UNIVERSITY OF THE SACRED HEART
NATURAL SCIENCES DEPARTMENT
SANTURCE, PUERTO RICO

COURSE DOCUMENT

COURSE TITLE **:** Organic Chemistry 2

CODE **:** Chem 302

PREREQUISITE **:** Chem 301

HOURS/CREDITS **:** Four credits per semester; three hours per week lectures and three hours per week laboratory sessions; hybrid on line course

COURSE DESCRIPTION

Study of conjugate systems, resonance, molecular orbitals, reactions of conjugate systems, and kinetic and thermodynamic control of a reaction. The following mechanisms will be studied: electrophilic and nucleophilic aromatic substitutions, nucleophilic additions to carbonyl groups, nucleophilic acyl substitution, conjugate additions and aldol condensations. The properties of carboxylic acids and derivatives, amines, phenols, and polycyclic aromatic hydrocarbons will be studied. Finally and introduction to biochemistry with emphasis on carbohydrates, lipids, amino acids and nucleic acids will be covered.

Regardin spectroscopic techniques, an introduction to UV-VIS spectroscopy, IR spectroscopy, ^{13}C-NMR and Mass spectrometry will be given. Structure determination is the main focus on these subjects.

This course has an on-line component and is directed to students enrolled in the chemistry, biology and health sciences programs. This course will give these students a general view of the chemical and biological processes that occur in the world.

JUSTIFICATION

Materials such as medicines, textiles, plastics, combustibles, food, and biological processes occur on a daily basis in our world. Because of all this, a student must take to this course to have a complete academic formation.

The purpose of this course is to prepare sutdents to understand the basic processes in biological system and our environment.

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OBJECTIVES

At the end of this course the students will be able to:

1. Describe unsaturated systems using pi molecular orbitals and the stability of such systems by means of resonance structures.
2. Explain the difference between kinetic and thermodynamic control in a reaction.
3. Explain reactions of conjugate systems and the factors that affect them.
4. Define an aromatic system and determine if a given molecule is either aromatic, antiaromatic or non aromatic.
5. Show the different electronic transitions that a molecule can by means of molecular orbitals, in the ultraviolet-visible region and calculate the maximun wavelength using the Woodward-Fieser rules.
6. Determine the molecular structure of an organic compound given its IR spectra and its molecular formula and assigned functional groups of that molecule to the given spectra.
7. Describe the chemical process that takes place inside a mass spectrometer and the importance of mass spectrometry to determine molecular structure.
8. Explain the basic principles of ^{13}C nuclear magnetic resonance and the importance in molecular structure determination.
9. Determine the molecular structure of an organic compound from its IR, NMR, UV-VIS and MS spectra.
10. Explain the mechanism of electrophilic aromatic substitution, the factors that affect a reaction that proceeds by that mechanism and point out the difference between the ortho, para and meta director in the substrate.
11. Give IUPAC names to aldehydes, ketones, carboxylic acids and their derivatives, amines, phenols, and polycyclic aromatic hydrocarbons.
12. Explain the mechanism of nucleophilic addition to carbonyl compounds and the electronic and steric factors that affect the reactivity of aldehydes and ketones.
13. Explain the keto-enol tautomer mechanism and predict the dominat structure.
14. Design organic synthetic routes based on nucleophilic addition mechanism.
15. Explain the aldol mechanism, conjugate nucleophilic addition and related mechanisms.
16. Design synthetic routes based on aldol mechanism, crossed aldol mechanism, Michael addition and Robinson annulation.
17. Name carboxilic acids and their derivatives using IUPAC nomenclature.
18. Explain the addition-elimination mechanism and the synthetic uses.
19. Name amines using IUPAC rules and explain their different synthetic routes.
20. Explain the chemical properties of amines as bases and the structural factors that affect

those.

