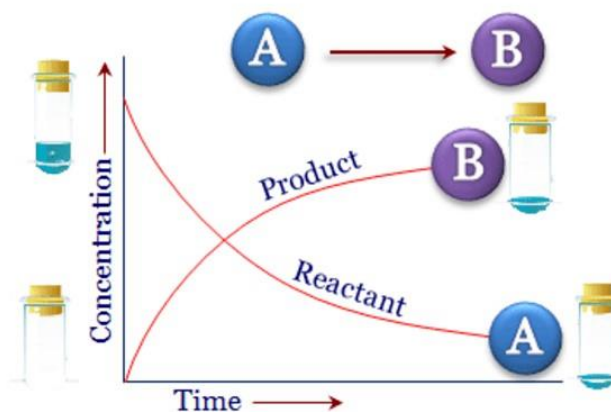# Chemical Kinetics

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The contents of this presentation is prepared to provide a brief idea about the topics, details will be discussed in the classes.
Contents have been collected from multiple textbooks and internet.

Rate of a Reaction

- **Reaction rate** is the change in the concentration of a reactant or a product with time (M/s).

$$A \longrightarrow B$$

$$\text{rate} = -\frac{\Delta[A]}{\Delta t} \qquad \Delta[A] = \text{change in concentration of A over time period } \Delta t$$
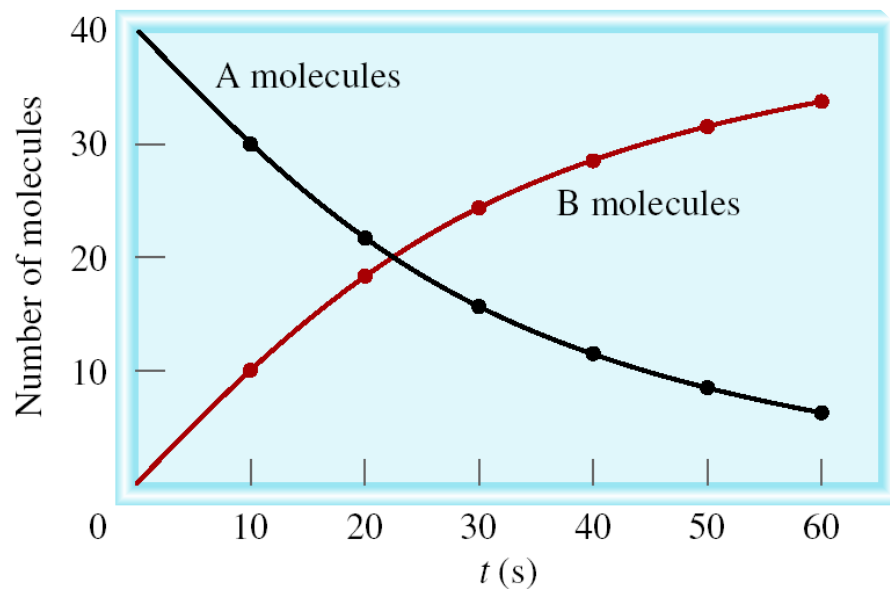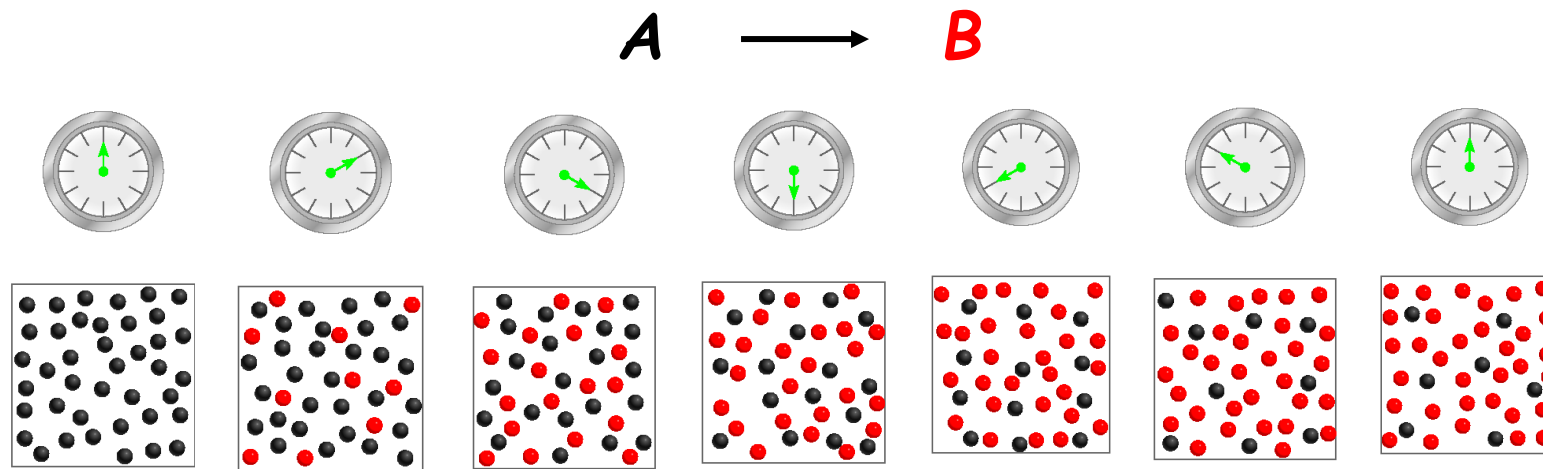
$$\text{rate} = \frac{\Delta[B]}{\Delta t} \qquad \Delta[B] = \text{change in concentration of B over time period } \Delta t$$

Because [A] decreases with time, **$\Delta[A]$ is negative**.

Unit: mole L^{-1} s^{-1}, mole L^{-1} min^{-1}, mole L^{-1} h^{-1} etc.
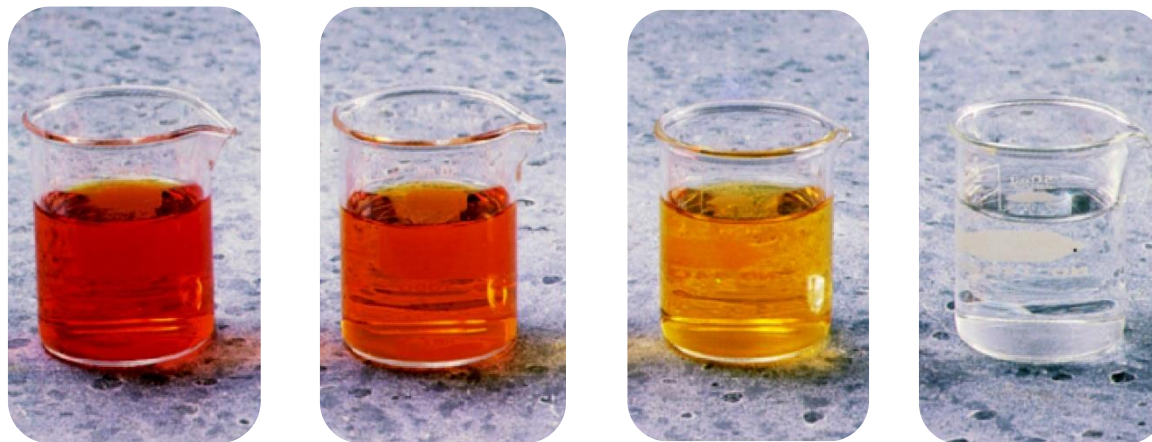
Rate of a Reaction

