

Dehydro halogenation of alkyl halides

1,2-Elimination

What is Dehydrohalogenation?

- Dehydrohalogenation is a type of elimination reaction where an alkyl halide ($R-CH_2-CHX-R'$) loses a hydrogen atom (H) and a halogen atom (X), usually from adjacent carbon atoms, resulting in the formation of an alkene.

General reaction:



- Requires a **base**, such as OH^- or an alkoxide ion
- Produces an alkene and a hydrogen halide (HX)

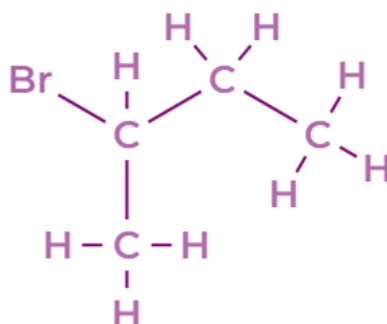
1,2-Elimination (β -Elimination)

- This is called 1,2-elimination or β -elimination because:
 - The halogen (X) is removed from the α -carbon (carbon bearing the halogen)
 - The hydrogen (H) is removed from the β -carbon (adjacent to the α -carbon)
 - A double bond forms between the α - and β -carbons

Example of 1,2-Elimination

Let's consider **2-bromobutane** reacting under basic conditions:

Structure of 2-bromobutane:



Reaction Conditions

- Under heat and strong base (e.g., KOH in ethanol), the following occurs:
 - The Br atom on carbon-2 acts as the leaving group.
 - One of the β -hydrogens is abstracted from carbon-3.
 - A double bond forms between carbon-2 and carbon-3.

Resulting Product



- The product is **but-2-ene**, a typical result of a 1,2-elimination process.
- Note: There can be stereoisomers in the products (*cis* and *trans* forms), especially in symmetrical alkenes.

Types of 1,2-Elimination Mechanisms

- 1,2-Elimination can proceed via two principal mechanistic pathways:

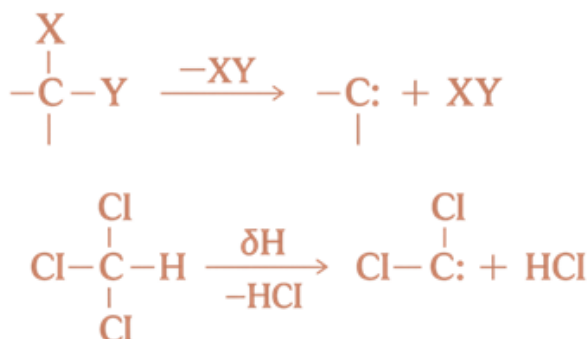
A. E2 Mechanism (Bimolecular Elimination)

B. E1 Mechanism (Unimolecular Elimination)

Why It's an Elimination

- Unlike substitution (where one group replaces another), elimination removes two atoms/groups entirely, forming a π -bond.
- The reaction reduces saturation (alkane $\rightarrow$ alkene)

Key Points of 1,2-Elimination



- Requires a base to abstract the β -hydrogen
- The halogen leaves as a leaving group
- Alkene is formed from the remaining carbons
- It's called β -elimination because the hydrogen is on the β -carbon
- Competes with substitution reactions under similar conditions

Regioselectivity and Multiple Products

- When more than one β -hydrogen is available, multiple alkenes can form.
- Their distribution depends on:
 - **Zaitsev's Rule:** The more substituted (stable) alkene is favored.
 - **Hofmann's Rule:** The less substituted alkene is favored when bulky bases are used.

General Conditions That Affect Elimination

- **Substrate:** Tertiary > secondary > primary (in terms of ease of elimination)
- **Base strength:** Strong base favors E2; weak base + heat favors E1

