

Comparison of the Mechanisms of Elimination Reactions (E1 and E2) in Alkyl Compounds

	E1	E2
Kinetics and Rate Law	First Order: Rate = $\kappa[R-X]^1$	Second Order: Rate = $\kappa[R-X]^1[Nu:]^1$
Rate-determining Step	Formation of carbocation	Anti-coplanar arrangement of the β -hydrogen and leaving group in the transition state.
Characteristics of Mechanism	<p>Two steps:</p> <p>Step 1:</p> $R-X \xrightarrow{RDS} R^+ + X^-$ <p>or</p> <p>Step 2:</p> <p>X can be the solvent.</p> <p>1st step is the slow step, rate-determining step. Bond breaking.</p>	<p>One step:</p> <p><i>Concerted</i> mechanism. Anti-coplanar arrangement of the β-hydrogen and leaving group.</p>
Effect of alkyl structure on rate	<p>Stability of carbocation is important:</p> $R_3C^+ > R_2HC^+ > RH_2C^+ \gg H_3C^+$ <p>Dehydration of 3° alcohols are classical examples of E1 reactions using H_2SO_4 and heat. Tertiary alkyl halides, especially, will undergo E1 eliminations in <i>protic</i> solvents with heat.</p>	<p>Regioselectivity plays an important role in the reaction rate. If there is no anti-coplanar β-hydrogen and leaving group no elimination occurs, then substitution is the most likely reaction, if possible.</p> <p>Tertiary alkyl halides undergo E2 even in the presence of weak bases, i.e., acetate.</p>
Effect of base on rate	Very weak bases are the favored reagents therefore <i>protic</i> solvents are preferred.	<p>The rate of the reaction is dependent on the nature and concentration of the base.</p> <p><i>Strong bases are preferred.</i></p>
Effect of solvent on rate	The rate of the reaction increases with solvent polarity and basicity. Solvent reduces electrostatic interaction in the transition state.	Polar aprotic solvents provide a faster rate. The nucleophile is not solvated in polar aprotic solvents, which makes them better nucleophiles.
Possible rearrangements	The reaction is under <i>thermodynamic control</i> , which results in high concentrations of the more stable alkene product. Intermediate carbocations can rearrange, especially 2° to 3°.	There reaction is under <i>kinetic control</i> . The product of the reaction results from the lowest energy transition state.