(8) **Today**

Sections 11.7 - 11.11: Elimination Reactions: E1, E2, ~~E1cB~~

Competition between S_N1, E1, S_N2, and E2

Next Class (9)

Chap 12: ~~Mass~~ Spectrometry and Infrared Spectroscopy

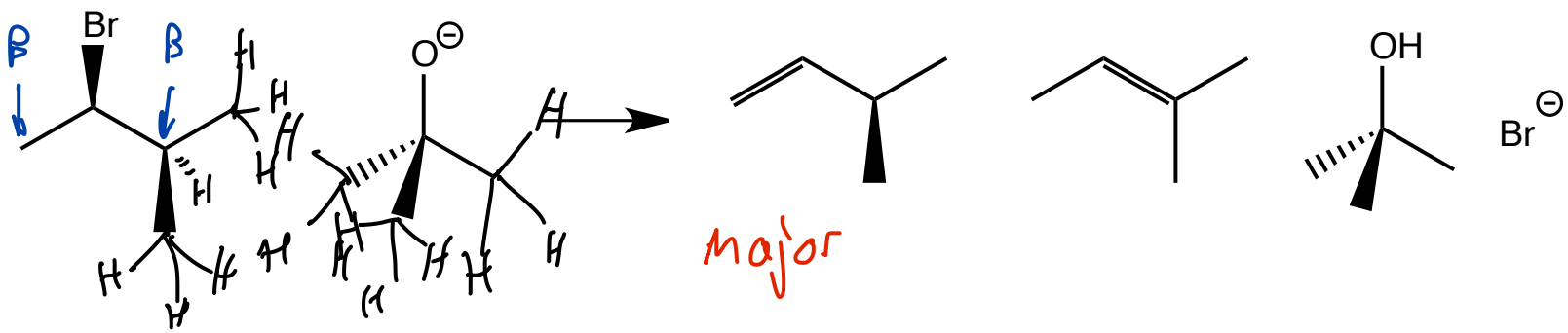
(10) **Second Class from Today**

Chap 12: Mass Spectrometry and Infrared Spectroscopy

Third Class from Today (11)

Chap 13 : Nuclear Magnetic Resonance Spectroscopy

major product ?



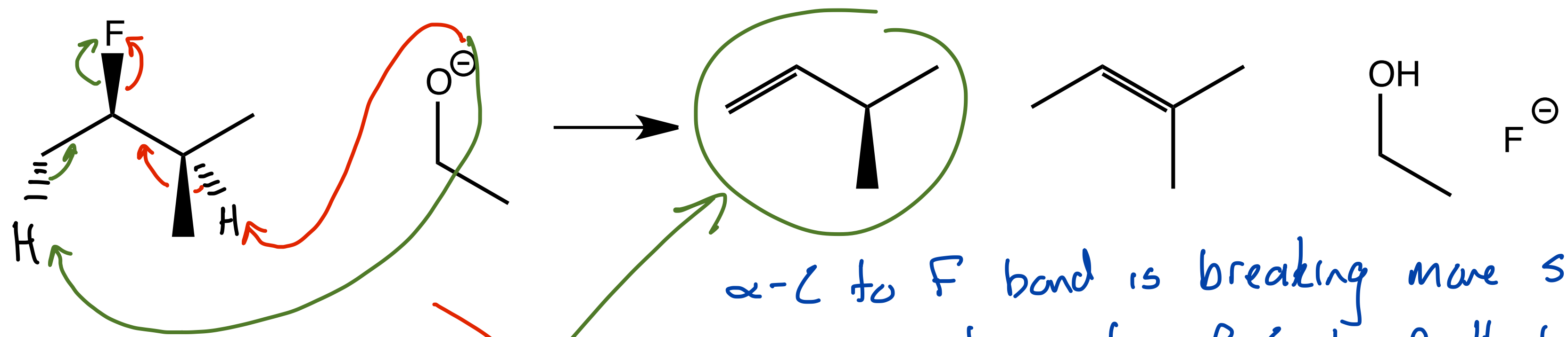
Kinetic control of product distribution. Product that forms fastest is major product. Typically, the most stable alkene forms fastest unless there is a kinetic problem

