

Mt. San Jacinto College
Integrated Course Outline of Record

Form B

Submitted by: Rosaleen Gibbons Date: 10/10/2019

Department	Subject	Course Number	Title
Chemistry	Chemistry CHEM	112	Organic Chemistry I

Units/Hours

Each lecture unit requires 1 hour per week of class time, and 2 hours per week of study outside of class.
Each laboratory unit requires 3 hours per week of class time.
Each activity unit requires 2 hours per week of class time and 1 hour per week of study outside of class.

Lecture Units

3.00

Lecture Contact Hours

48.00 - 54.00

Lecture Homework Hours

96.00 - 108.00

Lab Units

2.00

Lab Contact Hours

96.00 - 108.00

Lab Homework Hours

0

Total Units

5.00

Total Contact Hours

144.00 - 162.00

Stand Alone:

Program Applicable

AA/AS Degree General Ed Breadth Area(s):

A NATURAL AND PHYSICAL SCIENCES

General Education Justification:

Students will exhibit an understanding of Organic Chemistry and the role it plays in the chemistry of living systems and in the synthesis of new compounds(GELO1). Chem 112 incorporates the GELO competencies of Area A by introducing students to the scientific methods of investigation, evaluation and synthesis (GELO2, GELO6). Student investigate the fundamental properties of organic chemistry including the chemical, physical, and thermodynamic properties of organic chemical compounds (GELO4). The course investigates chemical structure and reaction using dehydration, dehydrohalogenation, evaluates chemical compounds using spectroscopy and nuclear magnetic resonance (GELO3), and measures physical properties of known and unknown substances to identify mass, density, frequency and wavelength (GELO5). The course emphasizes experimental methodology as related to organic chemical compounds (GELO2).

Maximum Enrollment:

24

Maximum Enrollment Justification:

Course has safety or compliance factors which influence the enrollment cap – check all that apply:

- * Course has safety or health reasons that the class should have a non-standard enrollment cap.
- * Course has specific standards outside of the college calling for a specific or capped class size.

Justification: CHEM112 is a combined lecture and laboratory course offered over a single-semester. Students perform laboratory experiments with a number of chemicals and reagents that are toxic, corrosive and/or irritants to the skin, eyes, and respiratory system. During each laboratory session, students are transporting these chemicals and reagents as well as glassware and other equipment from a dispensing area across the lab to their bench where they carry out procedures. Many labs also require the use of Bunsen burners with open flames. American Chemical Society (ACS) has recommended guidelines of 50 sq ft per student to ensure safety in the learning environment of a student chemistry laboratory. More than 24 students in the laboratory would constitute a safety hazard.

Grading Method:

Letter Grade or P/NP

TOP code:

1905.00

Can be Taken

1

time(s) for credit (max 4)

- Visual or Performing Arts course that is required to meet major requirements for UC/CSU

- Intercollegiate athletics course

- Academic/vocational competition course

Catalog Description:

(Please do not refer to transferability or degree, certificate, or employment concentration applicability. Please only describe the course).
(75 words or less in gray box below).

This course is the first of a two-semester sequence in organic chemistry. The topics covered include molecular properties, structure and bonding, stereochemistry, reactions and synthesis of alkane, alkenes, alkynes and alkyl halides, NMR and IR spectroscopy, and the chemistry of benzene and aromatic compounds.

Schedule Description:

(Please do not refer to transferability or degree, certificate, or employment concentration applicability. Please only describe the course).
(25 words or less in gray box below).

This is the first of two semesters of Organic Chemistry focusing on alkanes, alkenes, alkynes, organohalides, and benzene.

Need for the course:

This course is a transfer course to UC and CSU for Chemistry majors, premed, and Biochemistry majors.

Prerequisite(s):

Prerequisites go through a separate approval process. See Forms E1-E6 for details.
(For further clarification, contact the Prerequisite Subcommittee)

- CHEM 102 with a Grade of C or better.

Corequisite(s):

Corequisites go through a separate approval process. See Forms E1-E6 for details.

-none-

Recommend Preparation:

Recommended Preparation goes through a separate approval process. See Forms E1-E6 for details.

