Course Chem 343 Lecturer Coffman
Day Friday Date 11/06/15
Notes Taken By Nolan Blythe Total # of Pages 5

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S_N2 vs E2 rxns of Alkyl Halides....

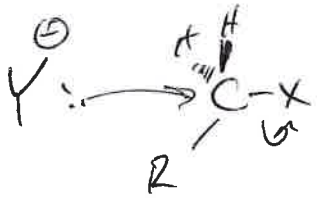
Identify, for specific cases, whether S_N2 predominates or E2 or both pathways are significant

Key Considerations

1) Alkyl Halide structure

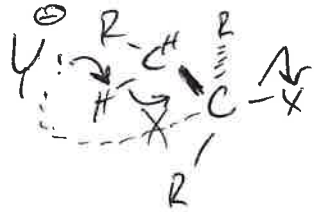
More alkyl substituents on C bearing the halide

$\Rightarrow$ E2 more likely rel. to S_N2



1° - S_N2 probable (but E2 possible)

vs.



3° - S_N2 doesn't occur

E2 if anything

2° - Anticipate mixtures!

(But not always...)

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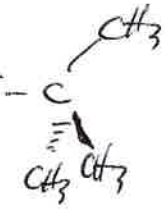
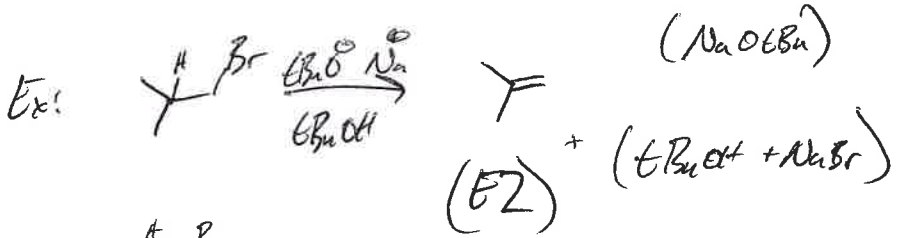
2) Nucleophile / base structure

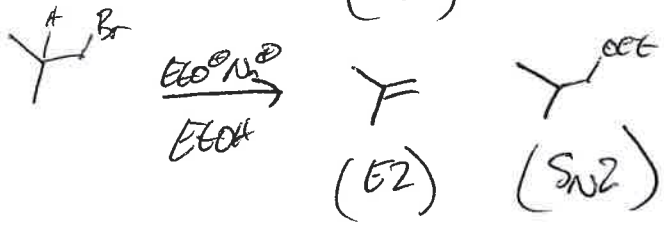
a) Steric bulk surrounding e⁻ rich atom favors E2 over SN2

"bulky base" Classic - t-butoxide

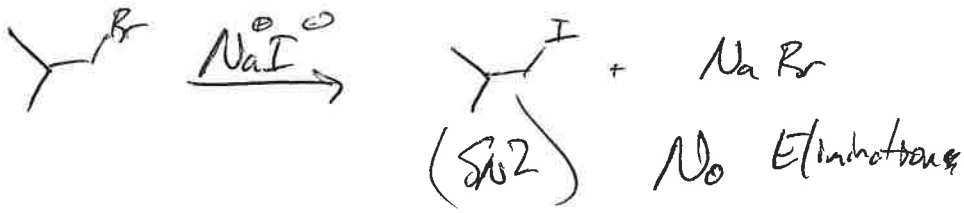


Ex:





b) Non-basic, electron-rich species ⇒ SN2



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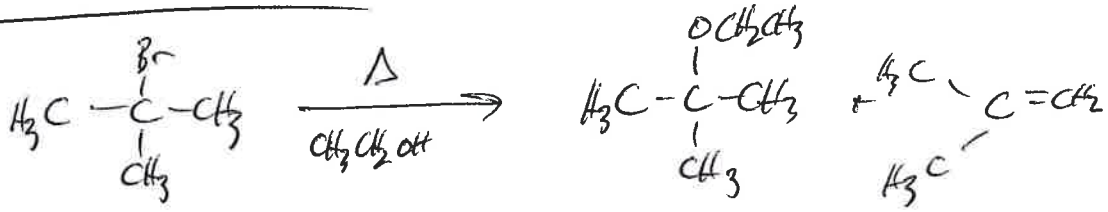
S_N1 + E_1 Rxns

Ex!



