SCH 4U

REACTION MECHANISMS & CATALYSTS

Raw materials →→→→→→→→→→→ House

Many intermediate steps

1. hole
2. foundation
3. walls
4. roof
5. electrical
6. plumbing

REACTION MECHANISM: = series of steps that make up overall reaction

= each step called an **ELEMENTARY REACTION**.

Eg. **Overall:** $2NO_{(g)} + O_{2(g)} \rightarrow 2NO_{2(g)}$

2-Step Mechanism: 1. $NO_{(g)} + O_{2(g)} \rightarrow \underline{NO_{3(g)}}$

2. $\underline{NO_{3(g)}} + NO_{(g)} \rightarrow 2NO_{2(g)}$

$NO_{3(g)}$ is a **reaction intermediate**.

- Does not appear in the overall reaction
- Formed in step 1.
- Consumed in later step.

MOLECULARITY = number of moles of reactants in an elementary step

- In above example, both steps are bimolecular
- Termolecular (3 reactants) = rare due to orientation
- Unimolecular (1 reactant)

Eg. $Cl_{2(g)} \xrightarrow{UV} 2Cl_{(g)}$

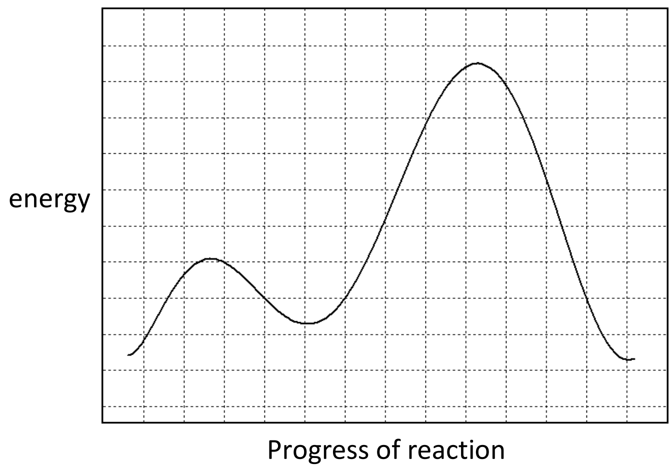
RATE-DETERMINING STEP = the one elementary step that is the slowest

Eg. Baking a cake

1. ingredients for cake → mixed ingredients (fast)

2. mixed ingredients → baked cake (slow) – rate-determining step

Reaction intermediate



PART 1: RATE-DETERMINING STEP & THE RATE LAW

Is a proposed reaction mechanism reasonable?

(A) Do the steps add up to the overall reaction?

(B) Are the steps reasonable in molecularity? (termolecular is slow)

(C) Is the rate law for rate-determining step consistent with overall experimental rate law?
(**NOTE**: for rate-determining step **ONLY**, the coefficients become the exponents)

Eg. 1 $2NO_{2(g)} + Cl_{2(g)} \rightarrow 2NO_2Cl_{(g)}$

Experimental rate = k[NO_2][Cl_2] -- 2nd order

Proposed Mechanism:

1. $NO_{2(g)} + Cl_{2(g)} \rightarrow NO_2Cl_{(g)} + Cl_{(g)}$ (slow)
2. $NO_{2(g)} + Cl_{(g)} \rightarrow NO_2Cl_{(g)}$ (fast)

(A)

(B)

(C)

Eg. 2 $2NO_{(g)} + 2H_{2(g)} \rightarrow N_{2(g)} + 2H_2O_{(g)}$

Experimental: $rate = k[NO]^2[H_2]$

Proposed Mechanism:

1. $2NO_{(g)} + H_{2(g)} \rightarrow N_2O_{(g)} + H_2O_{(g)}$ (slow)
2. $N_2O_{(g)} + H_{2(g)} \rightarrow N_{2(g)} + H_2O_{(g)}$ (fast)

(A)

(B)

(C)

