

SYLLABUS

TITLE:	Organic Chemistry II
CODE:	QUI 302
PREREQUISITE:	QUI 301
CREDITS:	4 credits 45 contact hours 45 hours of laboratory 1 term

DESCRIPTION

Study of molecular orbitals and aromatic systems. Aromatic electrophilic substitution mechanisms, nucleophilic carbonyl addition, acyl nucleophilic substitution, and enolate-related condensations are studied. The IUPAC nomenclature of benzene derivatives, aldehydes, ketones, carboxylic acids and their derivatives, and amines is discussed. An introduction to the chemistry of carbohydrates, lipids, amino acids, and nucleic acids is presented at the end. Ultraviolet-visible, infrared, ^{13}C nuclear magnetic resonance, and mass spectrometry are discussed. The elucidation of structures of organic compounds is emphasized by integrating all these techniques. This course is aimed at students with a concentration in chemistry, biology, biotechnology, and allied health sciences, who are trained to understand the biological and industrial processes of the world around us. The course requires independent use of the Science Media Lab.

JUSTIFICATION

Medicines, textiles, plastics, fuels, food and biological processes occur in the daily life of human beings. In these processes organic chemistry is present. Therefore, it is important that a student who is training as a scientist has knowledge about how organic chemistry works. The purpose of the course is to train students to understand organic chemistry and thus have a basis to understand the processes that occur in biological systems or in the environment. This branch of chemistry permeates everything that happens in our daily lives.

COMPETENCES

The course develops in the student the following competencies:

- **Critical Thinking**

- **Entrepreneurship and innovation**
- **Research and exploration**
- **Communication**
- **Ethical sense and social justice**

OBJECTIVES

At the end of the course the student will be able to:

1. Define an aromatic system and be able to determine if a molecule is aromatic, anti aromatic or non-aromatic.
2. Indicate the different electronic transitions that a molecule can carry out in the ultraviolet-visible region and calculate, using the Woodward-Fieser rules, the maximum wavelength expected to be observed in a molecule.
3. Given the infrared spectrum of a compound and its molecular formula, it is possible to assign absorption bands of the different functional groups that the molecule has to elucidate its structure.
4. Describe what a mass spectrometric experiment consists of and the usefulness of this technique to elucidate structures of organic compounds.
5. Explain the basic principles of ^1H and ^{13}C nuclear magnetic resonance and its usefulness in the elucidation of organic structures.
6. Elucidate the structure of an organic compound given its ^1H and ^{13}C nuclear magnetic resonance spectrum, infrared, mass and ultraviolet-visible.
7. Explain the mechanism of electrophilic aromatic substitution in benzene and the different monosubstitution products that are obtained in different reactions of this type.
8. Differentiate the different groups that orient ortho, meta and para in benzene when carrying out electrophilic aromatic substitution.
9. Design synthetic routes based on electrophilic aromatic substitution reactions and other reactions such as syntheses based on the diazonium salt.
10. Name aldehydes and ketones using IUPAC rules.
11. Explain the mechanism of nucleophilic addition to carbonyl and the electronic and structural factors that affect the reactivity of aldehydes and ketones under this mechanism.
12. Explain keto-enol tautomerism and predict the predominant form.

13. Carry out organic syntheses using the nucleophilic carbonyl addition mechanism and explain how the carbonyl group can be protected during a synthesis if necessary.
14. Describe by means of mechanisms the aldol condensations, crossed aldol, conjugated nucleophilic addition and differentiate them from the nucleophilic addition to carbonyl.
15. Write the IUPAC name of carboxylic acids and their derivatives such as acyl chlorides, esters, primary, secondary, and tertiary amides, carboxylic anhydrides, and nitriles.
16. Explain the acyl nucleophilic substitution mechanism, the factors that favor it, and synthesize derivatives of carboxylic acids from acyl chlorides and carboxylic anhydrides using this mechanism.
17. Write the IUPAC name of primary, secondary, and tertiary amines. Describe the different ways of synthesizing amines.
18. Explain the basicity of amines, the structural factors that affect it, and the reactions they carry out.
19. Draw and name the structures of a monosaccharide and those of the D-aldose and D-ketoses family and explain the different monosaccharide reactions.
20. Differentiate between a monosaccharide, a polysaccharide, a steroid, an amino acid and a lipid and their properties.
21. Describe the structure of polynucleotides associated with DNA and RNA.

