

Prepared by the Department of Natural Sciences & Applied Technology

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Effective: Fall 2014

1. Course Number: CHM251 / CHM251L

Course Title: Organic Chemistry I / Organic Chemistry I Laboratory

2. Description: This course covers organic nomenclature, bonding, structure, reaction theory, aliphatic hydrocarbons, functional groups, stereochemistry, aromatic hydrocarbons, alkyl halides, and reaction mechanisms. The laboratory emphasizes basic laboratory techniques for separation, purification and synthesis. (3 class hours/ 4 laboratory hours)

3. Student Learning Outcomes: (instructional objectives; intellectual skills):

Upon successful completion of this course, students are able to do the following.

- Draw and interpret Lewis, condensed, and line-angle structural formulas and show which atoms bear formal charges
- Draw resonance forms and use them to predict stabilities
- Calculate empirical and molecular formulas from elemental compositions
- Predict relative acidities and basicities based on structure, bonding and resonance of conjugate acid-base pairs
- Identify nucleophiles (Lewis bases) and electrophiles (Lewis acids), and write reactions for Lewis acid-base reactions
- Draw the structure of a single bond, a double bond and a triple bond.
- Predict the hybridization and geometry of the atoms in a molecule
- Draw three dimensional representation of a given molecule
- Identify constitutional isomers and stereo isomers
- Identify polar and non-polar molecules and predict which ones can engage molecular bonding
- Predict the general trend in the boiling points and solubilities of compounds based on their size, polarity and hydrogen bonding ability
- Identify the general classes of hydrocarbons and draw structural formulas for examples
- Identify the classes of compounds containing oxygen or nitrogen and draw structural formulas for examples
- Explain and predict trends in physical properties of alkanes
- Correctly name alkanes and bicyclic alkanes
- When given the name of an alkane, draw the structure and give the molecular formula
- Compare the energies of alkane conformation and predict the most stable conformation
- Compare the energies of cycloalkanes and explain ring strain
- Identify and draw *cis* and *trans* stereo isomers of cycloalkanes
- Draw accurate cyclohexane conformations and predict the most stable conformation of substituted cyclohexanes
- Explain the mechanism and energetics of the free-radical halogenation of alkanes
- Predict the products of halogenation of an alkane based on the selectivity of halogenation
- Calculate enthalpy changes from bond-dissociation enthalpies
- Determine the order of a reaction and suggest a possible mechanism based on its rate equation
- Use energy diagrams to discuss transition states, activation energies, intermediates, and the rate-determining step of a multi-step reaction
- Describe the structures of carbocations, free radicals, and the structural features that stabilize them. Explain which are electrophilic and which are nucleophilic
- Classify molecules as chiral or achiral and identify mirror planes of symmetry
- Identify asymmetric carbon atoms and name them using the (R) and (S) nomenclature
- Calculate specific rotations from polarimetry data
- Draw all stereoisomers of a given structure
- Identify enantiomers, diastereomers, and meso compounds
- Draw correct Fischer projections or asymmetric carbon atoms
- Explain how the physical properties differ for different types of stereoisomers

