Chem 164/261
Assignment & Lecture Outline 3:
Stereochemistry, Alkyl Halide Substitution (S_N1 & S_N2) and Elimination (E1 & E2) Reactions

Read

Organic Chemistry, L Wade, UA Custom Edition, 2013, Volume 1 (Chem 164/261)

- Functional Group List - Inside Front Cover (also Handout)
- Chapter 6 – Stereochemistry
- Chapter 7 – Alkyl Halides: Nucleophilic Substitution & Elimination Reactions

Problems: (do all "*solved problems"* in chapters listed below)

Do **Not** turn in, answers available in "Student Solutions Manual for Organic Chemistry" for LG Wade

- **Chapter 6:** 6.1 to 6.8; 6.12; 6.16; 6.19; 6.20; 6.25; 6.26; 6.28; 6.31
- **Chapter 7:** 7.2; 7.3; 7.7; 7.8a; 7.11; 7.12; 7.14; 7.17; 7.19; 7.20; 7.23; 7.30; 7.34; 7.41; 7.42; 7.43

Lecture Outline # 3

I. **Comparison of 2 Structures:**

Same Molecular Formula ? -> If Yes, Possibly Isomers or Identical
Same Arrangement (Sequence) of Groups ?
If No -> Structural Isomers
If Yes -> Superposable?
If Yes -> Identical Structures
If No -> Stereoisomers
Non-Superposable Mirror Images ?
If NO -> Diastereomers
If Yes -> Enantiomers

II. **Chirality and Stereoisomers**

A. The Concept of Chirality
1. Identification of chiral objects
a) achiral = not chiral
b) planes of symmetry within a molecule
2. Types of stereoisomers – enantiomers and diastereomers

B. Location of stereogenic (chiral) centres – 4 different groups on tetrahedral atom
1. Enantiomers & diastereomers
2. Meso compounds - chiral centers with plane of symmetry within molecule
3. Molecules with more than one chiral centre
4. Recognition of chiral centers in complex molecules - cholesterol - 8 chiral centres
Drawing the enantiomer of cholesterol and its potential 255 stereoisomers
5. Fischer projections

C. R and S nomenclature
    1. Rules for Assigning R and S configurations
    2. Treatment of multiple bonds

III. **Optical Rotation, Optical Purity, and Resolution of Enantiomers**

A. Optical Rotation
    1. Measurement, factors, and absolute rotation
    2. Optical purity and enantiomeric excess
    3. Physical Properties of Enantiomers and Diastereomers
    4. Racemic mixtures - 50-50 mixtures of enantiomers
    5. Optical Purity = enantiomeric excess (ee)

B. Separation (Resolution) of Enantiomers (e.g. Racemic mixtures)
    1. Creation of diastereomers
    2. Biological recognition

IV. **Nucleophilic Substitution Reactions (S_N1 and S_N2)**

A. General Features of Nucleophilic Substitution vs. Elimination Reactions
    1. Definitions: S_N1 and S_N2
    2. Mechanisms

B. S_N2 Reactions
    1. Stereochemistry - Walden Inversion (inversion of configuration)
    2. Substitution of Primary and Secondary Alkyl Halides
    3. Synthesis of alcohols, ethers, other halides, etc.
    4. Replacement of Acetylenic Hydrogen
        a. Acidity of Alkynes
        b. Alkylation – Substitution Reactions

C. S_N1 Reactions
    1. Stereochemical Aspects (loss of stereochemistry via carbocations)
    2. Substitution of Tertiary Alkyl Halides and Other Tertiary Carbons
    3. Synthesis of alcohols, ethers, halides

V. **Elimination Reactions - E1 & E2 Competition with Substitution Reactions (S_N1 and S_N2)**

A. El Mechanism - Saytzeff (Zaitsev) Rule, Leaving Groups

B. E2 Mechanism – Stereochemistry

C. Competition of Elimination Reactions (E2 and E1 versus S_N1 and S_N2)