$$A \longrightarrow B$$
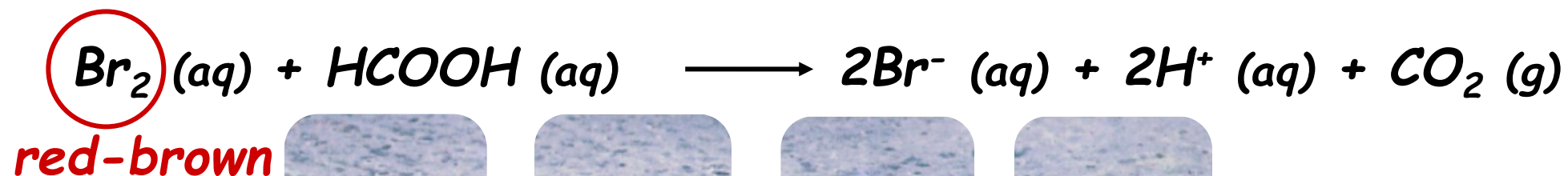

$$rate = -\frac{\Delta[A]}{\Delta t}$$

$$rate = \frac{\Delta[B]}{\Delta t}$$

Rate of a Reaction

Br_2 (aq) + HCOOH (aq) $\longrightarrow$ $2Br^-$ (aq) + $2H^+$ (aq) + CO_2 (g)

red-brown

time

393 nm light

Detector

$t_1 < t_2 < t_3$

Absorption

t_1

t_2

t_3

300   400   500   600

Wavelength (nm)
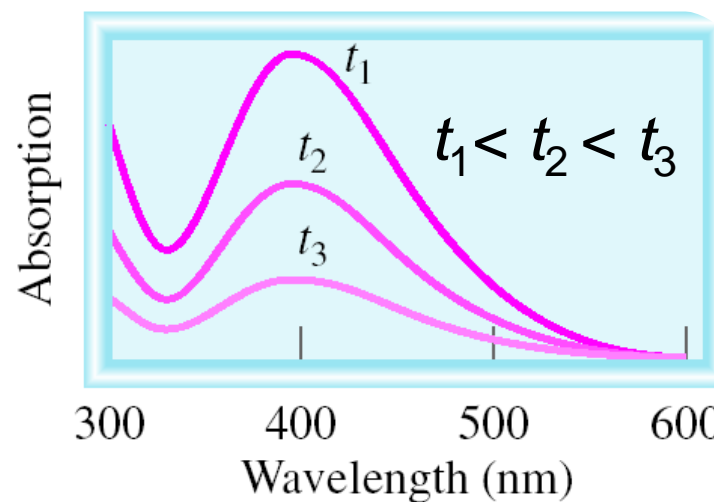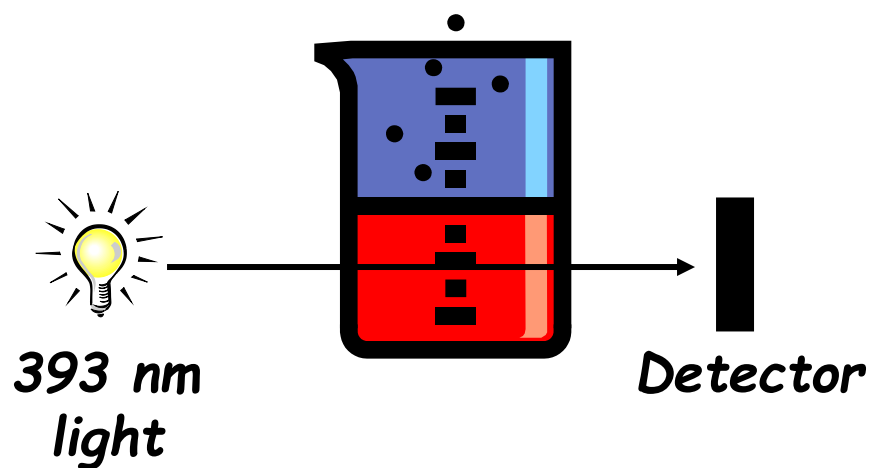
$\Delta[Br_2]$ a ΔAbsorption

Reaction Rates and Stoichiometry

$$2A \longrightarrow B$$
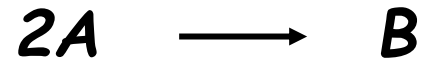
Two moles of A disappear for each mole of B that is formed.

$$\text{rate} = -\frac{1}{2}\frac{\Delta[A]}{\Delta t} \qquad \text{rate} = \frac{\Delta[B]}{\Delta t}$$

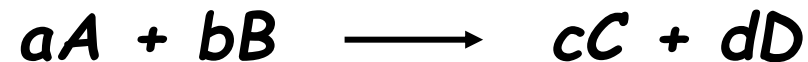$$aA + bB \longrightarrow cC + dD$$

$$\text{rate} = -\frac{1}{a}\frac{\Delta[A]}{\Delta t} = -\frac{1}{b}\frac{\Delta[B]}{\Delta t} = \frac{1}{c}\frac{\Delta[C]}{\Delta t} = \frac{1}{d}\frac{\Delta[D]}{\Delta t}$$

Reaction Rates and Stoichiometry

$$C_2H_4 + O_3 \rightarrow C_2H_4O + O_2$$
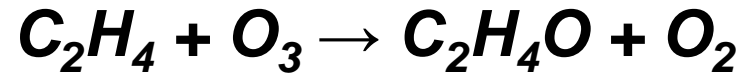
$[O_2]$ increases just as fast as $[C_2H_4]$ decreases.

$$Rate = -\frac{\Delta[C_2H_4]}{\Delta t} = -\frac{\Delta[O_3]}{\Delta t} = \frac{\Delta[C_2H_4O]}{\Delta t} = \frac{\Delta[O_2]}{\Delta t}$$

Reaction Rates and Stoichiometry

$$H_2 + I_2 \rightarrow 2HI$$

[HI] increases twice as fast as [H_2] decreases.

$$Rate = -\frac{\Delta[H_2]}{\Delta t} = -\frac{\Delta[I_2]}{\Delta t} = \frac{1}{2}\frac{\Delta[HI]}{\Delta t}$$
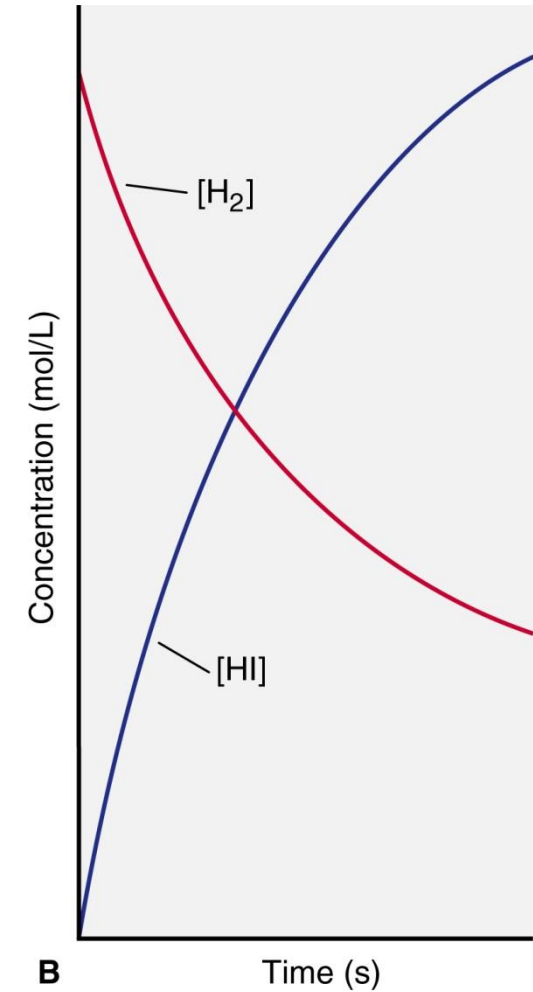
Reaction Rates and Stoichiometry