- Suggest how to separate different types of stereoisomers
- Correctly name alkyl halides and identify them as 1°, 2°, or 3°
- Predict the products of S_N1, S_N2, E1, and E2 reactions, including stereochemistry
- Draw the mechanisms and energy profiles of S_N1, S_N2, E1, and E2 reactions
- Predict and explain the rearrangement of cations in first-order reactions
- Predict which substitutions or eliminations will be faster, based on differences in substrate, base/nucleophile, leaving a group, or solvent
- Predict whether a reaction will be first-order or second-order
- Predict predominance of substitution or elimination, when possible
- Use Zaitsev's rule to predict major and minor elimination products
- Draw and name all alkenes with a given molecular formula
- Use the *E-Z* and *cis-trans* systems to name geometric isomers
- Use heats of hydrogenation to compare stabilities of alkenes
- Predict relative stabilities of alkenes and cycloalkanes, based on structure and stereochemistry
- Predict the products of dehydrohalogenation of alkyl halides, dehalogenation of dibromides, and dehydration of alcohols, including major and minor products
- Propose logical mechanisms for dehydrohalogenation, and dehalogenation, and dehydration reactions
- Predict and explain the stereochemistry of E2 eliminations to form alkenes; predict E2 reactions on cyclohexane systems
- Propose effective single-step and multi-step syntheses of alkenes
- Predict the products of additions, oxidations, reductions, and cleavages of alkenes, including orientation of reaction (regiochemistry) and stereochemistry
- Propose logical mechanisms to explain the observed products of alkene reactions, including regiochemistry and stereochemistry
- Use retrosynthetic and analysis to solve multi-step synthesis problems with alkenes as reagents, intermediates, or products
- Choose the preferred method when more than one method is possible for a chemical transformation, and explain its advantages
- Determine the structure of an unknown alkene using clues provided by products of reactions such as ozonolysis
- Name alkynes and draw structures from their names
- Explain why alkynes are more acidic than alkanes and alkenes; demonstrate how to generate nucleophilic acetylide ions and heavy-metal acetylides
- Propose effective single-step and multi-step syntheses of alkynes
- Predict the products of additions, oxidations, reductions, and cleavages of alkynes, including orientation of reaction (regiochemistry) and stereochemistry
- Use alkynes as starting materials and intermediates in one-step and multi-step syntheses
- Demonstrate how reduction of an alkyne leads to an alkene or alkane derivative with the desired stereochemistry
- Draw and name alcohols, phenols, diols, and thiols
- Predict relative boiling points, acidities, and solubilities of alcohols
- Demonstrate how to convert alkenes, alkyl halides, and carbonyl compounds to alcohols
- Use Grignard and organolithium reagents effectively for the synthesis of primary, secondary, and tertiary alcohols
- Propose synthesis and oxidation products of simple thiols
- Predict the products of the reactions of alcohols with oxidizing and reducing agents; Carboxylic acids chlorides; dehydrating reagents (e.g., H₂SO₄ and H₃PO₄); inorganic acids; inorganic hydrides
- Predict the products of reactions with alkoxide ions
- Propose chemical test to distinguish alcohols from other types of compounds
- Propose methods to convert alcohol to a related compound with a different functional group
- Predict the products of the pinacol arrangement and periodate cleavage of glycols
- Use retrosynthetic analysis to propose effective single-step and multi-step syntheses of compounds using alcohols as intermediates (especially those using Grignard and organolithium reagents to assemble the carbon skeletons)
- Draw and name ethers epoxides
- Predict relative boiling points and solubilities of ethers
- Explain how ether solvents stabilize electrophilic reagents and why they are compatible with organometallic reagents

- Devise efficient laboratory syntheses of ethers and epoxides, including the Williamson ether synthesis: alkoxyation-demurcuration; peroxyacid epoxidation; base-promoted cyclization of halohydrins
- Predict the products of reactions of ethers and epoxides, including cleavage and autoxidation of ethers; acid-and-base-promoted opening of epoxides; reactions of epoxides with organometallic reagents

4. Credits: 5 credits

5. Satisfies General Education Requirement: No

6. Prerequisites: A grade of C or higher in CHM102 or CHM152

7. Semester Offered: Fall

8. Suggested General Guidelines for Evaluation: Course grading procedures are detailed on a student handout. In summary, grades are based on quizzes, hourly exams, final exam, laboratory reports and notebook (20.0%) and evaluation of learned laboratory techniques and organization.

9. General Topical Outline:

CHM251 Organic Chemistry I Course Outline

A. Structure and Properties

1. Organic Chemistry
2. The Structural Theory
3. The Chemical Bond before 1926
4. Quantum Mechanics
5. Atomic Orbitals
6. Electronic Configuration: Pauli Exclusion Principle
7. Molecular Orbitals
8. The Covalent Bond
9. Hybrid Orbitals
 - a. sp
 - b. sp²
 - c. sp³
10. Unshared Pairs of Electrons
11. Intramolecular Forces
12. Bond Dissociation
 - a. Homolysis
 - b. Heterolysis
13. Polarity
 - a. Of Bonds
 - b. Of Molecules
14. Structure and Physical Properties
 - a. Melting Points
 - b. Intermolecular Forces
 - c. Boiling Point
 - d. Solubility
15. Acids and Bases
16. Isomerism

