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Course: Chemistry 341, Lecturer: Prof. Claus
Day: Friday, Date: 10/11/04
Notes Taken By: Chris [Redacted], Total Number of Pages: [Redacted]

Topics:
- The E1 and E2 Reactions
- Stereochemistry
- The E, Reaction

Predicting Substitution / Elimination Reactions

Four related runs in Ch. 6 (Sn2, Sn2, E1, E2)

\[
\begin{align*}
\text{Cl} & \quad \text{OH} \\
\text{H} & \quad \text{H} \\
\end{align*}
\]

Sn2 pathway: (minor product)

\[
\begin{align*}
\text{Cl} & \quad \text{OH} \\
\text{H} & \quad \text{H} \\
\end{align*}
\]

E2 pathway: Major product + (minor)

E, pathway: Mechanistic Thinking

Nucleophile is pair of electrons from C-C bond

E2: Elimination run, 2 = bimolecular (2nd order overall)

Is reverse of HCl addition to double bond

How can you rationalize E, product mix?

Conformation 1:

Conformation 2:

Terminal carbon

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Zaitsev's rule predicts $E_2$ mix. Elimination occurs to give the 'prenstabilized' alkene as the major product. Therefore, internal double bond is major product in $E_2$ reaction of 2-chloro-2-butane. Trans-2-butene is major (be able to predict).

More detailed Mechanistic picture:

- Specific geometry required called "anti peri-planar" (C-H bond 180° opposite C=C bond, in same plane).

- Newman: anti
- Newman: gauche

No other possible product (for internal double bond - Zaitsev's rule).

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Put it all together

1. Classify alkyl halide (primary, secondary, tertiary)
   a) Primary Alkyl halide
      - Think SN2 as major
      - E2 will be minor, competing rxn
      - E1 is major rxn with bulky, strong base (e.g., Me-Br + OH-)
   b) Secondary Alkyl halide (hardest to predict)
      - Think SN2 & E2 for major rxns
      - Look for factors that favor E2
        * Strong base (esp. bulky base)
      - Look for factors that favor Sn2
        * Good nucleophile ( lone pair + negative charge)
        * Not on list of strong bases
   c) 3° Alkyl halides
      - Think Sn1 or E2
      - Sn1 favored by weak bases (usually weak nucleophile, too)
      - E2 favored by strong bases

* E1 is rarer (low level) competing rxn
Predicting w/o pka table: (or, memorize this list!) (Also are strong nucleophiles)

- **Strong bases:**
  - OH
  - OR
  - NH₂
  - NHR (R = ethyl)
  - NR₂

**All strong bases are strong nucleophiles; not all strong nucleophiles are strong bases.**

**Bulky base:**  
R = big

**CH₃**

**Prototypical bulky, strong base:**

- **CH₃**
  - (Abb = OMe, e.g. KOMe, NaOMe)

Rsns also apply to cyclic molecules (Easier to predict with use of chair conformational drawing!)

**Br**

**CH₃**

- **H**

**E₂ favored**

Strong base, 2° halide

Could have formed on other side, too

- **CN**

- **Me**

**Sw 2**

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