UNIVERSIDAD DE CASTILLA - LA MANCHA

GUÍA DOCENTE

1. General information

Course: ORGANIC CHEMISTRY I
Code: 57309
Type: CORE COURSE
ECTS credits: 9
Degree: 398 - UNDERGRADUATE DEGREE PROGRAMME IN CHEMISTRY
Academic year: 2020-21
Center: 1 - FACULTY OF SCIENCE AND CHEMICAL TECHNOLOGY
Group(s): 20 23
Year: 2
Duration: AN
Main language: Spanish
Second language:
Use of additional languages:
English Friendly: Y
Web site:
Bilingual: N

Lecturer: **ENRIQUE DIEZ BARRA** - Group(s): **20 23**

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Lecturer: **MARIA DEL PILAR PRIETO NUÑEZ-POLO** - Group(s): **20 23**

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2. Pre-Requisites

It is recommended to have studied the subject Chemistry of the basic module and to have registered the subject Organic Chemistry II.

3. Justification in the curriculum, relation to other subjects and to the profession

The subject of Organic Chemistry is included in the module of Fundamentals of Chemistry in the Degree of Chemistry. It is designed to develop the concepts and fundamental data of Organic Chemistry, to show the experimental evidence that supports these concepts, to apply these data and concepts to the resolution of chemical problems and to demonstrate that this subject evolves rapidly and that it plays a key role in modern technological developments in very diverse fields, from biology to materials science, influencing in a fundamental way all aspects of daily life.

The subject Organic Chemistry I is compulsory, annual and corresponds to the second year of the degree in which the foundations of the different areas of Chemistry are initiated. The subject consists of 9 credits, of which 6 are theoretical and are studied in the first semester, and the remaining three are practical, being studied in the second semester. It is the first subject of Organic Chemsitry, and it deals with the basic concepts that will be extended in the subjects Organic Chemistry II, Organic Chemistry III and Extension of Organic Chemistry.

4. Degree competences achieved in this course

Course competences

Code	Description
CB02	Apply their knowledge to their job or vocation in a professional manner and show that they have the competences to construct and justify arguments and solve problems within their subject area.
E01	Understand and use chemical terminology, nomenclature, conventions and units
E03	Handle chemicals safely and with respect to the environment
E05	Know the chemical elements and their compounds, their forms of obtaining, structure, properties and reactivity, as well as the main techniques for their analysis
E06	Know the structural properties of chemical compounds, including stereochemistry, as well as the main structural research techniques

E09	Know the kinetics of chemical change, including catalysis and reaction mechanisms
G01	Know the principles and theories of Chemistry, as well as the methodologies and applications characteristic of analytical chemistry, physical chemistry, inorganic chemistry and organic chemistry, understanding the physical and mathematical bases that require
G02	Be able to gather and interpret data, information and relevant results, obtain conclusions and issue reasoned reports on scientific, technological or other problems that require the use of chemical tools
T03	Proper oral and written communication
T07	Ability to work as a team and, where appropriate, exercise leadership functions, fostering the entrepreneurial character
T11	Ability to obtain bibliographic information, including Internet resources

5. Objectives or Learning Outcomes

Course learning outcomes

Description

Acquire the ability to interpret the experimental results, relating each experimental stage with the theoretical knowledge acquired

Acquire the necessary practical training to apply it in your professional life. Know the main methods of isolation, purification and characterization of organic compounds

Acquire the ability to handle chemical reagents and organic compounds safely.

Acquire an awareness of environmental protection developing the idea that Organic Chemistry should be used to improve the quality of life.

Learn to work autonomously in a laboratory and know how to interpret the experimental results obtained.

Know the stereochemistry of the compounds

Know the structure of the main organic functional groups

Know the utility of the spectroscopic techniques in Organic Chemistry

Know the main aspects of the terminology and nomenclature in Organic Chemistry

Know the basic principles of Organic Chemistry.

To ensure that the student is able to search and select information in the field of Organic Chemistry and that he / she is capable of processing and presenting it adequately both orally and in writing, developing his / her synthesis capacity, being critical and objective

To develop in the student the capacity of initiative to pose and solve concrete problems of Organic Chemistry, as well as to interpret the obtained results

Develop your ability to teamwork

Recognize the main reactive intermediates and the influence of stereoelectronic effects on their stability and reactivity

Encourage and promote in the student all those values ¿¿and attitudes inherent to scientific activity.

