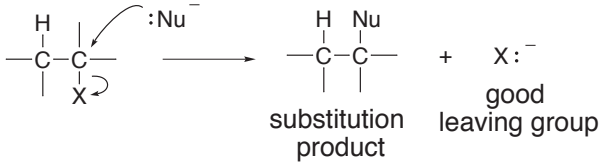
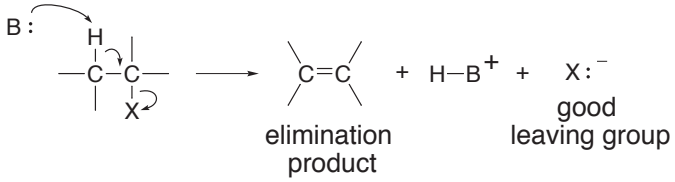
Chapter 8: Alkyl Halides and Elimination Reactions

♦ A comparison between nucleophilic substitution and β-elimination

Nucleophilic substitution—A nucleophile attacks a carbon atom (7.6).



β-Elimination—A base attacks a proton (8.1).

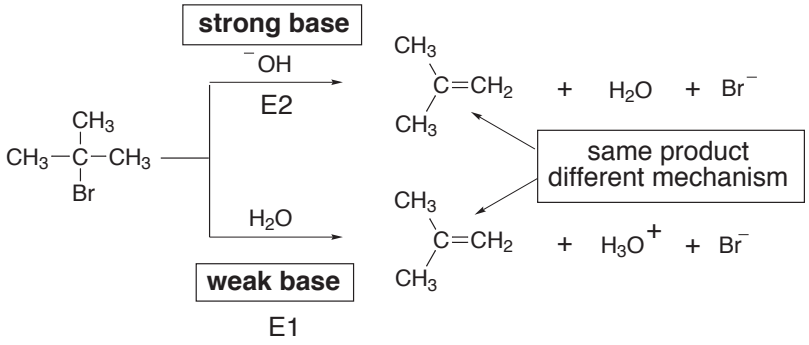


Similarities	Differences
• In both reactions RX acts as an electrophile, reacting with an electron rich reagent. • Both reactions require a **good leaving group X:⁻** willing to accept the electron density in the C–X bond.	• In substitution, a nucleophile attacks a single carbon atom. • In elimination, a Brønsted–Lowry base removes a proton to form a π bond, and two carbons are involved in the reaction.

♦ The importance of the base in E2 and E1 reactions (8.9)

The strength of the base determines the mechanism of elimination.

- Strong bases favor E2 reactions.
- Weak bases favor E1 reactions.



♦ E1 and E2 mechanisms compared

	E2 mechanism	E1 mechanism
[1] Mechanism	• One step (8.4B)	• Two steps (8.6B)
[2] Alkyl halide	• rate: $R_3CX > R_2CHX > RCH_2X$ (8.4C)	• rate: $R_3CX > R_2CHX > RCH_2X$ (8.6C)
[3] Rate equation	• rate = k[RX][B:] • second order kinetics (8.4A)	• rate = k[RX] • first order kinetics (8.6A)
[4] Stereochemistry	• anti periplanar arrangement of H and X (8.8)	• trigonal planar carbocation intermediate (8.6B)
[5] Base	• favored by strong bases (8.4B)	• favored by weak bases (8.6C)
[6] Leaving group	• better leaving group → faster reaction (8.4B)	• better leaving group → faster reaction (Table 8.4)
[7] Solvents	• favored by polar aprotic solvents (8.4B)	• favored by polar protic solvents (Table 8.4)
[8] Product	• more substituted alkene favored (Zaitsev Rule, 8.5)	• more substituted alkene favored (Zaitsev Rule, 8.6C)

♦ Summary chart on the four mechanisms: S_N1, S_N2, E1 or E2

Alkyl halide type	Conditions	Mechanism
1^o RCH_2X	strong nucleophile strong bulky base	**S_N2** **E2**
2^o R_2CHX	strong base and nucleophile strong bulky base weak base and nucleophile	**S_N2 + E2** **E2** **S_N1 + E1**
3^o R_3CX	weak base and nucleophile strong base	**S_N1 + E1** **E2**

♦ Zaitsev Rule

- β-Elimination affords the more stable product having the more substituted double bond.
- Zaitsev products predominate in E2 reactions except when a cyclohexane ring prevents trans diaxial arrangement.