SAGRADO
Universidad del Sagrado Corazón

SYLLABUS

TITLE: Organic Chemistry I

CODE: QUI 301

PREREQUISITE: QUI 102

CREDITS: 4 credits | 45 contact hours | 45 hours of laboratory | 1 term

DESCRIPTION

Study of the atomic and molecular structure of organic compounds. The course covers aspects related to the concept of isomerism, including stereoisomerism. The parameters that affect organic reactions are discussed. Substitution and elimination reactions related to alkyl halides and addition reactions related to alkenes and alkynes are studied.

The physical and chemical properties of alkanes, alkenes, alkynes, alkyl halides, alcohols, and ethers are discussed. Nomenclature, molecular structure, synthesis, and reactions of the compounds belonging to these families are emphasized.

An introduction to spectroscopic techniques as tools to elucidate structures of organic compounds is presented. The nuclear magnetic resonance technique is emphasized in the first part.

This course is aimed at students with a concentration in chemistry, biology, and allied health sciences, who are trained to understand the biological and industrial processes of the world around us. The student makes independent use of the Science Media Lab and Web tools.

JUSTIFICATION

Medicines, textiles, plastics, fuels, food, and biological processes occur in the daily life of human beings. These are examples of the importance of a student training in the natural sciences having knowledge of organic chemistry. 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.

COMPETENCES

The course develops in the student the following competencies:

- **Critical Thinking**
- **Research and exploration**
- **Communication**
- **Ethical sense and social justice**

OBJECTIVES

At the end of the course, students will be trained to:

1. Understand the atomic structure of the fundamental elements found in organic compounds and draw the Lewis structure of a compound emphasizing its geometric structure and the possible resonance structures that they may have.
2. Describe the intermolecular forces that occur in organic compounds alone or mixed with other compounds.
3. Define and give examples of the following types of isomers: conformers, enantiomers, connecting isomers, and diastereomers.
4. Name compounds that belong to the families of alkanes, cycloalkanes, alkenes, alkynes, alkyl halides, alcohols and ethers given the structure of the compound or draw the structure given the name.
5. Distinguish the enantiomers that are associated with a chiral compound as well as diastereomers and meso compounds that may be in a compound.
6. Explain the difference between kinetics and thermodynamics of an organic reaction, substitution, elimination, addition, and rearrangement reactions.
7. Explain the mechanisms of bimolecular (SN2) and unimolecular (SN1) nucleophilic substitution, unimolecular (E1) and bimolecular (E2) elimination and the factors that affect the reactions in which they appear.
8. Explain the reactions carried out by alkenes, alkynes, alcohols, ethers, and epoxides.
9. Propose a reasonable synthesis to obtain alkenes, polyenes, alkynes, alcohols, ethers, and epoxides.
10. Write a research proposal that solves a problem related to organic chemistry.

CONTENT

I. Introduction

A. Atomic structure
   1. Atomic orbitals
   2. Electronic configurations

B. Covalent bond
   1. Formation of the covalent bond
   2. Lewis structures
   3. Bond length
   4. Bond angle
   5. Resonance
   6. Molecular geometry
      a. Linear
      b. Angular
      c. Trigonal flat
      d. Tetrahedral
      e. Trigonal pyramidal
   7. Dipole moment and molecular structure

C. Intermolecular forces
   1. London
   2. Dipole-dipole
   3. Ion-dipole
   4. H bridge

D. Functional groups of families of organic compounds
   1. Alkanes
   2. Alkenes
   3. Alkynes
   4. Cycloalkanes
   5. Alkyl halides
      a. Primary
      b. Secondary
      c. Tertiary
   6. Alcohols
      a. Primary
      b. Secondary
      c. Tertiary
   7. Ethers
   8. Aromatics
   9. Aldehydes

10. Ketones
11. Carboxylic acids
12. Amines
    a. Primary
    b. Secondary
    c. Tertiary
13. Amides
    a. Primary
    b. Secondary
    c. Tertiary
14. Esters
15. Carboxylic anhydrides
16. Acyl chlorides
17. Nitriles

II. Alkanes and cycloalkanes

A. Properties
B. Structure
    1. Condensed formula
    2. Line formula
C. Nomenclature
    1. Alkanes and alkyl groups
    2. Cycloalkanes
    3. Bicyclic
D. Newman Conformations and Projections
    1. Ethane
        a. Staggered
        b. Eclipsed
    2. Butane
        a. Anti
        b. Gauche
        c. Eclipsed
E. Angular stress and conformations in cycloalkanes
    1. Cyclopropane
    2. Cyclobutane
    3. Cyclopentane
    4. Cyclohexane
        a. Chair conformation
        b. Boat conformation
        c. Axial and equatorial positions

F. Synthesis of alkanes
    1. Reduction of alkyl halides
    2. Synthesis Corey-Posner, Whitesides-House

III. Isomers and stereoisomers

A. Definition of the different types of isomers
    1. Constitutional isomers
    2. Geometric isomers
        a. Cis isomer
        b. Trans isomer
    3. Stereoisomers
        a. Enantiomers
        b. Diastereomers
        c. Meso compounds
B. Optical activity
    1. Polarimeter
    2. Specific rotation
    3. Racemic mixture
C. R-S assignment to chiral carbon
    1. Assignment of priorities
    2. Compounds with a single chiral carbon
    3. Compounds with two chiral carbons
D. Fisher projection
    1. Compounds with a single chiral carbon
    2. Compounds with two chiral carbons
        a. Enantiomers
        b. Diastereomers
        c. Meso compounds