6. Units / Contents

Unit 1: THE CHEMICAL BOND. Introduction to Organic Chemistry. Atoms, electrons and orbitals. Ionic Bonding. Covalent bonding: Lewis structures. Formal charges. Molecular orbitals. Molecular orbitals of the hydrogen molecule Electronic structure of the carbon atom: Hybridization sp3: The bond in methane. sp2 hybridization: The bond in ethylene sp hybridization: The bond in acetylene. Polar covalent bonding and electronegativity Dipole moment. Electronic effects: Inductive effect. Conjugative effect and resonance. Other types of bonding: influence on the physical properties of organic compounds Structural formulas of organic molecules. Types of isomers.

Unit 2: PERSPECTIVE OF ORGANIC REACTIONS. Concept of functional group. Main functional groups. Types of organic reactions. Reaction mechanisms: ionic and radical reactions, how they occur. Concept of electrophilic and nucleophilic Energy and transition state diagrams. Reaction intermediates: Structure of carbocations, free radicals, carbanions and carbenes. Stability of carbocations. Stability of free radicals. Stability of carbanions.

Unit 3: ALKANES AND CYCLOALKANES. Classes of hydrocarbons. Introduction to alkanes. Sources of alkanes and cycloalkanes. Concept of isomerism: Butanes, pentanes and higher alkanes. IUPAC nomenclature of alkanes and cycloalkanes. Concept of radical: Alkyl groups. Physical properties of alkanes and cycloalkanes. Combustion of alkanes. Oxidation-reduction in Organic Chemistry: Oxidation states.

Unit 4: CONFORMATIONS OF ALKANES AND CYCLOALKANES. Concept of conformation: conformational isomers. Conformational analysis of ethane, butane and higher alkanes. Conformational analysis of cycloalkanes. Small rings: cyclopropane and cyclobutane. Cyclopentane. Cyclohexane: Axial and equatorial bonds, ring inversion, conformational analysis of monosubstituted cyclohexanes. Conformational analysis of disustituted cyclohexanes. Medium and large rings. Polycyclic systems. Heterocyclic compounds.

Unit 5: STEREOCHEMISTRY. Optical activity. Polarimeter. Chirality. Molecules with a chiral center: Enantiomers. Racemic. Chiral center and asymmetric carbon atom. Symmetry in aquiral structures. Absolute and relative configuration. Fischer's projection formulas. Cahn-Ingold-Prelog R-S notation system Chiral molecules with two stereogenic centers: Diastereoisomers. Meso forms. Physical properties of stereoisomers. Pseudo-asymmetric centers. Epimers. Non-carbon stereogenic centers. Chirality without chiral centers. Resolution of racemics.

Unit 6: ALKENES. Nomenclature. Structure and bonding. E-Z stereoisomery. Sequence rules. Physical properties. Relative stability of alkenes: combustion heats Preparation of alkenes: Elimination reactions. Hydrogenation. Stereochemistry. Electrophilic addition reactions: Mechanism and orientation Addition of hydrogen halides. Regioselectivity: Markovnikov rule. Rearrangements. Addition of sulphuric acid. Hydration of alkenes catalyzed by acid. Oximercuriation-demercuriation. Hydroboration-oxidation. Mechanism. Addition of halogens. Mechanism: Halonium ions. Conversion of alkenes into halohydrines. Oxidation of Alkenes: Hydroxylation. Epoxidation. Ozonolysis. Oxidation with strong oxidizing agents. Hydrogen bromide radical addition: mechanism.

Unit 7: ALKYNES. Nomenclature. Structure and bonding. Sources of alkynes. Physical properties. Acetylene acidity and terminal alkynes. Preparation of Alkynes: Alkylation of acetylene and terminal alkynes. Elimination reactions. Reactions of Alkynes: Addition of halogen. Addition of hydrogen halides. Addition of water. Hydroboration-oxidation. Hydrogenation. Reduction with metal-ammonium. Oxidative ruture of alkynes.