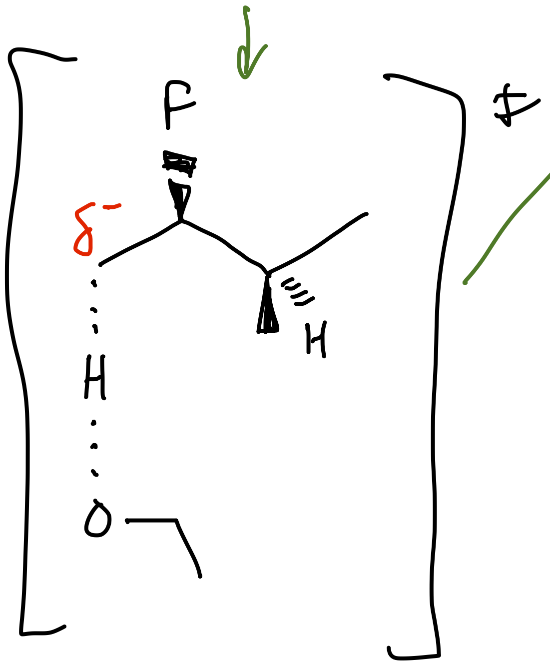
1. Big base exception $(CH_3)_3CO^{\ominus}$ or bigger
   can't make as much product because the base can't get at the β-H easily

2. Poor LG exception: F^-, NR_3 $N(CH_2)_3$

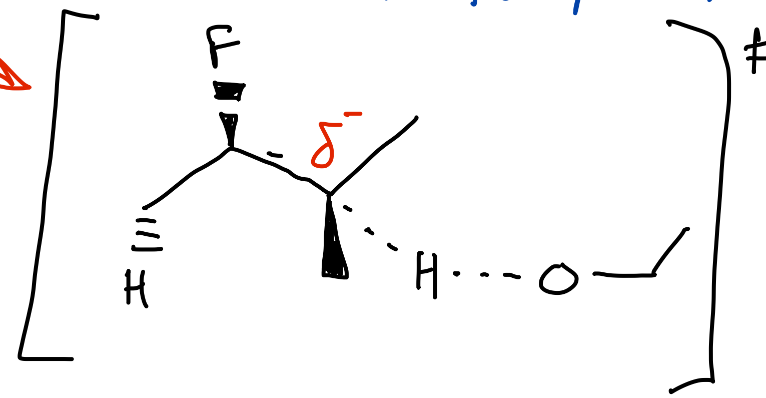
   build up of ⊖ on TS causes less substituted alkene to be major product

major





α-C to F bond is breaking more slowly than the β-C to β-H bond



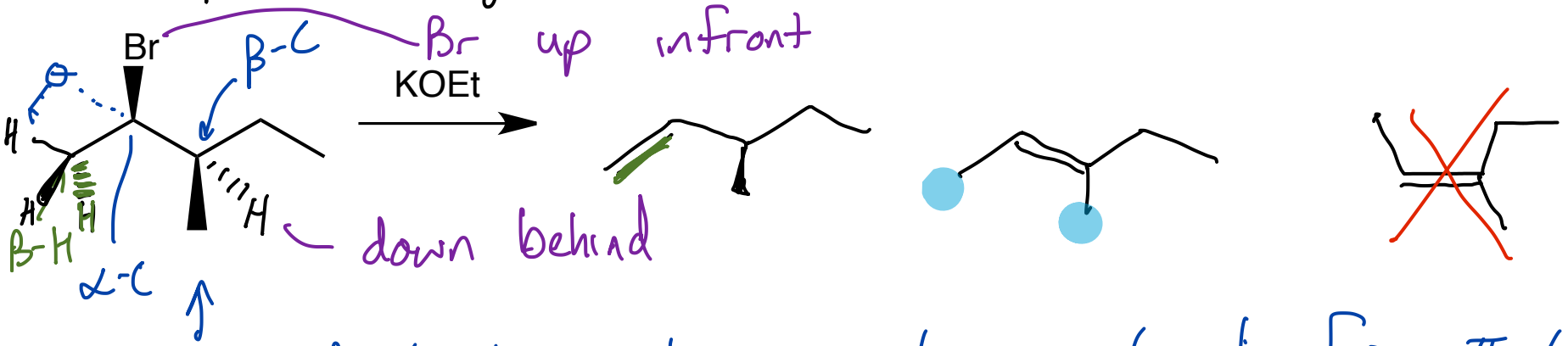
$\ominus$ charge builds up on β-C

★ δ^- builds up on 3° C atom ← "extra" e^- density around 3° C the δ^- is made more unstable

