Program Applicable

Effective Quarter: Fall 2016

I. Catalog Information

CHEM 12B **Organic Chemistry** **5 Unit(s)**

Prerequisite: CHEM 12A with a grade of C or better.

Advisory: EWRT 1A or EWRT 1AH or ESL 5.

Graded

Three hours lecture, six hours laboratory (108 hours total per quarter).

An exploration of the physical properties and chemical behavior of important classes of organic compounds, focusing on: polyenes; aromatic compounds; alcohols, thiols, and ethers; and aldehydes and ketones and their derivatives. Emphasis on retrosynthesis, spectroscopic structure determination, and reaction mechanism. Laboratory experiments involving the synthesis of simple compounds and the characterization of those compounds using chromatography and infrared (IR), ultraviolet-visible (UV-Vis), and nuclear magnetic resonance (NMR) spectroscopy. For chemistry majors or those in closely-allied fields such as biochemistry and chemical engineering.

Course Justification: This course is a major preparation requirement in the discipline of chemistry at all CSUs and UCs. This course belongs on the Biological Sciences Associates in Sciences degree. This is the second of three courses in the Organic Chemistry sequence of classes where students are introduced to topics in organic chemistry such as more advanced organic reactions, reaction mechanisms, and analysis of organic molecules.

- **Student Learning Outcome**: Apply molecular orbital theory to predict the outcome of selected chemical reactions.

- **Student Learning Outcome**: Apply resonance theory to predict the major and minor products of chemical reactions.

- **Student Learning Outcome**: Generate logical multi-step syntheses of increasingly complex molecules.

- **Student Learning Outcome**: Construct logical stepwise reaction mechanisms for increasingly complex chemical systems.

II. Course Objectives

A. Examine the key structural features and physical properties of important classes of organic compounds, especially: polyenes; aromatic compounds; alcohols, phenols, and ethers; thiols and sulfides; aldehydes and ketones; acetals and ketals; and imines and enamines.

B. Compose valid names for alcohols, ethers, thiols, aldehydes, ketones, benzene and its derivatives, and related organic compounds using both common and IUPAC nomenclature conventions.

C. Predict the reactivity of alcohols, ethers, thiols, aldehydes, ketones, benzene and its derivatives, and related organic compounds on the basis of their structure.

D. Create detailed reaction mechanisms and use those mechanisms to explain experimental observations or predict the most likely outcome of reactions of alcohols, ethers, thiols, aldehydes, ketones, benzene and its derivatives, and related organic compounds.

E. Construct detailed synthetic schemes for the interconversion of alcohols, ethers, thiols, aldehydes, ketones, benzene and its derivatives, and related organic compounds by functional group transformation using retrosynthetic analysis.

F. Examine the behavior of alcohols, ethers, thiols, aldehydes, ketones, benzene and its derivatives, and related organic compounds by utilizing the frameworks of kinetics, thermodynamics, and equilibrium.

III. Essential Student Materials

None

IV. Essential College Facilities

Fully equipped chemical laboratory including, at a minimum, the following: consumable chemicals, chemical balances, glassware, molecular models, melting point apparatus, laptops with data acquisition modules, fume hoods, chemical disposal facilities, lockable student storage areas, and laboratory technician.

V. Expanded Description: Content and Form

A. Examine the key structural features and physical properties of important classes of organic compounds, especially: polyenes; aromatic compounds; alcohols, phenols, and ethers; thiols and sulfides; aldehydes and ketones; acetals and ketals; and imines and enamines.

- **1.** Examine the effects of conjugation on molecular structure and electronic structure.
- **2.** Compare the reactivity of aldehydes and ketones

B. Compose valid names for alcohols, ethers, thiols, aldehydes, ketones, benzene and its derivatives, and related organic compounds using both common and IUPAC nomenclature conventions.

- **1.** Examine the guidelines for naming compounds based on current IUPAC committee recommendations for organic compounds.
  - **a.** Dienes and polyenes
  - **b.** Alcohols, thiols, and ethers
  - **c.** Aldehydes and ketones
  - **d.** Aromatic compounds
- **2.** Survey key examples of traditional or common nomenclature.
  - **a.** Common names of aldehydes and ketones, such as acetone and methyl ethyl ketone (MEK)
  - **b.** Common names of aromatic compounds, such as xylene, styrene, toluene, phenol, aniline, cumene, and acetophenone

C. Predict the reactivity of alcohols, ethers, thiols, aldehydes, ketones, benzene and its derivatives, and related organic compounds on the basis of their structure.