Unit 8: CONJUGATION AND POLYMERIZATION. The allyl group. Types of dienes. Bonding in allenes. Relative stabilities of alkadienes. Electronic delocalization of conjugated dienes. Preparation of dienes. Addition of hydrogen halides to conjugated dienes. Addition of halogens to dienes Diels-Alder reactions. Stereo-selectivity. Polymerization of alkenes and dienes.

Unit 9: ARENES AND AROMATICITY. Nomenclature. Sources of aromatic hydrocarbons. Benzene: structure and stability. Kekulé formulation of the structure of benzene. Description of the benzene bond by resonance. Aromaticity: Hückel's rule. Cyclobutadiene and cyclooctetraene. Anulenes. Aromatic ions. Heterocyclic aromatic compounds. Polycyclic aromatic hydrocarbons. Physical properties. Reduction reactions. Reactions in the side chain: halogenation of alkylbenzenes by free radicals Oxidation of alkylbenzenes. Preparation of alkylbenzenes. Addition reactions of alkyl benzenes.

Unit 10: REACTIONS OF ARENES. ELECTROPHILIC AROMATIC SUBSTITUTION. Electrophilic aromatic substitution of benzene. Mechanism of the electrophilic aromatic substitution. Nitration. Sulfonation. Halogenation. Friedel-Crafts Alkylation and acylation. Synthesis of alkylbenzenes by acylation-reduction. Reaction rated and orientation of the electrophilic aromatic substitution. Effects of substitutes in the electrophilic aromatic substitution: activating and deactivating substitutes. Halogens as substituents. Regioselective synthesis of disubstituted and polysubstituted aromatic compounds. Synthesis of polycyclic aromatic compounds. Substitution reaction in naphthalene. Substitution reaction in heterocyclic aromatic compounds.

Unit 11: SPECTROSCOPY. Electromagnetic radiation. Quantified energy states. Proton Nuclear Magnetic Resonance Spectroscopy (1H-RMN). Nuclear shielding and chemical shift. Chemical shift and molecular structure. Interpretation of proton NMR spectra. Spin-spin coupling. Splitting patterns. Carbon 13 Nuclear Magnetic Resonance (13C-NMR). Spectrum interpretation. Infrared (IR) spectroscopy. Ultraviolet-visible spectroscopy (UV-VIS). Mass

spectrometry.

7. Activities, Units/Modules and Methodology

Training Activity	Methodology	Related Competences (only degrees before RD 822/2021)	ECTS	Hours	As	Com	Description
Class Attendance (theory) [ON-SITE]	Lectures	CB02 E01 E05 E06 T03	1.08	27	Y	N	
Class Attendance (practical) [ON-SITE]	Practical or hands-on activities	E01 E03 E05 E06 G02 T03 T07	1.6	40	Y	Y	
Workshops or seminars [ON-SITE]	Problem solving and exercises	E01 E02 E03 E05 E07 T03	0.72	18	Y	N	
Group tutoring sessions [ON-SITE]	Group tutoring sessions	E01 T03	0.04	1	Y	N	
Study and Exam Preparation [OFF-SITE]	Self-study		5.36	134	N	-	
Progress test [ON-SITE]			0.08	2	Y	N	
Final test [ON-SITE]			0.12	3	Y	Y	
		Total:	**9**	**225**			
		Total credits of in-class work: 3.64					**Total class time hours: 91**
		Total credits of out of class work: 5.36					**Total hours of out of class work: 134**

As: Assessable training activity
Com: Training activity of compulsory overcoming (It will be essential to overcome both continuous and non-continuous assessment).

8. Evaluation criteria and Grading System

Evaluation System	Continuous assessment	Non-continuous evaluation*	Description
Assessment of problem solving and/or case studies	15.00%	0.00%	
Progress Tests	25.00%	0.00%	
Laboratory sessions	15.00%	15.00%	
Final test	45.00%	85.00%	
Total:	**100.00%**	**100.00%**	

According to art. 4 of the UCLM Student Evaluation Regulations, it must be provided to students who cannot regularly attend face-to-face training activities the passing of the subject, having the right (art. 12.2) to be globally graded, in 2 annual calls per subject , an ordinary and an extraordinary one (evaluating 100% of the competences).

