INVESTIGATION OF REACTION MECHANISM

- Actual pathway of reaction is called reaction mechanism
- Mechanism is only suggestive not conclusive
- Mechanism is based on available evidences

TYPES OF MECHANISMS

1. **HETEROLYTIC MECHANISMS**

   If a bond breaks in such a way that both electrons remain with one fragment

   - Nucleophilic Reactions
   - Electrophilic Reactions

2. HOMOLYTIC OR FREE-RADICAL MECHANISMS

If a bond breaks in such a way that each fragment gets one electron
Free radicals are formed

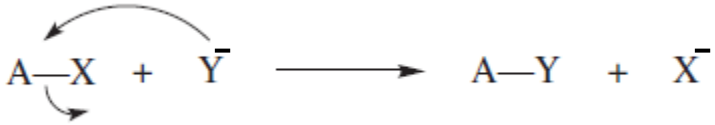
3. PERICYCLIC MECHANISMS

Electrons move in a closed ring
No intermediates, ions or free radicals are formed

TYPES OF REACTIONS

1. **SUBSTITUTIONS**

(i) Nucleophilic substitution

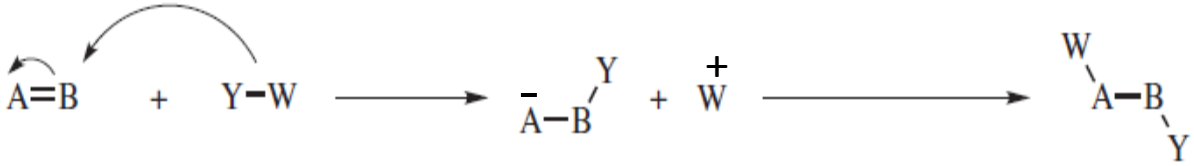


(ii) Electrophilic substitution

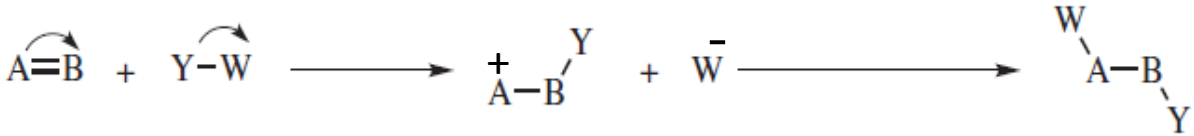
(iii) Free-radical substitution

2. **ADDITIONS**

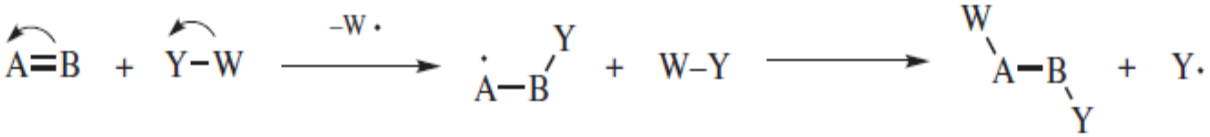
(i) Nucleophilic addition



(ii) Electrophilic addition



(iii) Free-radical addition



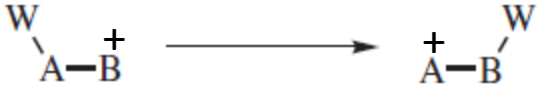
(iv) Simultaneous addition

3. ELIMINATIONS

Heterolytic or Pericyclic mechanisms

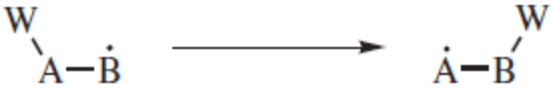
4. REARRANGEMENTS

(i) Nucleophilic



(ii) Electrophilic

(iii) Free-radical



5. REDOX REACTIONS

May be substitutions, eliminations, additions, rearrangements types
May be of some other type

6. COMBINATIONS OF THE ABOVE

Addition-Elimination, Oxidative-Addition, Reductive-Elimination etc.

INVESTIGATION OF REACTION MECHANISM: EVIDENCES

- Actual pathway of reaction is called reaction mechanism
- Mechanism is only suggestive not conclusive
- Mechanism is based on available evidences

EVIDENCES

1. Nature of Products

2. Thermodynamics and Kinetic Requirements

3. Study of Intermediates
   - (i) Isolation of intermediates
   - (ii) Detection of intermediates
   - (iii) Trapping of Intermediates
   - (iv) Addition of Suspected intermediates

4. Stereochemical studies

5. Isotopic Studies
   - (i) Isotopic labelling
   - (ii) Isotopic effect
   - (iii) Isotopic scrambling