## CHEMICAL KINETICS

By Deepak Kumar Mandal Email: dkmiitg@gmail.com

#### Content

- Rate of Reaction
- Order of Reaction
- Arrhenius Equation

### Introduction

- In chemical Kinetic, Reaction occurs in single step are Simple or Elementary reaction & those which take two or more steps are complex reaction.
- For elementary reaction order of reaction & molecularity are *generally* same.

#### Rate of Reaction

> Change in concentration of Reactant or Product per unit time called rate of Reac<sup>n</sup>.

$$A \xrightarrow{} P$$

$$t=0 \qquad a \qquad 0$$

$$t=t \qquad a-x \qquad x$$

$$rate \propto [Reactant]$$

$$=> r = k[a-x]$$

$$|$$

$$Rate Constant$$

$$Rate = \frac{dx}{dt}$$

$$rate = \frac{a - x - a}{dt} = \frac{-x}{t} = \frac{dx}{dt} (for A)$$

$$rate = \frac{x - 0}{dt} (for P)$$

#### Rate of Reaction

$$A + B ----> C + D$$

Rate of Reaction 
$$(r) = \frac{-d(A)}{dt} = \frac{-d(B)}{dt} = \frac{d(C)}{dt} = \frac{d(D)}{dt} = \frac{dx}{dt}$$

> Rate of disappearance of reactant = Rate of appearance of Product

eg. 
$$2A + 3B ---> C + 4D$$

$$rate = \frac{-1}{2} \frac{d[A]}{dt} = \frac{-1}{3} \frac{d[B]}{dt} = \frac{d[C]}{dt} = \frac{1}{4} \frac{d[D]}{dt}$$

 $\sim$  Conc<sup>n</sup> = P<sup>r</sup> at Temp<sup>r</sup> constant

### Order of Reaction

- No of molecules of reactant whose conc<sup>n</sup> determines the rate of reaction.
- > It is experimental value. It may be zero or fraction, -ve also.
- > It is derive from rate expression.

$$A \rightarrow P$$

$$R = K[A]^x$$

x = order of Reaction

### 1st order of Reaction

$$R = K[A]^x x = 1$$

$$kt = 2.303 \log \frac{a}{a - x}$$

> a= initial conc<sup>n</sup>; a-x=left conc<sup>n</sup>; k=time<sup>-1</sup>

$$t(1/2) = \frac{0.693}{K}$$

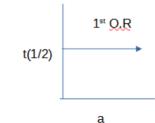
: Independent of initial concentration

$$t=t/2$$

$$a=a; a-x=a/2$$

$$k = \frac{2.303}{t(1/2)} \log \frac{a}{a/2} = \frac{0.693}{t(1/2)}$$

$$t(1/2) = \frac{0.693}{K}$$



 $A \rightarrow P$ 

$$r = k[a - x]$$

$$\frac{dx}{dt} = k[a-x]$$

$$\frac{dx}{a-x} = kdt$$

$$kt = 2.303 \log \frac{a}{a - x}$$

#### Zero order of Reaction

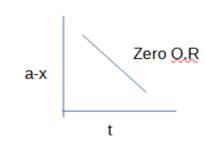
$$R = K[A]^x$$
 at  $x = 0$ 

• 
$$x = kt$$
 ;  $k = mole L^{-1} time^{-1}$ 

For If t=t/2 => x=a/2  

$$t(1/2) = \frac{a}{2k}$$
: t<sub>1/2</sub> ∝ a

Rate const. => depends only Temp<sup>r</sup>



$$r = k [a - x]^0$$
$$r = k$$

$$\frac{dx}{dt} = k$$

$$dx = k \cdot dt$$

$$x = kt$$

# Arrhenius Eqn

Relation between rate constant & Temperature

$$\kappa = Ae^{-Ea/RT}$$

$$\log K = \log A - \frac{Ea}{2.303 RT}$$

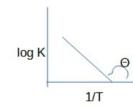
- ✓ A= Arrhenius Constant or Pre-exponential factor
- Ea = activation energy; R= gas const.; T= temp. In Kelvin

$$K = Ae^{-(Ea/RT)}$$

$$\ln K = \ln A - \frac{Ea}{RT}$$

$$2.303 \log K = 2.303 \log A - \frac{Ea}{RT}$$

$$\log K = \log A - \frac{Ea}{2.303 RT}$$



$$slope = tan\Theta = \frac{-Ea}{2.303 R}$$
$$y - intercept = log A$$

## Conclusion