PART 2: CATALYSTS

- Substance that speeds up a chemical reaction without being used up

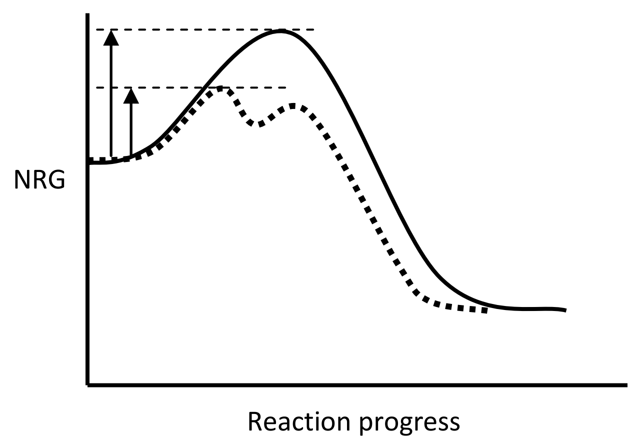
[**NOTE:** **INHIBITORS** are substances that slow down a chemical reaction without being used up]

Eg. $2H_2O_{2(aq)} \xrightarrow{MnO_2} O_{2(g)} + 2H_2O_{(l)}$

- Important economically

HOW IT WORKS:

1. lowers E_a, therefore more molecules have sufficient K.E. to react



2. provides alternate reaction mechanism

UNCATALIZED: $A + B \longrightarrow AB \quad (slow)$

CATALIZED: $A + B \xrightarrow{cat.} AB \quad (fast)$

1. $A + cat \rightarrow A - cat$
2. $A - cat + B \rightarrow AB + cat$

Each step is faster than overall uncatalized reaction

$A + B \xrightarrow{cat} AB$

A-cat is a reactant intermediate, but ***cat*** is regenerated.

