(8) **Today**

Sections 11.7 - 11.11: Elimination Reactions

Section 17.6: Alcohols and Elimination Reactions

Next Class (9)

Competition between S_N1, E1, S_N2, and E2

Chap 12: Mass Spectrometry and Infrared Spectroscopy

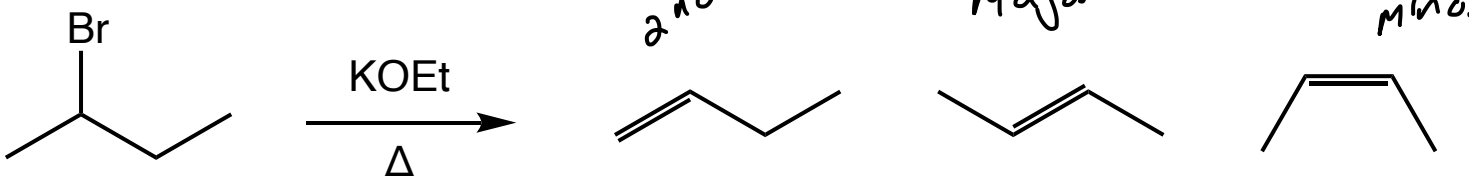
(10) **Second Class from Today**

Chap 12: Mass Spectrometry and Infrared Spectroscopy

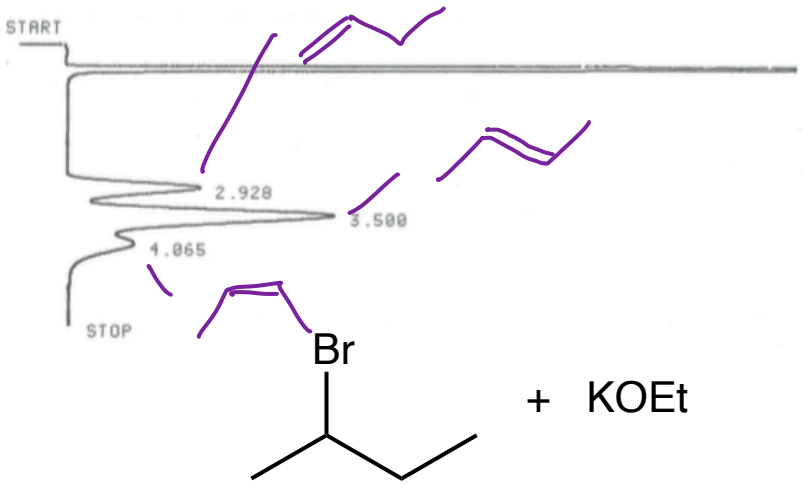
Third Class from Today (11)

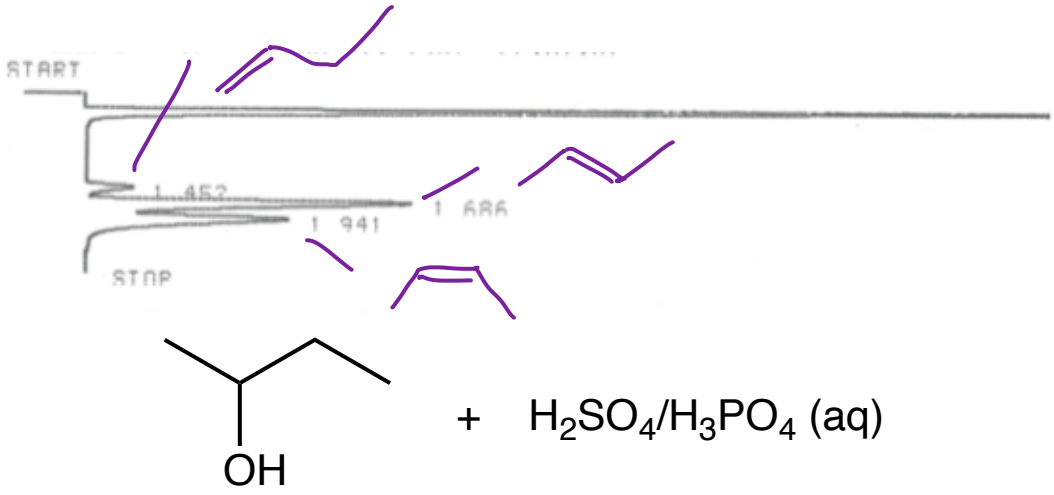
Chap 13 : Nuclear Magnetic Resonance Spectroscopy

not exactly the same product distribution as E1. Why different?



