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Recall: S_N2 reactions... Reactivity is influenced by:
 - Alkyl Halide structure (sterics)
 - Nucleophile reactivity
 - Solvation
 - Leaving group

Leaving group trends
 - For alkyl halides, I^\ominus best, F^\ominus worst

Thus, $R-I > R-Br > R-Cl [>>> R-F]$ F^\ominus is never an S_N2 LG

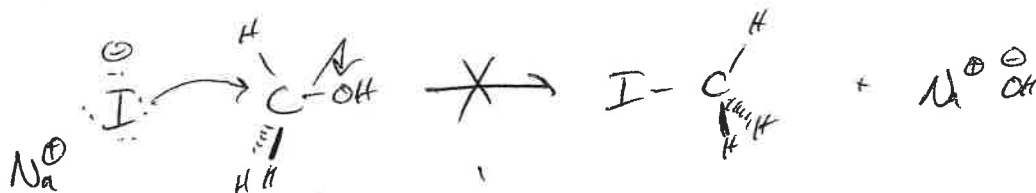
General trends -

Leaving groups that correspond to weak bases are generally good leaving groups (e.g., halides)

Leaving groups that correspond to strong bases are generally poor leaving groups

For example, OH^\ominus is never an S_N2 leaving group (too strong of a base)

Thus

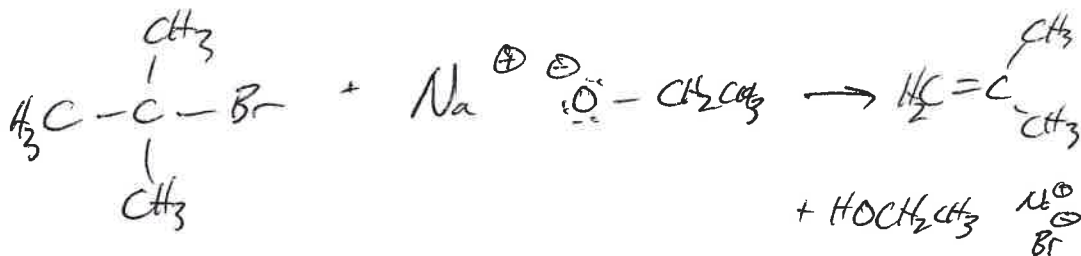


→ No Reaction

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Elimination

Recall:



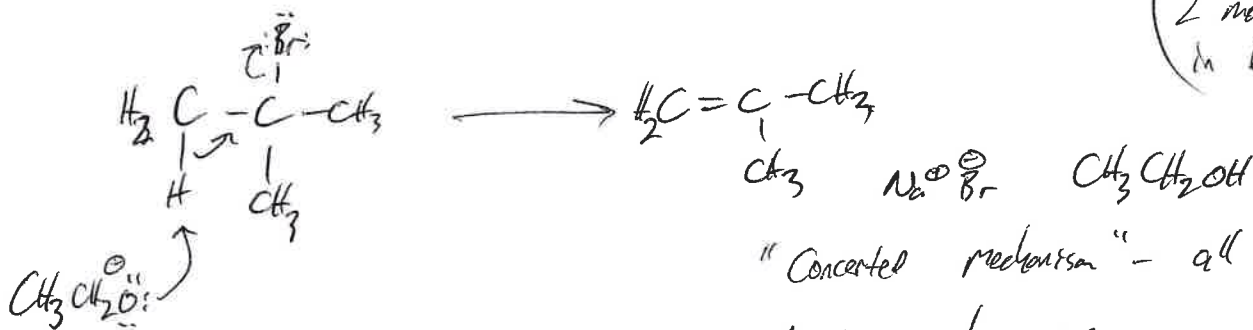
Rate Law

$$\text{rate} = k [(\text{CH}_3)_3\text{CBr}] [\text{Na}^+\text{O}^-]$$

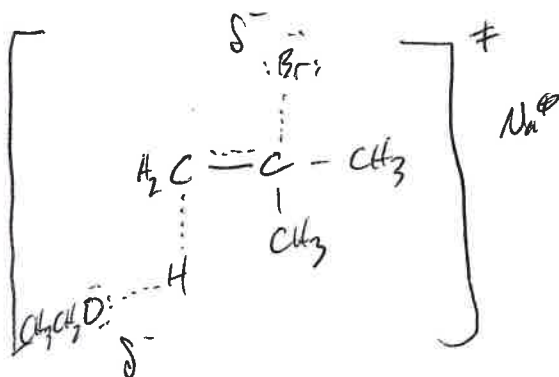
∴ Second order
 E2

Mechanistic Hypothesis:

"elimination" "bimolecular"
 (2 molecules involved in Rate-determining T.S.)