- *Write the rate expression for the following reaction:*

$$CH_4 \ (g) + 2O_2 \ (g) \longrightarrow CO_2 \ (g) + 2H_2O \ (g)$$
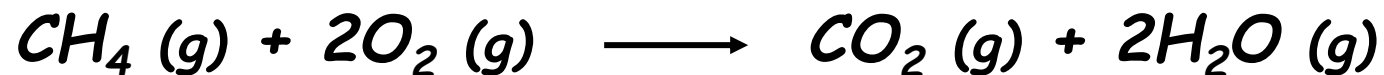
$$rate = -\frac{\Delta[CH_4]}{\Delta t} = -\frac{1}{2}\frac{\Delta[O_2]}{\Delta t} = \frac{\Delta[CO_2]}{\Delta t} = \frac{1}{2}\frac{\Delta[H_2O]}{\Delta t}$$
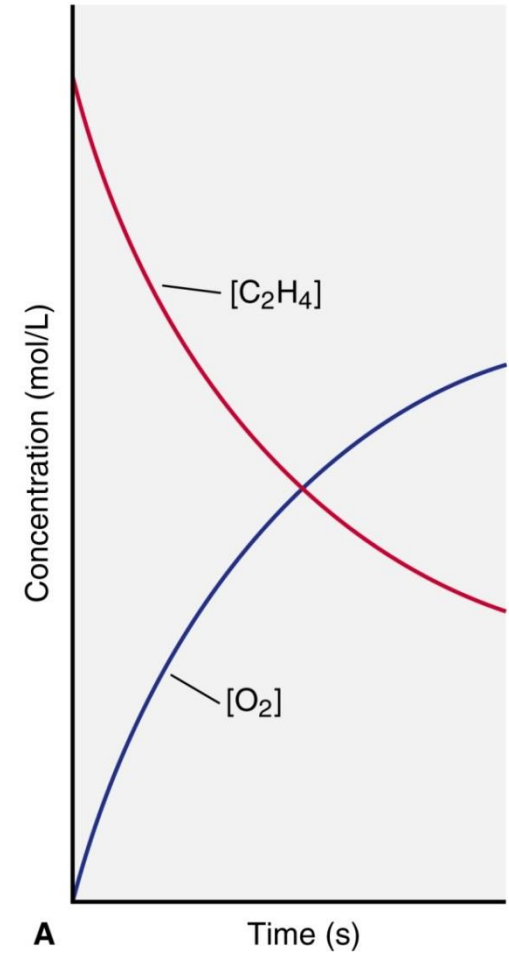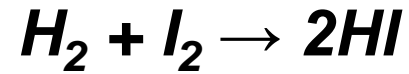
The Rate Law

- The rate law expresses the relationship of the rate of a reaction to the rate constant and the concentrations of the reactants raised to some powers.

$$aA + bB \longrightarrow cC + dD$$

$$Rate = k\ [A]^m\ [B]^n$$

- The term k is the rate constant, which is specific for a given reaction at a given temperature.

- The exponents m and n are reaction orders and are determined by experiment.
    - The values of m and n are not necessarily related in any way to the coefficients a and b.

The Order of a Reaction

- *The order of a reaction is defined as the sum of the powers of concentrations in the rate law.*

$$aA + bB \longrightarrow cC + dD$$
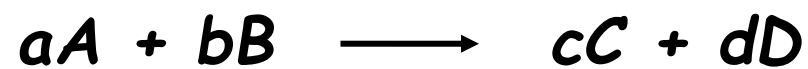
$$Rate = k\,[A]^m\,[B]^n$$

- *The order of such a reaction is (m + n)*

Examples of reaction order :

RATE LAW	REACTION ORDER
rate $= k\,[N_2O_5]$	1
rate $= k\,[H_2]\,[I_2]$	$1+1=2$
rate $= k\,[NO_2]^2$	2
rate $= k\,[[H_2]\,[NO]^2$	$1+2=3$
rate $= k\,[CHCl_3]\,[Cl_2]^{1/2}$	$1+\dfrac{1}{2}=1\dfrac{1}{2}$

Features of The Order of a Reaction

- *Reaction orders are always determined experimentally.*

- *Order is always defined in terms of reactant (not product) concentrations.*

- *The order of a reactant is not related to the stoichiometric coefficient of the reactant in the balanced chemical equation.*

- *A reaction has an individual order "with respect to" or "in" each reactant.*

The Order of a Reaction - Problems

Problem Many gaseous reactions occur in car engines and exhaust systems. One of these is

$$NO_2(g) + CO(g) \longrightarrow NO(g) + CO_2(g) \qquad Rate = k[NO_2]^m[CO]^n$$

(a) Use the following data to determine the individual and overall reaction orders.
(b) Calculate k using the data from experiment 1.

Experiment	Initial Rate (mol/L·s)	Initial [NO$_2$] (mol/L)	Initial [CO] (mol/L)
1	0.0050	0.10	0.10
2	0.080	0.40	0.10
3	0.0050	0.10	0.20

Solution (a) Calculating m in $[NO_2]^m$: We take the ratio of the rate laws for experiments 1 and 2, in which [NO$_2$] varies but [CO] is constant:

$$\frac{Rate\ 2}{Rate\ 1} = \frac{k[NO_2]_2^m[CO]_2^n}{k[NO_2]_1^m[CO]_1^n} = \left(\frac{[NO_2]_2}{[NO_2]_1}\right)^m \qquad or \qquad \frac{0.080\ mol/L \cdot s}{0.0050\ mol/L \cdot s} = \left(\frac{0.40\ mol/L}{0.10\ mol/L}\right)^m$$

This gives $16 = (4.0)^m$, so we have $m = \log 16/\log 4.0 = 2.0$. The reaction is second order in NO$_2$.

Calculating n in $[CO]^n$: We take the ratio of the rate laws for experiments 1 and 3, in which [CO] varies but [NO$_2$] is constant:

$$\frac{Rate\ 3}{Rate\ 1} = \frac{k[NO_2]_3^m[CO]_3^n}{k[NO_2]_1^m[CO]_1^n} = \left(\frac{[CO]_3}{[CO]_1}\right)^n \qquad or \qquad \frac{0.0050\ mol/L \cdot s}{0.0050\ mol/L \cdot s} = \left(\frac{0.20\ mol/L}{0.10\ mol/L}\right)^n$$

We have $1.0 = (2.0)^n$, so $n = 0$. The rate does not change when [CO] varies, so the reaction is zero order in CO.

Therefore, the rate law is

$$Rate = k[NO_2]^2[CO]^0 = k[NO_2]^2(1) = k[NO_2]^2$$

The reaction is second order overall.

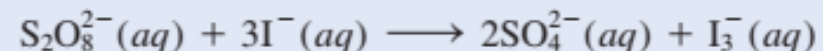(b) From experiment 1, rate = 0.0050 mol/L·s and [NO$_2$] = 0.10 mol/L. Calculating k:

$$Rate = k[NO_2]^2$$

$$k = \frac{rate}{[NO_2]^2} = \frac{0.0050\ mol/L \cdot s}{(0.10\ mol/L)^2}$$

$$= 0.50\ L/mol \cdot s$$

The Order of a Reaction - Problems

Practice Exercise The reaction of peroxydisulfate ion ($S_2O_8^{2-}$) with iodide ion (I^-) is

$$S_2O_8^{2-}(aq) + 3I^-(aq) \longrightarrow 2SO_4^{2-}(aq) + I_3^-(aq)$$

From the following data collected at a certain temperature, determine the rate law and calculate the rate constant.

