



INTER-AMERICAN UNIVERSITY OF PUERTO RICO
METROPOLITAN ENCLOSURE
Faculty of Science and Technology
Natural Sciences Department

Course for students of Biology, Biomedical Sciences, Natural Sciences, Microbiology,
Chemistry and Medical Technology

COURSE SYLLABUS

I. GENERAL INFORMATION

Course Title:	Organic Chemistry I
Code and Number:	CHEM 2221
Credits:	4 Credits
Requirement:	CHEM-1111
Academic term:	Trimester: 2021-33
Contact hours:	Three hours and 50 minutes per week
Professor:	Luis A. Arias, Ph.D.
Office:	419
Office hours:	Tuesday: 11:15- 12:15 Wednesday: 12:15-14:15
Office phone:	787-250-1912 Ext. 2323
Email	Through the BlackBoard Mail

II. Course description:

Theoretical and experimental study of the structural, physical and chemical characteristics of organic compounds. Emphasis is placed on the nomenclature, isomerism, synthesis and reactions of hydrocarbons, alcohols, alkyl halides and aromatic compounds. It requires 45 hours of lecture and 45 hours of classroom laboratory.

III. TERMINAL AND TRAINING OBJETIVES

- 1. General Aspects of the Structure** - Determine the fundamental characteristics of the chemical bond of the carbon compounds and their relationship with the molecular structure: isomerism (constitutional, conformational, stereoisomerism).
 - 1.1. Represent the electronic configurations of the elements of periods I and II of the periodic table in developed form, diagram and using the configurations of the corresponding noble gases.
 - 1.2. Classify the atomic orbitals of the elements of the first and second period according to their energy and symmetry.
 - 1.3. Represent graphically the formation of chemical bonds by interaction of atomic orbitals.
 - 1.4. Describe the type and geometrical characteristics of the sp , sp^2 and sp^3 hybrid orbitals for the elements of the second and third periods.
 - 1.5. Predict the molecular geometry of the hydrogenated compounds of the elements of the second period using the electronic pair repulsion model.
 - 1.6. Describe the type and geometrical characteristics of the bonds in the saturated and unsaturated carbon compounds: alkanes, alkenes, carbonyls, alkynes, alcohols, ethers, amines, alkyl halides, nitriles and aromatic compounds based on hybrid orbitals.
 - 1.7. Represent molecular structures by writing the different types of chemical formulas: molecular, structural, line and Lewis formulas including formal charges.
 - 1.8. Identify the different types of intermolecular forces and predict their effects on the physical properties of various compounds and states of matter.
 - 1.9. Write the Newman projections of the conformational isomers in alicyclic compounds and determine their relative potential energies.

- 1.10. Draw the conformational isomers of cyclohexane and determine their relative energies.
- 1.11. Draw the geometric isomers of 1,2-, 1,3- and 1,4-disubstituted cycloalkanes. Identify them as *cis-trans* and determine their relative stabilities.
- 1.12. Draw the geometric isomers of the alkenes, identify them as *cis-trans*, *E-Z* and determine their relative stabilities.
- 1.13. Identify the asymmetric atoms or stereogenic centers. Draw a pair of enantiomers in your Fischer and three-dimensional projections.
- 1.14. Determine the absolute configuration (R, S) of each enantiomer and its effect on the polarized light in the plane.
- 1.15. Calculate the specific rotation of an enantiomer.
- 1.16. Define the concept of racemic mixture.
- 1.17. Calculate the specific rotation of pure enantiomers and / or their mixtures. Determine the percent enantiomer excess (% ee).
- 1.18. Draw the Fischer projections of diastereomers and meso compounds with at least two chiral centers.
- 1.19. Predict the reactions that can produce optically active compounds.
- 1.20. Establish the correlation between chemical reactivity and molecular structure of mon-substituted and some di-substituted derivatives of benzene.