21. Explain the chemical properties of polycyclic aromatic compounds.
22. Draw and name monosacharides form the D-aldoses and D-ketoses and explain the reactions of these compounds.
23. Explain the difference between monosacharides, polysacharides, steroids, amino acids and lipids in terms of structurarl properties.
24. Describe the structures of DNA and RNA.

CONTENIDO

I. Conjugate Systems
   A. Resonance
   B. Molecular Orbitals
      1. Allyl System
      2. 1,3-butadiene System
   C. Classification of Dienes
      1. Conjugate
      2. Cumulated
      3. Isolated
   D. Preparation of Dienes
   E. 1,2 and 1,4 electrophilic additions of dienes
   F. Kinetic and Thermodynamic Control
   G. Diels-Alder Reaction
      1. Diene Conformation
         a. S-cis conformation
         b. S-trans conformation
      2. Electron withdraing and Electron donating groups
      3. Stereochemistry
      4. Mechanism
   H. Ultraviolet-Visible Spectroscopy (UV-VIS)
      1. Electronic Transitions
      2. Instrumentation
      3. Solvent Effect

4. Woodward-Fieser Rules

II. Aromaticity
   A. The bencene molecule
   B. Structure of Bencene. Molecular Orbitals
   C. Properties of Aromatic Compounds
      1. Electron delocalization
      2. Planar Cyclic Structure
      3. Molecular orbitals: The Polygon Rule
      4. Number of Pi electrons
   D. Aromatic, Antiaromatic and Nonaromatic compounds
   E. Examples

III. Infrared Spectroscopy
   A. Vibrational Modes
      1. Symmetric and Asymmetric stretch
      2. Bending
         a. Rocking
         b. Scissoring
         c. Wagging
         d. Twisting
   B. Instrumentation
      1. Sources
      2. Cells
         a. NaCl
         b. KBr
         c. Solvents
   C. Oscillator
      1. Force Constant
      2. Wavenumber
   D. Espectrum
      1. Fingerprint region
      2. Broad bands
      3. Sharp bands

E. Functional Groups
    1. Alcanes
    2. Alkenes
    3. Alkynes
    4. Alcohols
    5. Ketones
    6. Aldehydes
    7. Carboxylic acids and derivatives
    8. Nitriles
    9. Amines
    10. Bencene derivatives
F. Carbinyl wavenumber variations
    1. Resonance effect
    2. Inductive effect
    3. Angular strain
    4. Hydrogen Bonds
G. Examples

IV. Mass Spectrometry
A. Instrumentation
    1. Ionization Chamber
    2. Mass Analyzer
    3. Mass Spectrum
        a. Relative Abundance
        b. Mass to charge ratio, m/z
B. Fragmentation Patterns
    1. Alcanes
    2. Alkenes
    3. Alkynes
    4. Alcohols
    5. Ethers
    6. Aromatics
C. McLafferty Rearrangement

1. Aldehydes
2. Ketones
3. Carboxylics acids
4. Esters
5. Amides
6. Anhydrides

D. Halogenated Compounds
1. Isotopic Effect of Cl
2. Isotopic Effect of Br

E. Examples

V. Nuclear Magnetic Resonance Spectroscopy of ^{1}H and ^{13}C

A. Magnetic Anisotropy
1. Carbonyl Group
2. Alkenes
3. Alkynes
4. Aromatics

B. Splitting Patterns: Exceptions to the N+1 Rule

C. Nuclear Magnetic Resonance ^{13}C
1. Principles
2. Nuclear Spin of ^{13}C
3. Chemical Shift in ^{13}C-NMR
4. ^{13}C NMR Spectra
5. Examples
6. Structure determination using UV, IR, NMR and MS.

