Organic Reactions and Mechanisms

The key differences between **SN1** and **SN2** reactions are outlined below:

1. Mechanism

- **SN1 (Unimolecular Nucleophilic Substitution)**:
  - Proceeds in two steps:
    1. The leaving group departs, forming a carbocation intermediate.
    2. The nucleophile attacks the carbocation to form the product.
- **SN2 (Bimolecular Nucleophilic Substitution)**:
  - Proceeds in a single step, where the nucleophile attacks the substrate simultaneously as the leaving group departs, forming a transition state.

2. Kinetics

- **SN1**: Follows **first-order kinetics**, with the rate determined solely by the concentration of the substrate (alkyl halide):

$$\text{Rate} = k[\text{alkyl halide}]$$

- **SN2**: Follows **second-order kinetics**, with the rate depending on both the substrate and the nucleophile:

$$\text{Rate} = k[\text{alkyl halide}][\text{nucleophile}]$$

3. Stereochemistry

- **SN1**: Since the carbocation intermediate is planar, the nucleophile can attack from either side, resulting in a **racemic mixture** (if the substrate is chiral).
- **SN2**: The nucleophile attacks from the opposite side of the leaving group (backside attack), leading to **inversion of configuration** (Walden inversion), resulting in one specific stereoisomer.

4. Substrate Preference

- **SN1**: Favored by **tertiary** alkyl halides because they form stable carbocations. Stability order: Tertiary > Secondary > Primary (Primary carbocations are too unstable).
- **SN2**: Favored by **primary** alkyl halides due to lower steric hindrance. Reactivity order: Methyl > Primary > Secondary > Tertiary (Tertiary substrates are too hindered for backside attack).

5. Nucleophile

- **SN1**: The strength of the nucleophile is **less important** since it does not affect the rate of the reaction (only the stability of the carbocation matters).
- **SN2**: Requires a **strong nucleophile** since the nucleophile participates in the rate-determining step.

6. Solvent

- **SN1**: Favored by **polar protic solvents** (e.g., water, alcohols) that stabilize the carbocation intermediate and the leaving group.
- **SN2**: Favored by **polar aprotic solvents** (e.g., acetone, DMSO) that do not solvate the nucleophile, leaving it free to attack the substrate.

7. Reaction Conditions

- **SN1**: Best for bulky, sterically hindered substrates with good leaving groups and in polar protic solvents.
- **SN2**: Best for unhindered substrates with a strong nucleophile in polar aprotic solvents.

8. Examples

- **SN1 Example**:

$$(\mathrm{CH_3})_3\mathrm{CBr} \rightarrow (\mathrm{CH_3})_3\mathrm{C^+} + \mathrm{Br^-} \quad (\mathrm{Step\ 1})$$

$$(\mathrm{CH_3})_3\mathrm{C^+} + \mathrm{H_2O} \rightarrow (\mathrm{CH_3})_3\mathrm{COH_2^+} \rightarrow (\mathrm{CH_3})_3\mathrm{COH} \quad (\mathrm{Step\ 2})$$

- **SN2 Example**:

$$\mathrm{CH_3Br} + \mathrm{OH^-} \rightarrow \mathrm{CH_3OH} + \mathrm{Br^-}$$

Summary Table:

Property	SN1	SN2
Mechanism	Two steps (carbocation intermediate)	Single step (simultaneous attack)
Rate law	First-order, rate = k[alkyl halide]	Second-order, rate = k[alkyl halide] [nucleophile]
Stereochemistry	Racemization (loss of stereochemistry)	Inversion of configuration
Substrate preference	Tertiary > Secondary > Primary	Methyl > Primary > Secondary
Nucleophile	Weak nucleophiles can work	Strong nucleophile required
Solvent	Polar protic (stabilizes carbocation)	Polar aprotic (enhances nucleophilicity)
Reaction conditions	Bulky substrates, good leaving group, polar protic solvents	Unhindered substrates, strong nucleophiles, polar aprotic solvents

Understanding these differences helps in predicting which reaction pathway (SN1 or SN2) a given substrate will follow under specific conditions.