2. Aspects of Nomenclature - Name organic compounds applying the IUPAC systematic rules and through some trivial names.

- 2.1 Identify the most important functional groups in organic compounds.
- 2.2. Write the IUPAC name of alkanes, cycloalkanes and bicyclic compounds.
- 2.3 Write the IUPAC name of the alcohols and classify them as primary, secondary or tertiary.
- 2.4 Write the IUPAC name of the halogenated alkanes and cycloalkanes, classify them as primary, secondary, tertiary, benzylic, aryl, vinyl.
- 2.5 Write the IUPAC name of the amines and classify them as primary, secondary or tertiary.
- 2.6 Write the IUPAC name of the most common symmetric and non-symmetric ethers.
- 2.7 Write the IUPAC name of the alkenes and cycloalkenes.
- 2.8 Write the IUPAC name of the alkynes.
- 2.9 Write the IUPAC name of the aromatic compounds derived from benzene and the principal anulenes.
- 2.10 Write the IUPAC name of compounds with more than one functional group and including stereoisomeric centers

3. Mechanisms of Reaction - Write the mechanisms and predict the structure of the products of nucleophilic substitution reactions, elimination, electrophilic aromatic and radical substitution, electrophilic addition, reduction and molecular transpositions.

- 3.1 Write the mechanism of electrophilic addition reactions to alkenes: addition of hydrogen halides, addition of $\text{H}_2\text{O} / \text{H}_2\text{SO}_4$, ($\text{ROH} / \text{H}_2\text{SO}_4$) hydroxy (alkoxy) mercuration-demercuration, addition of borane, addition of halogens, Addition of HBr / ROOR .
- 3.2 Apply the Markovnikov rule to non-symmetric alkenes.
- 3.3 Identify the steps in the preparation of compounds of the anti-Markovnikov type, determining in each case the regiochemistry (regioselectivity) and the stereochemistry (stereoselectivity) of the reactions.
- 3.4 Write the mechanism and determine the stereochemistry of the catalytic hydrogenation of alkenes.
- 3.5 Write the mechanism of the halogenation of an alkane. Identify the determinant steps of the radical reaction.
- 3.6 Write the mechanisms of the substitution reactions in the alkyl halides, alcohols and ethers. Discuss the competitive aspects that determine the regiochemistry and stereoselectivity of the reactions based on the following factors: the structure of the substrate, the nature of the nucleophile, the nature of the leaving group, the nature of the solvent and the temperature of the reaction.

- 3.7 Write the mechanisms of the elimination reactions in the alkyl halides and alcohols. Discuss the competitive aspects that determine the regiochemistry and stereoselectivity of the reactions based on the following factors: the structure of the substrate, the nature of the base, the nature of the leaving group, the nature of the solvent and the temperature of the reaction or the catalyst.
- 3.8 Write the general mechanism of electrophilic substitution in an aromatic system and applying to the description of the following reactions: halogenation, nitration, alkylation and Friedel-Crafts acylation, sulfonation.

4. Kinetics and thermodynamics-Determine the fundamental characteristics of kinetics of first and second order reactions, their thermodynamic and activation parameters.

- 4.1 Describe electrophilic addition reactions by means of energy profiles, identifying reactants, transition states, intermediate species and products. Identify the determining step of each reaction by comparing its energies of activation and considering the rearrangements or transpositions.
- 4.2 Describe the unimolecular and bimolecular reactions of nucleophilic substitution by means of energy profiles, identifying reactants, transition states, intermediate species and products. Identify the determining step of each reaction by comparing its activation energies.
- 4.3 Describe the unimolecular and bimolecular reactions of elimination by means of energy profiles, identifying reactants, transition states, intermediate species and products. Identify the determining step of each reaction by comparing its activation energies.
- 4.4 Determine the factors that favor the unimolecular or bimolecular course of a nucleophilic substitution reaction taking into account as decisive criteria the relative stabilities of intermediate chemical species and transition states.
- 4.5 Determine the factors that favor the unimolecular or bimolecular course of an elimination reaction taking into account as decisive criteria the reaction conditions, the relative stabilities of the intermediate chemical species and that of the transition states. Discuss the anti-periplanar transition state and emphasize the distribution of Hofmann and Zaitsev products.
- 4.6 Relate the molecular structures of the transition states with the intermediate species, reactants or products based on the Hammond postulate.
- 4.7 Establish the kinetic relationship between the halogens (selectivity) and the reactivity of primary, secondary, tertiary, and benzylic hydrogens.
- 4.8 Describe the electrophilic aromatic substitution reactions by means of energy profiles, identifying reactants, transition states, intermediate species and products. Identify the determining step of each reaction by comparing its activation energies.
- 4.9 Compare and contrast the energy profiles of the bimolecular nucleophilic substitution and elimination reactions with those of the electrophilic aromatic substitution reactions.

