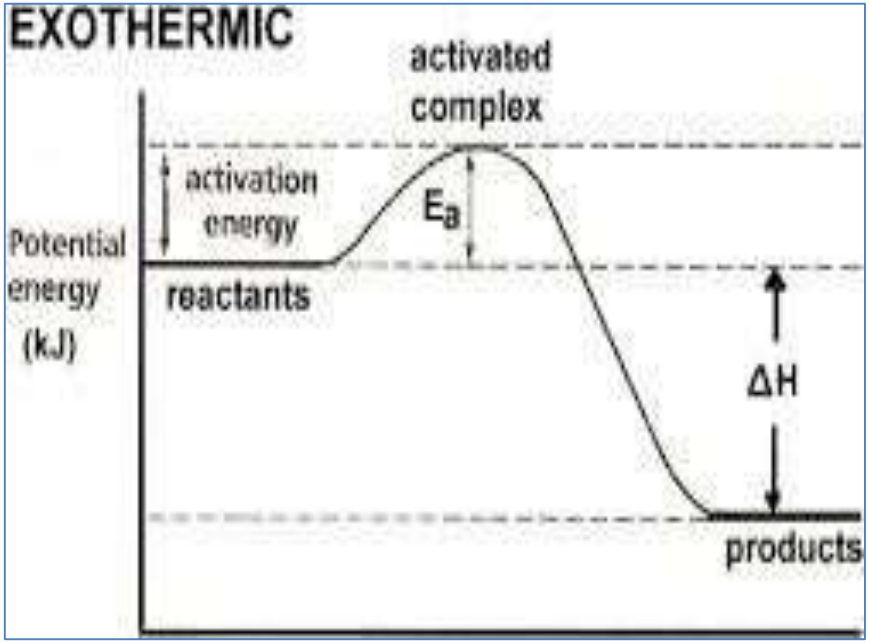
Ethanol — Acetaldehyde — Acetic acid

Reaction Intermediate: A reaction intermediate is a species produced during an elementary step of reaction but does not appear in the net reaction equation.

Example: In decomposition of N_2O_5, NO_3 is said to be a reaction intermediate.

Potential energy diagram

A **potential energy diagram** plots the change in potential energy that occurs during a chemical reaction.