VI. Electrophilic Aromatic Substitution

A. General Mechanism
1. Arenium ion
2. Arenium Stabilization
3. Energy Reaction profile

B. Monosubstitution Reactions
1. Halogenation
2. Nitration

3. Sulfonation
4. Friedels-Craft Alkylation
5. Friedels-Craft Acylation

C. Ortho-Para Directors

D Meta Directors

E. Resonance and Inductive Effects.

F. Side chain Reactions of Bencene Derivatives
1. Oxidations
2. Reductions

G. Diazonium salt Formation
1. Experimental Conditions
2. Synthetic Routes

H. Organic Synthesis using Electrophilic Aromatic Substitution.

VII. Aldehydes y Ketones

A. Physical Properties of Aldehydes and Ketones

B. Keto-Enol Tautomerism

C. Preparation of Aldehydes and Ketones
1. Oxidation of Primary Alcohols
2. Addition of Water to Alkenes
3. Oxidation of Secondary Alcohols

D. Reactions of Aldehydes and Ketones
1. Mechanism of Carbonyl Nucleophilic Addition
   a. Steric Effect
   b. Inductive Effect
2. Addition of HCN: formation of cyanohydrines
3. Addition of alcohols: formation of acetals and ketals
4. Addition of phosphorous ylide: The Wittig Reaction
5. Addition of 1,2-ethanediol: Protecting Carbonyl Groups
6. Condensations with Amine Derivatives

E. Qualitative Analysis
1. Tollens's Test
2. Iodoform Test's

VIII. Aldol Condensation

A. Aldol Condensation
   1. Mechanism
   2. Formation of Unsaturated α,β System
   3. Synthetic Routes using Aldol Condensation
      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. Crossed Aldol Condensation

C. Practical Crossed Aldol Condensation

D. Clainsen-Schmidt Condensation

E. Cyclizations

F. Conjugate Additions
   1. Michael Addition
   2. Robinson Annulation

G. Aldol Condensation in Acidic Media

H. Synthetic routes using β diketones

IX. Carboxylic acids and their Derivatives

A. Physical Properties of Carboxylic acids

B. IUPAC Names of Carboxylic Acids

C. Preparation of Carboxylic Acids
   1. Oxidations of Alcohols, alkylbencenes and aldehydes.
   2. Grignard Reactions with CO_2
   3. Acids Hydrolysis of Nitriles.
   4. Purification of Carboxylic Acids

D. Reactions of Carboxylic Acids
   1. Preparation of Acyl Chloride from Carboxylic Acids
   2. Decarboxilation
   3. Deshydration of Dicarboxylic Acids
   4. Synthesis of Acyl Chlorides using $SOCl_2$, PCl_3 y PCl_5

E. Preparation of Carboxylic Acids Derivatives
   1. Structure of Carboxylic Acids Derivatives

a. Acyl Chlorides
b. Acid Anhydrides
c. Nitriles
d. Esters
e. Amides
(1) Primary
(2) Secundary
(3) Tertiary

2. Addition-Elimination Mechanism
3. Reactivity of Derivatives
4. Preparation of Carboxylic Acid Derivatives from AcylChlorides
5. Preparation of Carboxylic Acid Derivatives from Acid Anhydrides
6. Hydrolysis of Esters in acid ans basic media
7. Preparation of Nitriles

X. Amines

A. Physical Properties
B. Basicity of amines
1. Basic Strngth
2. Amines vs. amides
C. Nomenclatura of Amines
D. Preparation of Amines
1. Sustitución nucleofílica S_N2
2. Reaction of alkyl halides with azides followed by reduction
3. Reduction of Nitro Groups
4. Gabriel Synthesis
5. Reductive Amination
6. Reduction of nitriles and amides
7. Reduction of Oximes
8. Hoffman Rearragement
E. Purification of Amines
F. Reactions of Amines
1. Oxidación with H_2O_2

2. Cope Elimination
3. Hoffman Elimination

XI. Nucleophilic Aromatic Substitution
   A. Mechanism of addition-elimination
   B. Mechanism of elimination-addition
   C. Examples

