Chem Kinetics

Lecture Notes on the Concepts of Rate of a Chemical Reaction

Definition of Reaction Rate

The rate of a chemical reaction is defined as the change in the concentration of reactants or products per unit time. It is a measure of how quickly reactants are converted into products in a chemical reaction.

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

Where $[A]$ is the concentration of the reactant, and Δt is the change in time. The negative sign indicates the decrease in the concentration of the reactant over time. Conversely, if the rate is expressed in terms of product formation, it is given by:

$$\text{Rate} = \frac{\Delta[B]}{\Delta t}$$

Where $[B]$ is the concentration of the product.

Rate Expressions and Units

The rate of a reaction can be expressed in various ways, depending on the phase and nature of the reactants and products. For a general reaction:

$$\text{A} \rightarrow \text{B}$$
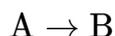
The rate expression in terms of the reactant A and the product B can be written as:

$$\text{Rate} = -\frac{d[A]}{dt} = \frac{d[B]}{dt}$$

The units of the rate of reaction are typically expressed as concentration per unit time. For reactions in solutions, the units are:

$$\text{mol L}^{-1}\text{s}^{-1}$$

For gas-phase reactions, the concentration is often expressed in terms of partial pressures, and the units are:

$$\text{atm s}^{-1}$$

Instantaneous and Average Rates

Average Rate: The average rate of reaction over a time interval is the change in concentration divided by the time interval. It is given by:

$$\text{Average Rate} = -\frac{[A]_2 - [A]_1}{t_2 - t_1}$$

Where $[A]_1$ and $[A]_2$ are the concentrations of A at times t_1 and t_2, respectively.

Instantaneous Rate: The instantaneous rate of reaction is the rate at a particular moment in time. It is determined by taking the derivative of concentration with respect to time:

$$\text{Instantaneous Rate} = -\frac{d[A]}{dt}$$

The instantaneous rate at any time t can be obtained by calculating the slope of the tangent to the concentration vs. time curve at that point.

Initial Rate Method

The initial rate method involves measuring the rate of reaction at the very beginning, where the concentrations of reactants are known and have not significantly changed. This method is useful for determining the order of a reaction and the rate constant. The initial rate is calculated using the slope of the tangent to the concentration vs. time curve at $t = 0$.

For a reaction:

$$\mathrm{A} + \mathrm{B} \rightarrow \mathrm{Products}$$
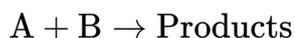
The rate law can be expressed as:

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

Where k is the rate constant, and m and n are the orders of the reaction with respect to reactants A and B. By measuring the initial rates for different initial concentrations of the reactants, the values of m, n, and k can be determined.

Summary

- **Reaction Rate:** Change in concentration per unit time.
- **Rate Expressions:** Negative for reactants, positive for products.
- **Units:** Typically $\mathrm{mol\ L^{-1}s^{-1}}$ for solutions and $\mathrm{atm\ s^{-1}}$ for gases.
- **Average Rate:** Change in concentration over a time interval.
- **Instantaneous Rate:** Rate at a specific moment, determined by the slope of the tangent to the concentration-time curve.
- **Initial Rate Method:** Used to determine reaction order and rate constant by measuring the rate at the start of the reaction.