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

COURSE SYLLABUS

I. GENERAL INFORMATION

Course Title:	Organic Chemistry I
Code and Number:	CHEM 2221
Credits:	4 credits
Requirement:	CHEM 1111
Academic term:	
Contact hours:	
Professor:	
Office:	
Office hours:	
Office phone:	
Email	

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 closed 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, sp2 and sp3 hybrid orbitals for the elements of the second period.
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 stereogénicos 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 H2O / H2SO4, (ROH / H2SO4) 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 of 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. CONTENT- Themes / Sub-themes-Sections of the text.

1. Structure and bond, acids and bases. 1.1-1.16; 2.1-2.12; 8.3-8.6
Electronic configurations for the elements of the second and third period, Lewis structures, formal charges, molecular formulas, condensed and skeletal, polarity of bonds and molecules, hybridization, lengths and angles of bonding, molecular geometry, isomers. Acid-base reactions of Brønsted-Lowry and according to Lewis. Resonance structures: Represent ion structures and molecules with pi bonds, compare their chemical stability and represent the resonance hybrid.

2. Introduction to organic compounds, nomenclature and physical properties: 3.1-3.15
General structures of functional groups (alkenes, alkynes, arenes, RX, RNH2, ROH, RCHO, R2CO, RCOOH, RCO2R). IUPAC nomenclature of branched alkanes, bicycloalkanes, alcohols, ethers and amines. Intermolecular forces and effect on boiling and melting points and solubility in water or organic solvents. Representation, conformational analysis and potential energy profiles of acyclic structures and relative stability between conformers based on dihedral angle, torsion tension, steric hindrance and hydrogen bridges. More stable conformation and IUPAC nomenclature of disubstituted cyclohexanes.

3. Alkenes: 5.2-5.4 5.5
General structure of an alkene (Review: Geometry, hybridization, bond angles, nucleophilicity). General molecular formula of alkenes, importance, draw isomeric alkenes, *cis* / *trans* stereochemistry, E / Z, IUPAC nomenclature of alkenes and cycloalkene. Chemical reactivity.

PARTIAL EXAMINATION I - DATE:

4. Stereochemistry: 4.1-4-4.16
R / *S* chirality and optical activity of carbons and other asymmetric atoms, enantiomers, diastereomers, Fischer projections, meso compounds, chirality in addition reactions to alkenes.

5. Reactions of alkenes and energy diagram or profiles: 6.1-6.9; 6.12-6.18, 13.3, 13. 7
Write the chemical equations for the basic reactions of the alkenes; hydrohalogenation, dihalogenation, hydration/alcoholation, hydroxy/alkoximercuration-demercuration, 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 (With HX, H_3O^+ / ROH_2^+, heat, X_2, X_2/H_2O, HBr / ROOR). Chirality in addition reactions to alkenes.

6. Structure, nomenclature, acidity and reactions of alkynes: 7.1-7.6; 7.9-7.12
Nomenclature and classification of alkynes, relative acidity, reactions (hydrohalogenation, dihalogenation, low or no Lindlar conditions) and acetylide anions and their transformations.

SECOND PARTIAL EXAM - DATE

7. Free radicals: 13.1-13.10- Task
Structural characteristics and stability of free radicals, mechanistic steps in the halogenation of alkanes or i

8. Substitution reactions in alkyl halides, alcohols, ethers: 9.1-9.8; 11.1, 11.2; 11.6
Relative reactivity and mechanisms of alkyl halides and alcohols in nucleophilic substitution reactions SN

9. Elimination reactions in alkyl halides and alcohols: 10.1-10; 10 9, 10.10; 11.4
Relative reactivity and mechanisms of the alkyl halides and alcohols in elimination reactions E1, E2, fact

THIRD PARTIAL EXAM - DATE:

10. Aromaticity and reactions of benzene: 8.1-8.3; 8.7-8.13; 19.1-19.11
Structural characteristics of benzene, aromaticity rules, non-aromatic and anti-aromatic character, effect of aromaticity on acidity or basicity, nomenclature of mono, di, etc. substituted benzene derivatives. Direct reactions, mechanisms and energy profiles for aromatic electrophilic substitution reactions to ber

11. Reactions of substituted benzenes 19.12-19.20; 19.25
Effect of substituents (inductive, resonant, activating or deactivating, ortho / para director or meta) on the reactivity of the benzene ring towards the second and / or third aromatic electrophilic substitution. Synthesis of mono, di or tri-substituted benzene derivatives in a maximum of 3 steps.