-none-

Other Enrollment Criteria:

-none-

Learning Objectives:

(please number each objective and express in behavioral terms)

Upon the completion of the course the student will be able to do the following:

1. Analyze the structure of atoms using modern atomic theory, valence bond theory and molecular orbital theory, and evaluate the fundamental properties of compounds including acid-base, thermodynamic, kinetic, and physical properties to describe physical and chemical characteristics, deduce compound names using the IUPAC system, and identify functional groups.
2. Evaluate generalized reactions, and categorize various reactions as addition, substitution, condensation, elimination, or oxidation-reduction.
3. Formulate the three dimensional structure of molecules, predict possible isomers, and analyze the chemistry that leads to enol-keto tautomerism in addition to recognition and characterization of stereochemistry, and the optical activity of a compound.
4. Scrutinize in detail the chemistry and structure of the families of alkanes, cyclic hydrocarbon compounds, alkenes, alkynes, alkyl halides, and benzene with emphasis on reactions and reaction mechanisms.
5. Observe regiochemistry and Markovnikov's Rule, and apply Hammond's postulate and potential energy when evaluating carbocations, stable intermediates, and transition states.
6. Apply the general principles and patterns of alkene reactions to form halohydrins, alcohols, alkanes, carbonyls, carboxylic acids, cyclopropane, epoxide, and polymers, and alkyne reactions to form halohydrins, alkenes, alkanes, carbonyls, carboxylic acids, and amines.
7. Analyze and deduce chain elongation reactions such as Grignard and organo coupling with Gilman reagent, as well as the properties of nucleophiles, electrophiles, leaving groups, and solvents as they pertain to substitution and elimination reactions such as, SN1, SN2, E1, and E2.
8. Investigate the general properties of electromagnetic radiation to determine molecular structure by analyses of infrared (IR) spectroscopy, ultraviolet/visible (UV-VIS) spectroscopy, and nuclear magnetic resonance (NMR) spectroscopy; in addition, utilize mass spectrometry (MS) for molecular identification, as well as gas chromatography (GC).
9. Interpret cyclic-planar geometry, conjugation, and Huckel's rule relative to identification of aromatic, non-aromatic, and anti-aromatic compounds, and evaluate aromatic ring activation/deactivation through interpretation of resonance and analyses of reactivity in the ortho, meta, and para sites of benzene and other aromatic compounds efficiently synthesized by mechanisms that add one, two, or more substituents by electrophilic aromatic substitution.

Laboratory Objectives

1. Practice lab safety, wear proper personal protective equipment (PPE), utilize Safety Data Sheets (SDS), observe chemical hazards and use proper chemical hygiene, in addition to explaining and demonstrating correct procedures for safe handling and disposal of hazardous waste.
2. Construct microscale glassware (microbell, picnometer, magnetic spin bar, evacuated capillary, microburette), and demonstrate specific precautions when using needles and sharps; assemble taper glassware apparatus and safely conduct experimental procedures.
3. Operate electrical equipment such as but not limited to melt temps, vortexes, and centrifuges according to manufacturer instructions, and extract accurate data from refractometers, polarimeters, and analytical balances to the correct level of

instrument precision.

4. Operate, analyze, and interpret GC, FT-IR, UV-VIS, and NMR data and results both manually and with the use of software.
5. Accurately determine physical properties in the laboratory, and in the field to the correct level of instrument precision.
6. Perform simple distillation, extraction, sublimation, crystallization, and evaporation techniques in addition to various chromatography techniques, including but not limited to thin layer chromatography and gas chromatography.
7. Employ a variety of solubility and chemical tests and identify functional groups based on observations of results.
8. Carry out single-step synthesis reactions at the microscale and semi-microscale levels with purification and characterization of product(s).
9. Maintain a proper laboratory notebook and organized computational files of analytical data/results.
10. Construct a clear/concise scientific laboratory report with experiential objectives, procedures, data/results, conclusions, and ACS formatted references for each experiment throughout the semester.