Experiment	$[S_2O_8^{2-}]$ (M)	$[I^-]$ (M)	Initial Rate (M/s)
1	0.080	0.034	2.2×10^{-4}
2	0.080	0.017	1.1×10^{-4}
3	0.16	0.017	2.2×10^{-4}

Molecularity of a Reaction

- *Chemical reactions are classified into two types-*

  ✓ *Elementary reactions -   occurs in a single step*

  ✓ *Complex reactions -   occurs in two or more steps*

- *For elementary reactions, molecularity is defined as the number of molecules involved in the reaction.*

- *Examples:*

$$Br_2 \longrightarrow 2Br \qquad \qquad \text{Unimolecular}$$

$$H_2 + I_2 \longrightarrow 2HI \qquad \qquad \text{Bimolecular}$$
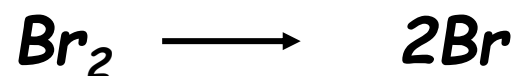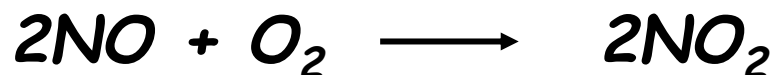
$$2NO + O_2 \longrightarrow 2NO_2 \qquad \qquad \text{Termolecular}$$

Molecularity of a Complex Reaction

- *Most chemical reactions are complex reactions. These occur in a series of steps.*

- *Each step is an elementary reaction.*

- *Some of the steps will be fast, others will be slow. A reaction can proceed no faster than its slowest step.*

- *Thus the slowest step is the* **rate determining step** *of the reaction.*

- *Molecularity of a complex reaction is defined as the number of molecules or atoms taking part in the rate-determining step.*

$$2N_2O_5 \longrightarrow 4NO_2 + O_2$$
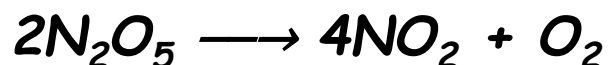
Step 1: $2N_2O_5 \longrightarrow 2NO_2 + 2NO_3$; Fast

Step 2: $NO_2 + NO_3 \longrightarrow NO_2 + NO + O_2$; Slow

Step 3: $NO + NO_3 \longrightarrow 2NO_2$; Fast

Thus step 2 in the above mechanism is rate-determining and has molecularity '2' which could be considered as the molecularity of the decomposition reaction of N_2O_5.
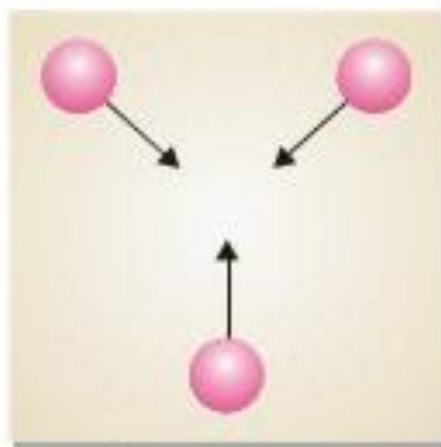
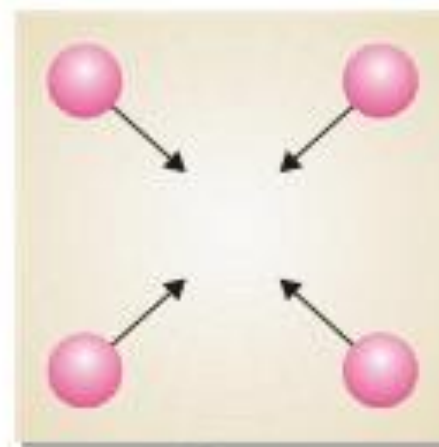# Why High Molecularity Reactions are Rare?

- *The rate of a chemical reaction is proportional to the number of collisions taking place between the reacting molecules.*

- *The chances of simultaneous collision of reacting molecules will go on decreasing with increase in number of molecules.*
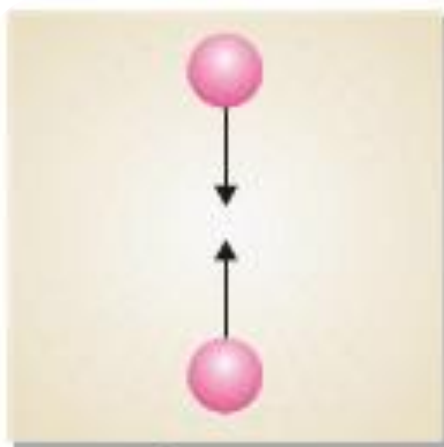
Common   Less common   Rare

Order and Molecularity of Reaction

Order	Molecularity
Sum of powers of the concentration terms in the rate law expression.	Number of reactant molecular involved in a reaction
It is experimentally determined value.	It is a theoretical concept.
It can have a fractional value.	It is always a whole number.
Order of reaction can be zero.	Molecularity can never be zero.
Order of reaction can change with conditions like temperature, pressure, concentration etc.	For a chemical reaction, molecularity is always same.

Zero Order Reaction

- A zero order reaction is one whose rate is independent of concentration.

- A reactant whose concentration does not affect the reaction rate is not included in the rate law.

- The concentration of such a reactant has the power 0. Thus $[A]^0 = 1$.

- Let's consider the following zero order reaction,

$$A \longrightarrow product$$

Initial conc. a 0

Final conc. $(a-x)$ x

Rate of reaction, $dx/dt = k_0 [A]^0 = k_0 (a-x)^0 = k_0$

$\qquad$ or, $dx = k_0 dt$

$\qquad$ or, $x = k_0 t \qquad$ (by integrating)

$\qquad$ or, $k_0 = x/t$

Zero Order Reaction - Graphs
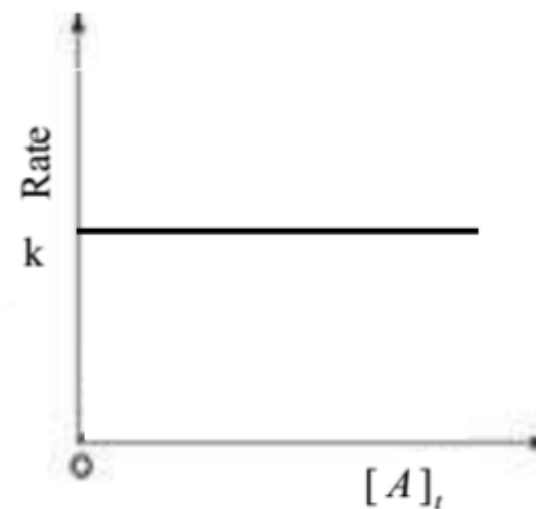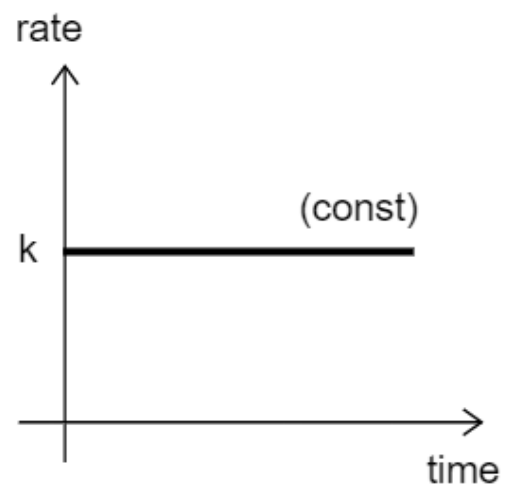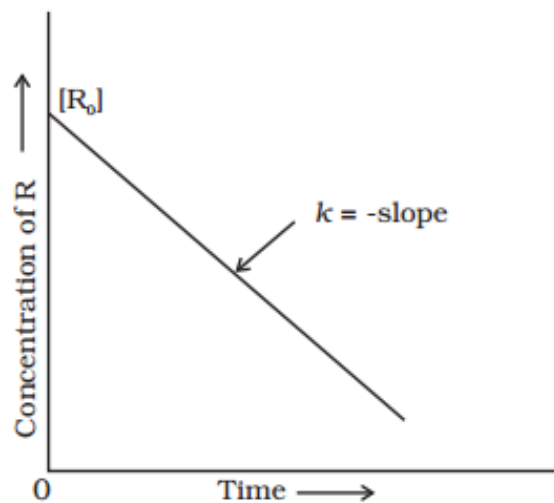
First Order Reaction