COMPREHENSIVE FINAL EXAM: Subjects: 1-9 (80 pts), 10-11 (45 pts) DATE: June /1st/ 2018

VI. ACTIVITIES

Conference
Board
Student participation
Laboratory experiments
Practice exercises

VII. EVALUATION CRITERIA

The evaluation of the course consists of:

A. A part of theory composed of three partial exams, of 100 points each; besides the end of 125 points. These exams will correspond to 70% of the final grade.

It is not eliminated, nor does it substitute any of the partial exams. If you miss a partial exam, you must make arrangements to answer it during the teacher's office hours and, at most, one week after the group has taken the exam. The final exam is mandatory for all students.

If you take advantage of the tutoring service offered by “Fortalece tu Ciencia”, at the end of the quarter you could accumulate up to 10 points that would be added to the worst partial test.

In preparation for the final exam of 125 points, there is a bank of questions available through BlackBoard, which is recommended to be resolved as the topics are developed and discussed. This bank of questions is also useful for all partial exams.

B. The second component of the course evaluation is the laboratory or experimental practice which correspond to 30% of the final grade and must be approved with 60% or more in order to pass the course.

C. The evaluation scale to be applied in final grade is chemistry-1: A 85-100, B 75-84, C 65-74, D 55-64.

VIII. ETHICAL VALUES

It is expected that 100% of the students show a behavior of total honesty when completing and delivering the assignments. 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.

IX. EDUCATIONAL RESOURCES:

a) Textbook:

Organic Chemistry, P. Y. Bruice, 7th Edition, Prentice Hall 2014. ISBN 978-0-321-803322-1.

b) Laboratory manual:

Manual of Organic Chemistry I, A. Alzérreca, L. Arias, F. Shalabi and I. Rosado, Fourth Edition, San Juan, Puerto Rico- Version of March 2018.

c) Electronic resources

1. http://www.pearsonhighered.com/thechemistryplace/books.html (accessed December/2017)
2. Animations for substitution reactions http://www.chemtube3d.com/sn2_benzylchloride_sh_secondary.html (accessed Dec/2017)
3. Virtual text- Provides information about the complete Organic course (I and II), including exercises and resolved quizzes. http://www2.chemistry.msu.edu/faculty/reusch/VirtTxtJml/intro1.htm (accessed December/2017)
4. **Animations on chirality** http://www.khanacademy.org/science/organic-chemistry/stereochemistry-topic/chirality- R, Sm/v/introduction-to-chirality (accessed 1 / Dec / 2017)
5. For any organic theme, including videos and animations, go to: http://www.khanacademy.org/science/organic-chemistry (accessed December/2017)
6. Tutorial in English narrated by Dr. Thomas Poon: www.ochem.com (accessed Dec / 2017)

X. BIBLIOGRAPHY

a) Books

1. Organic Chemistry, P. Y. Bruice, Sexta Edición, Prentice Hall **2010**, ISBN 13: 978-0-321- 66313-9
2. A Small Scale Approach to Organic Laboratory Techniques D. L. Pavia, G. M. Lampman, G. S. Kriz, R. G. Engel, Third Edition, Brook/Cole Cengage, **2011**, ISBN-13:978-1-4390-4932-7.

b) Computer program:

1. Scigress (a copy is provided for all students who wish to do so

XI. 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 Office of the Professional Counselor, Mr. José Rodríguez, located in the University Orientation Program.

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).

March/23/2018