



E2 Mechanism

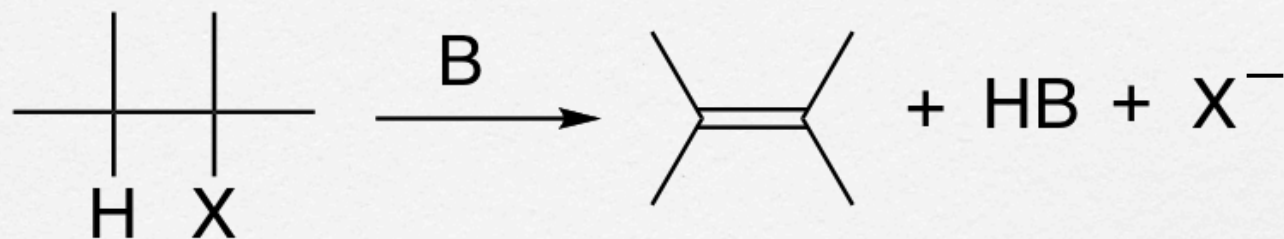
UCI Chem 51A
Dr. Link

Goals

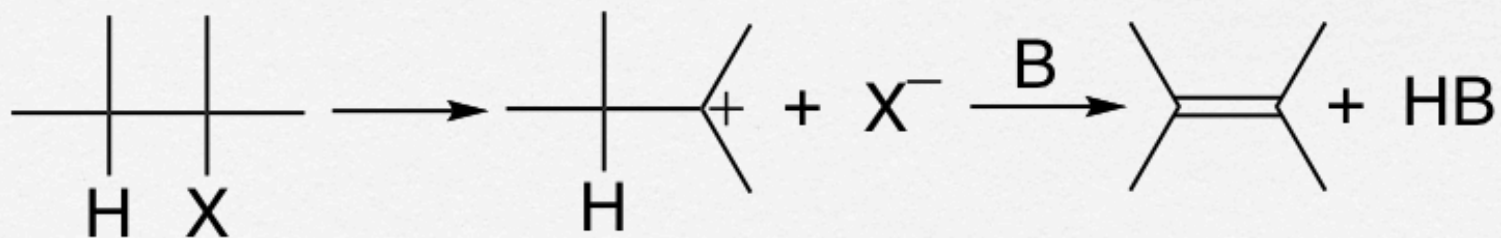
- After this lesson you should be able to
 - Identify and draw the E2 mechanism
 - Describe the experimental evidence that supports the E2 mechanism
 - Identify alkyl halides that are likely to undergo E2 reaction
 - Identify bases that promote the E2 mechanism
 - Identify solvents that promote the E2 mechanism
 - Explain the regioselectivity of the E2 mechanism
 - Explain the stereochemical outcome of the E2 mechanism
 - Predict the outcome of E2 reactions

Making Alkenes: 2 Possible Pathways

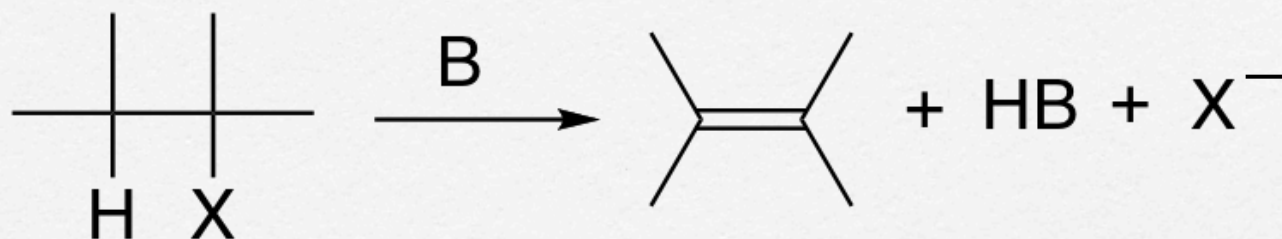
All at Once



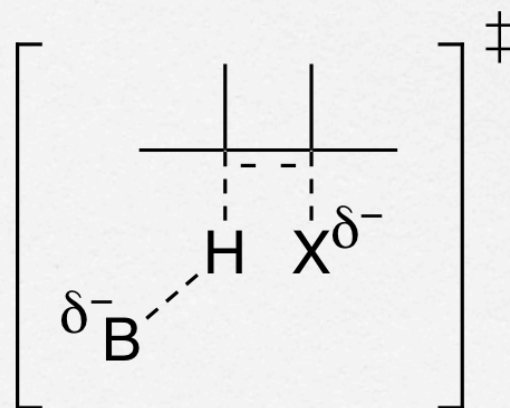
One Step at A Time



E2 Fundamentals



Transition State*



How Do We Know?