Course Content:

(please number the outline of main topics and subtopics)

1. Structure and Bonding
 1. electron orbitals and shells
 2. ground state electron configurations
 3. ionic bonds and valence shell electrons
 4. ionization energy
 5. electron affinity
 6. covalent bonds
 7. Lewis structures
 8. hybridization of atomic orbitals
 9. bond lengths and bond energies
2. Molecular Properties
 1. electronegativity
 2. dipoles and polarity
 3. structure determination
 4. formal charges
 5. oxidation numbers
 6. resonance structures
 7. acid and base properties
 8. equilibrium
 9. free energy
 10. enthalpy
 11. entropy
 12. bond dissociation energy
 13. heats of reaction
3. Reactions Overview
 1. addition reactions
 2. substitution reactions
 3. elimination reactions
 4. condensation reactions
 5. reaction mechanisms
 6. activation energy
 7. reaction rates
 8. intermediates
 9. transition states
 10. potential energy diagrams
 11. synthesis of organic compounds
4. Alkanes and Cyclic Hydrocarbons
 1. IUPAC naming system

2. aliphatic hydrocarbons
3. alkyl groups
4. other functional groups
5. isomers
6. stereochemistry
7. physical and chemical properties
8. naming cycloalkanes
9. cis-trans isomerism
10. anti and gauche conformations
11. Bayer Strain Theory
12. mono and disubstituted cycloalkanes
13. IUPAC Nomenclature

5. Alkenes

1. nomenclature
2. physical and chemical properties
3. structure
4. degree of unsaturation
5. laboratory and industrial preparation
6. elimination reactions, which include alcohol dehydration reactions, dehydrohalogenation reactions, and dehydration reactions
7. electronic structure and stability
8. electrophilic addition reactions, which include hydration reactions, oxymercuration reactions, and hydroboration reactions
9. Markovnikov's rule
10. oxidation and reduction reactions
11. polymerization reactions
12. use of alkenes in synthesis
13. IUPAC Nomenclature

6. Alkynes

1. nomenclature
2. physical and chemical properties
3. structure
4. degree of unsaturation
5. laboratory and industrial preparation
6. dihalide elimination reactions
7. electronic structure and stability
8. electrophilic addition reactions, which include hydration reactions, and hydroboration reactions
9. oxidation and reduction reactions
10. alkylation reactions
11. use of alkynes in synthesis
12. IUPAC Nomenclature

7. Stereochemistry

1. physical properties of stereoisomers
2. enantiomers
3. chirality
4. specific rotation
5. optical activity
6. diastereomers
7. meso compounds
8. racemic mixtures
9. isomerism
10. Fisher projections
11. stereochemistry of addition reactions

8. Alkyl Halides

1. nomenclature
 2. physical and chemical properties
 3. structure
 4. preparation
 5. halogenation of alkanes, alkenes, and alcohols
 6. preparation of Grignard reagents and organometallic compounds
 7. oxidation-reduction reactions
 8. first and second order nucleophilic substitution reactions
 9. elimination reactions
 10. kinetics of substitution reactions
 11. steric effects
 12. attacking groups and leaving groups effects
 13. solvent effects
 14. use of alkyl halides in synthesis
 15. IUPAC Nomenclature
9. Infrared Spectroscopy (IR)
1. regions of the spectrum
 2. frequency
 3. wavelength
 4. amplitude
 5. using IR to identify an unknown compound
10. Nuclear Magnetic Resonance Spectroscopy (NMR)
1. the nature of absorption
 2. Proton NMR
 3. characterizing of molecular structure
 4. chemical shifts
 5. spin-spin splitting patterns
 6. coupling constants
 7. integrating spectra to determine the number of hydrogen atoms in a compound
 8. Carbon-13 NMR
 9. magnetic resonance imaging (MRI)
 10. uses of NMR in determining the structure of a compound
11. Ultraviolet spectroscopy (UV) and Conjugated Systems
1. preparation of conjugated dienes
 2. structure and stability
 3. electrophilic addition reactions
 4. kinetics of addition reactions
 5. Diels Alder reactions
 6. uses of UV spectroscopy in structure determination
 7. HOMO-LUMO transitions
12. Benzene and Aromatic Compounds
1. sources of benzene
 2. nomenclature
 3. resonance forms
 4. molecular orbital description
 5. Hückel $4n + 2$ rule
 6. IR, UV, and NMR spectroscopy of aromatic compounds
 7. electrophilic aromatic substitution reactions
 8. halogenation reactions
 9. alkylation reactions
 10. acylation reactions
 11. Friedel-Crafts reactions
 12. nucleophilic aromatic substitution reactions
 13. oxidation and reduction reactions