- Let's consider a first order reaction,

$$A \longrightarrow product$$

Initial conc.   a   0

Final conc.   (a-x)   x

Rate of reaction, $dx/dt = k\,[A] = k\,(a-x)$

By integration and mathematical simplification,

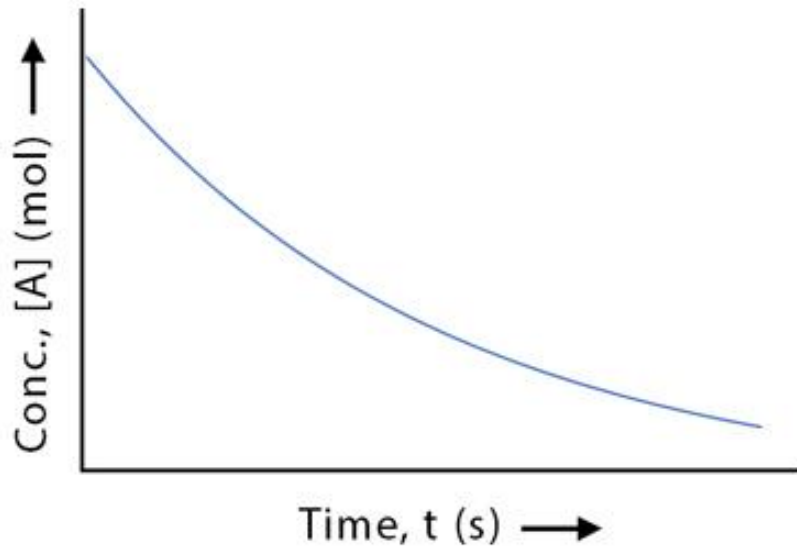$$kt = \ln \frac{[A]_o}{[A]} \qquad\qquad kt = \ln \frac{a}{a-x}$$
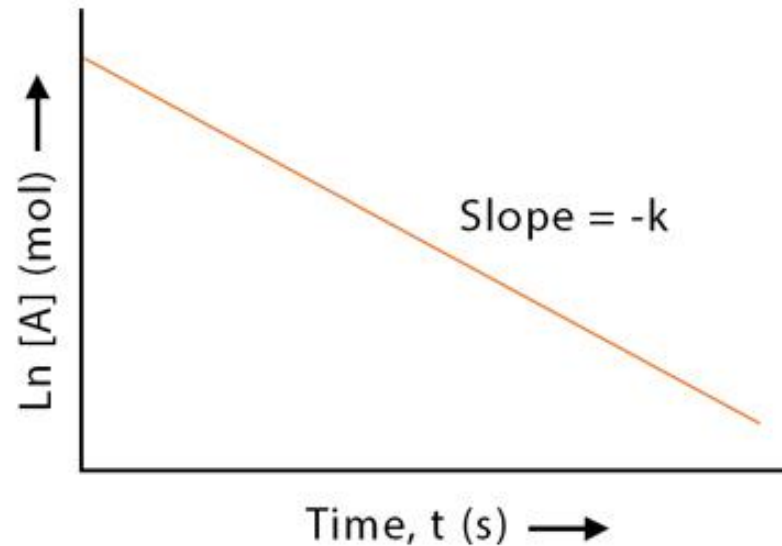
$$k = \frac{2.303}{t} \log \frac{[A]_o}{[A]} \qquad\qquad k = \frac{2.303}{t} \log \frac{a}{(a-x)}$$

First Order Reaction - Graphs

$$[A] = [A]_o \exp (-kt)$$

Slope = -k

$$\ln [A] = \ln [A]_o - kt$$

First Order Reaction – Half Life

$$t = \frac{2.303}{k} \log \frac{[A]_o}{[A]} \qquad\qquad t = \frac{2.303}{k} \log \frac{a}{(a-x)}$$

When $t = t_{1/2}$, $[A] = [A]_o/2$ or $x = a/2$; then we can write,

$$t_{1/2} = \frac{2.303}{k} \log \frac{[A]_o}{[A]_o/2} \qquad\qquad t_{1/2} = \frac{2.303}{k} \log \frac{a}{(a-a/2)}$$

$$\text{or, } t_{1/2} = \frac{2.303}{k} \log 2 \qquad\qquad t_{1/2} = \frac{2.303}{k} \log 2$$
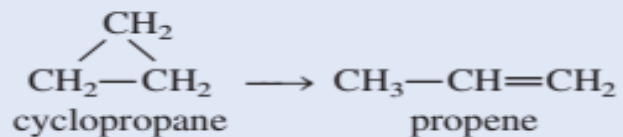
$$\text{or, } t_{1/2} = \frac{0.693}{k}$$

Half life of a first order reaction does not depend on the initial concentration of the reactant
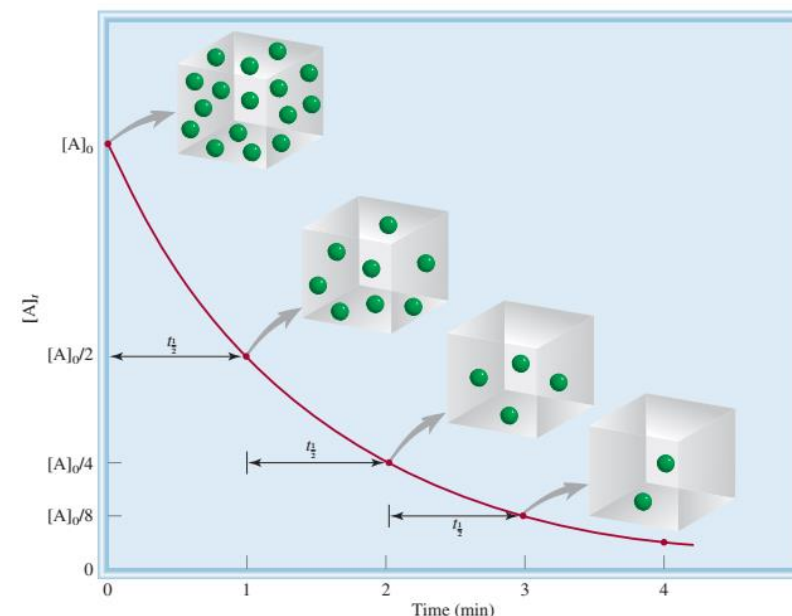
First Order Reaction – Problems

The conversion of cyclopropane to propene in the gas phase is a first-order reaction with a rate constant of 6.7×10^{-4} s^{-1} at 500°C.

$$CH_2 \diagdown CH_2 \diagup CH_2 \longrightarrow CH_3 - CH = CH_2$$

cyclopropane   propene

(a) If the initial concentration of cyclopropane was 0.25 M, what is the concentration after 8.8 min? (b) How long (in minutes) will it take for the concentration of cyclopropane to decrease from 0.25 M to 0.15 M? (c) How long (in minutes) will it take to convert 74 percent of the starting material?

Solution (a) In applying Equation (13.4), we note that because k is given in units of s^{-1}, we must first convert 8.8 min to seconds:

$$8.8 \text{ min} \times \frac{60 \text{ s}}{1 \text{ min}} = 528 \text{ s}$$

We write

$$\ln [A]_t = -kt + \ln [A]_0$$
$$= -(6.7 \times 10^{-4} \text{ s}^{-1})(528 \text{ s}) + \ln (0.25)$$
$$= -1.74$$

Hence, $[A]_t = e^{-1.74} = 0.18 \ M$

(b) Using Equation (13.3),

$$\ln \frac{0.15 \ M}{0.25 \ M} = -(6.7 \times 10^{-4} \text{ s}^{-1})t$$

$$t = 7.6 \times 10^2 \text{ s} \times \frac{1 \text{ min}}{60 \text{ s}}$$

$$= 13 \text{ min}$$

(c) From Equation (13.3),

$$\ln \frac{0.26}{1.00} = -(6.7 \times 10^{-4} \text{ s}^{-1})t$$

$$t = 2.0 \times 10^3 \text{ s} \times \frac{1 \text{ min}}{60 \text{ s}} = 33 \text{ min}$$

First Order Reaction – Problems

Practice Exercise The reaction 2A $\longrightarrow$ B is first order in A with a rate constant of 2.8×10^{-2} s^{-1} at 80°C. How long (in seconds) will it take for A to decrease from 0.88 M to 0.14 M?

First Order Reaction – Problems

The decomposition of ethane (C_2H_6) to methyl radicals is a first-order reaction with a rate constant of $5.36 \times 10^{-4}\,s^{-1}$ at 700°C:

$$C_2H_6(g) \longrightarrow 2CH_3(g)$$

Calculate the half-life of the reaction in minutes.