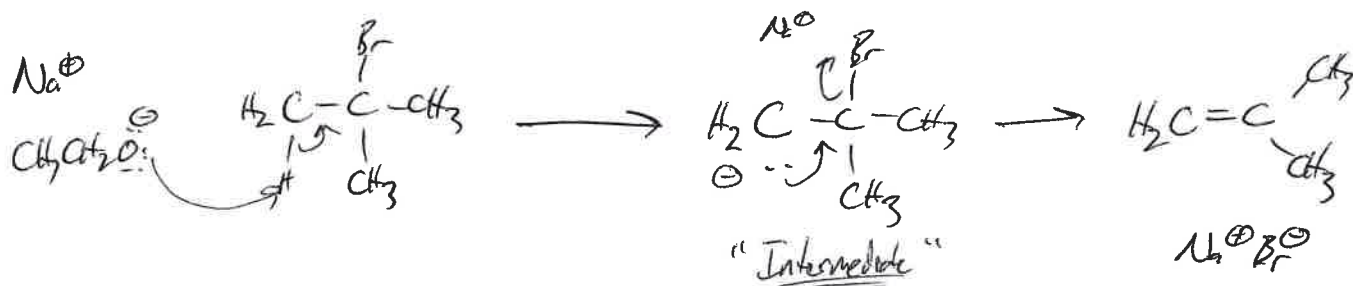


"Concerted mechanism" - all electrons moving at once

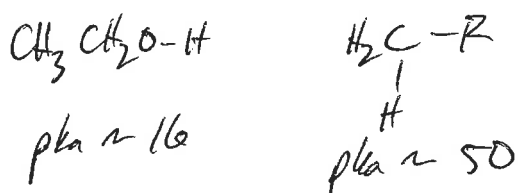


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Consider an alternative hypothesis (known to be **INCORRECT**)

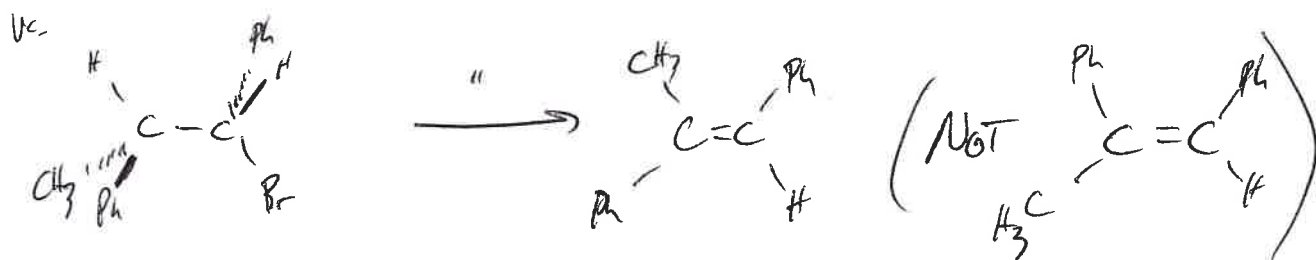
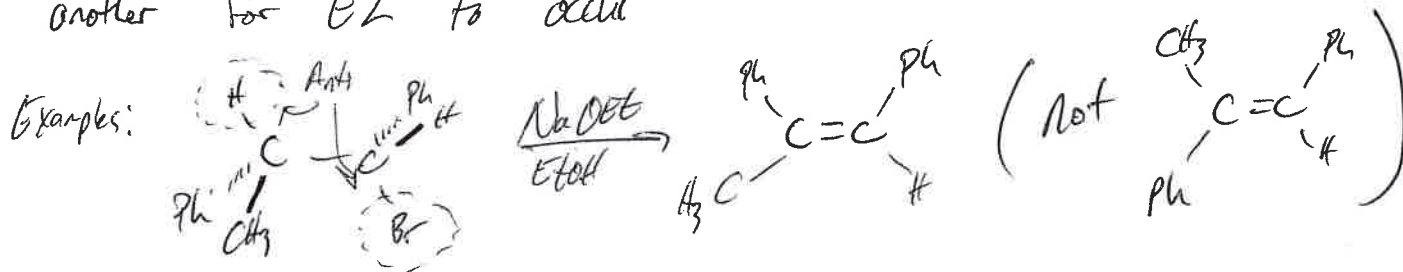