HOMOGENEOUS CATALYST

- Catalyst same phase as reactants

Eg. $2SO_{2(g)} + O_{2(g)} \xrightarrow{NO_{2(g)}} 2SO_{3(g)}$

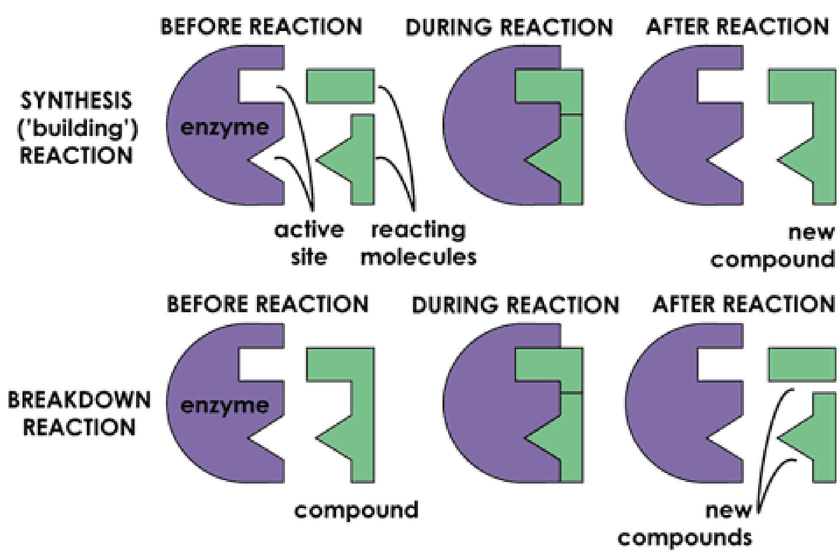
HETEROGENEOUS CATALYST

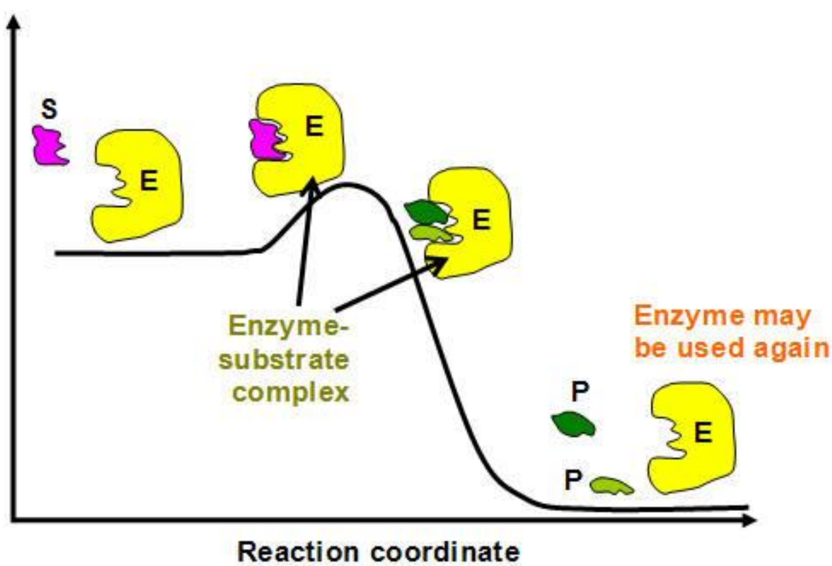
- Catalyst different phase as reactant

Eg. $2H_2O_{2(aq)} \xrightarrow{MnO_{2(s)}} O_{2(g)} + 2H_2O_{(l)}$

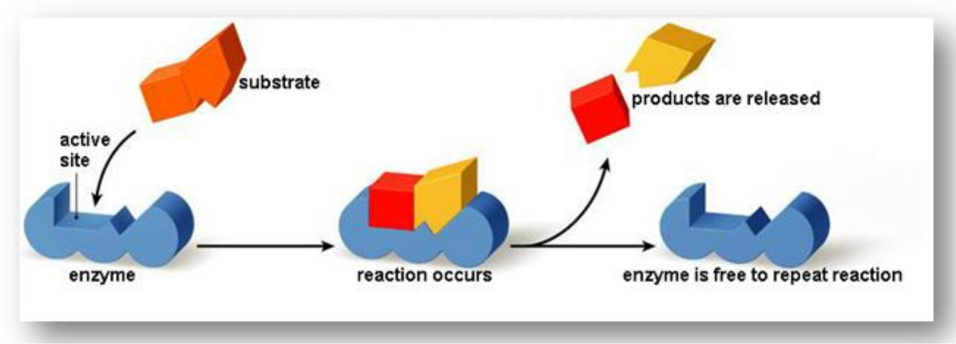
ENZYMES

- Biological catalysts (proteins)
- 2 theories: ① **Lock & key model**
  ② **Induced-fit model**

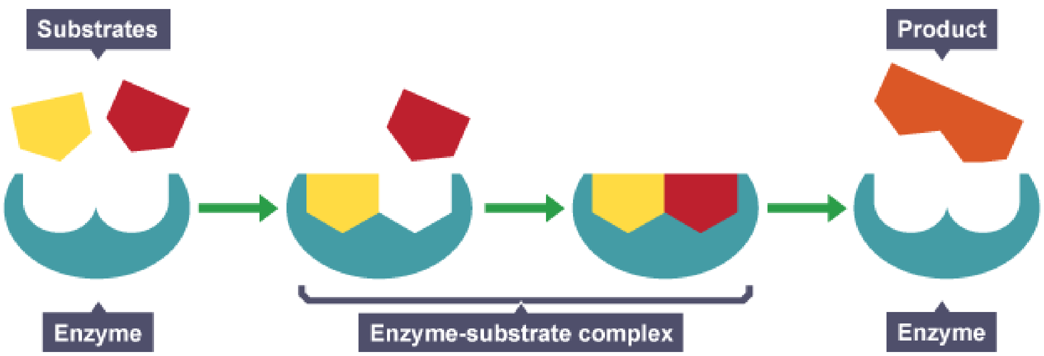




① LOCK & KEY MODEL



② INDUCED FIT MODEL



SIMILARITIES AND DIFFERENCES BETWEEN ENZYMES AND CATALYSTS

SIMILARITIES	DIFFERENCES
◆ Both are needed in minute quantities	◆ Enzymes are complex proteins while catalysts are simple inorganic molecules
◆ Both accelerate the rate of a reaction, but cannot initiate one	◆ Enzymes have a very high molecular weight while catalysts have a low molecular weight
◆ Both of them bring about a decrease in the activation energy	◆ Enzymes catalyse only biological reactions
◆ Both of them temporarily combine with the substrate molecule	◆ Enzymes catalyse specific types of reactions while catalysts have a wide range
◆ Both of them do not undergo any change in their composition and hence, can be used again and again	◆ Enzymes are significantly affected by temperature and pH, but not so in the case of catalysts
◆ Both of them do not alter the nature and quantity of the end products	◆ Enzymes are regulated by specific substances called cofactors, but not so in the case of catalysts
◆ The reaction accelerated by both of them is reversible	◆ Enzymes can be easily inactivated but not so in the case of catalysts