CONTENT

- I. Aromaticity
 - A. Resonance
 - B. Molecular orbital theory
 1. Fundamentals
 - a. Binding, anti-bonding and non-bonding orbitals
 - b. Nodes
 - c. HOMO and LUMO
 2. Molecular orbitals pi
 3. Allyl system
 4. 1,3-butadiene system
 - C. Case of the benzene molecule
 1. Molecular orbitals pi

- 2. Degenerate orbitals
 - D. Structure of benzene
 - E. Properties of an aromatic system
 - 1. Delocalization of pi electrons
 - 2. Planar cyclic structure
 - 3. $4n + 2$ pi electrons
 - 4. Energy diagram of pi molecular orbitals
 - F. Properties of an antiaromatic system
 - 1. Electron delocalization
 - 2. Planar cyclic structure
 - 3. $4n$ pi electrons
 - 4. Energy diagram of molecular orbitals
 - G. Ultraviolet-visible spectroscopy (UV-VIS)
 - 1. Electronic transitions
 - 2. Instrumentation
 - 3. Transmittance and absorbance
 - 4. Absorption spectrum and λ MAX
 - 5. Effect of solvent on λ MAX
 - 6. Woodward-Fieser Rules
 - a. polyenes
 - b. ketones and conjugated aldehydes
 - c. benzene derivatives
- II. Infrared spectroscopy
- A. Vibrational modes
 - 1. Symmetrical and asymmetric lengthening
 - 2. Bends
 - a. Rocking chair
 - b. Scissors
 - c. Turn
 - d. Wag
 - B. Oscillator
 - 1. Spring force constant
 - 2. Wave number
 - C. Infrared spectrum
 - 1. Useful region
 - 2. Wide bands
 - 3. Acute bands
 - D. Functional groups and wave number
 - 1. Alkanes

2. Alkenes
 3. Alkynes
 4. Alcohols
 5. Ketones
 6. Aldehydes
 7. Carboxylic acids and their derivatives
 8. Nitriles
 9. Amines
 10. Benzene derivatives
- E. Variations in the frequency of carbonyl absorption
1. Resonance effect
 2. Inductive effect
 3. Angular stress
 4. Hydrogen bridges
- F. Examples
- III. Mass spectrometry
- A. Instrumentation
1. Ionization chamber
 2. Mass separator
 3. Mass spectrum
 - a. Mass to load ratio, m/z
 - b. Relative abundance
 - c. Molecular ion
 - d. Base peak
- B. Patterns of fragmentation
1. Alkanes
 2. Alkenes
 3. Alkynes
 4. Alcohols
 5. Ethers
 6. Aromatics
- C. McLafferty rearrangement
1. Aldehydes
 2. Ketones
 3. Carboxylic acids
 4. Esters
 5. Amides
 6. Anhydrous
- D. Halogenated compounds

1. Isotopic patterns of chlorinated compounds
 2. Isotopic patterns of brominated compounds
- E. Examples of mass spectra

IV. Introduction to ^1H and ^{13}C Nuclear Magnetic Resonance

- A. Establishment rate
1. Meaning
 2. Formula to calculate it
- B. Nuclear spin
- C. Magnetic field
- D. NMR process
- E. Hydrogen shielding
- F. Chemical shift
- G. Proton equivalence
1. Homotopic hydrogens
 2. Enantiotopic hydrogens
 3. Diastereotopic hydrogens
- H. Spin-spin coupling
1. Types of signals
 - a. Singlet
 - b. Doublet
 - c. Triplet
 - d. Quartet
 - e. Multiplete
 2. Coupling constant
- I. Kinetics of a process and NMR.
- J. Structure elucidation
- K. Magnetic anisotropy
1. Carbonyl
 2. Alkenes
 3. Alkynes
 4. Aromatics
- L. Doubling patterns that do not follow the $N + 1$ rule
- M. ^{13}C MRI
1. Principles
 2. ^{13}C nuclear spin
 3. Characteristic chemical shifts
 4. ^{13}C NMR spectrum
 5. Examples