pKa consideration cast doubt on this alt. hypothesis



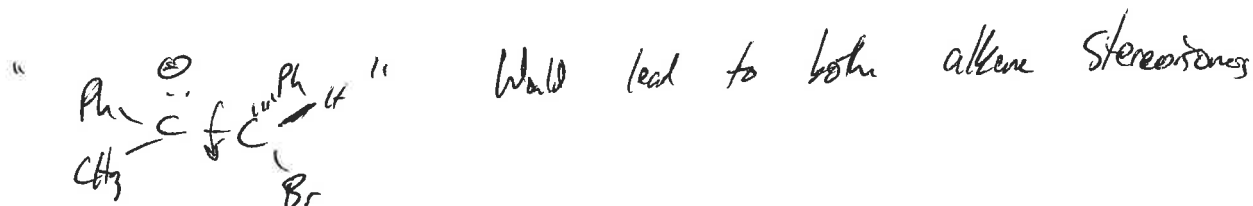
Stereochemical evidence invalidates the alternative (i.e. stepwise - nonconcerted) mechanism hypothesis

In general, H + ~~LG~~ LG (Br, here) must be anti to one another for E2 to occur

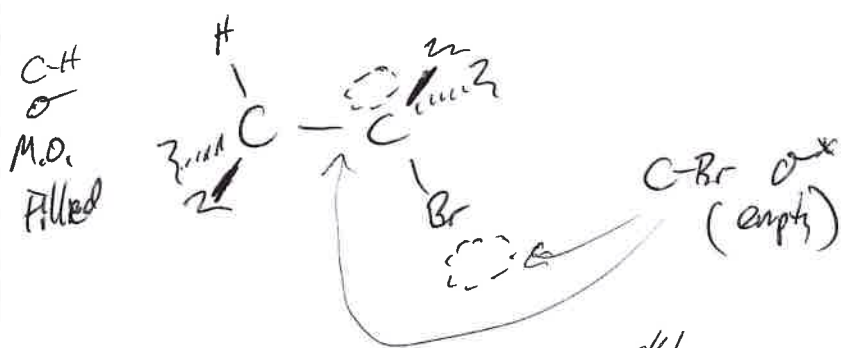


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Disproves existence of carbocation intermediate such as

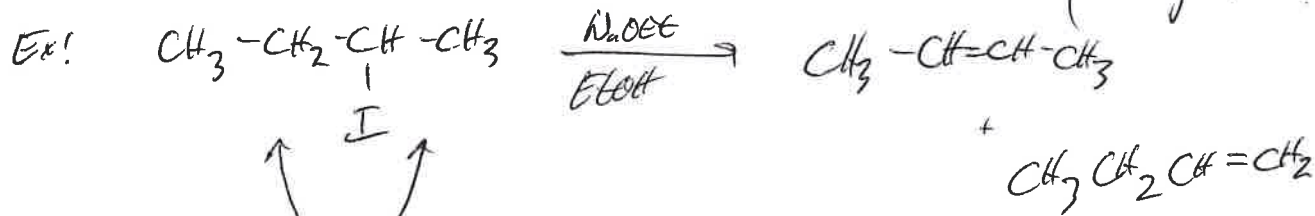


Rationale for concerted mech from Mol. orbitals



These two M.O. are perfectly aligned when C-H + C-Br are anti

E2 rxns can, depending on alkyl halide structure, generate multiple products ("regioisomers")



two different sets of β hydrogens

"Zaitsev's rule" - major vs. minor \Rightarrow expect product mixture

Note: Two perspectives in organic reactivity
 - Reactivity + mechanism (fundamental)
 - Synthetic utility