Is the most stable product always still the major product?

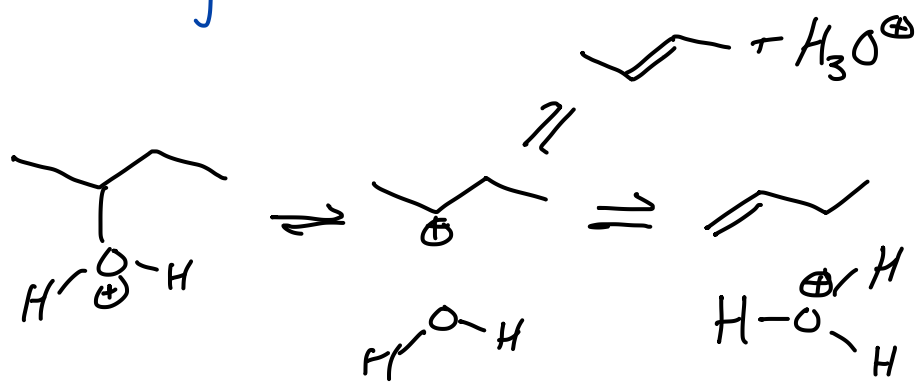


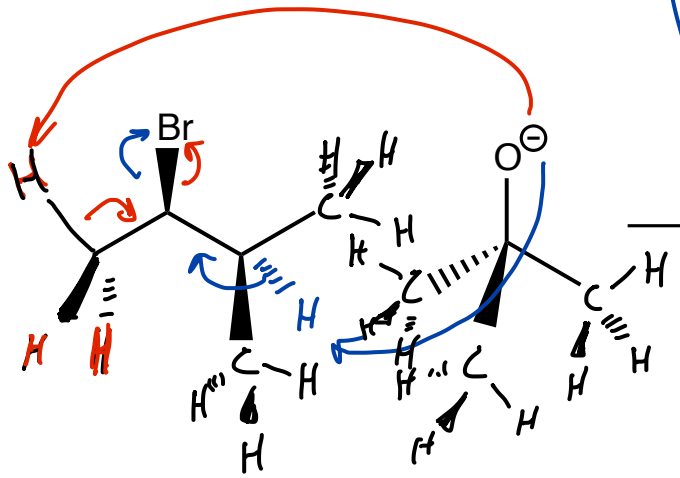


Kinetic control - Fastest forming

the product that forms the fastest is the major product

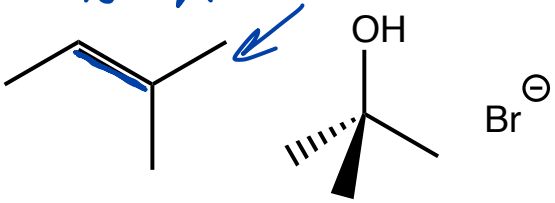
thermodynamic control - most stable





major product

Kinetic problem makes it harder to make this

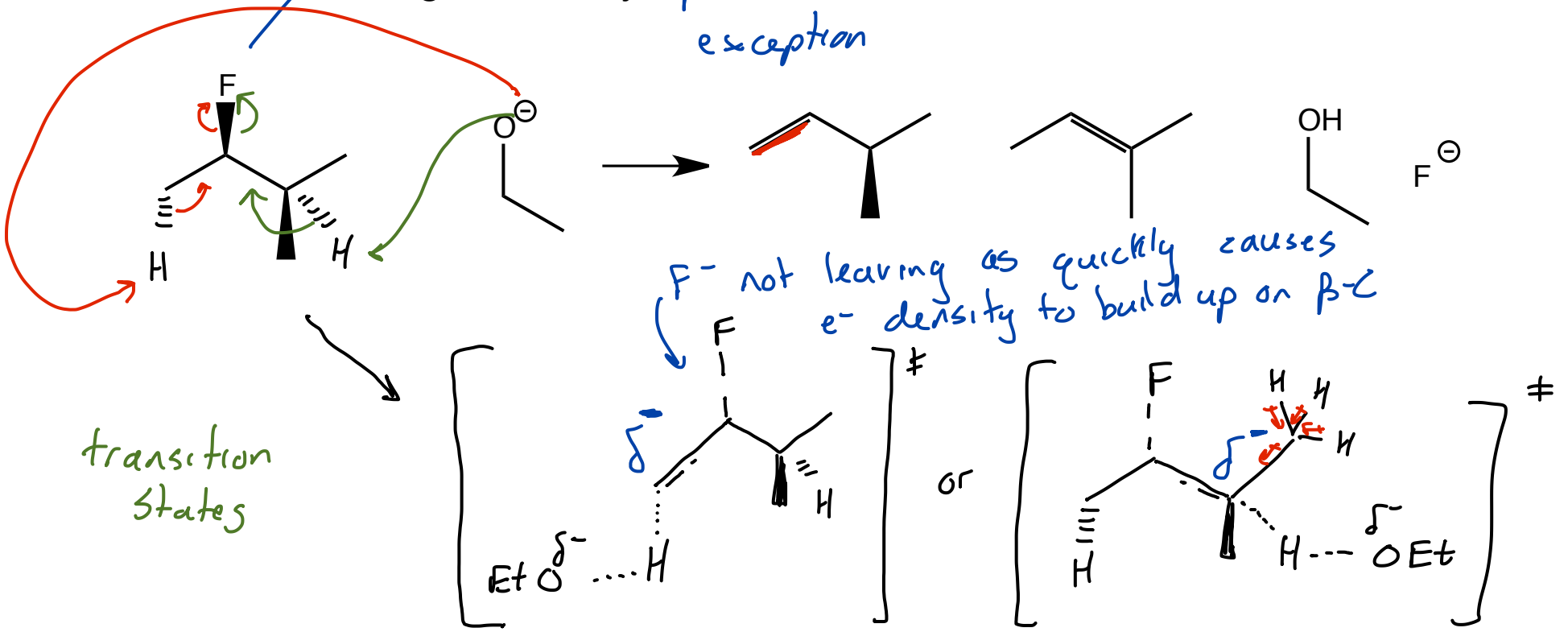


reaction is kinetically controlled ... product that forms fastest is major product.