5. Organic Synthesis - Propose synthetic methods for obtaining alkyl halides, alkenes, alkynes, alcohols and organometallic compounds, including synthetic sequences of moderate level.

- 5.1 Write the chemical equations of the different methods of obtaining alkenes: elimination of alkyl halides and dehydration of alcohols
- 5.2 Given a chemical reaction, diagram the corresponding chemical equation.
- 5.3 Explain the mechanisms and laws of rapidity of substitution and elimination reactions.
- 5.3 Explain the stereochemical consequences of these reactions.
- 5.4 Illustrate the energy profiles and identify the reactants, transition states, intermediaries and products.
- 5.5 Write the chemical equations of the different methods of obtaining alkynes: elimination of alkyl dihalides and vinyl halides; by SN2 type reactions using acetyl anions.
- 5.6 Write the products and determine the stereochemistry of: the catalytic hydrogenation of alkynes and the reduction with alkali metals (Li, Na).

- 5.7 Write the structure of the dehydration products of the non-symmetrical alcohols and determine the main product.
- 5.8 Illustrate by means of specific reactions, the use of N-bromosuccinimide (NBS) in the synthesis of organic bromides.
- 5.9 Write the chemical equations of the different methods of obtaining alkyl halides: halogenation of alkanes, allylic halogenation, hydrohalogenation of alkenes, hydrohalogenation of alkynes, substitution in alcohols.
- 5.10 Classify nucleophilic substitutions in unimolecular and bimolecular reactions. Write their equations, mechanisms, laws of reaction speed, explain their stereochemical consequences.
- 5.11 Write the structure of the dehydrohalogenation products of unsymmetrical alkyl halides and determine the main product.
- 5.12 Write the structure of electrophilic substitution products in benzene and monosubstituted and some disubstituted derivatives.
- 5.13 Write the sequence of reactions for the synthesis of compounds in a minimum of two or three steps.

6. Correlation of Chemical Reactivity and Molecular Structure - Establish the relationship between chemical reactivity and the molecular structure of several systems.

- 6.1 Identify acids and bases according to the Brønsted-Lowry and Lewis theories.
- 6.2 Identify the strong and weak acids and bases based on the constants pK_a , pK_b , K_a and K_b .
- 6.3 Write acid-base equations and determine the direction of the equilibrium of each reaction using the values of the acid constants.
- 6.4 Predict and compare the physical properties of alcohols, ethers, amines and alkyl halides against alkanes.
- 6.5 Discuss the competitive aspects that determine the course of nucleophilic substitution reactions and elimination based on the following factors: the structure of the substrate, the nature of the nucleophile or the base, the nature of the leaving group, the nature of the solvent and the temperature of the reaction.
- 6.6 Compare the relative stability between alkenes based on the degree of substitution, heat of hydrogenation and / or computational calculations.
- 6.7 Apply the Hückel rule to predict the aromaticity of annuli and their ions.
- 6.8 Establish the differences between the aromatic, non-aromatic and anti-aromatic character.
- 6.9 Establish the correlation between acid strength and molecular structure of phenols using inductive and/or resonance effects.
- 6.10 Classify the benzene substituents in activators and deactivators depending on the speed of the reaction and its orienting effect to determine the aromatic electrophilic di- and tri-substitution products.
- 6.11 Establish the correlation between acid strength and molecular structure of phenols using inductive and / or resonance effects.

7. Experimental techniques of preparation, purification and identification of organic compounds at the laboratory level.

- 7.1 Use experimental techniques in the preparation, purification and identification of organic compounds.
- 7.2 Isolate organic products and subject them to purification techniques such as: extraction, distillation, recrystallization and chromatography (column and thin layer).
- 7.3 Apply synthetic methods in the preparation of simple organic compounds.
- 7.4 Choose among sources and forms of access to bibliographic information related to physical constants, and the chemical properties of organic compounds.

8. Molecular Modeling - Apply molecular modeling computer programs.

- 8.1 Establish a relationship between physical and chemical properties and molecular structure through molecular modeling by computer.
- 8.2 Emphasize the use of molecular modeling with and without computer programs for the conformational analysis and compare the stability between isomers.
- 8.3 Use computerized programs to predict the reactivity and position of attack for benzene and its derivatives in a substitution reaction aromatic electrophilic.