$H_2O^{\oplus}CH_2CH_3$ $:\ddot{Br}:^{\ominus}$

Observe - Rate Law

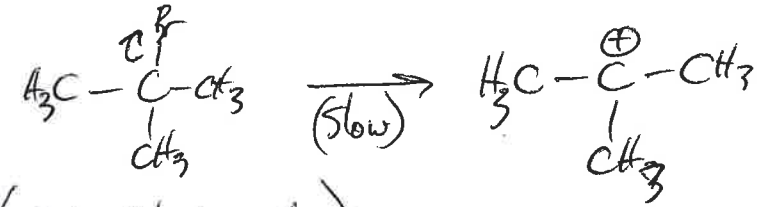
$$\text{Rate} = k[(CH_3)_3CBr]$$

1st order! Rate depends only on [alkyl halide]

S_N1 + $E1$

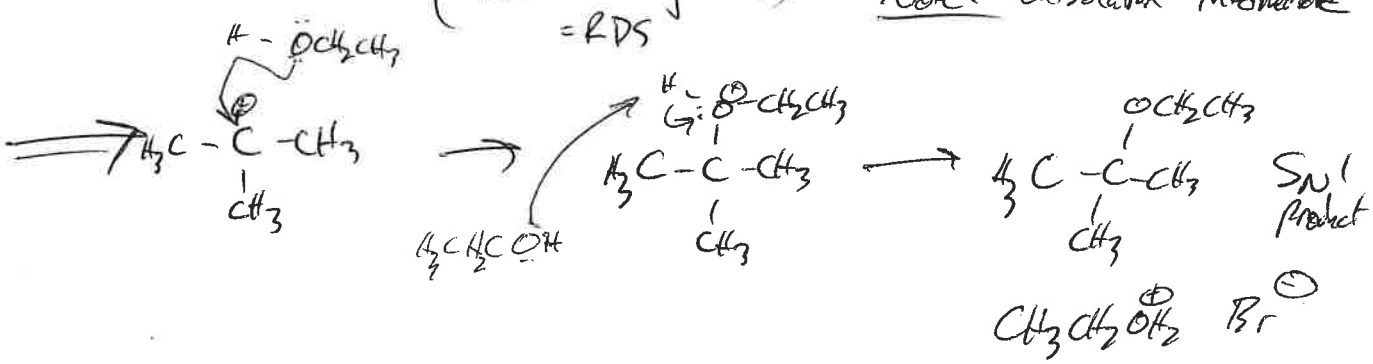
First order!

Mech Hypothesis:



(Rate-determining step) = RDS

Note: Carbocation intermediate



S_N1 product

$CH_3CH_2\overset{\oplus}{O}H_2$ $Br^{\ominus}$

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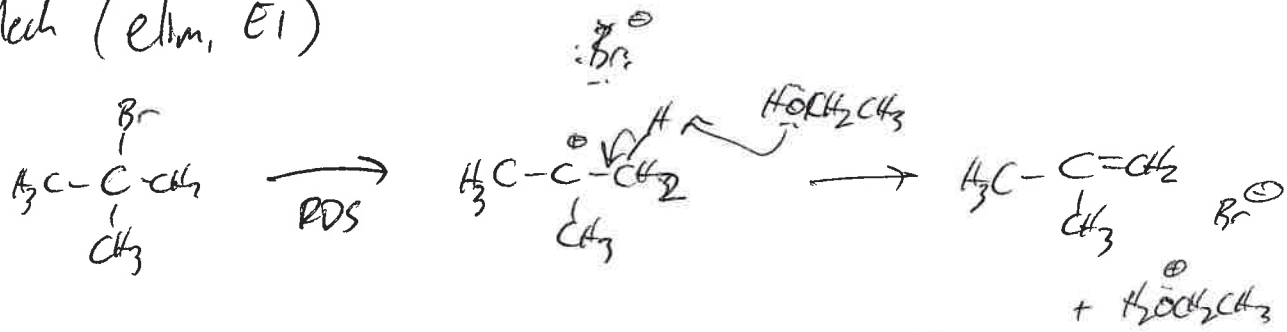
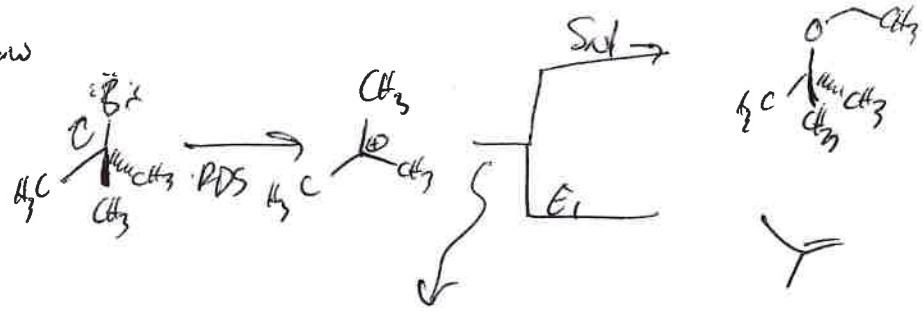
Mech (elim, E1)



Redraw



Product determing step

Reactivity Trends

1) 3° alkyl Halides are most prone to SN1 E1 pathways (2° ok, 1° never)

Rationale: 3° C⊕ more stable than 2° C⊕. (No 1° C⊕)

("Hammond Postulate")

2) SN1/E1 Reactivity* is favored by polar, protic solvents

(* of alkyl halides)

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Rotatable