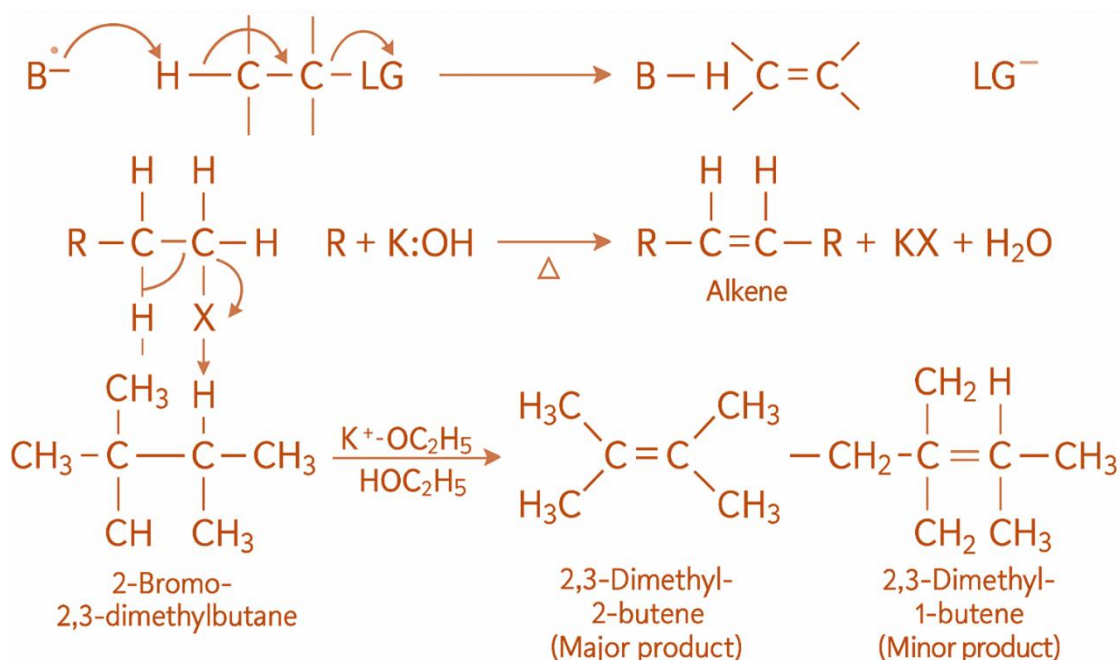
- **Leaving group:** Better leaving group ($I^- > Br^- > Cl^-$) favors elimination
- **Solvent and temperature:** Polar protic solvents and heat favor E1; aprotic + strong base favors E2

Kinetics of the E2 Mechanism

General Reaction:



Example:



Rate Law (E2):

$$\text{Rate} = k [\text{Alkyl Halide}][\text{Base}]$$

- **Second-order overall:** The reaction rate depends on the concentration of two reactants.
- This reflects a single-step, concerted mechanism (both the base and the substrate are involved in the transition state).

Implications of the Rate Law:

- Doubling the concentration of the base doubles the rate.
- Doubling the alkyl halide concentration also doubles the rate.
- Changing the solvent or temperature can affect the rate, but concentration changes are directly reflected in the speed of reaction.

Transition State (E2):

- The reaction occurs through a single transition state where:

- The base begins to abstract the β -hydrogen,
- The π -bond begins to form between α and β carbons,
- The leaving group (X^-) starts to depart from the α -carbon.
- All of this happens simultaneously (concerted).

Kinetics of the E1 Mechanism

General Reaction:

Alkyl halide $\rightarrow$ carbocation intermediate $\rightarrow$ alkene

Example:



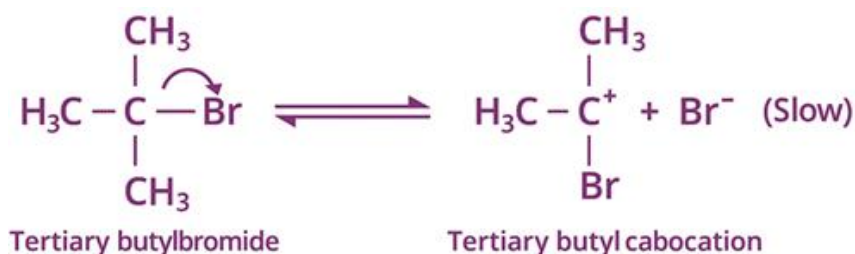
Rate Law (E1):

$$\text{Rate} = k [\text{Alkyl Halide}]$$

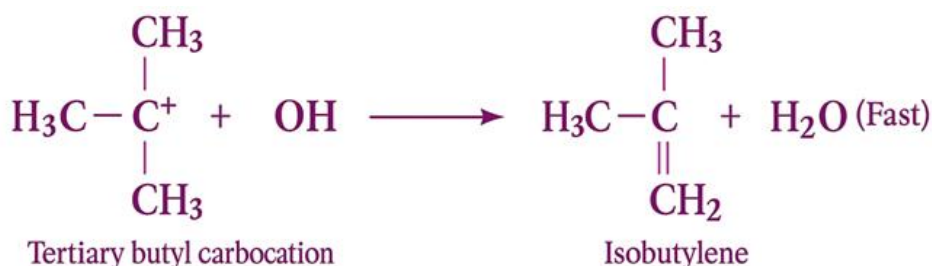
- **First-order overall:** The rate depends only on the concentration of the substrate (the alkyl halide).
- The base does not appear in the rate-determining step.