- **1.** Investigate the influence of delocalization on the reactivity of polyenes and other linearly conjugated systems.
  - **a.** Conjugated systems

1. Conjugated versus unconjugated polyenes
2. Cumulenes
3. Conjugated ions

b. Review of resonance

1. Writing resonance structures
2. Blending of resonance forms to more accurately represent molecular structure

c. Molecular orbitals in conjugated systems

1. Generation of delocalized molecular orbitals through combination of atomic orbitals
2. Bonding, non-bondings, and anti-bonding orbitals

2. Assess the relationship between structure and reactivity in pericyclic reactions

a. Determination of frontier (HOMO/LUMO) orbital geometry

b. Conrotatory versus disrotatory cyclization geometries

c. Suprafacial versus antarafacial addition

d. Thermal versus photochemical reactions

e. The Diels-Alder reaction

3. Examine the effects of aromaticity on chemical reactivity.

a. Aromatic compounds

1. Observation of aromaticity through heats of hydrogenation
2. Structural effects of aromaticity on bond length and strength
3. Resonance structures of aromatic compounds

b. Aromaticity

1. Structural prerequisites for aromaticity
2. Molecular orbital explanation for the Huckel [4n + 2] rule
3. Aromatic stabilization and anti-aromatic destabilization of cyclic molecules
4. Frost circles
5. Effects of antiaromaticity on molecular structure, such as the non-planarity of cyclooctatetraene and the thermodynamic instability of cyclobutadiene

4. Estimate the acidity of organic molecules.

a. Acidity of alcohols

1. Inductive effects
2. Trends in acidity

b. Acidity of aromatic compounds

1. Resonance stabilization of benzoate
2. Resonance stabilization of phenoxide

3. Substituent effects

D. Create detailed reaction mechanisms and use those mechanisms to explain experimental observations or predict the most likely outcome of reactions of alcohols, ethers, thiols, aldehydes, ketones, benzene and its derivatives, and related organic compounds.

1. Examine the effects of delocalization on reaction mechanism.
   - **a.** Conjugate (1,4) versus vicinal (1,2) addition
   - **b.** Electrophilic aromatic substitution versus electrophilic addition to alkenes
2. Explore the major reactions of aromatic compounds.
   - **a.** Electrophilic aromatic substitution
     1. Halogenation
     2. Nitration
     3. Sulfonation
   - **b.** Friedel-Crafts alkylation
     1. Carbocation migration
     2. Ring activation
   - **c.** Friedel-Crafts acylation
     1. Acylinium ion
     2. Ring deactivation
   - **d.** Nucleophlic aromatic substitution
   - **e.** Reduction
     1. Stability of benzene towards catalytic hydrogenation
     2. Reduction of nitro groups
   - **f.** Benzyne
3. Investigate the reactions of alcohols, thiols, and ethers.
   - **a.** Dehydration of alcohols
   - **b.** Conversion of alcohols into leaving groups
     1. Thionyl chloride
     2. Phosphorus tribromide
     3. Tosyl chloride and related sulfonyl halides
     4. Stereochemical consequences of leaving group formation
   - **c.** Oxidation of alcohols
     1. Chromate oxidation
     2. Pyridinium chlorochromate (PCC)
     3. Swern oxidation

- **d.** Epoxide formation and reaction
  1. Formation of epoxides from alkenes using peroxyacids
  2. Acid-catalyzed ring-opening
  3. Base-promoted ring-opening
- **e.** Protecting groups for alcohols
  1. Protecting group synthetic stratagy
  2. Trimethysilyl (TMS) ethers and related silyl ethers
  3. Tetrahydropyran (THP) ethers
  4. Benzyl ethers (optional)
  5. Deprotection conditions
- **f.** Crown ethers
- **g.** Thiols
  1. Nucleophilicity
  2. Disulfide formation

4. Survey the major reactions of aldehydes and ketones.

- **a.** Reactivity of the carbonyl bond
  1. Electrophilicity of carbon
  2. Cationic versus anionic reactions and mechanisms
- **b.** Hydrates, acetals, and ketals
  1. Formation
  2. Use of acetals and ketals as protecting groups
- **c.** Formation of imines, enamines, hydrazones, and oximes
- **d.** Oxidation
  1. Over-oxidation of hydrates of aldehydes
  2. Tollens' reagent
- **e.** Reduction
  1. Sodium borohydride and lithium aluminum hydride
  2. Wolff-Kishner reaction
  3. Reduction of imines
- **f.** Alkylation
  1. Formation and reaction of Grignard reagents
  2. Conjugate addition of organocuprates
  3. Functional group compatibility

- **g.** Wittig reaction
  - **1.** Ylide formation
  - **2.** Cyclic mechanism
- **h.** Cannizzaro reaction and relationship to NADH mechanism (optional)

E. Construct detailed synthetic schemes for the interconversion of alcohols, ethers, thiols, aldehydes, ketones, benzene and its derivatives, and related organic compounds by functional group transformation using retrosynthetic analysis.

- **1.** Evaluate the utility of Grignard and Wittig reactions in the synthesis of larger molecules by the formation of new carbon-carbon bonds.
- **2.** Explore the use of alcohols as key synthetic intermediates.
- **3.** Investigate the use of oxidation and reduction reactions in multistep synthesis.

F. Examine the behavior of alcohols, ethers, thiols, aldehydes, ketones, benzene and its derivatives, and related organic compounds by utilizing the frameworks of kinetics, thermodynamics, and equilibrium.

