Reaction Mechanisms

Chapter 6.6

Reaction Mechanisms

- The sequence of events that describes the actual process by which reactants become products is called the reaction mechanism
- The balanced chemical equation for the reaction specifies only the reactants and products, and gives no information on the mechanism

- Most chemical reactions occur by a sequence of simpler reactions

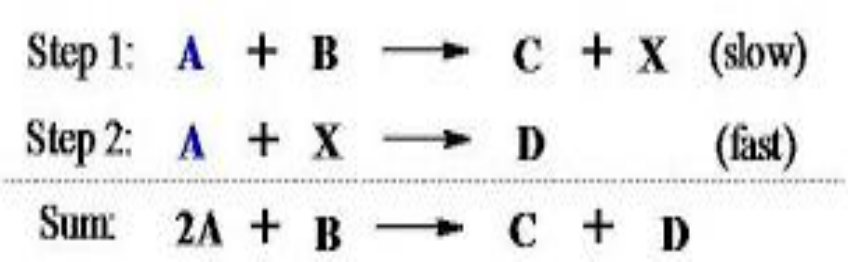
Reaction Mechanisms

$$2A + B \longrightarrow C + D$$

Rate = k[A][B]

- A **reaction mechanism** is a series of elementary steps by which a chemical reaction occurs

A **reaction intermediate** is a chemical species that is neither a reactant or product but is formed and consumed in the reaction



The **rate-determining step** is the step in the reaction mechanism that determines the rate of the overall reaction (the slowest step in the mechanism)

- An **elementary step** is a step involving a one-two- or three-entity collision that cannot be explained by simpler reactions

Rate Law and Elementary Reactions

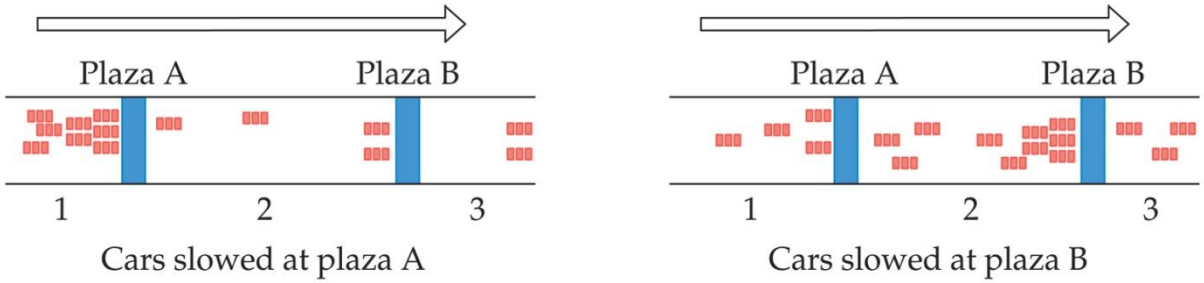
- Rate Law equations can be written directly from the balanced equations representing elementary steps

Molecularity	Elementary Reaction	Rate Law
*Uni*molecular	$A \longrightarrow$ products	Rate $= k[A]$
*Bi*molecular	$A + A \longrightarrow$ products	Rate $= k[A]^2$
*Bi*molecular	$A + B \longrightarrow$ products	Rate $= k[A][B]$
*Ter*molecular	$A + A + A \longrightarrow$ products	Rate $= k[A]^3$
*Ter*molecular	$A + A + B \longrightarrow$ products	Rate $= k[A]^2[B]$
*Ter*molecular	$A + B + C \longrightarrow$ products	Rate $= k[A][B][C]$

- The molecularity of a process tells how many individual entities are involved in the process (Termolecular steps are very rare because the chances of three molecules coming into contact at the same time are miniscule)

Rate Determining Step

- In a multistep process, one of the steps will be slower than all others
- The overall reaction cannot occur faster than this slowest, rate-determining step



- The rate law equation for the overall reaction is the same as the rate law equation for the rate-determining step

Reaction Mechanisms

- In order for a reaction mechanism to be plausible, it must satisfy two requirements:

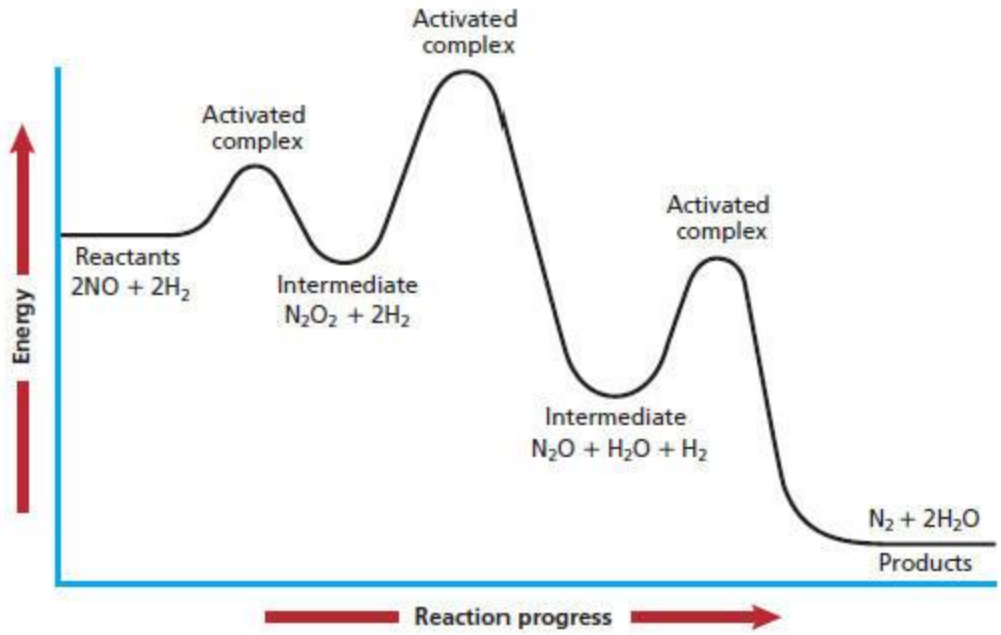
1. Summing the elementary steps in the reaction mechanism must give the overall balanced equation for the reaction
2. The reaction mechanism must agree with the experimentally determined rate law

Reaction Mechanism Example

$2NO_{(g)} + 2H_{2(g)}$ --- > $N_{2(g)} + 2H_2O_{(g)}$ rate = $k[H_2]$

The mechanism for the above reaction occurs in three steps:

$$2NO \rightarrow N_2O_2 \quad \text{(fast)}$$
$$N_2O_2 + H_2 \rightarrow N_2O + H_2O \quad \text{(slow)}$$
$$N_2O + H_2 \rightarrow N_2 + H_2O \quad \text{(fast)}$$



Practice

Answer the following questions about the two step mechanism below:

$$O_3 \longrightarrow O_2 + O \quad \text{(slow)}$$
$$O + O_3 \longrightarrow 2O_2 \quad \text{(fast)}$$

1. What is the rate law equation for each elementary step?
2. What is the molecularity of each elementary step?
3. What is the overall chemical reaction?
4. What is the rate law equation for the overall reaction?
5. Draw an energy diagram to show the progress of this reaction

Arrhenius Equation

- It is clear from the rate law expression that rate of reaction is affected by concentration
- Rate = $k[A]^m[B]^n$
- But what about the other factors that affect reaction rate?
- They are accounted for in the rate constant, k

$$k = Ae^{-\frac{E_a}{RT}}$$

HOMEWORK

Required Reading:

p. 383-387

(remember to supplement your notes!)

Questions:

p. 386 #1-3

p. 387 #1-9