B. Methane

1. Hydrocarbons
2. Structure of Methane
3. Physical Properties
4. Source
5. Reactions
6. Oxidation: Heat of Combustion
7. Chlorination: A Substitution Reaction

8. Control of Chlorination
9. Reactions with other Halogens: Halogenation
10. Relative Reactivity
11. Reaction Mechanisms
12. Mechanism of Chlorination: Free Radicals
13. Chain Reactions
14. Inhibitors
15. Heat of Reaction
16. Energy of Activation
17. Progress of Reaction: Energy Changes
18. Rate of Reaction
19. Relative Rates of Reaction
20. Relative Reactivities of Halogens toward Methane
21. An Alternative Mechanism for Halogenation
22. Structure of the Methyl Radical
23. Transition State
24. Reactivity and the Development of the Transition State
25. Chlorofluorocarbons and the Ozone Layer
26. Molecular Formulas and Empirical Formulas
27. Qualitative Elemental Analysis
 - a. Carbon
 - b. Hydrogen
 - c. Halogen
28. Molecular Weights and Empirical Weights

C. Alkanes

1. Classification by Structure: The Family
2. Structure of Ethane
3. Conformations and Torsional Strain
4. Propane and the Butanes
5. Conformations of n-Butane - Van der Waals Repulsion
6. Higher Alkanes - The Homologous Series
7. Nomenclature
 - a. Alkyl Groups
 - b. Common Names
 - c. IUPAC Names
8. Classes of Carbon and Hydrogen Atoms
9. Physical Properties
10. Industrial Source and Laboratory Preparation
11. The Grignard Reagent: An Organometallic Compound
12. Coupling of Alkyl Halides with Organometallic Compounds
13. Reactions
14. Halogenation
 - a. Mechanism
 - b. Orientation
 - c. Relative Reactivities of Alkanes
 - d. Ease of Abstraction of Hydrogens
15. Stability of Free Radicals
16. Ease of Formation of Free Radicals
17. Transition State for Halogenation
18. Orientation and Reactivity
19. Reactivity and Selectivity
20. Non-Rearrangement of Free Radicals - Isotopic Tracers
21. Combustion
22. The Greenhouse Effect
23. Pyrolysis
24. Determination of Structure
25. Analysis of Alkanes

D. Stereochemistry I. Stereoisomers

1. Stereochemistry and Stereoisomerism
2. Isomer Number and Tetrahedral Carbon
3. Optical Activity - Plane Polarized Light
4. The Polarimeter
5. Specific Rotation
6. Enantiomerism
 - a. The Discovery
 - b. And the Tetrahedral Carbon
 - c. And Optical Activity
7. Chirality and the Chiral Center
8. Enantiomers
9. The Racemic Modification
10. Configuration
11. Specification of Configuration: R and S
12. Sequence Rules
13. Diastereomers
14. *Meso* Structures
15. Specification of Configuration: More Than One Chiral Center
16. Conformational Isomers
17. Reactions Involving Stereoisomers
18. Generation of a Chiral Center: Synthesis and Optical Activity
19. Reactions of Chiral Molecules
 - a. Bond-Breaking
 - b. Relating Configurations
 - c. Generation of a Second Chiral Center
 - d. With Optically Active Reagents - Resolution
 - e. Mechanism of Free Radical Chlorination
20. Optical Purity