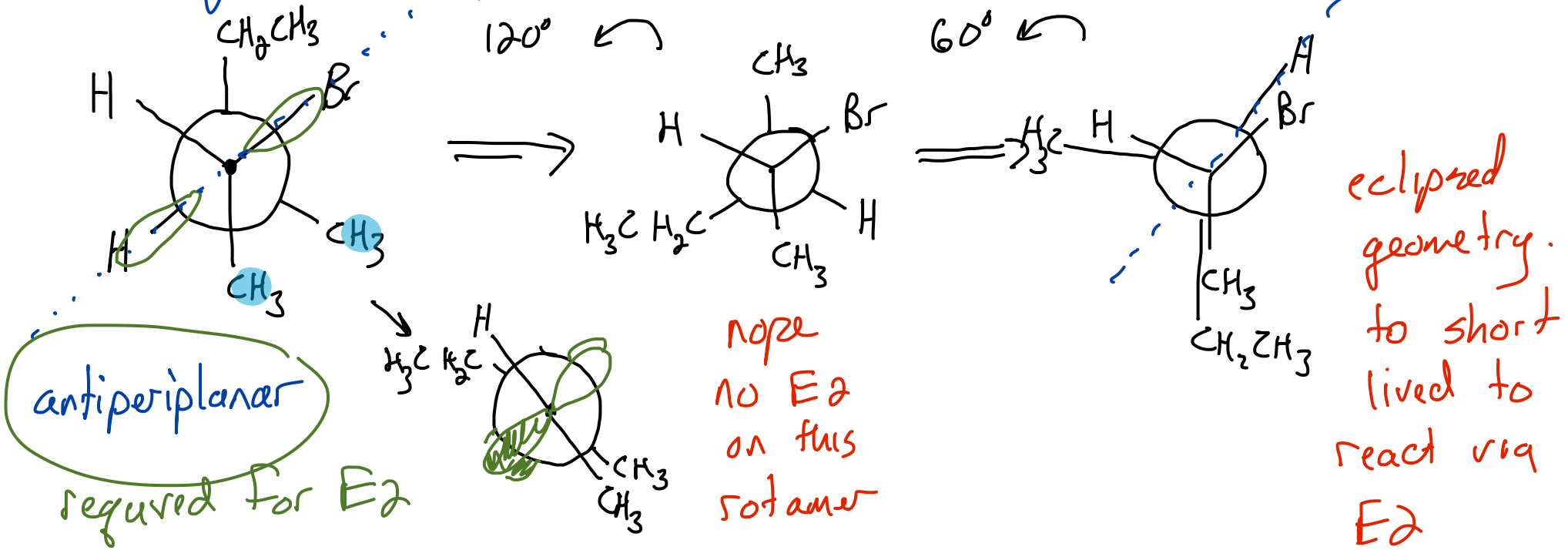
★ δ^- builds up on 1° C atom

more stable

Specific arrangement of LG + β-H required

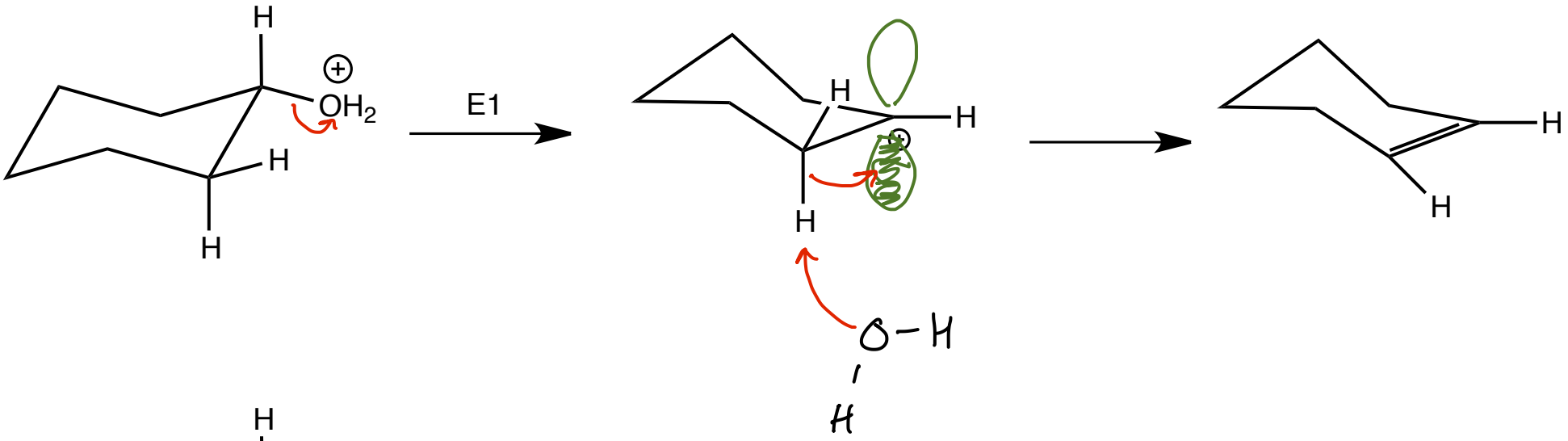


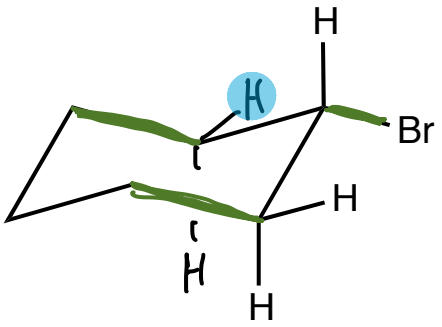
molecule needs to be in the correct geometry to form π bond in a single step



Elimination: The Stereochemistry of the Mechanisms Compared

Sections 11.7 - 11.11, 17.6



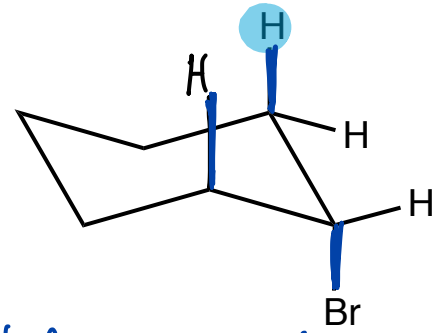


E2

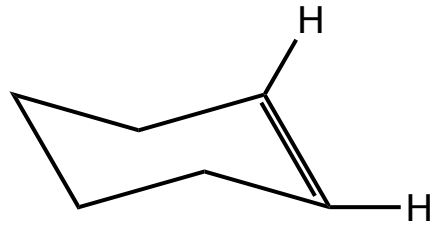
Nope

E2 rxn cannot occur when LG is in equitorial position

ring flip

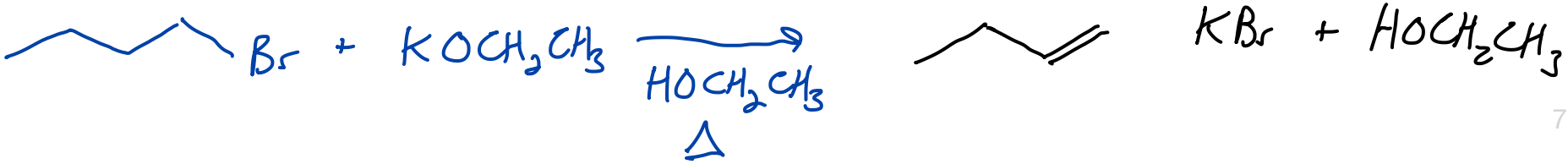


E2



LG in axial position is antiperplanar to axial positions of B-C's

E2	E1
Two molecules collide in a 1 step mechanism	Dissociation of **one molecule** controls the rate of a two step reaction
bimolecular rate determining step	**unimolecular** rate determining step
periplanar arrangement required antiperiplanar arrangement prefered	C^+ formation leads to all possible stereoisomers equilibrium ... isomerization
Kinetic Control Most substituted alkene is major product unless there is a kinetic problem -alignment not possible -gauche interactions in TS — makes some harder to form -big base and crowed β-H } less substituted alkene -poor LG	Thermodynamic Control Most stable alkene is the major product Equilibrium process can lead to isomerization
1°, 2°, 3° substrates	2° alkyl, 2° allylic/benzylic, 3° substrates no 1° C^+
Strong base required ^-OH or stronger	Weak bases required
polar aprotic or protic solvent	polar protic solvent



Elimination: Issues with Acid Catalyzed Elimination of Alcohols

Sections 11.7 - 11.11 and 17.6