14. catalytic hydrogenation
15. use in synthesis of other organic compounds
16. substituent effects, inductive effects, and resonance effects in reactions
17. IUPAC Nomenclature

Lab Content:

(please number the outline of main topics and subtopics)

Students work independently in the laboratory completing experiments and manipulating equipment, while handling and observing the physical appearance, properties, chemical reactivity, and hazards of volatile organic compounds. Safety in the lab is a priority, and all students must pass a safety exam before they are released to perform wet lab experiments. As part of the safety exam, students must demonstrate the ability to work autonomously and productively in a chemistry lab setting; laboratory assignments require hands on manipulations, visual, and auditory abilities.

1. Safety
 - a. General Laboratory Safety
 - b. Personal Protective Equipment (State and Federal requirements)
 - c. SDS and Chemical Hygiene (Safety Data Sheets, Aldrich catalog, CRC, and Merck index)
 - d. Handling and Disposal of Hazardous Waste (State and Federal requirements)
 - e. Glassware and Sharps
 - f. Accident Safety
 - g. Safety Equipment
2. Laboratory Equipment
 - a. Standard Taper Glassware
 - b. Support Apparatus
 - c. Construct glassware (micro-burets, -pycnometer, -bells, stir bars, evacuated capillaries)
 - d. Electrical Equipment, not limited to: hot plates, melt temps, centrifuges, vortexes, ovens
 - e. Refractometers
 - f. Polarimeters
 - g. Analytical balances
 - h. Compressed Gas Cylinders
3. Instrumentation and Associated Software
 - a. GC (Gas Chromatography)
 - b. FT-IR (Fourier Transform Infrared Spectroscopy)
 - c. NMR (Nuclear Magnetic Resonance Spectroscopy)
 - d. UV-VIS (Ultraviolet-Visible Spectroscopy)
4. Techniques - Beginning
 - a. Determination of Physical Properties (evacuated & unevacuated mp, bp, density, etc.,)
 - b. Simple Distillation and Distillation using advanced techniques
 - c. Solvent Extraction
 - d. Sublimation
 - e. Crystallization
 - f. Chromatography (TLC and GC)
5. Single-step Synthesis, purification techniques and product analyses (E1 Elimination, Catalytic Hydrogenation, Benzoin, Cannizzaro Reaction)
 - a. Microscale
 - b. Semi-microscale
 - c. Macroscale
6. Molecular Modeling (recognition and identification of functional groups, hybridization, geometry, and IUPAC nomenclature)
7. Laboratory Notebook and Computational Data Files
 - a. Derivation of clear/concise experimental objectives
 - b. Retention, understanding and interpretation of mechanisms
 - c. Streamlining and organization of preparation and procedures

- d. Tabular formatting of chemical hazards, data, observations, and results
- e. Problem solving and troubleshooting
- f. Data analyses including calculations of theoretical and percent yields
- g. Critical evaluation/discussion of experimental conclusions in comparison to current literature
- h. Proper formatting of references according to American Chemical Society (ACS)
- i. Analyses of analytical spectral data in comparison to current literature

Methods of Instruction:

Methods of instruction may include, but are not limited to the following:

- **Method:** Lecture
Integration: Lecture will utilize whiteboard, power point, spectroscopy, molecular models, demonstrations, and multimedia in an interactive discussion-based, problem solving forum to prepare students for active participation in experimental procedures in the lab. Lecture material will be used to convey concepts of organic chemistry such as identifying and naming compounds, how to synthesize new compounds, and how to isolate and characterize molecules with various functional groups.
- **Method:** Multi-Media
Integration: Computer simulations and other multi-media will be used to demonstrate proper laboratory techniques such as how to perform attenuated total reflectance (ATR) FT-IR. Additionally simulation and multi-media resources will be utilized to observe virtual mechanisms during multi-step syntheses reactions.
- **Method:** Molecular Modeling
Integration: Laboratory model kits and molecular modeling software programs will be used to create three-dimensional representations of organic molecules and demonstrate how reactions occur.
- **Method:** Activity
Integration: Group assignments, projects, and homework will be used to evaluate, analyze, compare and contrast various mechanisms of syntheses, explain the chemical behavior of reactive species that drive a reaction forward, characterize physical, chemical, and analytical data/results, and develop intuitive understanding of spectroscopic data in real time.
- **Method:** Lab Activities
Integration: Laboratory experimentation will provide a hands on opportunity to unite lecture material with real-world chemistry at the microscale, semi-microscale, and macroscale levels using updated protocols and equipment in a controlled laboratory environment, and in the field to convey active learning. Students will (1) collect scientific data while performing lab experiments, (2) format and write lab reports using scientific methods including an organized presentation of data and results, and (3) demonstrate application of knowledge through post-laboratory analysis. All laboratory activities will focus on laboratory skills, experimental techniques, proper use of equipment, safe lab practices and chemical hygiene, waste disposal, and quality of data/results.

Methods of Evaluation:

A student's grade shall be determined by the instructor using multiple measures of performance related to the course objectives. Methods of evaluation may include but are not limited to the following:

- **Method:** Homework
Integration: Homework will be used to assess student familiarity of physical properties, chemical reactivity and synthesis of new compounds containing various functional groups, and to generate discussion.
- **Method:** Lab Practicums and Exams
Integration: Practicums and Exams are conducted to assess student knowledge of safe practices, policies, and chemical hygiene in addition to student learning and practical application of the course material. Students will evaluate experimental data, calculate and analyze results such as expected and unexpected percent yields and percent errors, troubleshoot problems, and propose alternative procedures, techniques, and/or equipment to describe and explain potential improvements.
- **Method:** Final Performance
Integration: The final exam will assesses the students' comprehensive understanding of the identification, physical properties, chemical reactivity, and synthesis, of organic compounds containing various functional groups in addition to structure/function relationships of biochemical molecules.

- **Method:** Group Projects

Integration: Student's work will be assessed in small groups of 3 or 4 as they undertake intellectually challenging syntheses reactions and utilize spectral data to acquire or identify products using brainstorming by leveraging multiple resources and engaging in collaborative efforts.

- **Method:** Written Laboratory Assignments

Integration: Pre-laboratory assignments and formal laboratory reports will be assessed to determine student engagement and performance in evaluation and interpretation of laboratory exercises in which distillation, extraction, synthesis, purification, and characterization of compounds will be conveyed in an organized format, including an objective, table of physical properties/hazards, chemical reaction, protocol, data/results, calculations, discussion and conclusions, references, and appendix written clear and concise with appropriate scientific language, and acknowledgment of literature values.

- **Method:** Exams/Tests

Integration: Lecture midterm exams will be utilized to monitor student progress throughout the course, and modify teaching practices to better serve student learning and engagement.

Examples of Assignments:

Students will be expected to understand and critique college level texts or the equivalent. Reading and writing, as well as out of class assignments are required. These assignments may include but are not limited to the following:

Given below are sample questions that may appear on homework, midterm exams, or on the final exam. Questions are given for each section of the course outline. (Taken from McMurray, Organic Chemistry, 8th. ed.)

1. Structure and Bonding.

1. Draw the Lewis structure of a vinyl chloride molecule.
2. Draw all the bonds in propene and indicate the hybridization of each carbon atom.
3. Give the ground state electron configuration of an aluminum atom.
4. Which of the following compounds have covalent bonds and which have ionic bonds? CH_4 , CH_2Cl_2 , LiI , KBr , MgCl_2 , Cl_2 .

2. Molecular Properties.

1. Make a three-dimensional drawing of dichloromethane and predict whether it has a dipole moment.
2. What is the pH of a 0.500 M aqueous solution of benzoic acid, $\text{pK}_a = 4.19$?
3. Show how acetaldehyde can act as a Lewis base.
4. Alcohols can act either as weak acids or as weak bases. Formulate the reactions of methyl alcohol with the strong acid, HCl , and with the strong base, NaNH_2 .

