S_N1 vs. S_N2

UCI Chem 51A
Dr. Link

Goals

- After this lesson you should be able to
  - Identify reaction conditions that favor either S_N1 or S_N2 mechanisms
  - Predict the outcome of a nucleophilic substitution reaction based on the electrophile, nucleophile, and reaction conditions

S_N2 Summary

* Rate = 2nd order
* Mechanism = 1 step
* Electrophile: Me>1°>2°, no 3°
* LG = good LG required
* Nu = strong Nu favors S_N2
* Solvent = polar aprotic favors S_N2
* Stereochemistry = backside attack, inversion

Nice summary video from University of Surrey!

http://www.youtube.com/watch?NR=1&feature=endscreen&v=h5xvaP6blZI

S_N1 Summary

* Rate = 1st order
* Mechanism = 2 steps
* Electrophile: benzyl, ally, 3° > 2°...
    * no 1°, no methyl
* LG = good LG required
* Nu = weak Nu favors S_N1
* Solvent = polar protic solvent favors S_N1
* Stereochemistry = racemization of stereocenter

University of Surrey summary video
http://www.youtube.com/watch?v=JmcVgE2WKBE

What Happens In A Flask?

* LOTS of molecules in a typical reaction
* Do they all follow the same path?
    * Not necessarily!

We choose conditions that favor one path and disfavor others!

Which Mechanism Is It?

- Depends on
  - Electrophile
  - Nucleophile
  - Solvent
- Both S_N1 and S_N2 require good LG

The Electrophilic Carbon & R Groups

Primary/Methyl

SN1 SN2

Secondary

SN1 SN2

Tertiary

SN1 SN2

Allylic

SN1 SN2

Benzylic

SN1 SN2

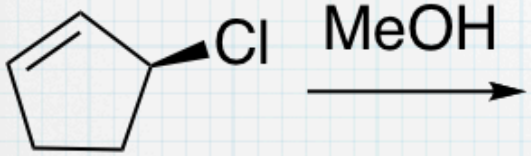
The Nucleophile

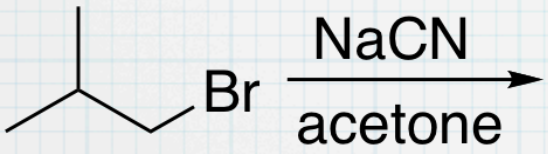
- Strong Nu favors S_N2
  - Generally charged!
- Weak Nu favors S_N1
  - S_N2 slower if Nu is weak, allowing time for S_N1 to happen
  - Generally not charged or weaker of the charged Nu

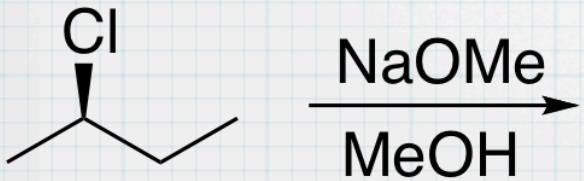
The Solvent

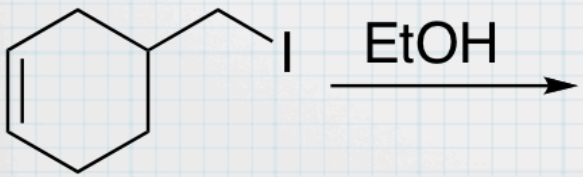
* Polar aprotic solvent favors S_N2
* Polar protic solvent favors S_N1
    * Lowers E_a for carbocation formation
    * Disfavors S_N2 because of solvation of Nu

Examples



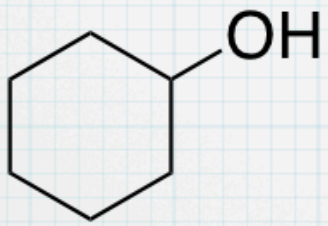






A Glimpse of Your Future: Synthesis

* How could we make this molecule?



Wrapping Up

* Practice predicting the outcome of nucleophilic substitution reactions
* Practice deciding what types of reaction condition and reactants should be used to favor one type of substitution over another
* Practice working backward from products to reactants