IV. Organic reactions

A. Kinetics of a reaction
    1. Law of speed
    2. Speed constant
        a. Collisions
        b. Orientation during collision
        c. Activation energy
        d. Temperature
        e. Arrhenius equation
    3. Mechanism of a reaction
        a. SN2

b. SN1
4. Energy contour diagram
a. Transition state
b. Intermediary
c. Hammond postulate

B. Thermodynamics of a reaction
1. State of equilibrium
2. ΔH, ΔS, ΔG of a reaction
3. Exoenergetic and endoenergetic reaction

C. Acids and bases
1. Bronstead-Lowry definition
2. Lewis definition
3. Acid-base strength
a. Resonance effect
b. Inductive effect
c. Steric effect
d. Hybridization effect

D. Classification of reactions
1. Substitution
2. Addition
3. Elimination
4. Rearrangement
5. Oxi Reduction

V. Substitution Reactions and Alkyl Halides

A. Properties
B. Nomenclature
C. Bimolecular nucleophilic substitution (SN2)
1. Substrate
2. Reagent
3. Law of speed
4. Factors that affect an SN2 reaction
a. Substrate type
b. Solvent
1) Protic solvent
2) Polar aprotic solvent
c. Nucleophile
d. Outgoing group
5. Stereochemistry of the SN2 reaction
6. Synthetic use of SN2

D. Unimolecular nucleophilic substitution (SN1)
    1. Mechanism of the reaction and its law of speed
    2. Factors affecting the SN1 reaction
        a. Substrate type
            1) Structure of the carbocation
            2) Carbocation stability
        b. Solvent
        c. Nucleophile
        d. Outgoing group
    3. Stereochemistry of the SN1 reaction
        a. Racemic mixture
        b. Investment vs retention

VI. Alkenes and alkynes

A. Physical properties
B. Nomenclature
    1. Z isomer
    2. E isomer
    3. Cycloalkenes
C. Stability of alkenes
D. Stereochemistry of cycloalkenes
E. Synthesis of alkenes: E2 mechanism
    1. Speed law
    2. Factors that favor the E2 mechanism
    3. Stereochemistry
    4. Zaitsev's rule
F. Synthesis of alkenes: E1 mechanism
    1. Law of speed
    2. Factors that favor it
    3. Stereochemistry
G. SN2 vs E2 and SN1 vs E1
H. Synthesis of Alkenes: Dehydration of Alcohols
    1. Mechanism
    2. Migration of carbocations
I. Reactions of alkenes
    1. Mechanism of electrophilic addition
        a. Electrophile
        b. Electrophile vs nucleophile
    2. Markovnikov's rule
    3. Regioselective reaction

4. Stereochemistry of the mechanism of addition
5. Electrophilic addition reactions
    a. Adding H_2SO_4
    b. Adding H_2O / H +
    c. Adding halogens
        1) Stereochemistry
    d. Halogenation in water
6. Regioselective vs stereospecific reaction
7. Alkene oxidations
    a. Syn hydroxylation
    b. Ozonolysis
    c. Other oxidations

J. Nomenclature of alkynes
K. Physical properties of alkynes
L. Acidity of alkynes
M. Synthesis of alkynes
    1. Synthesis from alkenes
    2. Synthesis via $NaNH_2$ combined with SN2 reaction
N. Reactions of alkynes
    1. Adding halogens
    2. Adding HX
    3. Alkyne oxidations
    4. Hydrogenation of alkynes
        a. Syn addition
        b. Anti addition

VII. Conjugated systems

A. Classification of dienes and polyenes
    1. Conjugates
    2. Accumulated
    3. Isolated
B. Preparation of dienes
C. 1.2 and 1.4 addition of electrophiles to dienes
D. Kinetic and thermodynamic control
E. Diels-Alder reaction
    1. Conformation of the diene
        a. S-cis conformation
        b. S-trans conformation
    2. Electron donor and electron attractor groups
    3. Stereochemistry

4. Mechanism

VIII. Alcohols and ethers

A. Physical properties of alcohols and ethers
B. Nomenclature of alcohols
   1. Common nomenclature
   2. IUPAC Nomenclature
C. Synthesis of alcohols
   1. Hydration of alkenes
   2. Oxymercuration-demercuration
   3. Hydroboration-oxidation
   4. Grignard reagent
   5. Reduction of aldehydes and ketones
D. Reactions of alcohols
   1. Reactivity of the OH group
   2. Acidity of alcohols
   3. Conversion of alcohols to mesylates and tosylates
   4. Mesylates and tosylates in SN2 reactions.
   5. Alkyl phosphates
   6. Conversion of alcohols to alkyl halides
E. Nomenclature of ethers
   1. Common ethers
   2. Crown ethers
F. Synthesis of ethers
   1. Dehydration of alcohols
   2. Williamson synthesis
G. Reactions of ethers

LABORATORY EXPERIENCES

A. Laboratory Safety and "Safety Data Sheets"
B. Recrystallization and Melting Point (Miniscale)
C. Recrystallization and Melting Point (Microscale)
D. Distillation and Boiling Point (Miniscale)
E. Distillation and Boiling Point (Microscale
F. Extraction (Miniscale)
G. Extraction (Microscale)
H. Dehydration from an alcohol

I. Sn2 reaction: Synthesis of 1-bromobutane

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	25%
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. Cengage Learning.

REFERENCES

Yurkanis, P. (2016). *Organic Chemistry* (8va. ed.). Pearson.

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://wwwiupac.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.