- Kinetics

- $\text{rate} = k [\text{R-X}] [\text{Base}]$

- RDS 2nd order

- Intermediates

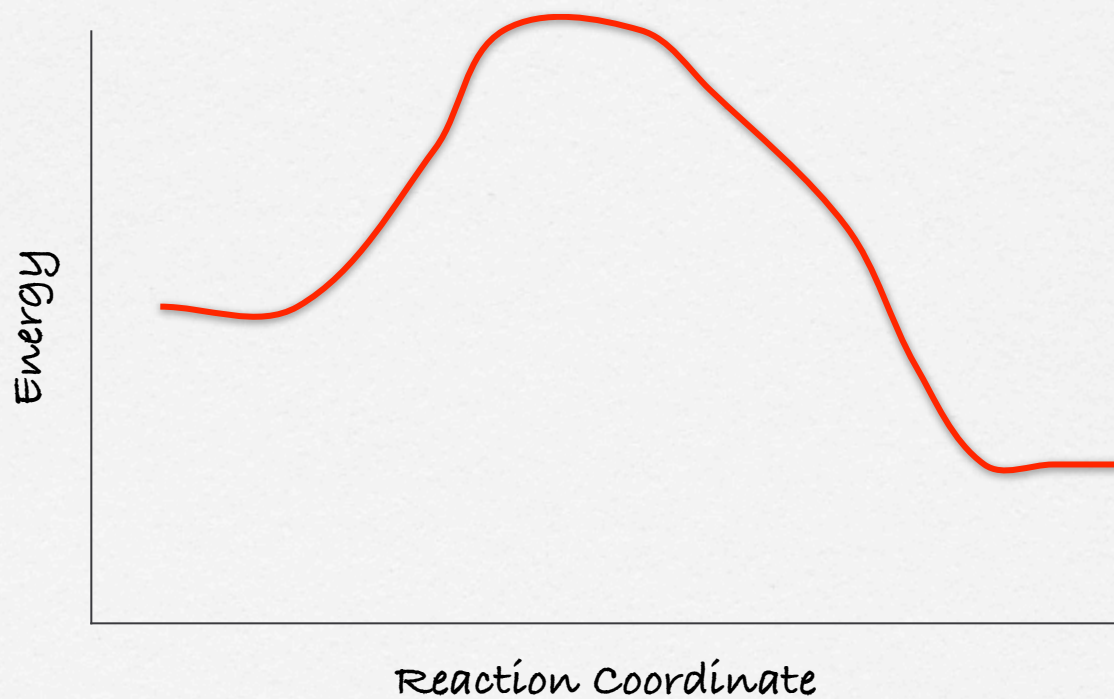
- No evidence of any intermediates

- Stereochemistry

- Preference for removing specific $\beta\text{-H}$

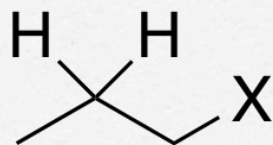
The Leaving Group

- Good leaving group needed for E2.

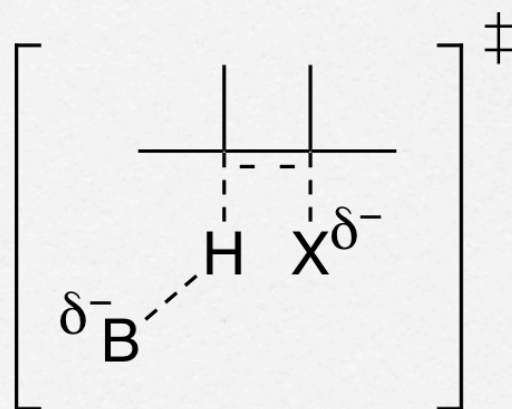
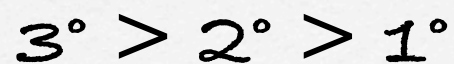


The Alkyl Halide

β -H REQUIRED!