3. Reactions Overview.

1. Draw and name all monochloro products you might obtain from the reaction of 2-methylpentane with chlorine.
2. Which of the following species would you expect to behave as electrophiles, and which as nucleophiles? H^+ , OH^- , NH_3 , Mg^{2+} .
3. Calculate ΔH° for each step in the gas-phase radical substitution reaction of chlorine with methane.
4. Sketch a reaction energy diagram for a two-step reaction with an endothermic first step and an exothermic second step. Label all parts of the diagram corresponding to reactant, product, and intermediate.

4. Alkanes and Cyclic Hydrocarbons.

1. Draw structures of the five isomers of hexane and name each.
2. Make a graph of the potential energy versus the angle of bond rotation for propane, and assign values to the energy maxima.
3. Which is the more efficient fuel on a per-gram basis, cyclopropane or cyclohexane? Explain.
4. Using molecular models and structural drawings, explain why trans-decalin is rigid and cannot ring-flip, whereas cis-decalin can easily ring-flip.

5. Alkenes.

1. Draw the structure of 3,4-diisopropyl-2,5-dimethyl-3-hexene.
2. Predict the product of the reaction of cyclohexene with hydrochloric acid.
3. Propose a mechanism to account for the formation of 1-bromo-1-ethylcyclohexane on reaction of

vinylcyclohexane with HBr.

4. A compound of formula $C_{10}H_{14}$ undergoes catalytic hydrogenation but absorbs only 2 equivalents of hydrogen. How many rings does the compound have?
5. What product(s) would you expect from the reaction of cyclopentene with NBS and water? Show the stereochemistry.
6. Simmons-Smith reaction of cyclohexene with diiodomethane gives a single cyclopropane product, but reaction with 1,1-diiodoethane gives a mixture of two isomeric methylcyclopropane products. What are the two products, and how do they differ?

6. Alkynes.

1. There are seven isomeric alkynes with the formula C_6H_{10} . Draw them, and name them according to IUPAC rules.
2. What product would you obtain by hydration of 2-methyl-4-octyne?
3. How would you prepare cis-2-butene starting with 1-propyne, an alkyl halide, and any other reagents needed?
4. Beginning with acetylene and any alkyl halides needed, how would you synthesize 2,2-dimethylhexane?
5. Hydrocarbon A has the formula $C_{12}H_8$. It absorbs 3 equiv of hydrogen on catalytic reduction over a palladium catalyst to give B (C_9H_{18}). On ozonolysis, only two products are formed: oxalic acid and succinic acid. Formulate these reactions and propose structures for A and B.

7. Stereochemistry.

1. Alanine, an amino acid found in proteins, is chiral. Draw the two enantiomers of alanine using the standard convention of wedged, solid, and dashed lines.
2. Chloramphenicol, a powerful antibiotic isolated in 1949 from the *Streptomyces venezuelae* bacterium, is active against a broad spectrum of bacterial infections and is particularly valuable against typhoid fever. Assign R,S configurations to the stereogenic centers in chloramphenicol.
3. What kind of isomers are there in the pair (S)-5-chloro-2-hexene and chlorocyclohexane?
4. What is the stereochemistry of the product that results from addition of Br_2 to cyclohexene? Is the product optically active? Explain.
5. Draw a compound that fits the following description: a chiral carboxylic acid with the formula $C_5H_{10}O_2$.

8. Alkyl Halides.

1. Taking the known relative reactivities of 1 $^\circ$, 2 $^\circ$, and 3 $^\circ$ hydrogen atoms into account, what product(s) would you expect to obtain from monochlorination of 2-methyl-butane? What would the approximate percentage of each product be?
2. How would you prepare 2-chloro-2-methylpropane from the appropriate alcohol?
3. Organic solvents such as benzene, ether, and chloroform are neither protic nor strongly polar. What effect would you expect these solvents to have on SN_2 reactions?
4. How can you account for the fact that 3-bromo-1-butene and 1-bromo-2-butene undergo SN_1 reaction at nearly the same rate even though one is a secondary halide and the other is primary?

9. IR Spectroscopy.

1. Calculate the energy of a gamma ray with wavelength 5.0×10^{-9} cm.
2. How might you use IR spectroscopy to distinguish between CH_3CH_2OH and CH_3OCH_3 ?
3. Carvone is an unsaturated ketone responsible for the odor of spearmint. It has an intense infrared absorption at 1690 cm^{-1} . What kind of ketone does carvone contain?
4. Propose a structure for a compound that meets the following description: A non-optically active compound C_5H_9N with an IR absorption at 2215 cm^{-1} .

