Course 343 Lecturer Gellman

Day 11/7/11 Monday Date

Notes Taken By SCS Total # of Pages 2

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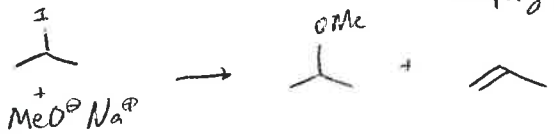
Recall: Reactions of Alkyl Halides : substitution and/or elimination

SN2 : $MeO^{\ominus}Na^{\oplus}$ + I~ → MeO~ + $Na^{\oplus}I^{\ominus}$

E2 : $MeO^{\ominus}Na^{\oplus}$ + I⊥ → ‖ + MeOH + $Na^{\oplus}I^{\ominus}$

- Possible to have both reactions competing!

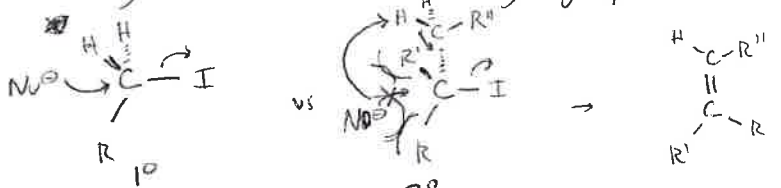


- How to predict when SN2 or E2 or both are favored?

∴ Considerations

① Structure of alkyl halide (1°, 2°, or 3°)

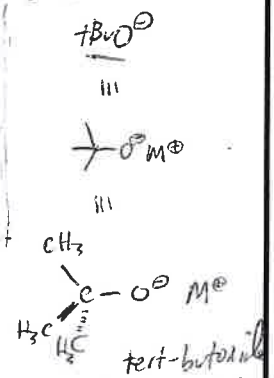
→ increasing steric bulk near leaving group disfavors SN2, favors E2



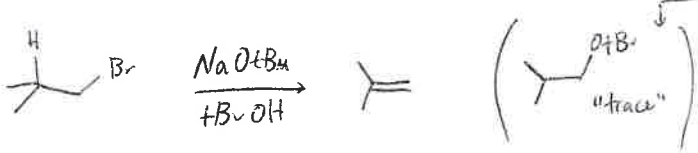
-too crowded for backside attack

② Structure of nucleophile/base

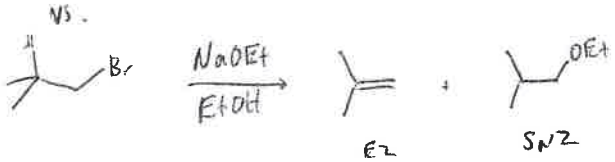
→ increasing bulk favors E2 over SN2 "bulky base" ⇒



ex)



vs.



∴ bulkier base favors E2

Course 343 Lecturer Gellman

Day Monday Date 11/7/16

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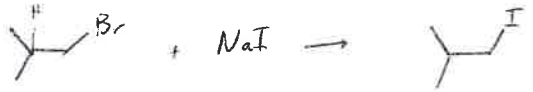
③ Balance of Nucleophilicity vs Basicity of Anionic Component

- most halides are good nucleophiles but weak bases

ex)

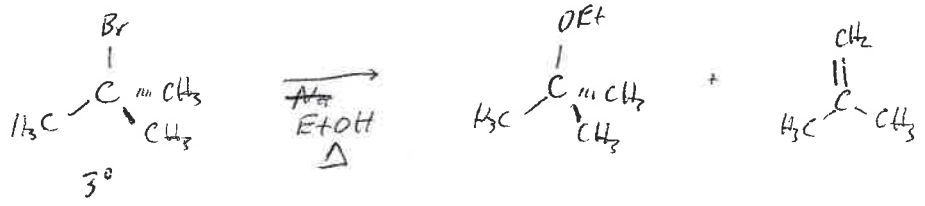


Note: ~~either~~ unlike $Cl^{\ominus}$, $Br^{\ominus}$, & $I^{\ominus}$, $F^{\ominus}$ is pretty basic & can do E2

- ^{18}F important for PET imaging

S_N1 & $E1$

ex)



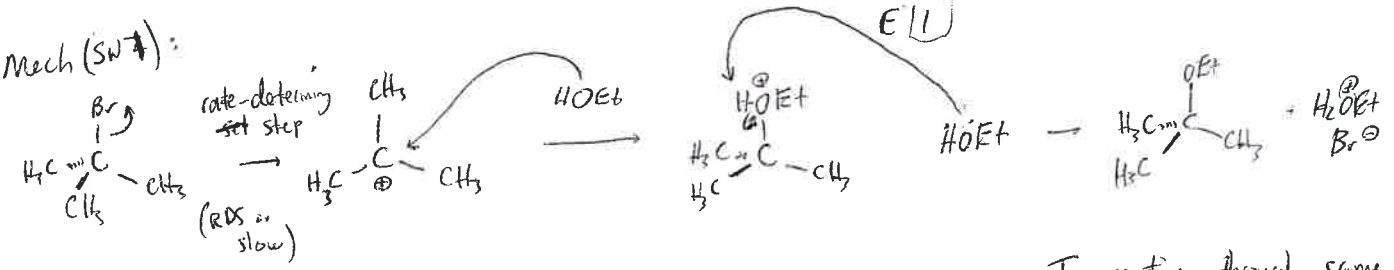
Note: no alkoxides, just the neutral alcoholic solvents

- Kinetics analysis:

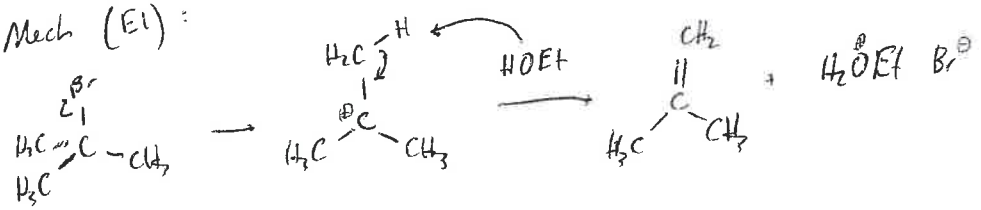
for both reactions.. rate = $k[(CH_3)_3CBr]$ ∴ S_N1 = unimolecular

E1

- Mech (S_N1):



- Mech (E1):



- Two reactions through same carbocation intermediate
- ~~Rxn~~ Product-determining step follows carbocation formation

- Rxn conditions determine ~~of~~ which path E1 vs S_N1