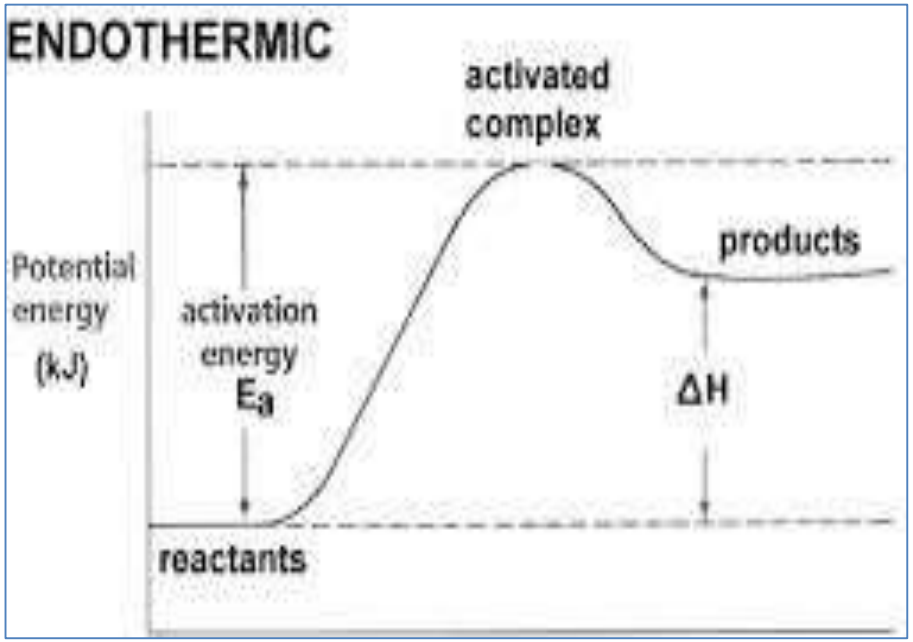
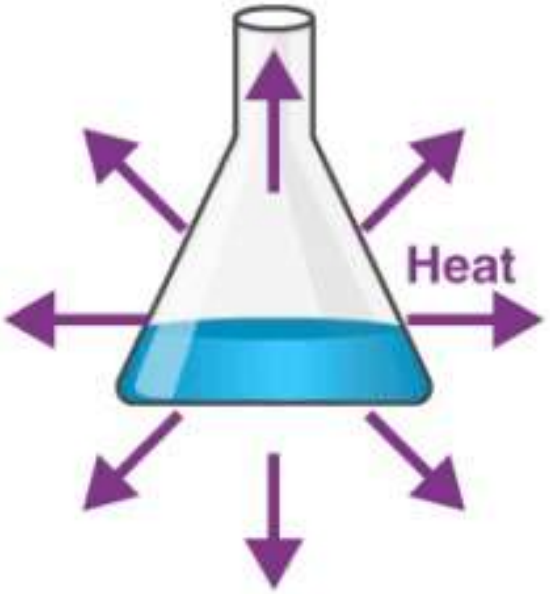
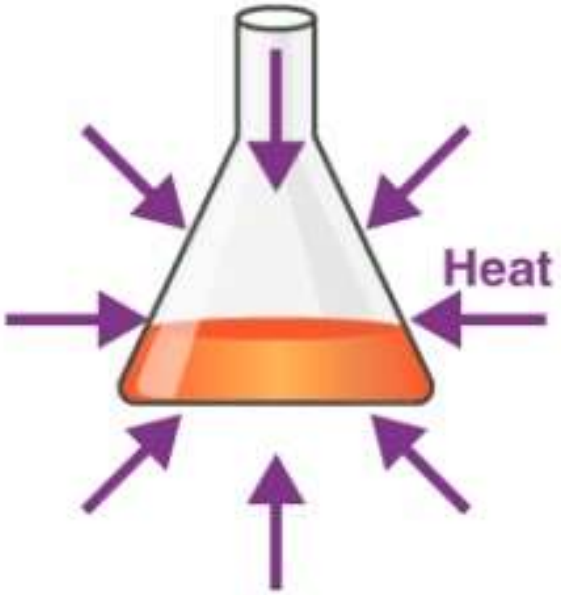


Fig :Potential energy diagram for exothermic and endothermic reaction





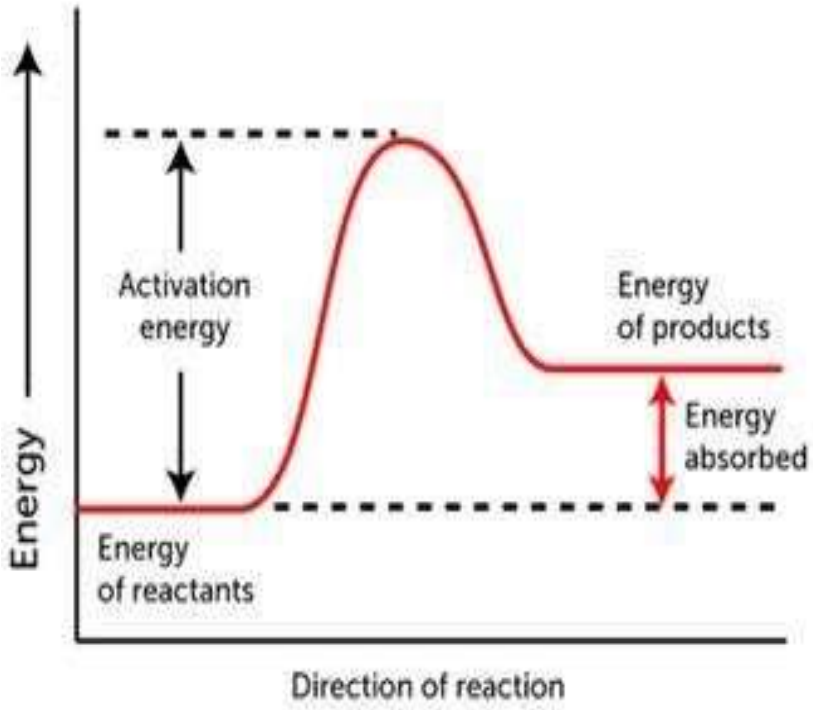
Exothermic Reactions

A reaction that releases energy from the system in the form of heat.