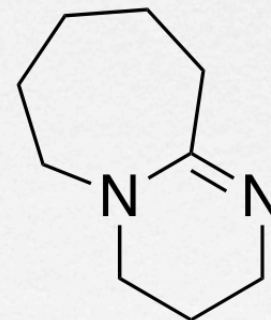
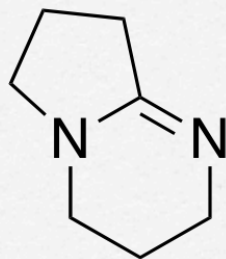
Reactivity Order



The Base

- E2 favored by strong base!
- usually charged

New Bases!



The Solvent

□ E2 favored by polar aprotic solvents

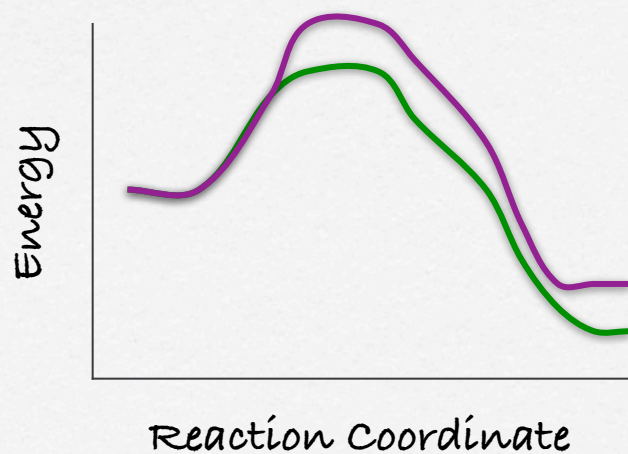
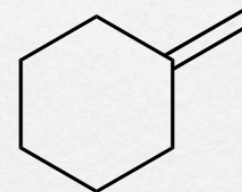
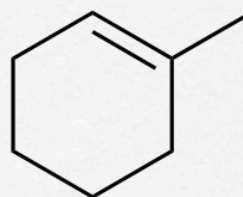
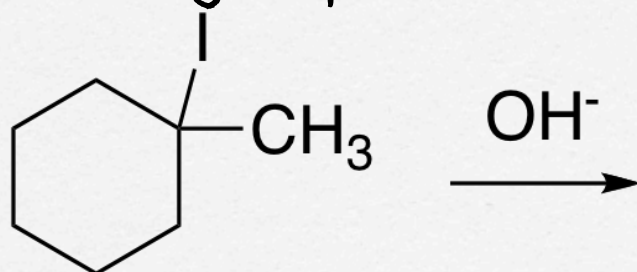
Polar protic solvents cage the base and
decrease reactivity

Regioselectivity & Stereoselectivity

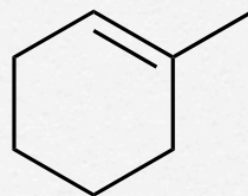
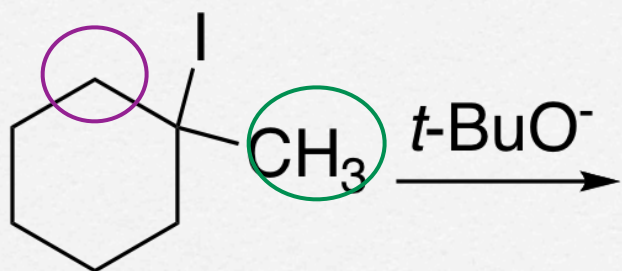
- What happens when there are multiple β -H's that can be removed?
- Regioselectivity: formation of one constitutional isomer is favored over another
- Stereoselectivity: formation of one stereoisomer is favored over another