- **1.** Explore the contrast of kinetic versus thermodynamic control in chemical reactions.
  - **a.** Reaction coordinate diagrams of systems experiencing kinetic versus thermodynamic control
  - **b.** Effects of temperature on product distribution
- **2.** Predict the reactivity of aromatic compounds in electrophilic substitution reactions
  - **a.** Ortho/para-directors
    - **1.** Resonance stabilization of reaction intermediate
    - **2.** Activators versus deactivators
  - **b.** Meta-directors
    - **1.** Avoidance of resonance destabilization
    - **2.** Ring deactivation
- **3.** Investigate the reversibility of reactions involving carbonyl-containing compounds
  - **a.** Reversibility of cationic (acid-catalyzed) reactions
  - **b.** Irreversibility of anionic (base-promoted) reactions
  - **c.** Keto-enol tautomerization
    - **1.** Relative stability of ketones versus enols
    - **2.** Relative stability of imines versus enamines

VI. Assignments

A. Required readings from the textbook and laboratory manual

B. Discretionary written problems from each lecture chapter and laboratory experiment

C. Written laboratory reports for each experiment performed in the laboratory

VII. Methods of Instruction

0. Lecture and visual aids
   Laboratory demonstrations
   Discussion of assigned readings
   Discussion of problem solving performed in class
   Quiz and examination review performed in class
   Homework assignments
   Collaborative learning and small group exercises
   Laboratory experience which involves students in formal exercises of data collection and analysis
   Laboratory discussion sessions and quizzes that evaluate the experiments performed

VIII. Methods of Evaluating Objectives

- **A.** At least three one-hour written examinations designed to periodically assess the students' ability to apply concepts and skills acquired through one of more modes of instruction, such as lecture, assigned readings, small group discussions, or homework problems.
- **B.** At least one written laboratory examination designed to assess the students' ability to apply concepts and skills acquired through conducting laboratory experiments and preparing written laboratory reports.
- **C.** Regular homework assignments and/or lecture quizzes designed to periodically assess the students' progress in acquiring key concepts and skills.
- **D.** Laboratory reports for each experiment performed, which will be used to assess the ability of a student to clearly and logically express the qualitative or quantitative results of an experiment. Laboratory reports will include an analysis of any relevant spectral or physical data and, optionally, a discussion of theoretical or experimental concepts applied in the experiment.
- **E.** Comprehensive final lecture exam designed to assess the students' ability to critically apply concepts and skills introduced throughout the course.
- **F.** One-hour in-class final lab examination designed to assess the students' ability to apply concepts and skills acquired through conducting laboratory experiments and preparing written laboratory reports.

IX. Texts and Supporting References

- **A.** Examples of Primary Texts and References
  1. *Klein, David. "Organic Chemistry", 2e. Wiley, 2015.
  2. *Gilbert, John C. and Martin, Stephen F. "Experimental Organic Chemistry: A Miniscale and Microscale Approach", 6e. Brooks/Cole, 2015.
- **B.** Examples of Supporting Texts and References
  1. Smith, Janice G. "Study Guide/Solutions Manual for Organic Chemistry", 4e. McGraw-Hill, 2014.

X. Lab Topics

- **A.** Laboratory methodology
  1. Maintaining a laboratory notebook
  2. Writing laboratory reports
- **B.** Chemical safety
  1. Materials safety data sheets (MSDS)

2. Chemical disposal
   a. Separation of waste streams
   b. Proper disposal methods
   c. Environmental hazards of improper waste disposal
3. Laboratory environment
   a. Maintaining laboratory cleanliness
   b. Chemical labeling
   c. Segregation of chemicals by hazard
   d. Secondary containment
4. Personal safety
   a. Safety goggles
   b. Limiting chemical exposure
   c. Safety showers
   d. Eyewash stations
   e. Proper use of fire extinguishers
5. Emergency situations
   a. Fires
   b. Earthquakes
   c. Evacuation prodecures

C. Analyze spectroscopic data to determine the structure of organic compounds.
1. Review the central concepts of spectroscopy.
2. Analyze organic compounds using infrared (IR) spectrophotometry.
   a. Effects of conjugation on bond stretching
   b. Interpretation of IR spectra
3. Analyze organic compounds using ultraviolet-visible (UV) spectrophotometry.
4. Elucidate the structure of organic compounds using nuclear magnetic resonance spectroscopy (NMR).
   a. Deshielding effects of aromatic compounds
   b. Interpretation of NMR spectra

D. Laboratory experiments
1. Investigation of kinetic versus thermodynamic control of product distribution in chemical reactions, such as the competing synthesis of two semicarbazones
2. Synthesis of an alkene via a Diels-Alder reaction
3. Investigation of the reactivity of aromatic compounds via bromonation

4. Nitration of aromatic compounds
5. Friedel-Crafts acylation of aromatic compounds
6. Synthesis of an alcohol such as triphenylmethanol via Grignard alkylation
7. Oxidation of an alcohol such as cyclododecanol
8. Reduction of a ketone or aldehyde such as camphor
9. Synthesis of an alkene via Wittig reaction