XII. Polycyclic Aromatic Compounds (PAH) and Phenols
   A. Properties of PAH
   B. Biphenyls
      1. Nomenclature
      2. Reactions
   C. Benzenoids
      1. Nomenclature
      2. Reactions
   D. Phenols
      1. Nomenclature
      2. Physical Properties
      3. Acidity of Phenols
      4. Preparation of Phenols
      5. Reactions
      6. Quinones

XIII. Carbohydrates
   A. Classification of Carbohydrates
      1. Monosacharides
      2. Polisacharides
   B. Classification of Monosacharides
      1. Ketoses
      2. Aldoses
   C. D and L Configuration of Sugars
   D. Family of D-aldoses y D-ketoses
   E. Erithro y threo Stereoisomers
   F. Epímers

G. Cyclic Structures of Monosacharides
    1. Glucose Molecule
    2. Fructose Molecule
    3. Piranose y Furanose
H. Anomers
    1. α and β Anomers.
    2. Mutarotation
I. Reactions of Monosacharides
    1. Epimerization
    2. Reductions: alditols
    3. Oxidations
        a. Water and Bromine
        b. Nitric Acid
        c. Tollens' Test
        d. Benedict's Test
    4. Formation of Glucosides
    5. Formation of esters
    6. Reactions with Phenylhydrazine: Osazones
    7. Ruff's Degradation
    8. Kiliani-Fisher Synthesis
    9. Reactions with HIO_4
J. Disacharides and polisacharides
    1. Sacarose
    2. Maltose
    3. Lactose
    4. Cellulose
    5. Starch

XIV. Special Topics

A. Lípids
    1. Waxes
    2. Fatty Acids
    3. Triglicerides

4. Phospholipids
5. Steroids
6. Prostaglandines
7. Terpens
    a. Nomenclature
    b. Classification
8. Terpenoids

B. Amino acids
1. Structure
2. Stereochemistry
3. Zwitterions.
4. Isoelectric Point
5. Synthesis of amino acids
    a. Hell-Volhard-Zelinski Reaction
    b. Gabriel Synthesis-malonic esters.
    c. Strecker's Synthesis
6. Reactions of Amino Acids
    a. Carboxylic Group Esterification
    b. Acylation of the Amino Group
    c. Nynhidrine reaction
7. Peptide Structure.
8. Amino Acid Sequence determination

C. Nucleic Acids
1. Nucleotides y ribonucleotides
2. Nucleosides y ribinucleosides
3. Amines Bases
4. Phosphate Groups Grupos
5. DNA Structure.

INSTRUCTIONAL STRATEGIES

On line Course
Overheads

Lectures
Laboratories
Problem Sets
Class Discussions

EVALUATION

Partial exams	30%
Assistance	5%
Problem Sets	10%
Forum	10%
Laboratory	25%
Final test	20%
Total	100%

BIBLIOGRAPHY

Text

Wade, L.G. Jr., Organic Chemistry, 5ta ed, Prentice may, 2003.

Laboratory Manual: Química Orgánica, Manual de laboratorio, escala micro Primera Parte 3ra edición

References

Paula Yurkanis Bruice, Organic Chemistry, 2ndEd. (2004) Prentice Hall

Solomon, T.W., Fundamentals of Organic Chemistry, 5ta ed, John Wiley & Sons, Inc

The electronic database to which the Madre Maria Teresa Guevara Library is subscribed in conjunction with COBIMET includes documents, articles from journals, periodicals, and other information resources related to the course topics. To use these resources follow the next steps:

To access the library Web Page **from any place inside the campus**:

- Go to **http://biblioteca.sagrado.edu/**,
- Go to **Biblioteca Virtual** link and a page will appear from which access to the database will be granted. The database is organized according to discipline and in alphabetical order.

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- Enter your user name and password (The user name and password are requested in the Library).
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Electronic addresses

http://chemistry.about.com

http://academicinfo.net/chemorganic.html

http://www.iupac.org

If any student needs special accommodation he or she must request it to the Associate Dean of Students Affairs with special needs. The student should also notify the professor.

February 2008