Solution For a first-order reaction, we only need the rate constant to calculate the half-life of the reaction. From Equation (13.6)

$$t_{\frac{1}{2}} = \frac{0.693}{k}$$

$$= \frac{0.693}{5.36 \times 10^{-4}\,s^{-1}}$$

$$= 1.29 \times 10^3\,s \times \frac{1\ min}{60\ s}$$

$$= 21.5\ min$$

First Order Reaction – Problems

SOLVED PROBLEM. From the following data for the decomposition of N_2O_5 in CCl_4 solution at 48°C, show that the reaction is of the first order

t (mts)	10	15	20	∞
Vol of O_2 evolved	6.30	8.95	11.40	34.75

SOLUTION

For a first order reaction the integrated rate equation is

$$\frac{1}{t} \log \frac{V_\infty}{V_\infty - V_t} = k$$

In this example, $V_\infty = 34.75$

t	$V_\infty - V_t$	$\dfrac{1}{t} \log \dfrac{V_\infty}{V_\infty - V_t}$	=	k
10	28.45	$\dfrac{1}{10} \log \dfrac{34.75}{28.45}$	=	0.00868
15	25.80	$\dfrac{1}{15} \log \dfrac{34.75}{25.80}$	=	0.00862
20	23.35	$\dfrac{1}{20} \log \dfrac{34.75}{23.35}$	=	0.00863

Since the value of k is fairly constant, it is a **first order reaction**.

First Order Reaction – Problems

SOLVED PROBLEM 5. For a certain first order reaction $t_{0.5}$ is 100 sec. How long will it take for the reaction to be completed 75% ?

SOLUTION

Calculation of k

For a first order reaction

$$t_{1/2} = \frac{0.693}{k}$$

or

$$100 = \frac{0.693}{k}$$

$\therefore$

$$k = \frac{0.693}{100} = 0.00693 \text{ sec}^{-1}$$

Calculation of time for 75% completion of reaction

The integrated rate equation for a first order reaction is

$$k = \frac{2.303}{t} \log \frac{[A]_0}{[A]}$$

or

$$t = \frac{2.303}{k} \log \frac{[A]_0}{[A]}$$

When $\dfrac{3}{4}$ initial concentration has reacted, it is reduced to $\dfrac{1}{4}$

Substituting values in the rate equation

$$t_{3/4} = \frac{2.303}{0.00693} \log \frac{[A]_0}{\frac{1}{4}[A]_0}$$

$$= \frac{2.303}{0.00693} \log 4 = \textbf{200 sec}$$

First Order Reaction – Problems

SOLVED PROBLEM 6. A first order reaction is one-fifth completed in 40 minutes. Calculate the time required for its 100% completion.

SOLUTION

Calculation of k

For a first order reaction

$$k = \frac{2.303}{t} \log \frac{[A]_0}{[A]}$$

After 40 mts, the initial concentration is reduced to $\frac{4}{5}$ That is,

$$[A] = \frac{4}{5}[A]_0$$

Substituting values in the equation above

$$k = \frac{2.303}{40} \log \frac{[A]_0}{\frac{4}{5}[A]_0}$$

or

$$k = \frac{2.303}{40} \log 5 - \log 4 = 0.00558 \, mt^{-1}$$

Calculation of time required for 100% completion

We know that for first order reaction

$$k = \frac{2.303}{t} \log \frac{[A]_0}{[A]}$$

$$t = \frac{2.303}{k} \log \frac{[A]_0}{[A]}$$

If reaction is 100% complete in, say, t_1 time, we have, $[A] = 0$. Thus,

$$t_1 = \frac{2.303}{0.00558} \log \frac{[A]_0}{0} = \infty$$

Second Order Reaction

- Let's consider a second order reaction,

$$2A \longrightarrow \text{product}$$

Rate of reaction, $dx/dt = k\,(a-x)^2$

$$\text{or, } \int \frac{dx}{(a-x)^2} = \int k\,dt \quad \text{or, } \frac{1}{a-x} = kt + I \text{ -------- (1)}$$

When $t = 0$, $x = 0$; therefore, $I = 1/a$

Then, equation (1) will be, $\quad \frac{1}{a-x} = kt + \frac{1}{a}$

$$\text{or, } k = \frac{1}{t}\,\frac{x}{a(a-x)} \quad \text{----------- (2)}$$

When $t = t_{1/2}$, $x = a/2$; then equation (2) becomes –

$$t_{1/2} = \frac{1}{k\,a}$$

While half-life of a first order reaction is independent of initial concentration, half-life of a second order reaction depends on initial concentration.
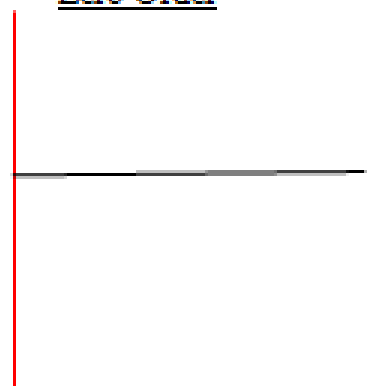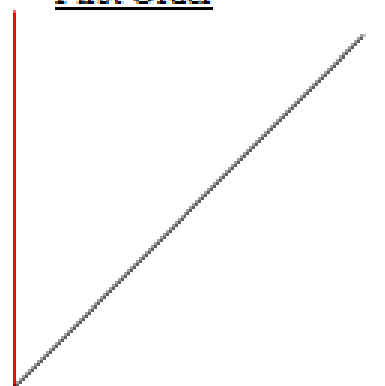
Second Order Reaction
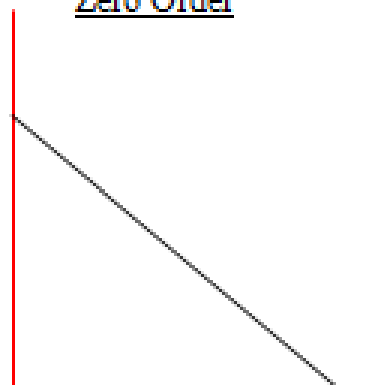
Pseudo-Order Reaction

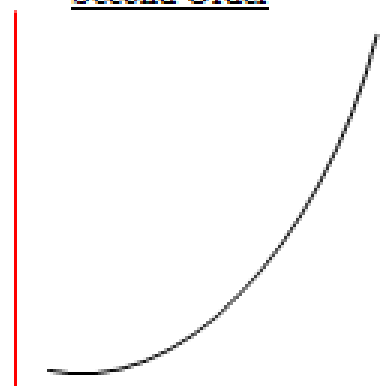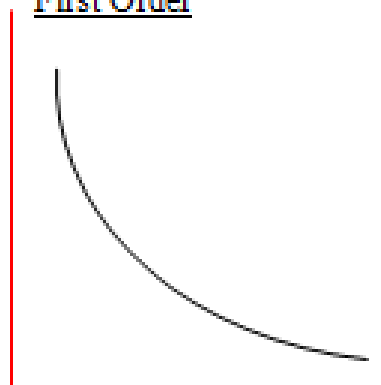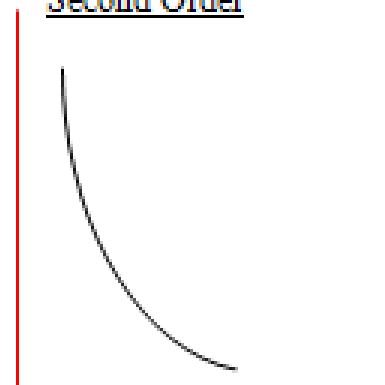- A reaction in which one of the reactants is present in a large excess shows an order different from the actual order.

- The experimental order which is not the actual one is referred to as the pseudo-order.

- Let's consider a reaction, $A + B \longrightarrow$ product

Then, rate = k [A] [B]

If B is present in large extent, its concentration practically remains unchanged over the course of the reaction. Therefore,

rate = k' [A]   where, k' = k[B]

Thus, the actual order of the reaction was second-order, but in practice it is first order reaction. Hence it is said to be pseudo first order reaction.