9. Assignments, course calendar and important dates

Not related to the syllabus/contents

Hours	**hours**
Class Attendance (practical) [PRESENCIAL][Practical or hands-on activities]	40
Study and Exam Preparation [AUTÓNOMA][Self-study]	134

Unit 1 (de 11): THE CHEMICAL BOND. Introduction to Organic Chemistry. Atoms, electrons and orbitals. Ionic Bonding. Covalent bonding: Lewis structures. Formal charges. Molecular orbitals. Molecular orbitals of the hydrogen molecule Electronic structure of the carbon atom: Hybridization sp3: The bond in methane. sp2 hybridization: The bond in ethylene sp hybridization: The bond in acetylene. Polar covalent bonding and electronegativity Dipole moment. Electronic effects: Inductive effect. Conjugative effect and resonance. Other types of bonding: influence on the physical properties of organic compounds Structural formulas of organic molecules. Types of isomers.

Activities	**Hours**
Class Attendance (theory) [PRESENCIAL][Lectures]	4
Workshops or seminars [PRESENCIAL][Problem solving and exercises]	2

Unit 2 (de 11): PERSPECTIVE OF ORGANIC REACTIONS. Concept of functional group. Main functional groups. Types of organic reactions. Reaction mechanisms: ionic and radical reactions, how they occur. Concept of electrophilic and nucleophilic Energy and transition state diagrams. Reaction intermediates: Structure of carbocations, free radicals, carbanions and carbenes. Stability of carbocations. Stability of free radicals. Stability of carbanions.

Activities	**Hours**
Class Attendance (theory) [PRESENCIAL][Lectures]	2
Workshops or seminars [PRESENCIAL][Problem solving and exercises]	1

Unit 3 (de 11): ALKANES AND CYCLOALKANES. Classes of hydrocarbons. Introduction to alkanes. Sources of alkanes and cycloalkanes. Concept of isomerism: Butanes, pentanes and higher alkanes. IUPAC nomenclature of alkanes and cycloalkanes. Concept of radical: Alkyl groups. Physical properties of alkanes and cycloalkanes. Combustion of alkanes. Oxidation-reduction in Organic Chemistry: Oxidation states.

Activities	**Hours**
Class Attendance (theory) [PRESENCIAL][Lectures]	1
Workshops or seminars [PRESENCIAL][Problem solving and exercises]	1

Unit 4 (de 11): CONFORMATIONS OF ALKANES AND CYCLOALKANES. Concept of conformation: conformational isomers. Conformational analysis of ethane, butane and higher alkanes. Conformational analysis of cycloalkanes. Small rings: cyclopropane and cyclobutane. Cyclopentane. Cyclohexane: Axial and equatorial bonds, ring inversion, conformational analysis of monosubstituted cyclohexanes. Conformational analysis of disustituted cyclohexanes. Medium and large rings. Polycyclic systems. Heterocyclic compounds.

Activities	**Hours**
Class Attendance (theory) [PRESENCIAL][Lectures]	2
Workshops or seminars [PRESENCIAL][Problem solving and exercises]	1

Unit 5 (de 11): STEREOCHEMISTRY. Optical activity. Polarimeter. Chirality. Molecules with a chiral center: Enantiomers. Racemic. Chiral center and asymmetric carbon atom. Symmetry in aquiral structures. Absolute and relative configuration. Fischer's projection formulas. Cahn-Ingold-Prelog R-S

