Day-12

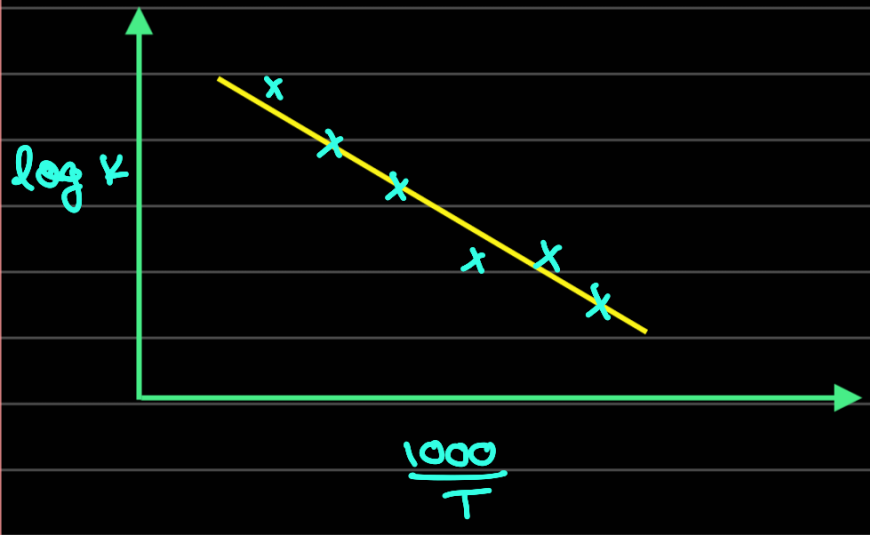
→ $k = A_0 \exp.\left(\frac{-E_a}{R_u T}\right)$

E_A → Activation energy
A_0 → Pre-exponential factor / frequency factor

Actually, $K = A_0 T^{\beta} \exp.\left(\frac{-E_A}{R_u T}\right)$

(β → any constant)

$E_A/R_u = T_A$ (Activation Temp.)



→ Molecularity : No. of reactant molecules in an elementary reaction.

- Unimolecular – $O_2 \longrightarrow O + O$ (Dissociation)
- Bimolecular – $H + OH \longrightarrow H_2O$
- Trimolecular – $O + O + M \longrightarrow O_2 + M$ (Recombination)

For elementary reaction,

order = molecularity

(Not true for global reaction)

Eg: Fuel + a Oxidizer ⟶ Products

$$\frac{d[\text{Fuel}]}{dt} = -K(T)\,[\text{Fuel}]^n[\text{Ox}]^m$$

overall order = $n+m$

n, m can be fractions

→ Elementary reactions:

$$H_2 + O_2 \underset{K_{r_1}}{\overset{K_{f_1}}{\rightleftharpoons}} HO_2 + H \qquad \text{(A)}$$

$$H + O_2 \underset{K_{r_2}}{\overset{K_{f_2}}{\rightleftharpoons}} OH + O \qquad \text{(B)}$$

K_{f_1}, K_{f_2} ⟶ elementary forward rate constants

K_{r_1}, K_{r_2} ⟶ elementary reverse rate constants

$$\frac{d[O_2]}{dt} = -K_{f_1}[H_2][O_2] = K_{r_1}[HO_2][H] \qquad \text{(1)}$$

$$\frac{d[O_2]}{dt} = -K_{f_2}[H][O_2] = K_{r_2}[OH][O] \qquad \text{(2)}$$

Net $\frac{d[O_2]}{dt}$ = (1) + (2)