Example: $CH_3COOC_2H_5 + H_2O \longrightarrow CH_3COOH + C_2H_5OH$
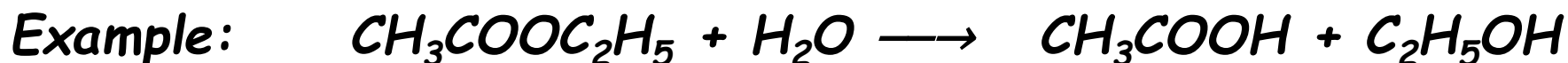
Units of rate constant

- **Zero order reaction**

$$k = dx/dt$$

Unit: mole L^{-1} time^{-1}

1st order reaction

$$k = \frac{2.303}{t} \log \frac{a}{(a-x)}$$

Unit: time^{-1}

2nd order reaction

$$k = \frac{1}{t} \frac{x}{a(a-x)}$$

Unit: L mole^{-1} time^{-1}

Determination of Order of a Reaction

❑ *Using integrated rate equation*

❑ *Graphical method*

❑ *Using half-life*

❑ *Differential method*

❑ *Ostwald's isolation method*

Determination of Order of a Reaction

❏ *Using integrated rate equation*

- For a particular reaction, A ⟶ product, 'a' is the initial concentration, (a-x) is the concentration at time t.

- The experimental value of a, (a-x) and t for different time interval are then substituted in the integrated rate equation for zero, 1st, 2nd or 3rd order reactions.

- The rate equation which yields a constant value of k corresponds to the correct order of the reaction.

- This method of ascertaining the order of a reaction is essentially a method of hit-and-trial but still used extensively to find the order of simple reactions.

Determination of Order of a Reaction
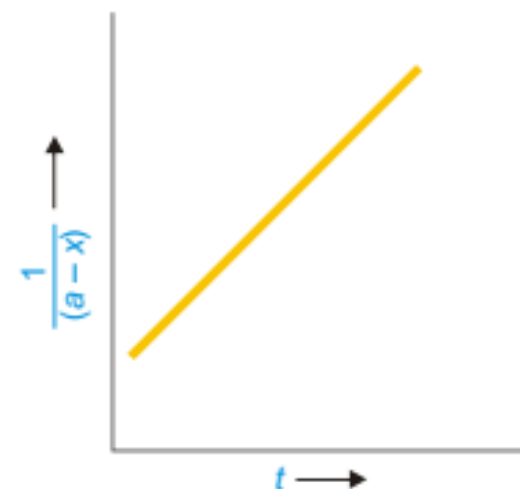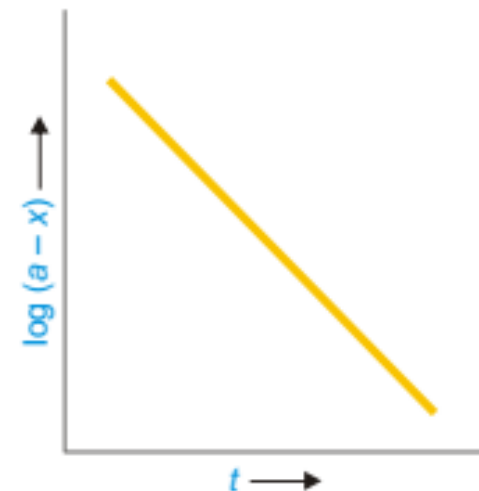
❑ *Graphical Method*

▪ **For 1st order reaction, the rate equation is –**

$$\ln a/(a-x) = kt$$

or, $\ln (a-x) = -kt + \ln a$

For 2nd order reaction,

$$1/(a-x) = kt + 1/a$$

Determination of Order of a Reaction

❑ *Using Half-life*

$$\text{Half life} \propto \frac{1}{[A]} \text{ for 2nd order reaction}$$

$$\text{Similarly, Half life} \propto \frac{1}{[A]^2} \text{ for 3rd order; Half life} \propto \frac{1}{[A]^{n-1}} \text{ for nth order}$$

Let the initial concentrations in the two experiments be $[A_1]$ and $[A_2]$, while times for completion of half change are t_1 and t_2 respectively.

$$\text{Then, } t_1 \propto \frac{1}{[A_1]^{n-1}} \quad \text{and } t_2 \propto \frac{1}{[A_2]^{n-1}}$$

$$\frac{t_2}{t_1} = \left[\frac{A_1}{A_2}\right]^{n-1}; \text{ or, } (n-1) \log\left[\frac{A_1}{A_2}\right] = \frac{t_1}{t_2}; \text{ or, } n = 1 + \frac{\log\left(\frac{t_1}{t_2}\right)}{\log\left[\frac{A_1}{A_2}\right]}$$

Determination of Order of a Reaction

❑ **The Differential Method**

The rate of a reaction of nth order is, $-\dfrac{dc}{dt} = k\,C^n$

Where, C is the concentration at any instant. For two reactions performed with two initial concentrations, we can write,

$$-\frac{dc_1}{dt} = k\,C_1^n \text{ and } -\frac{dc_2}{dt} = k\,C_2^n$$

Taking logs for both cases, $\log\left(-\dfrac{dc_1}{dt}\right) = \log k + n \log C_1$ ----------- (1)

and $\log\left(-\dfrac{dc_2}{dt}\right) = \log k + n \log C_2$ -------------(2)

Subtracting (2) from (1), we have,

$$n = \frac{\log\left(-\frac{dc_1}{dt}\right) - \log\left(-\frac{dc_2}{dt}\right)}{\log C_1 - \log C_2}$$

Determination of Order of a Reaction

❑ Ostwald's Isolation Method

- This method is employed in determining the order of complicated reactions by 'isolating' one of the reactants so far as its influence on the rate of reaction is concerned.

- Let's consider a reaction ,   A + B + C → product

- The order of the reaction with respect to A, B and C is determined.

- For the determination of the order of reaction with respect to A, B and C are taken in a large excess so that their concentrations are not affected during the reaction.

- The order of the reaction is then determined by using any of the methods described earlier.

- Likewise, the order of the reaction with respect to B and C is determined.

- Therefore, $n = n_A + n_B + n_C$

Collision Theory of Reaction Rates

- *A chemical reaction takes place only by collisions between the reacting molecules.*

- *The two main conditions for a collision between the reacting molecules to be productive are –*

  - *The colliding molecules must posses sufficient kinetic energy to cause a reaction.*