E. Alkyl Halides - Nucleophilic Aliphatic Substitution

1. Homolytic and Heterolytic Chemistry
2. Relative Rates of Competing Reactions
3. Structure - The Functional Group
4. Classification and Nomenclature
5. Physical Properties
6. Preparation
7. Nucleophilic Aliphatic Substitution
 - a. Reactions
 - b. Nucleophiles and Leaving Groups
 - c. Rate of Reaction: Effect of Concentration
 - d. Kinetics - Second-Order and First-Order Reactions
 - e. Duality of Mechanisms
8. S_N2 Reaction
 - a. Mechanism and Kinetics
 - b. Stereochemistry - Inversion of Configuration
 - c. Reactivity - Steric Hindrance
9. S_N1 Reaction
 - a. Mechanism and Kinetics
 - b. Stereochemistry
 - c. Reactivity
10. S_N2 vs S_N1
11. Carbocations
 - a. Structure
 - b. Stabilities - Accommodation of Charge. Polar Effects
 - c. Ease of Formation
 - d. Rearrangement
12. Analysis of Alkyl Halides

F. Alcohols and Ethers

1. Introduction
2. Alcohols
 - a. Structure
 - b. Classification
 - c. Nomenclature
 - d. Physical Properties
 - e. Industrial Source
 - f. Fermentation of Carbohydrates
 - g. Ethanol
 - h. Preparation of Alcohols
 - i. Reactions of Alcohols
 - j. Alcohols as Acids and Bases
 - k. Reactions of Alcohols with Hydrogen Halides. Acid Catalysis
 - l. Formation of Alkyl Sulfonates
 - m. Oxidation of Alcohols
3. Ethers
 - a. Structure and Nomenclature
 - b. Physical Properties
 - c. Preparation of Ethers
 - i. Industrial
 - ii. Laboratory - Williamson Synthesis
 - d. Reactions of Ethers - Acid Cleavage
 - i. S_N1 Type
 - ii. S_N2 Type
 - e. Analysis of Alcohols
 - f. Analysis of Ethers

G. Role of the Solvent

1. Role of the Solvent
2. Secondary Bonding
3. Solubility
 - a. Non-ionic Solutes
 - b. Ionic Solutes
 - i. Protic Solvents
 - ii. Aprotic Solvents
4. The S_N1 Reaction - Role of the Solvent: Ion-Dipole Bonds
5. The S_N2 Reaction
 - a. Role of the Solvent
 - i. Protic Solvents
 - ii. Aprotic Solvents
 - b. Phase Transfer Catalysis
6. S_N2 vs S_N1: Effect of the Solvent
7. Solvolysis: Nucleophilic Assistance by the Solvent

H. Alkenes I. Structure and Preparation

1. Unsaturated Hydrocarbons
2. Structure of Ethylene - The Carbon-Carbon Double Bond
3. Propylene
4. Hybridization and Orbital Size
5. The Butylenes
6. Geometric Isomerism
7. Higher Alkenes
8. Names of Alkenes
9. Physical Properties
10. Chemistry of Vision
11. Industrial Source
12. Preparation
13. Dehydrohalogenation of Alkyl Halides - 1,2-Elimination

14. Kinetics of Dehydrohalogenation
15. The E-2 Mechanism
 - a. Kinetics
 - b. Absence of Rearrangements
 - c. Isotope Effects
 - d. Absence of Hydrogen Exchange
 - e. The Element Effect
 - f. Orientation
 - g. Reactivity
16. The E-1 Mechanism
17. Evidence for the E-1 Mechanism
18. Elimination: E-2 vs E-1
19. Elimination vs Substitution
20. Dehydration of Alcohols

I. Alkenes II: Reactions of the Carbon-Carbon Double Bond

1. Reactions of the Alkenes
2. Reactions of the Carbon-Carbon Double Bond
3. Hydrogenation - Heat of Hydrogenation
4. Heat of Hydrogenation and Stability of Alkenes
5. Addition of Hydrogen Halides - Markovnikov's Rule
6. Addition of Hydrogen Bromide
7. Addition of Water - Hydration
8. Addition of Sulfuric Acid
9. Electrophilic Addition
 - a. Mechanism
 - b. Rearrangements
 - c. Orientation
 - d. Reactivity
10. Addition of Halogens
11. Mechanism of Addition of Halogens
12. Halohydrin Formation
13. Addition of Alkenes - Polymerization
14. Addition of Alkanes
15. Oxymercuration-Demercuration
16. Hydroboration-Deboronation
17. Mechanism of Hydroboration
18. Free Radical Addition Mechanism
19. Orientation of Free Radical Addition
20. Other Free Radical Additions
21. Free Radical Polymerization of Alkenes
22. Hydroxylation - Formation of 1,2 Diols
23. Cleavage: Determination of Structure by Degradation
24. Analysis of Alkenes