IV. COMPETENCES- This course covers the following competencies for the BS Program in Chemistry.

1. Demonstrate knowledge and understanding of the physical properties and chemical behavior of matter based on its composition and structure.
2. Demonstrate knowledge and understanding of chemical reactions based on their mechanisms and the factors that affect them.
- 7 Act in accordance with ethical standards and the laws that regulate the practice of Profession.

V. COURSE CONTENT

TEXTBOOK: ORGANIC CHEMISTRY: JANICE GORZYNSKI SMITH **SIXTH EDITION**

Unit-Topics	Thematic content	Chapter (sections)
1. Structure and bond	The periodic table, electronic configurations for the elements of the second and third period, Lewis structures, octet rule, formal charges, molecular formulas, condensed and skeletal, polarity of bonds and molecules, hybridization, bond lengths and angles, molecular geometry, isomers, electronegativity.	Chap.1 (1.1 - 1.14)
2. Acid and bases	Acids and bases reactions according to Brønsted-Lowry and Lewis.	Chap. 2 (2.1-2.8)
3. Resonance	Resonance structures: represent ion structures and molecules with pi bonds, compare their chemical stability and represent the resonance hybrid.	Chap. 1 (1.6) Chap. 16 (16.2-16.5)
4. Introduction to organic compounds, nomenclature and physical properties	General structures of functional groups, nomenclature of branched alkanes, cycloalkanes, bicycloalkanes, intermolecular forces and effect on the boiling and melting points and solubility in water or organic solvents, conformational analysis of acyclic and cyclic structures, dihedral angle, relative stability between conformers and profiles of potential energy, oxidation of alkanes, lipids.	Chap. 3 (3.1-3.9) Chap 4 (4.1-4.15)
EXAM # 1		
5. Stereochemistry, Isomers: the arrangement of atoms in space (it will be covered in the laboratory period)	Nomenclature and <i>cis / trans</i> isomerism, <i>R / S</i> chirality and optical activity of carbons and other asymmetric atoms, enantiomers, enantiomer mixture composition, diastereomers, Fischer projections, meso compounds.	Chap. 5 (5.1 –5.13)
6. Understanding organic reactions	Equations and types of organic reactions, breaking and bond formation, dissociation energies, thermodynamics, enthalpy, entropy, energy profiles, reaction kinetics.	Chap. 6 (6.1-6.11)
7. Alkyl Halides, Alcohols, Ethers: Substitution Reactions	Nomenclature and properties of alkyl halides, alcohols and ethers, relative reactivity and mechanisms of alkyl halides and alcohols in nucleophilic substitution reactions SN1, SN2, factors that affect the speed and / or control the stereochemistry of the reactions (substrate, nucleophile, leaving group, solvent, temperature, catalyst), synthesis.	Chap. 7 (7.1-7.18) Chap. 9 (9.1 -9.7, 9.11-9.13)
8. Alkyl Halides and Alcohols: Elimination Reactions	Relative reactivity and mechanisms of the alkyl halides in elimination reactions E1, E2, factors that affect the speed and / or control the stereochemistry of the reactions (substrate, base, leaving group, solvent, temperature, catalyst)	Chap. 8 (8.1-8.11) Chap. 9 (9.8-9.10)
EXAM #2		