Zaitsev Rule

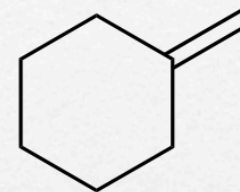
- Zaitsev rule: Most stable alkene will be major product



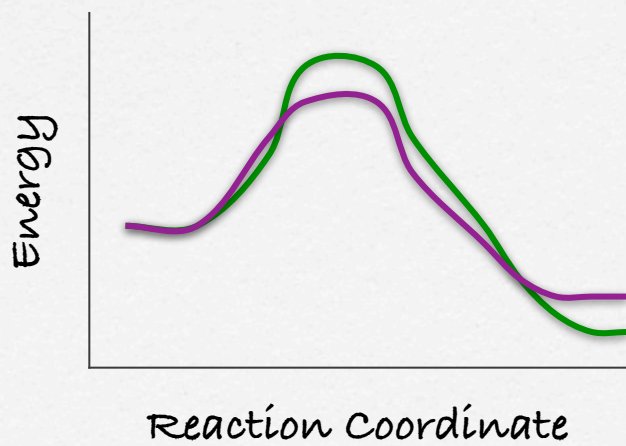
Always Zaitsev Rule?



most stable



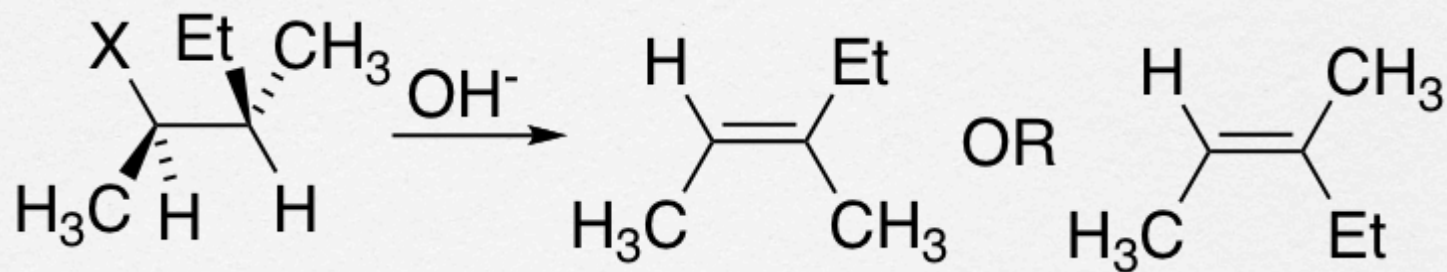
least stable



STERICS!!!

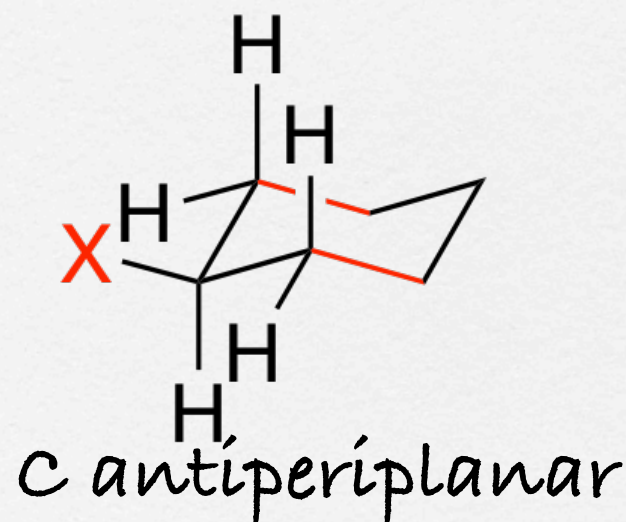
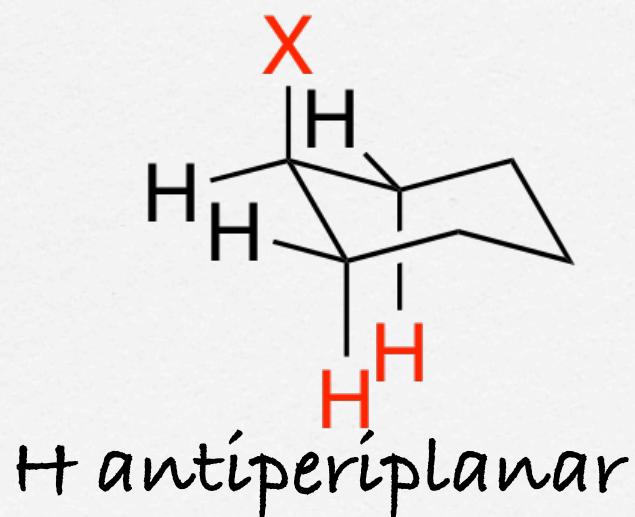
Stereochemistry & E2