10. NMR Spectroscopy.

1. 2-chloropropene shows signals for three kinds of protons in its 1H NMR spectrum. Explain.
2. Methyl 2,2-dimethylpropanoate has two peaks in its 1H NMR spectrum. What are their approximate chemical shifts?
3. Draw the structure for a compound with the following splitting pattern: C_3H_7Cl , with one doublet and one septet.
4. Propose a structure for a compound that fits the following description: a hydrocarbon with seven lines in its ^{13}C NMR spectrum.

11. UV Spectroscopy and Conjugated Systems.

1. If pure vitamin A has a wavelength of maximum absorption at 325 nm (= 50,100) in a cell with a path length of 1.00 cm, what is the vitamin A concentration in a sample whose absorbance at 325 nm is $A = 0.735$?
2. The π -molecular orbital diagram for an allylic radical is similar to that for an allylic carbocation. Which orbitals do the three π -electrons occupy?
3. Draw a segment of the polymer that might be prepared from 2-phenyl- 1,3-butadiene.
4. Dimethyl butynedioate undergoes a Diels-Alder reaction with (2E,4E)- hexadiene. Show the structure and stereochemistry of the product.

12. Benzene and Aromatic Compounds.

1. Draw the structure of p-bromochlorobenzene.
2. Pyridine is a flat, hexagonal molecule with bond angles of 120° . It undergoes electrophilic substitution rather than addition and generally behaves like benzene. Draw an orbital picture of pyridine to explain its properties.
3. Bromination of toluene gives a mixture of three bromotoluene products. Draw and name them.
4. What is the major monosubstitution product from the Friedel-Crafts reaction of benzene with 1-chloro-2-methylpropane in the presence of $AlCl_3$?
5. Write resonance structures for phenol to show the electron-donating resonance effect of the hydroxyl group.
6. Propose a synthesis of 4-chloro-1-nitro-2-propylbenzene from benzene.

SAMPLE LABORATORY ASSIGNMENT.

An example laboratory exercise is given (exerpted from Mayo, Pike, and Trumper, Microscale Organic Laboratory, 6th. ed., John Wiley and Sons, 2013, pp 153-163).

Introduction.

Read the general discussion on IR and NMR spectrographic techniques given in the laboratory text. Plan ahead so that you know how to operate all of the analytical equipment used in the experiment (IR, GC, etc.). Also, read the discussion section and make sure you understand the reactions and related chemistry for the experiment.

Experimental Procedure.

Part A: Cyclohexanol (Estimated time for the experiment is 1.5 hours)

1. In a tared 5.0-mL conical vial equipped with an air condenser, place 100 μ L of cyclohexanone followed by 250 μ L of methanol. Shake to obtain a homogeneous solution. Add 300 μ L of sodium borohydride reducing solution dropwise, with swirling in the hood. Let stand at room temperature for 15 minutes.
2. Isolate the product as follows. Using a calibrated Pasteur pipet, add 1.0-mL of cold, dilute hydrochloric acid dropwise. Extract the aqueous mixture with three 0.5-mL portions of methylene chloride. Separate the layers, and remove the methylene chloride layer. Transfer the organic phase to a Pasteur filter pipet containing 500 mg of anhydrous sodium sulfate.
3. Weigh the product and calculate the percent yield. Determine the refractive index and boiling point of the cyclohexanol product.
4. Obtain the IR spectrum of your sample using the capillary film sampling technique. Interpret the results. Compare the IR spectra of the reactant and product.
5. Purify the reaction product by preparative gas chromatography.
6. Perform the ceric nitrate test and 2,4-dinitrophenylhydrazine test on both the starting ketone and the alcohol product.