For a base to react with the H^+ it needs to be able to get close to the H^+ ... in this case it is hard to get at the blue β-H because of all the CH_3 groups.

Since there is no steric crowding at the primary β-H's it's easier/faster for this big base to react there.

N based LG too poor LG exception



F⁻ not leaving as quickly causes e⁻ density to build up on β-C

The buildup of ⊖ charge is more stable on the 1° β-C because there is less e⁻ density on neighboring atoms to destabilize the ⊖ charge.

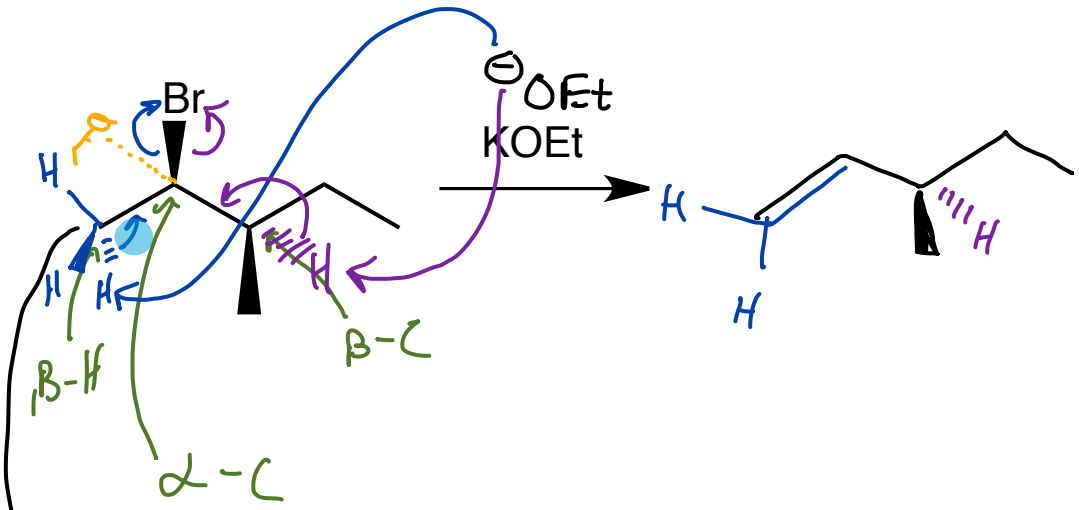
not so good LG { K_a of $HNR_3^{\oplus} \sim 10^{-11}$; K_a of $HF \sim 10^{-4}$