Themes	Thematic content	Chapter (sections)
9. Alkenes: Structure, nomenclature and reactions of alkenes	Cis / trans nomenclature and isomerism, alkene E / Z, alkene nucleophilicity, energy profiles versus progress for exo or endothermic reactions. Write the chemical equations for the basic reactions of the alkenes; hydrohalogenation, dihalogenation, hydration / alcoholation, hydroboration-oxidation, catalytic hydrogenation, addition Markovnikov and antimarkovnikov, rearrangement and relative stability of carbocations and alkenes, regioselectivity and stereoselectivity of additions to alkenes, mechanism of reactions.	Chap. 10 (10.1-10.18) Chap 12 (12.13-12.14)
10. Alkynes: Structure, nomenclature, acidity and reactions.	Nomenclature and classification of alkynes, relative acidity, reactions (hydrohalogenation, dihalogenation, reduction under Lindlar conditions or alkaline metals in liquid ammonia) and acetylide anions and their transformations.	Chap.11 (11.1 – 11.12) Chap. 12 (12.5)
11. Free radicals	Structural characteristics and stability of free radicals, mechanistic stages in the halogenation of alkanes or in benzylic or allylic positions, effect of free radicals on biological cells.	Chap 15 (15.1-15.13)
EXAM 3		
12.Aromaticity and reactions of benzene.	Structural characteristics of benzene, aromaticity rules, non-aromatic and antiaromatic character, effect of aromaticity on acidity or basicity, nomenclature of monosubstituted, disubstituted derivatives, etc.	Chap 17 (17.1-17.3, 17.5 -17.11)
13.Reactions of aromatic compounds.	Mechanisms and energy profiles for electrophilic aromatic substitution reactions to benzene (nitration, sulfonation, halogenation, alkylation and Friedel-Crafts acylation), reactions in ring substituents (S _N 1, S _N 2, oxidation, reduction, benzylic halogenation), effect of substituents (inductive, resonance, activating or deactivating, ortho / para director or meta) in the reactivity of the benzene ring towards the second and / or third aromatic electrophilic substitution. Synthesis of di or tri substituted benzene derivatives in a maximum of 3 steps.	Chap. 18 (18.1-18.16)
FINAL EXAM- 125 pts. Themes 1-11 (80), 12, 13 (45)		

VI. ACTIVITIES

Conference

Board

Group exercises (2-3) to review the previous class.

Short tests in person or through Blackboard and /or Connect (McGraw Hill)

Learn Smart and Prep (Resources through the Connect platform (McGraw Hill)

Exams

Participation of students on the whiteboard

Laboratory experiments

Practice exercises

VII. EVALUATION CRITERIA

1. The evaluation of the course consists of:

A. A theory part composed of three (3) partial exams, a final exam, short test and assignments. These evaluation criteria correspond to 75% of the final grade.

B. A part of experimental practice corresponding to 25% of the final grade which must be approved with a minimum of 60%.

Evaluation criteria	Value	% of final grade
Partial Exam # 1	100	17
Partial Exam # 2	100	15
Partial Exam # 3	100	15
FINAL EXAM Comprehensive	125	18
Assignments in Connect	100	5
Short tests in Connect	100	5
Laboratory	100	25
TOTAL	725	100

2. Access to the Connect Chemistry McGraw Hill platform **is required**. To buy this access you must go to the library of the enclosure. Access to this platform will facilitate compliance with the evaluation criteria, Assignments and Short Tests. Below the link to access the section of your course in Connect.

SECTION MONDAYS AND WEDNESDAY (10-12 am) CRN 10836

<https://connect.mheducation.com/class/l-arias-encarnacion-chem-2221-2021-33-crn-10836-monday-wednesday>

3. The student will have the opportunity to accumulate up to 6 points taking quizzes and 6 points from assignments through connect. Quizzes will have deadlines and up to 20 minutes to be completed. Assignments won't have time limit but they will have deadline.
4. There will be no double counting of exams, nor special works to substitute deficient results or improve your final average in the course. It is also not required that you present excuses if you do not show up for a partial exam. In that case, what you should do is take care of your personal situation and present yourself during office hours for the reposition, no later than one week after the exam.
5. A poor grade (54 % or less in the conference and 59 % or lower in the laboratory) means the non-approval of the course.
6. The following evaluation scale will be applied in the final grade.

100-85 A
84-75 B
74-65 C
64-55 D
54-0 F

VIII. EDUCATIONAL RESOURCES

a) Text book:

Organic Chemistry, Smith J.G. 6th Edition, McGraw-Hill Education, 2020. ISBN: 978-1-260 11910-7.

b) Manual for the laboratory:

LABORATORY MANUAL FOR ORGANIC CHEMISTRY I, L. Arias, and I. Rosado, San Juan, Puerto Rico **VERSION OF FEBRUARY 2021**.

b) Electronic resources.