Part B: Cis-and trans-4-tert-butylcyclohexanol (Estimated time is 2.0 hours for the experiment and 15 minutes for the GC analysis)

1. In a tared 3.0-mL conical vial equipped with an air condenser, place 50 mg of 4-t-butylcyclohexanone followed by 50 μ L of methanol. Shake to obtain a homogeneous solution. Add 100 μ L of sodium borohydride reducing solution dropwise, with swirling. Let stand at room temperature for 10 minutes.
2. Isolate the product as follows. Using a calibrated Pasteur pipet, add 1.0-mL of cold, dilute hydrochloric acid dropwise. Extract the aqueous mixture with three 0.5-mL portions of methylene chloride. Separate the layers, and remove the methylene chloride layer by allowing a gentle stream of nitrogen gas to impinge on the surface of the vial while it is warmed in a sand bath in the hood. Transfer the organic phase to a Pasteur filter pipet containing 250 mg of anhydrous sodium sulfate.

3. Weigh the solid product and calculate the percent yield. Determine the melting point of the product.
4. Obtain the IR spectrum of your sample using the capillary film melt technique and interpret the results. Also, obtain the NMR spectrum of your sample.
5. Separate the cis and trans isomers using gas chromatography. Determine the percentage of each isomer by determining the area under the curve.

Answer the questions assigned. Sample questions are given.

1. Suggest a chemical test that would allow you to distinguish between t-butyl alcohol and 1-butanol, both of which give a positive ceric nitrate test.
2. The reduction of 4-t-butylcyclohexanone is a stereoselective reaction. Which isomer predominates? Assuming that NMR data are not available, is it still possible to arrive at a rough estimate of the product ratio? How would you go about making this measurement? Suggest a value.
3. Sketch the NMR spectrum you would expect to observe for the following compounds. (a) acetone, (b) 1,1,2-tribromoethane, (c) ethyl chloride, (d) 2-iodopropane, (e) 1-bromo-4-methoxybenzene.

LABORATORY REPORT REQUIREMENTS:

1. *Prelab*. This portion of the lab report includes your name, date, course number (.25 points), the complete title of the experiment (exactly as it appears in the manual) 0.25 points, and the Objective (3 points). Also included is a table of chemicals and reagents with the appropriate physical and chemical properties for each substance. Table headers should be: MW, MP, BP, Density, refractive index, amount, hazards, and the table should have a number and title (Table 1: Physical and Chemical Properties of Reagents) 2 points. Table 1 is followed by Chemical Reactions (using structures not chemical formulas); if there are no reactions, this section will contain Structures (1 point). The experimental Procedure (2 points) is given in outline form, numbered, or with bullets. Each separate technique has a subheading. The prelab is periodically checked by the professor before any actual work is performed in the laboratory and is required before you begin an experiment!
2. Data and Results section (3 points) is completed during the lab and includes the date and time that the results were obtained. Include all data, observations, measurements, and results in tabular format labeled: Table #: Title (.25 points). Analytical results, such as spectral data/results should be attached at the end of the report, and labeled: Figure #: Title (.25 points). You may also be asked to turn in your product, TLC, or other materials with your lab report.
3. Calculations This section should directly follow the Data and Results section. ALL calculations for ALL trials should be in this section, neatly organized with subheadings in the same chronological order as the experiment is performed with proper significant figures (2-3 points).
4. Discussion and Conclusions This section should include a summary of the data and results of the experiment, including all experimental data (give the average if multiple trials were conducted), calculated yield, % errors, comparison to literature values (give the literature values), physical data/results, chemicals tests results, graphical values, and any other necessary information required to summarize the data and results as they apply to the 'Objectives' of this lab. This section, like all other sections should be in chronological order. Lastly, point out any problems that may have affected your overall experiment and how the experiment could be improved. Such improvements should describe peer reviewed methods and/or sophisticated instrumentation from literature sources that you have researched. Stating that you will clean glassware, make less mistakes, or be more careful next time is not acceptable (4 points).
5. References: Give a list of references in ACS formatted style (2 points). Answer any questions that may be assigned as a part of the lab.

Textbooks:

- Vollhardt, P., Schore, N (2018). *Organic Chemistry: Structure and Function*, 8th W. H. Freeman. ISBN: 978-1319176976
- Mayo, Pike, and Forbes (2013). *Microscale Organic Laboratory*, 6th ed. John Wiley and Sons. ISBN: 978-0-471-21502-8

Other Resources:

Minimum Qualification

- Chemistry (Masters Required)