K_a of $HBr \sim 10^{9}$ } very weak base } good LG

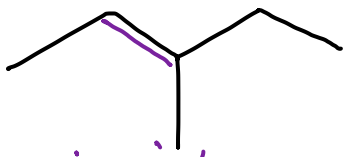
$F^- + NR_3$ vs Br^-

Elimination: The Stereochemistry of the E2 Mechanism

Sections 11.7 - 11.11, 17.6

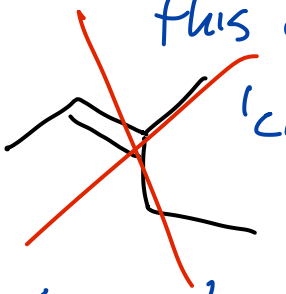


get this one 'cuz



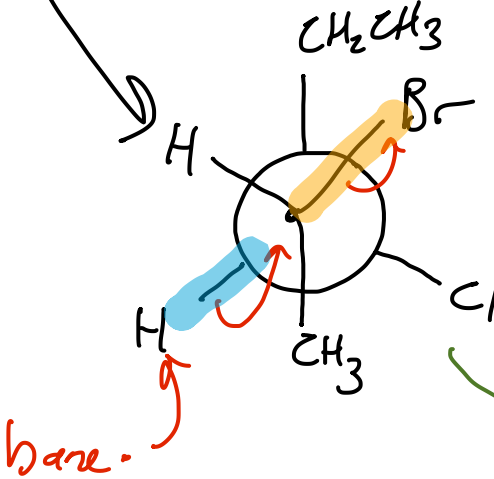
antiperiplanar transition state

don't get this one 'cuz

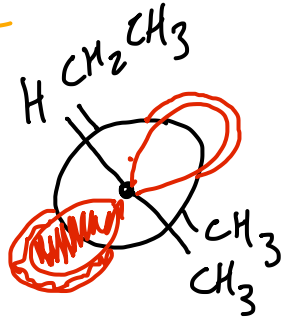


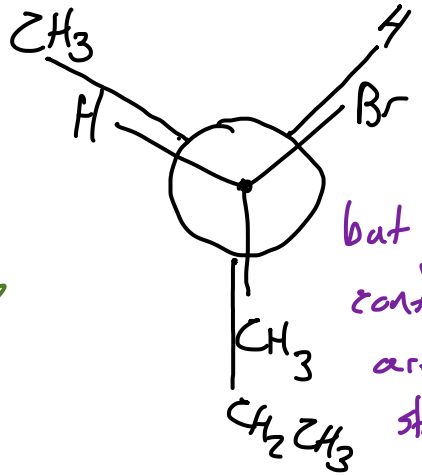
syn perplanar ≠ TS too unlikely to form

Since the rxn occurs in 1 step a specific alignment of the β-H + the LG is required... The β-C to β-H bond and the α-C to LG bond must be coplanar

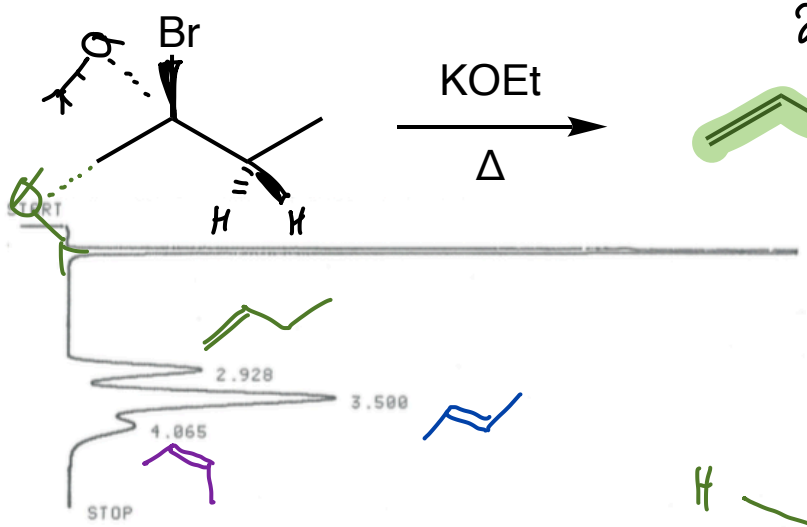


antiperiplanar





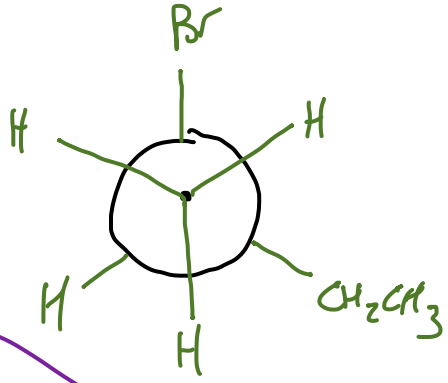
eclipsed version is coplanar but eclipsed conformations are not stable