1. <http://connect.mheducation.com> (Accessed February 27, 2021)
2. <http://www.prenhall.com/bruice> (Accessed February 27, 2021)
3. For purification techniques and melting points in the lab, nomenclature tutorial, or retrosynthesis <http://www.organicworldwide.net/> (Accessed February 27, 2021)
4. Alkene problems (Accessed February 27, 2021)
http://www.uam.es/departamentos/ciencias/qorg/docencia_red/qo/l9/reac_p.html
5. Others- Designed and assigned by the instructor

IX. BIBLIOGRAPHY

Books

1. Organic Chemistry, Organic Chemistry, P. Y. Bruice, Seventh Edition, Prentice Hall 2014. ISBN 13: 978-0-321-80322-1

2. Organic Chemistry, M. A. Fox and J. K. Whitesell, Tercera Edición, Jones and Bartlett Publishers **2004**. ISBN 0763721972.
3. Advanced Organic Chemistry, F. A. Carey and J. Sundberg, Cuarta Edición, Plenum Publishers 2001. ISBN 00306462443.
4. Advanced Organic Chemistry, March, J. Smith, M. B. Wiley-Interscience, Quinta Edición 2001, ISBN 04715890.
5. Organic Chemistry, P. Y. Bruice, Cuarta Edición, Prentice Hall 2001, ISBN 0130178516.
6. Organic Chemistry, F. A. Carey, McGraw-Hill Science 2002, ISBN 0072521708
7. Organic Chemistry, L. G. Wade and L. G. Jr. Wade, Prentice Hall, Fifth Edition 2002. ISBN 013033832X.
8. Macroscale and Microscale Organic Experiments, Kenneth L. Williamson, D.C. Houghton Mifflin Company, Fourth Edition 2002, ISBN 0618197028.
9. Experimental Organic Chemistry: A Miniscale and Macroscale Approach, J. C. Gilbert, S. F. Martin, Brooks College, Third Edition 2001, ISBN 00303440632.

Computers with Internet access and programs:

1. ChemDraw/CHEM 3D
2. <http://connect.mheducation.com>

X. SPECIAL NOTES

1. Auxiliary services or special needs

Any student requiring auxiliary services or special assistance must request them at the beginning of the course or as soon as he / she acquires knowledge that he / she needs them, through the corresponding register, in the Orientation Office with Mrs. María de Los Angeles Cabello, Office 111.

2. Honesty, fraud and plagiarism

The lack of honesty, fraud, plagiarism and any other inappropriate behavior in relation to academic work constitute major infractions sanctioned by the General Student Regulations. Major infractions, as provided in the General Student Regulations, may result in the suspension of the University for a defined period of more than one year or permanent expulsion from the University, among other sanctions.

3. Use of electronic devices

Cell phones and any other electronic device that could interrupt teaching and learning processes or alter the environment conducive to academic excellence will be disabled. The pressing situations will be attended, as appropriate. The use of electronic devices that allow accessing, storing or sending data during evaluations or examinations is prohibited.

4. Compliance with the provisions of Title IX

The Federal Higher Education Act, as amended, prohibits discrimination based on sex in any academic, educational, extracurricular, athletic or any other program or employment, sponsored or controlled by a higher education institution regardless of whether it is performed inside or outside the campus of the institution, if the institution receives federal funds. As provided by the current federal regulations, a Title IX Assistant Coordinator has been designated in our academic unit to provide assistance and guidance in relation to any alleged incident constituting discrimination based on sex or gender, sexual harassment or sexual assault. You can contact the Assistant Coordinator, Mr. George Rivera, at (787)250-1912 extension 2262 or 2147 or email griverar@metro.inter.edu. The Normative Document entitled **Rules and Procedures for Addressing Alleged Violations of the Provisions of Title IX** is the document that contains the institutional rules to analyze any complaint

filed based on this type of claim. This document is available on the website of the Inter-American University of Puerto Rico (www.inter.edu).

XI. ETHICAL VALUES

It is expected that 100% of the students show a behavior of total honesty when completing and delivering the assignments and laboratory reports. Plagiarism will not be allowed in any of its modalities, 0% of cases of dishonesty are expected.

NOTE: It is important to be clear that the different forms of plagiarism or improper use of works in the laboratory, ideas or words of another person without consent or recognition, is an academic infraction with very serious consequences. See the General Regulations for students of the Inter-American University of Puerto Rico-2004, p.60 and onwards for examples of the types of plagiarism and the sanctions that apply. In this course, this type of practice will be penalized when evaluating your work.

March 4, 2021