- Bond breaking & bond forming simultaneous
- TS[‡] must be antiperiplanar



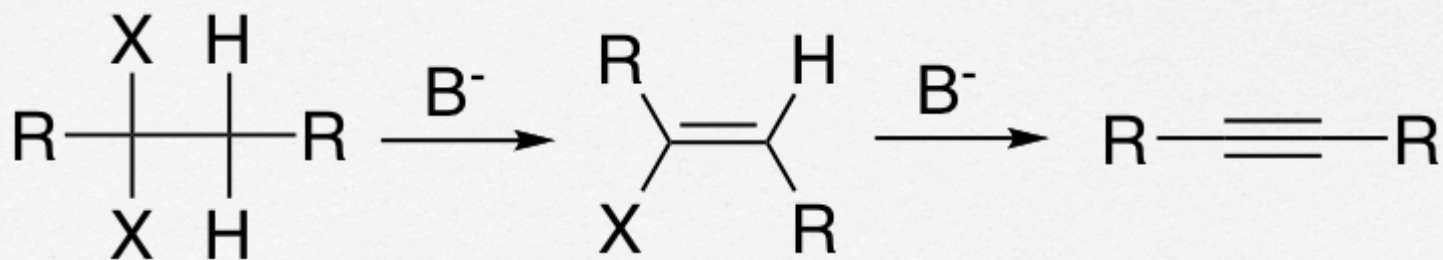
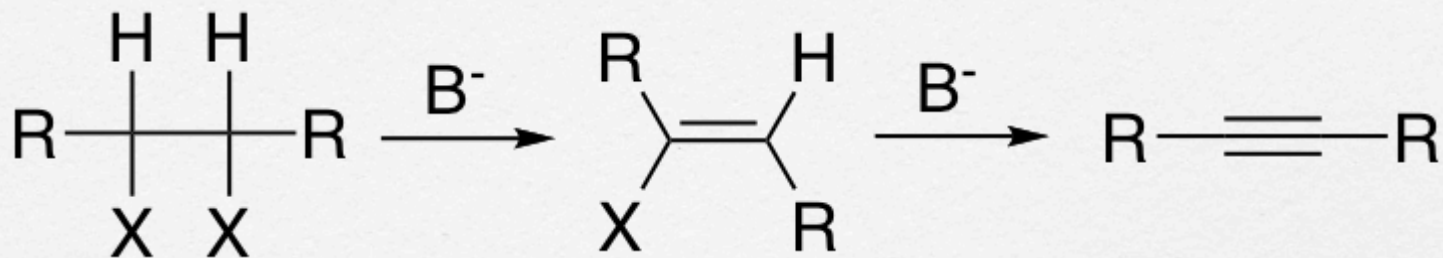
Ring Systems & E2 Stereochemistry

- How do we get antiperiplanar relationships in cyclohexane rings?



E2 & sp^2 Carbons

□ E2 can happen at sp^2 C



E2 Summary

- Rate = 2nd order
- Mechanism = 1 step
- LG = good LG required
- R-X = β -H required, $3^\circ > 2^\circ > 1^\circ$
- Base = Strong base favors E2
- Solvent = polar aprotic solvent favors E2
- Regioselectivity = usually most stable alkene favored*
- Stereochemistry = antiperiplanar TS[‡]

Wrapping Up

- Practice drawing E2 mechanism
- Practice identifying alkyl halides that can undergo E2 reactions
- Practice drawing products of E2 reactions
- Practice identifying major and minor products of E2 reactions