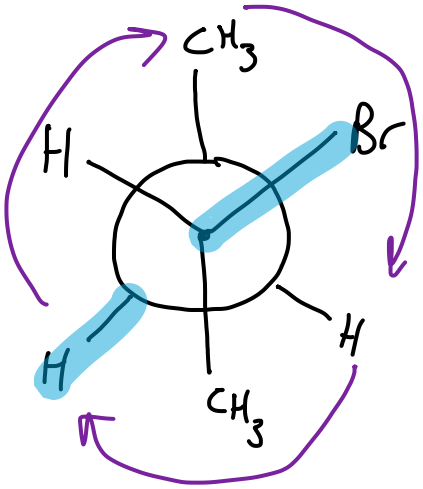


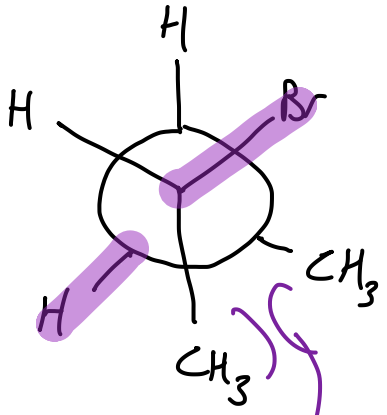
KOEt

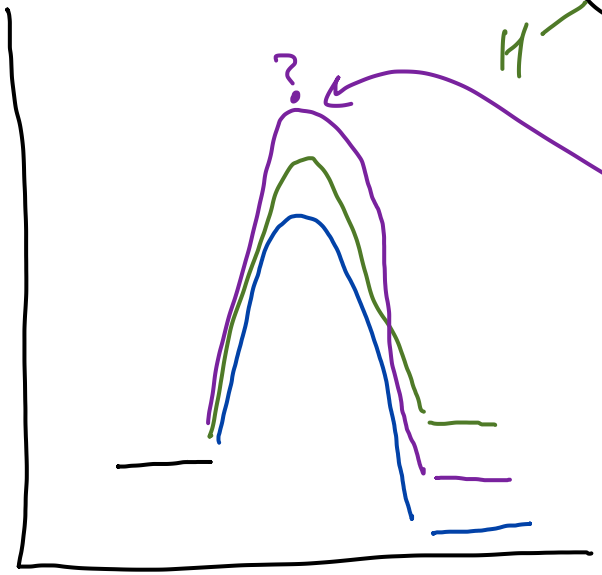
Δ

2nd 1st 3rd



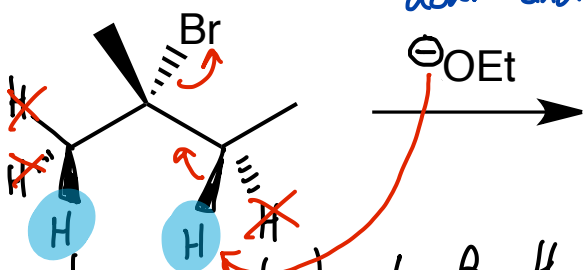


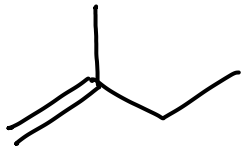


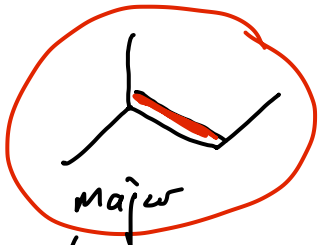


gauche interaction causes energy of this TS to be higher

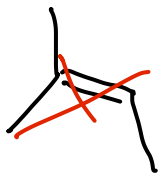
Br is up and behind the screen and can do E2 with β-H that is down and in front







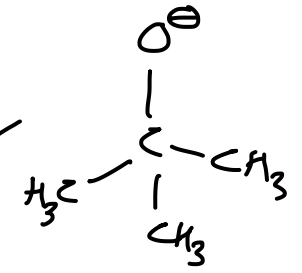
these are the same so don't draw both



base abstract β-H that is antiperiplanar with LG

e⁻ that were in β-H to β-C bond fall in to form α-C to β-C π bond and LG leaves.

Most stable alkene is major product unless....

1. less substitute alkene if... big base 
2. less substituted alkene if... poor LG (F^-, NR_3)
3. No β-H to line up or if gauche interactions cause higher E