6. Elucidation of structures of organic compounds using UV, IR, NMR and MS
- V. Aromatic electrophilic substitution
- A. General mechanism
 1. Formation of the arenium ion
 2. Stabilization of the arenium ion
 3. Recovery of aromaticity
 - B. Monosubstitution reactions
 1. Halogenation
 2. Nitration
 3. Sulfonation
 4. Friedels-Craft alkylation
 5. Friedels-Craft acylation
 - C. Ortho and Para counselors
 - D. D Target coaches
 - E. Resonance and inductive effect on orientation in the product.
 - F. Reactions of benzene derivatives with R groups and asylum
 1. Oxidations
 2. Reductions
 - G. Reactions using the diazonium salt
 1. Conditions
 2. Synthetic routes from the diazonium salt
- VI. Aldehydes and ketones
- A. Physical properties of aldehydes and ketones
 - B. Keto-enol tautomerism
 - C. Preparation of aldehydes and ketones
 1. Oxidation of primary alcohols
 2. Adding water to alkynes
 3. Oxidation of primary and secondary alcohols
 - D. Reactions of aldehydes and ketones
 1. Mechanism of nucleophilic addition to carbonyl
 - a. Reactivity via steric effect
 - b. Reactivity via inductive effect
 2. Addition of HCN: formation of cyanohydrins
 3. Addition of alcohols in an acid medium: formation of ketals and acetals
 4. Addition of phosphorane: Wittig's reaction
 5. Addition of 1,2-ethanediol: protection of carbonyl groups in synthesis

6. Addition of hydroxylamine, hydrazine, phenylhydrazine and phenyl semicarbazone
- E. Qualitative tests for aldehydes and ketones
 1. Tollens test
 2. Iodoform test
- VII. Condensations using enolates
 - A. Aldol condensation
 1. Mechanism
 2. Formation of the α , β unsaturated system
 3. Synthetic routes from the aldol product and the α , β unsaturated system.
 - a. Reduction with NaBH_4 and LiAlH_4
 - b. Reduction with H_2 in Pd-C and Ni
 4. Nomenclature of hydroxyaldehydes, hydroxyketones and diketones
 - B. Cross aldol condensation
 - C. Practical cross aldol condensation
 - D. Claisen-Schmidt condensation
 - E. Cyclizations
 - F. Nucleophilic addition to the β carbon of an α , β unsaturated system
 1. Adding Michael
 2. Robinson's nullification
 - G. Aldol condensation in acid medium
 - H. Synthesis Using β -dicarbonyls
- VIII. Carboxylic acids and their derivatives
 - A. Physical properties of carboxylic acids
 - B. IUPAC Nomenclature of Carboxylic Acids
 - C. Preparation of carboxylic acids
 1. Oxidation of alcohols, alkylbenzenes and aldehydes.
 2. Grignard reaction with CO_2
 3. Acid hydrolysis of nitriles.
 4. Purification of carboxylic acids
 - D. Carboxylic acid reactions
 1. Preparation of acyl chlorides from carboxylic acids
 2. Decarboxylation
 3. Dehydration of carboxylic diacids
 4. Formation of acyl chlorides from SOCl_2 , PCl_3 and PCl_5
 - E. Preparation of carboxylic acid derivatives
 1. Structure of carboxylic acid derivatives
 - a. Acyl chlorides

- b. Acid anhydrous
- c. Nitriles
- d. Esters
- e. Amides
 - 1) Primary
 - 2) Secondary
 - 3) Tertiary
- 2. Mechanism of acyl nucleophilic substitution
- 3. Order of reactivity of the different derivatives
- 4. Preparation of carboxylic acid derivatives from acyl chlorides
- 5. Preparation of carboxylic acid derivatives from acid anhydrous
- 6. Hydrolysis of esters and amides in acidic and basic medium
- 7. Preparation and hydrolysis of nitriles

IX. Amines

- A. Physical properties
- B. Basicity of amines
 - 1. Basic strength
 - 2. Amines vs. amides
- C. Nomenclature of amines
- D. Preparation of amines
 - 1. SN2 nucleophilic substitution
 - 2. Reaction of alkyl halides with azide followed by reduction
 - 3. Reduction of nitro compounds
 - 4. Gabriel's Synthesis
 - 5. Substitution with NH₃ derivatives and reduction
 - 6. Reduction of nitriles and amides
 - 7. Reduction of oximes
 - 8. Hoffman rearrangement
- E. Purification of amines
- F. Reactions of amines
 - 1. Oxidation with H₂O₂
 - 2. Cope Elimination
 - 3. Hoffman Elimination