  - *The reacting molecules must collide with proper orientation.*

Effective collision   Ineffective collision
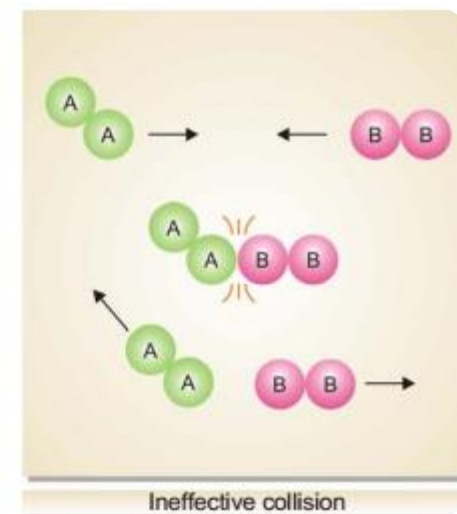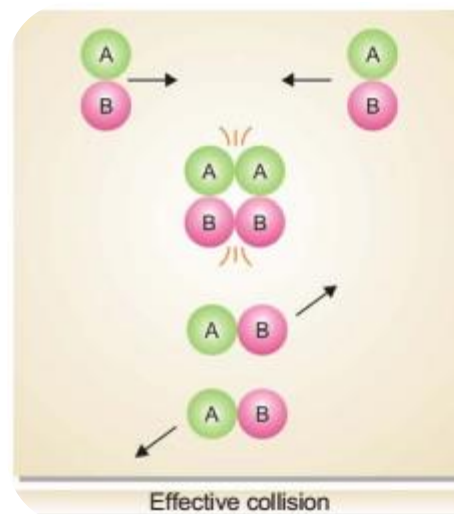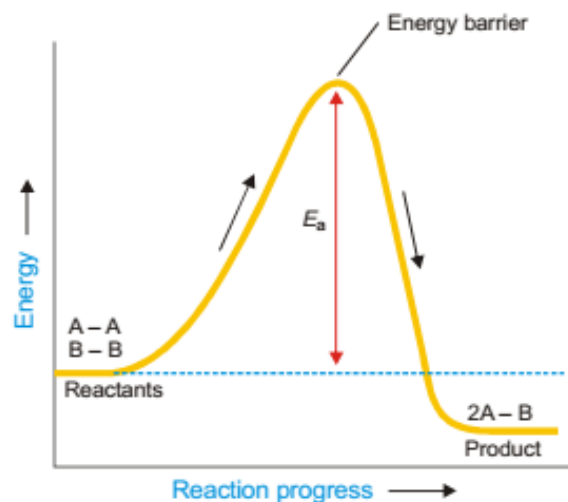
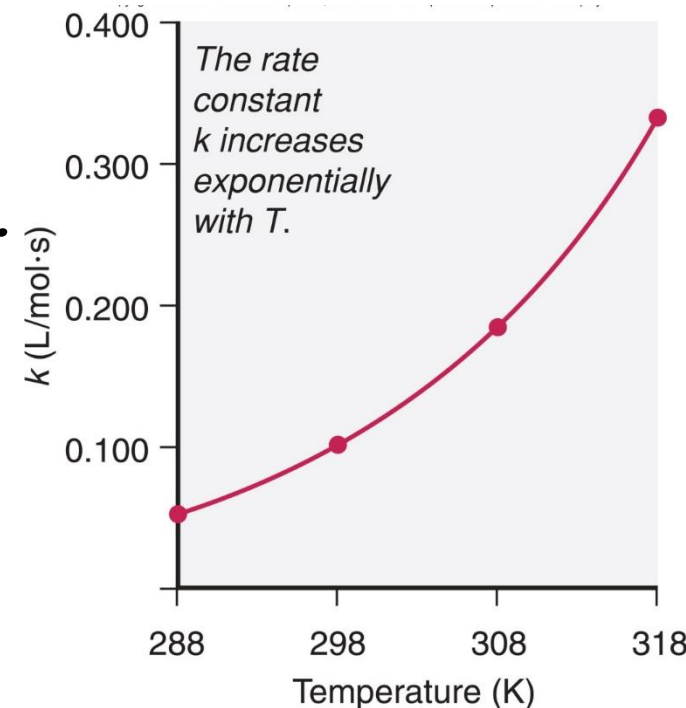# Temperature and Rate Constant

- Temperature has a dramatic effect on reaction rate. For many reactions, an increase of 10°C will double or triple the rate.

- Experimental data shows that k increases exponentially as T increases. This is expressed in the Arrhenius equation:

$$k = Ae^{-E_a/RT}$$

k = rate constant, A = constant, E_a = activation energy.

Higher *T* ⟶ **larger *k*** ⟶ **increased rate**

Reaction rate and k increase exponentially
as T increases.

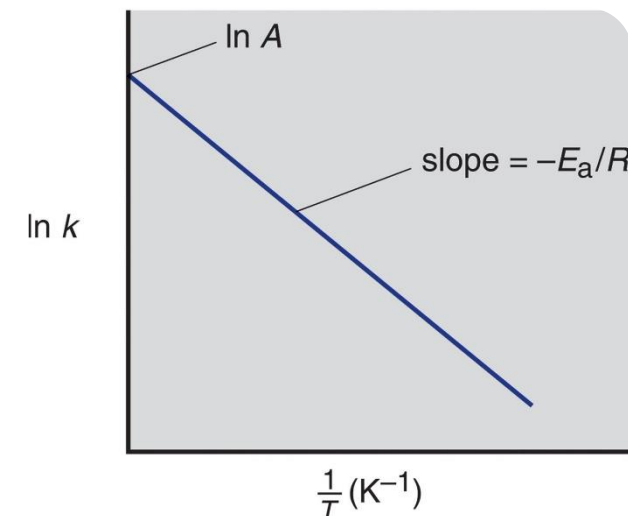The rate constant k increases exponentially with T.

Temperature and Rate Constant

- E_a can be calculated from the Arrhenius equation.

$$k = Ae^{-E_a/RT}$$

$$\ln k = \ln A \; \frac{-E_a}{R}\left(\frac{1}{T}\right)$$
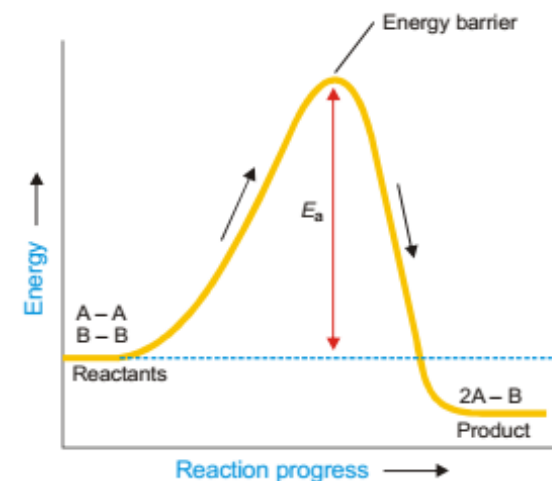
straight-line form

- If k_1 and k_2 are rate constants at temperature T_1 and T_2, then the above equation will be -

$$\ln \frac{k_2}{k_1} = -\frac{E_a}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$$

- Activation energy (E_a) is defined as the minimum amount of energy required by a reacting molecule to get converted into product.

Temperature and Rate Constant - Problem

- The decomposition of hydrogen iodide, $2HI(g) \rightarrow H_2(g) + I_2(g)$, has rate constants of 9.51×10^{-9} L/mol·s at 500 K and 1.10×10^{-5} L/mol·s at 600 K. Find E_a.
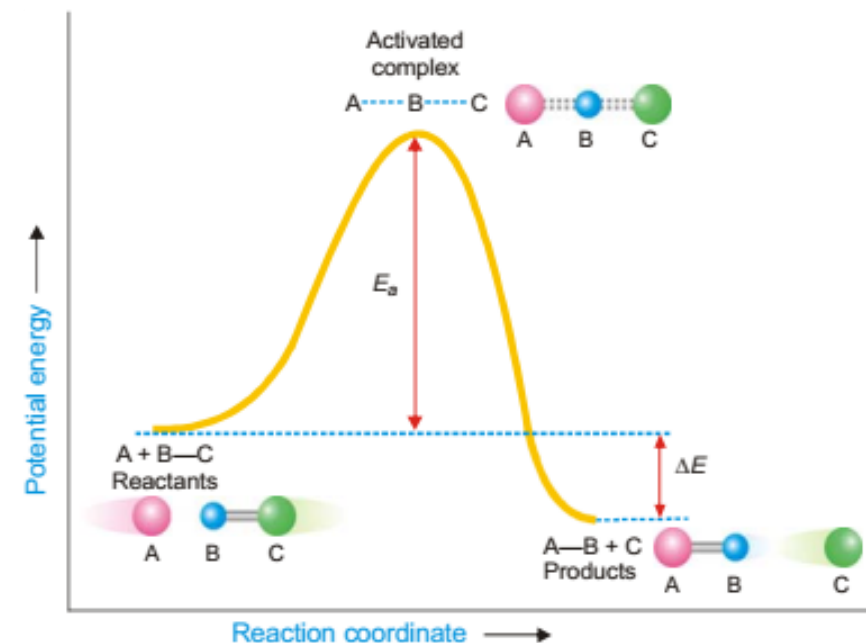
- Solution

$$\ln \frac{k_2}{k_1} = -\frac{E_a}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$$

Ans: $= 1.76 \times 10^5$ J/mol $= 1.76 \times 10^2$ kJ/mol

Transition State Theory

- *An effective collision between particles leads to the formation of a transition state or activated complex.*

- *During the collision, the reactant molecules form a transition state or activated complex which decomposes to give the products.*

- *The transition state is an unstable species that contains partial bonds.*

- *It's a transitional pathway between reactants and products.*

- *Transition states cannot be isolated.*

Thank You