UNIVERSITY OF THE SACRED HEART
NATURAL SCIENCES DEPARTMENT

COURSE DOCUMENT

COURSE TITLE: Organic Chemistry 1

CODE: Chem 301

PREREQUISITE: Chem 102

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

COURSE DESCRIPTION

DESCRIPTION

Study of the atomic and molecular structure of organic compounds. This course discusses isomerism, organic reactions such as substitution and elimination reactions, physical and chemical properties of alkanes, alkenes, alkynes, alkyl halides, alcohols, and ethers, nomenclature of these compounds NMR, and organic synthesis.

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.

OBJECTIVES

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

1. Explain the atomic structure of the elements commonly foud in organic compounds and the describe the molecules these formed in geometrical and resonance terms.

Define the following concepts and give examples of conformers, enantiomers, constitucional isomers and diastereomers.

2. Give IUPAC and common names to compounds from the following familias: alkanes, cycloalkenes, alkenes, alkynes, alkyl halides, alcohols, and ethers.
3. Differentiate all the enantiomers that a compound can have as well as the diastereomers and meso compounds that might be on a compound.
4. Explain the difference between the kinetics and thermodynamics in an organic chemical reaction, and the different types of these reactions such as substitution, addition, elimination and rearrangement.
5. Explain the SN1, SN2, E1 and E2 mechanisms and the factors that affect these reactions.
6. Explain the importance that NMR has in molecular structure determination.
7. Explain the reactions that alkanes, alkenes, alkynes, alcohols ethers and epoxides undergo.
8. Propose a reasonable synthetic route to obtain alkanes, alienes, alkynes, alcohols and ethers.

COURSE CONTENT

I. Introduction

- A. Atomic Structure
  - 1. Atomic Orbitals
  - 2. Electronic configurations
- B. Covalent Bond
  - 1. Covalent bond formation
  - 2. Lewis Structures
  - 3. Bond length
  - 4. Bond angle
  - 5. Resonance
  - 6. Molecular Geometry
    - a. Linear
    - b. Bent
    - c. Trigonal plane
    - d. Tetraedral
    - e. Trigonal pyramidal
  - 7. Dipole Moment and Molecular Structure
- C. Intermolecular Forces
  - 1. London

2. Dipole-dipole
3. Ion-dipole
4. Hydrogen Bond

D. 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

E. Functional Groups of Organic compounds
1. Alkanes
2. Alkenes
3. Alkynes
4. Cicloalkanes
5. Alkyl Halides
    a. Primary
    b. Secondary
    c. Tertiary
6. Alcoholes
    a. Primary
    b. Secondary
    c. Tertiary
7. Ethers
8. Aromatic compounds
9. Aldehydes
10. Ketone
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. Property

B. Structure

1. Condensed Formula
2. Bond-line Formula

C. Nomenclature

1. Alkanes
2. Cycloalkanes
3. Bicyclic compounds

D. Conformations and Newman Projections

1. Ethane
   a. Alternate
   b. Eclipsed
2. Butane
   a. Anti
   b. Gauche
   c. Eclipsed

E. Angular Strain and Conformations in Cycloalkanes

1. Cyclopropane
2. Cyclobutane
3. Cyclopentane
4. Cyclohexane
   a. Chair Conformation
   b. Boat Conformation
   c. Axial and Equatorial Positions

F. Alkane Synthesis

1. Alkyl Halides reduction with acid and zinc

2. Corey-Posner,Whitesides-House synthetic route

III. Isomers and Stereoisomers

A. Classification of isomers

1. Constitutional isomers
2. Geometric isomers
    a. Cis isomers
    b. Trans isomers
3. Stereoisomers
    a. Enantiomers
    b. Diastereomers
    c. Meso compounds

B. Optical activity

1. Polarimeter
2. Specific rotation
3. Racemic Mixture

C. R-S Configurations

1. Priorities
2. Compounds with a single chiral carbon
3. Compound with two chiral carbons

D. Fisher Projections

1. Compounds with a single chiral carbon
2. Compound with two chiral carbons
    a. Enantiomers
    b. Diastereoisomers
    c. Meso compounds

IV. Organic Reactions

A. Chemical Kinetics

1. Rate Law
2. Rate Constant
    a. Collisions
    b. Collision Orientation
    c. Activation Energy
    d. Temperature
    e. Ahrrenius' Equation

3. Reaction Mechanism
    a. S_N2
    b. S_N1
4. Reaction Energy Profile
    a. Transition State
    b. Intermediaries
    c. Hammond's Postulate

B. Termodynamics
1. The Equlibrium State
2. ΔH, ΔS, ΔG
3. Exoenergetic and endoenergetic reactions

V. Alkyl Halides
A. Properties
B. Nomenclature
C. Preparation
D. Aliphatic Nucleophilic Substitution (S_N2)
1. Substrate
2. Reagent
3. Rate Law
4. Factors affecting S_N2 mechanism
    a. Substrate Structure
    b. Solvent
        (1) Protic Solvents
        (2) Polar Aprotic Solvent
    c. Nucleophile
    d. Leaving Group
5. Stereochemistry of S_N2
6. Synthetic Applications of S_N2