Why First-Order?

- The E1 mechanism occurs in **two steps**:
 1. **Ionization:** The halide leaves, forming a carbocation. This is the slow, rate-determining step.



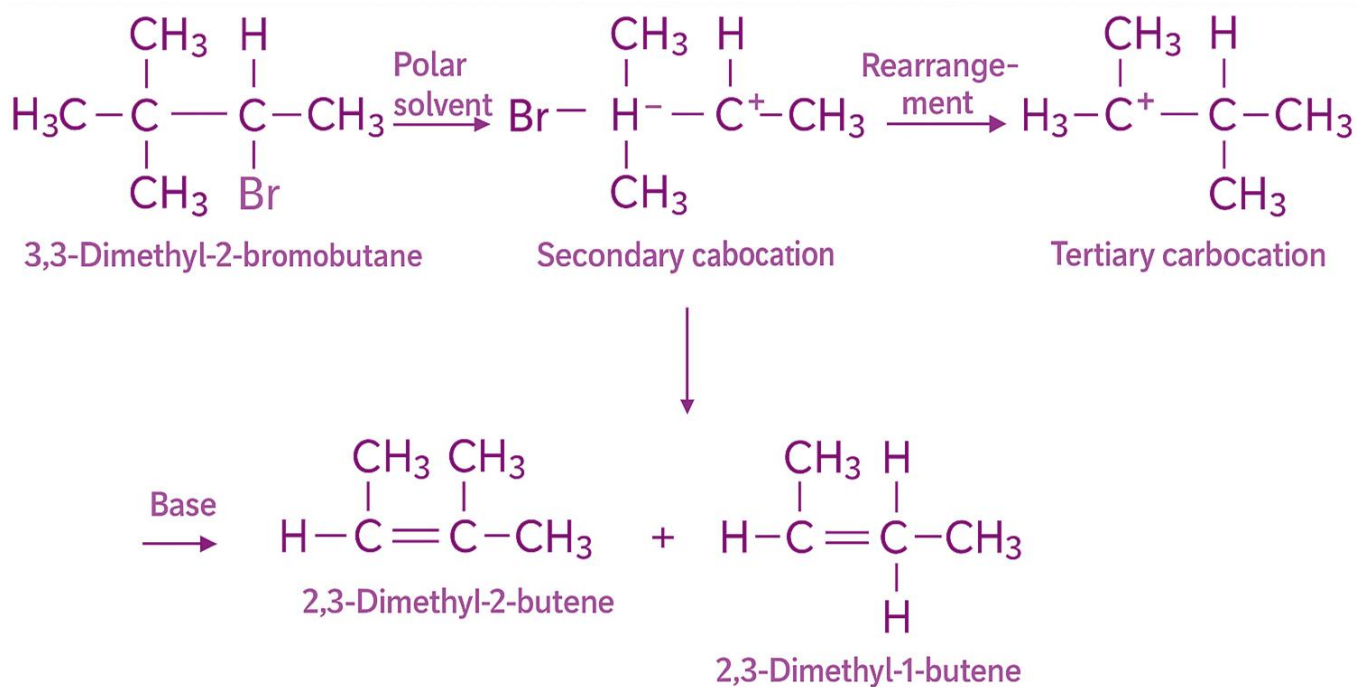
2. **Deprotonation:** A base abstracts the β -hydrogen, forming the alkene. This is a fast step.



- Since only the first step (formation of the carbocation) determines the rate, the base plays **no role** in the kinetics.

Transition State (E1):

- The transition state involves only the departure of the leaving group (X^-) and formation of the carbocation.
- The elimination of the β -H occurs after the rate-limiting step.



E2 Mechanism (Elimination Bimolecular)

Overview of E2 Mechanism

- The E2 mechanism (Elimination, bimolecular) is a concerted reaction in which:
 - a base removes a β -hydrogen,
 - a π -bond (double bond) forms between the α - and β -carbons, and
 - a leaving group (halide) departs—all in one single step.
- This is a fundamental reaction in organic chemistry, widely used for the synthesis of alkenes from alkyl halides, especially when strong bases are present.

General Form of the E2 Reaction

- Let's consider a generic alkyl halide:



- R = alkyl group
- X = leaving group (typically Br^- , Cl^- , I^-)
- Base^- = strong base (e.g., ^-OH , ^-OR , $^-\text{NH}_2$, tert-butoxide)
- Product = alkene



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