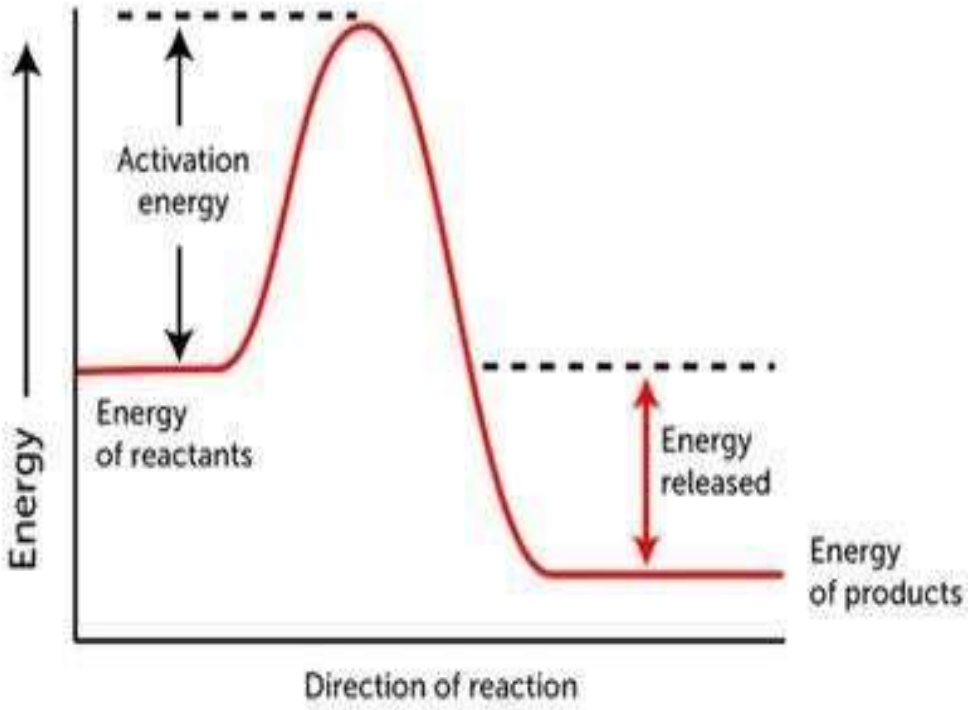
Endothermic Reaction

A reaction that the system absorbs energy from its surrounding in the form of heat.

Endothermic Reaction



Exothermic Reaction



Exothermic Reaction:

$$C(g)+O_2(g)\rightarrow CO_2(g)+HeatEnergy$$

$$NaOH(aq)+HCl(aq)\rightarrow NaCl(aq)+H_2O(l)+Energy$$

Endothermic Reaction:

$$N_2(g)+O_2(g)\xrightarrow{Heat}2NO$$

$$C(s)+H_2O(l)\xrightarrow{Heat}CO(g)+H_2(g)$$

	Endothermic reaction	Exothermic reaction
Definition	Chemical reaction where energy is absorbed.	Chemical reaction where energy is released in the form of heat.
Origin of energy	From the environment	Of the system
Potential energy	Lower in reactants than in products.	Higher in reactants than in products.
Production	Not spontaneous	Spontaneous
Internal energy change	$\Delta E > 0$; internal energy change greater than zero.	$\Delta E < 0$; internal energy change less than zero.
Temperature	Decreases	Increases
Examples	Reactions in photosynthesis and synthesis in general.	A burning match, combustion reactions.

Terms of potential energy (PE) diagram

Endothermic Reactions: the reactants have less potential energy than do the products.

Exothermic Reactions: the reactants have more potential energy than the products have.

Activation energy, E_a: The minimum energy required to initiate a chemical reaction. So the energy required by reactant molecule to be converted into product is called activation energy, E_a.
It is the difference in energy between reactant and transition state.

Activated complex: Activated complex is a grouping of atoms of reactant molecule that is unstable and breaks up or decompose at a definite rate to give the products of the reaction.
All the reactants proceed through formation of an intermediate activated complex or transition state before forming product **(transition state theory).** Activated complex has higher potential energy than reactants or products.

$$AB + C \longrightarrow \underset{\text{activated complex}}{A.....B.....C} \longrightarrow AC + B$$

In spite of collision between molecules reactions cant take place unless the energy barrier is crossed

Thank You All