E. Unimolecular Nucleophilic Substitution (S_N1)
1. Mecanism amd the rate law
2. Factores affecting S_N1
    a. Substrate Struture
        (1) Carbocation Structure
        (2) Carbocation Stability

b. Solvent

c. Nucleophile

d. Leaving Group

3. Stereochemistry of S_N1

a. Racemic Mixture

b. Inversion vs Retention

F. E2 Mechanism

1. Rate Law

2. Factors affecting it

3. Stereochemistry

G. E1 Mechanism

1. Rate Law

2. Factors affecting it

3. Stereochemistry

H. S_N2 vs E2 y S_N1 vs E1

J. Synthetic applications of E2

VI. Introduction to Nuclear Magnetic Resonance (NMR)

A. Index of Hydrogen Deficiency

1. Definition and meaning

2. Mathematical formula

B. Nuclear Spin

C. Magnetic Field

D. NMR Process

E. Shielding

F. Chemical Shift

G. Equivalent Protons

1. Homotopic hydrogens

2. Enantioropic hydrogens

3. Diastereotopic hydrogens

H. Spin-Spin Coupling

1. Types of Signals

a. Singlets

b. Doublets

c. Triplets

- d. Quartets
- e. Multiplets

2. Coupling Constant

I. NMR and Kinetics

J. Structure determination from an NMR Spectrum

VII. Alkenes and Alkynes

A. Physical Properties

B. Nomenclature

1. Z Isomers
2. E Isomers
3. Cicloalkenes

C. Stability of alkenes

D. Stereochemistry of Cicloalkenes

E. Alkene Synthesis

1. Hydrogenation of Alkynes
   - a. Syn addition
   - b. Anti addition
2. E2
   - a. Zaitsev's rule
3. Dehydration of alcohols
   - a. Mechanism
   - b. Migration of carbocations
4. Debromination

F. Reactions of Alkenes

1. Mechanism of Addition
   - a. Electrophiles
   - b. Electrophiles and Nucleophiles
2. Markovnikov's Rule
3. Regioselective Reactions
4. Stereochemistry of Addition Reactions
5. Addition Reactions
   - a. Addition of H_2SO_4
   - b. Addition of $H_2O/H+$
   - c. Addition of halogens

(1) Stereochemistry

d. Halogenation in water

6. Regioselective and Stereospecific Reactions

7. Oxidations of Alkenes

a. Syn Hydroxylation

b. Ozonolysis

c. Other oxidations

G. Nomenclature of Alkynes

H. Physical Properties of Alkynes

I. Acidity of Alkynes

J. Synthesis of Alkynes

1. Synthesis from alkenes

2. Synthesis from $NaNH_2$ and S_N2

K. Reactions of Alkynes

1. Addition of Halogens

2. Addition of HX

3. Oxidations of Alkynes

VIII. Alcohols and Ethers

A. Physical Properties of alcohols

B. Classification

1. Primary

2. Secondary

3. Tertiary

C. Nomenclature of Alcohols

1. Common Names

2. IUPAC Names

D. Synthesis of Alcohols

1. Hydration of Alkenes

2. Oxymercuration-Demercuration

3. Hydroboration-Oxidation

4. Grignard Reagent

5. Reduction of Aldehydes and Ketones

E. Reactions of Alcohols

1. Reactivity of the OH Group

2. Acidity of Alcohols
3. Transformation of Alcohols into Mesylates and Tosylates
4. Mesylates and Tosylates in S_N2 reactions.
5. Alkyl Phosphates
6. Transformation of Alcohols into Alkyl Halides

F. Physical Porperties of Ethers

G. Nomenclature of Ethers

1. Common Ethers
2. Crown Ethers

H. Synthesis of Ethers

1. Dehydration of alcohols
2. Williamson's synthesis
3. Sililation

I. Reactions of Ethers

J. Epoxides

1. Structure
2. IUPAC Name
3. Synthesis
4. Reactions

INSTRUCTIONAL STRATEGIES

Overheads
Lectures
Laboratory
Problem Sets
Discussions in classroom
On line resources

EVALUATION

Partial Exams	30%
Assistance	5%
Problem Set	10%
Forum	10%
Laboratory	25%
Final Test	20%
Total	100%

REFERENCES

Text

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

Direcciones electrónicas

http://chemistry.about.com

http://academicinfo.net/chemorganic.html

http://www.iupac.org

http://www.chem.ucla.edu/~webspectra/

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.

To access from any place outside the campus

- Write the following address **http://biblioteca.sagrado.edu/**,
- Select the link **Biblioteca Virtual** and a page will appear from which access to a database will be granted. The database is organized according to discipline and in alphabetical order.
- Enter your user name and password (The user name and password are requested in the Library).
-

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
Cualquier estudiante que necesite acomodo razonable deberá solicitarlo al Decano Asociado de Asuntos Estudiantiles.

febrero 2008