J. Stereochemistry II.

1. Organic Chemistry in Three Dimensions
2. Stereochemistry of Addition of Halogens to Alkenes
 - a. The *syn*- Addition
 - b. The *anti*- Addition
3. Mechanism of the E-2 Reaction
4. Stereochemistry of the E-2 Reaction
 - a. The *syn*- Elimination
 - b. The *anti*- Elimination
5. Stereospecific Reactions
6. Stereospecific vs Stereoselective Reactions

K. Conjugation and Resonance - Dienes

1. The Carbon-Carbon Double Bond as a Substituent
2. Free Radical Halogenation of Alkenes: Substitution vs Addition

3. Free Radical Substitution in Alkenes
 - a. Orientation
 - b. Reactivity
 - c. Allylic Rearrangement
4. Symmetry of the Allyl Radical
5. The Theory of Resonance
6. The Allyl Radical as a Resonance Hybrid
7. Stability of the Allyl Radical
8. Orbital Picture of the Allyl Radical
9. Using the Resonance Theory
10. Resonance Stabilization of Alkyl Radicals - Hyperconjugation
11. The Allyl Cation as a Resonance Hybrid

12. Nucleophilic Substitution in Allylic Substrates: S_N1
 - a. Reactivity
 - b. Allylic Rearrangement
13. Stabilization of the Carbocations: The Resonance Effect
14. Nucleophilic Substitution in Allylic Substrates - S_N2
15. Nucleophilic Substitution in Vinylic Substrates
16. Dienes
 - a. Structure
 - b. Properties
 - c. Stability
 - d. Resonance
17. Resonance in Alkenes - Hyperconjugation
18. Ease of Abstraction of Conjugated Dienes: Orientation of Elimination
19. Electrophilic Addition to Conjugated Dienes: 1,4-Addition
20. 1,2-Addition vs 1,4-Addition: Rate vs Equilibrium
21. Free Radical Polymerization of Dienes. Rubber and Rubber Substitutes
22. Isoprene and the Isoprene Rule
23. Analysis of Dienes

L. Alkynes

1. Introduction
2. Structure
3. Higher Alkynes - Nomenclature
4. Physical Properties of Alkynes
5. Preparation of Alkynes
 - a. Industrial
 - b. Laboratory
6. Reactions of Alkynes
7. Reduction of Alkynes
8. Electrophilic Addition to Alkynes
9. Hydration of Alkynes - Tautomerism
10. Acidity of Alkynes
11. Reactions of Metal Acetylides
12. Formation of Carbon-Carbon Bonds - Role Played by Organometallic Compounds
13. Analysis of Alkynes

M. Cyclic Aliphatic Compounds

1. Open Chain and Cyclic Compounds
2. Nomenclature
3. Preparation
 - a. Industrial
 - b. Laboratory
4. Reactions
5. Reactions of Small Rings
6. Bayer Strain Theory
7. Heats of Combustion and Relative Stabilities of the Cycloalkanes

8. Orbital Picture of Angle Strain
9. Factors Affecting Stability of Conformations
10. Conformations of Cycloalkanes
11. Conformations of Cyclohexane
 - a. Axial Positions
 - b. Equatorial Positions
12. Stereoisomers of Cyclic Compounds
 - a. *Cis* and *Trans* Isomers
 - b. Conformational Analysis
13. Stereochemistry of Elimination from Cycloalkanes
14. Carbenes: Methylene; Cycloaddition
15. Addition of Substituted Carbenes: 1,1-Elimination
16. Cyclic Ethers
17. Crown Ethers: Host-Guest Relationship

18. Epoxides
 - a. Structure
 - b. Preparation
19. Cleavage of Epoxides
 - a. Acid Catalyzed: *Anti*- Hydroxylation
 - b. Base Catalyzed
20. Orientation of Cleavage of Epoxides
21. Analysis of Alicyclic Compounds