Greener S_N1 Reaction

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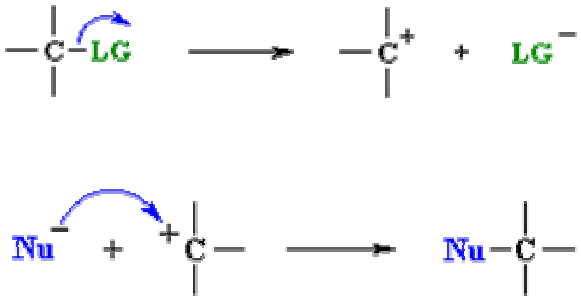
Outline

- Introduce S_N1 reaction mechanism
- S_N1 as a student lab
- Typical S_N1 lab and its problems
- Alternative substrate and analysis
- Alternative procedure and data
- Results

S_N1 – Unimolecular Substitution



Grasping the Mechanism

- Fundamental hands-on learning
- And why not be GREEN

Typical non-Green S_N1 reaction

- Shake for 20 min. in separatory funnel
- Workup procedure
  - Wash, dry, distill
- Analyze
- Product yield → 90 % (so they say)
  - Flammable and harmful
  - LD_{50} of 1g/kg (Caffeine's LD_{50} is .13g/kg)

Problems

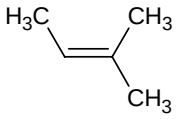
- *tert*-butyl alcohol
- Conc. HCl (12 M)
- Excess 3:1 HCl used

Alternative substrate

- *tert*-amyl alcohol

Alternative Substrate Analysis

- E1 product - 2-methyl 2-butene



  - Boiling point – 35-38 degrees
  - Refractive index – 1.3870

- S_N1 Product yield - 69 % *tert*-amyl chloride
  - Boiling point – 83 degrees
  - Refractive index – 1.4045

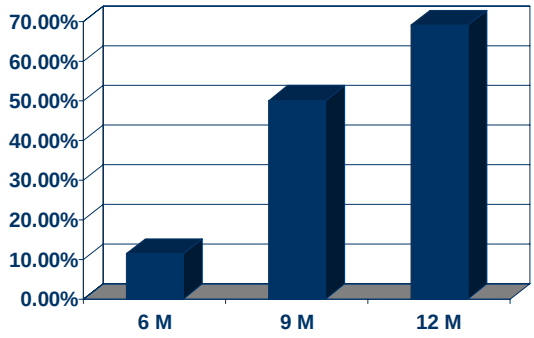
Alternative procedure

- Lower Conc.
  - Safer for students
  - Non-fuming
- Lower Molar Ratio
  - Less excess acid waste

Lower Concentration

- Concentrated HCl (12 M) – fuming
  - Must use in the fume hood
- 75 % HCl (9 M) – inconsistent vapors
  - Can be used on the bench, capped often
- 50 % HCl (6 M) – non-fuming, no vapors
  - Can be used on the bench, uncapped

Concentration vs. % Yield



Lower Molar Ratio

	3:1 Acid	2:1 Acid
6 M	11.5 %	N/A
9 M	50 %	52 %
12 M	69 %	68 %

- By definition an equilibrium reaction can't be 1:1

Results

- Any reaction with *tert*-amyl alcohol instead of *tert*-butyl alcohol is safer for your future children
- 2:1 molar ratio of acid yields the same amount as 3:1 and uses less material, which, in turn, produces less waste
- Tradeoffs with concentration of acid – the higher the yield, the higher the risk – a middle ground 9 M has a high yield and is less hazardous