X. Carbohydrates

- A. Classification of carbohydrates
 - 1. Monosaccharides
 - 2. Polysaccharides
- B. Classification of monosaccharides

1. Ketose
 2. Aldosas
 - C. D and L configuration of sugars
 - D. Family of D-aldoses and D-ketoses
 - E. Cyclic structures of monosaccharides
 1. Glucose case
 2. Case of fructose
 3. Pyranous and furanose
 - F. Anomers in monosaccharides
 1. α anomer and β anomer
 2. Mutarrotation
 - G. Monosaccharide reactions
 1. Epimerization
 2. Reductions: alditols
 3. Oxidations
 - a. Bromine water
 - b. Nitric acid
 - c. Reactions with HIO₄
 4. Ruff degradation
 5. Kiliani-Fisher synthesis
- XI. Introduction to lipids, amino acids and nucleotides
- A. Lipids
 1. Waxes
 2. Fatty acids
 3. Triglycerides
 4. Steroids
 5. Prostaglandins
 6. Terpenes
 - B. Amino acids
 1. Structure of an amino acid
 2. Stereochemistry
 3. Zwitterionic form.
 4. Peptide bond and structure of a polypeptide
 - C. Nucleic Acids
 1. Nucleotides and ribonucleotides
 2. Nucleosides and ribonucleotides
 3. Nitrogen bases
 4. Phosphate groups
 5. Polynucleotides

LABORATORY EXPERIENCES

- A. Synthesis of Cyclohexanol
- B. Esterification fisher
- C. Aromatic Substitution
- D. Aspirin Synthesis
- E. Double Link Reduction
- F. Synthesis of Sulfenilamide
- G. Saponification
- H. Reaction of carbonyl groups
- I. Carboxylic acids and their derivatives

METHODOLOGY

The following strategies of the active learning methodology are recommended:

- Written research proposal
- Laboratory
- Solution of a problem posed
- Web-supported education
- Bibliographic research
- Simulations
- Problem-based learning
- Web-supported learning
- Bibliographic research
- Conceptual maps
- Use of Web resources and tools: Blog
- Conference
- Flipped classroom
- Phenomenon-based learning: observation, discussion and analysis of processes, problems or phenomena
- Collaborative learning and teamwork
- Independent use of Media Lab
- Procedure-oriented coaching and problem solving
- Demonstration and practical exercises
- Self-assessment and peer assessment
- Application of theories, ...
- Graphs and functions

EVALUATION

Participation	15%
Partial Assignment	30%
Compositions	10%
Project or final exam	20%
Immersive Experience	<u>25%</u>
Total	100%

LEARNING ASSESSMENT

The institutional assessment rubric is applied to the core activity of the course.

BIBLIOGRAPHY

TEXT

Wade, L.G., Jr. & J. W. Simek (2016). *Organic Chemistry* (9na ed). Pearson.

LABORATORY MANUAL

Gilbert, J. (2015). *Experimental Organic Chemistry: A Miniscale & Microscale Approach*.
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Solomon, T.W., C. B. Fryhle & S. A. Snyder (2013). *Organic Chemistry* (11va ed.). John
Wiley & Sons, Inc.

Carey, F. A. & R. Giuliano (2016) *Organic Chemistry*, (10ma ed.), McGraw Hill.

ELECTRONIC REFERENCES

<http://chemistry.about.com>

<http://academicinfo.net/chemorganic.html>

<http://www.iupac.org>

<http://www.webspectra.chem.ucla.edu/>

Find more information resources related to the course topics on the library page
<http://biblioteca.sagrado.edu/>

REASONABLE ACCOMMODATION

To obtain detailed information on the process and the required documentation, you must visit the corresponding office. To guarantee equal conditions, in compliance with the ADA (1990) and the Rehabilitation Act (1973), as amended, all students who need reasonable accommodation services or special assistance must complete the process established by the Vice Presidency for Academic Affairs.

ACADEMIC HONESTY, FRAUD AND PLAGIARISM

Any student who misses the policy of honesty, fraud and plagiarism is exposed to the following sanctions: he will receive a zero mark in the evaluation and / or repetition of the work in the seminar, a note of F (*) in the seminar: suspension or expulsion as established in the Academic Honesty Policy document (DAEE 205-001) effective August 2005.

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