notation system Chiral molecules with two stereogenic centers: Diastereoisomers. Meso forms. Physical properties of stereoisomers. Pseudo-asymmetric centers. Epimers. Non-carbon stereogenic centers. Chirality without chiral centers. Resolution of racemics.	
Activities	**Hours**
Class Attendance (theory) [PRESENCIAL][Lectures]	3
Workshops or seminars [PRESENCIAL][Problem solving and exercises]	2
Unit 6 (de 11): ALKENES. Nomenclature. Structure and bonding. E-Z stereoisomery. Sequence rules. Physical properties. Relative stability of alkenes: combustion heats Preparation of alkenes: Elimination reactions. Hydrogenation. Stereochemistry. Electrophilic addition reactions: Mechanism and orientation Addition of hydrogen halides. Regioselectivity: Markovnikov rule. Rearrangements. Addition of sulphuric acid. Hydration of alkenes catalyzed by acid. Oximercuriation-demercuriation. Hydroboration-oxidation. Mechanism. Addition of halogens. Mechanism: Halonium ions. Conversion of alkenes into halohydrines. Oxidation of Alkenes: Hydroxylation. Epoxidation. Ozonolysis. Oxidation with strong oxidizing agents. Hydrogen bromide radical addition: mechanism.	
Activities	**Hours**
Class Attendance (theory) [PRESENCIAL][Lectures]	5
Workshops or seminars [PRESENCIAL][Problem solving and exercises]	3
Unit 7 (de 11): ALKYNES. Nomenclature. Structure and bonding. Sources of alkynes. Physical properties. Acetylene acidity and terminal alkynes. Preparation of Alkynes: Alkylation of acetylene and terminal alkynes. Elimination reactions. Reactions of Alkynes: Addition of halogen. Addition of hydrogen halides. Addition of water. Hydroboration-oxidation. Hydrogenation. Reduction with metal-ammonium. Oxidative ruture of alkynes.	
Activities	**Hours**
Class Attendance (theory) [PRESENCIAL][Lectures]	2
Workshops or seminars [PRESENCIAL][Problem solving and exercises]	2
Group tutoring sessions [PRESENCIAL][Group tutoring sessions]	1
Progress test [PRESENCIAL][]	2
Unit 8 (de 11): CONJUGATION AND POLYMERIZATION. The allyl group. Types of dienes. Bonding in allenes. Relative stabilities of alkadienes. Electronic delocalization of conjugated dienes. Preparation of dienes. Addition of hydrogen halides to conjugated dienes. Addition of halogens to dienes Diels-Alder reactions. Stereo-selectivity. Polymerization of alkenes and dienes.	
Activities	**Hours**
Class Attendance (theory) [PRESENCIAL][Lectures]	2
Workshops or seminars [PRESENCIAL][Problem solving and exercises]	1
Unit 9 (de 11): ARENES AND AROMATICITY. Nomenclature. Sources of aromatic hydrocarbons. Benzene: structure and stability. Kekulé formulation of the structure of benzene. Description of the benzene bond by resonance. Aromaticity: Hückel's rule. Cyclobutadiene and cyclooctetraene. Anulenes. Aromatic ions. Heterocyclic aromatic compounds. Polycyclic aromatic hydrocarbons. Physical properties. Reduction reactions. Reactions in the side chain: halogenation of alkylbenzenes by free radicals Oxidation of alkylbenzenes. Preparation of alkylbenzenes. Addition reactions of alkyl benzenes.	
Activities	**Hours**
Class Attendance (theory) [PRESENCIAL][Lectures]	2
Workshops or seminars [PRESENCIAL][Problem solving and exercises]	1
Unit 10 (de 11): REACTIONS OF ARENES. ELECTROPHILIC AROMATIC SUBSTITUTION. Electrophilic aromatic substitution of benzene. Mechanism of the electrophilic aromatic substitution. Nitration. Sulfonation. Halogenation. Friedel-Crafts Alkylation and acylation. Synthesis of alkylbenzenes by acylation-reduction. Reaction rated and orientation of the electrophilic aromatic substitution. Effects of substitutes in the electrophilic aromatic substitution: activating and deactivating substitutes. Halogens as substituents. Regioselective synthesis of disubstituted and polysubstituted aromatic compounds. Synthesis of polycyclic aromatic compounds. Substitution reaction in naphthalene. Substitution reaction in heterocyclic aromatic compounds.	
Activities	**Hours**
Class Attendance (theory) [PRESENCIAL][Lectures]	3
Workshops or seminars [PRESENCIAL][Problem solving and exercises]	3
Unit 11 (de 11): SPECTROSCOPY. Electromagnetic radiation. Quantified energy states. Proton Nuclear Magnetic Resonance Spectroscopy (1H-RMN). Nuclear shielding and chemical shift. Chemical shift and molecular structure. Interpretation of proton NMR spectra. Spin-spin coupling. Splitting patterns. Carbon 13 Nuclear Magnetic Resonance (13C-NMR). Spectrum interpretation. Infrared (IR) spectroscopy. Ultraviolet-visible spectroscopy (UV-VIS). Mass spectrometry.	
Activities	**Hours**
Class Attendance (theory) [PRESENCIAL][Lectures]	1
Workshops or seminars [PRESENCIAL][Problem solving and exercises]	1
Final test [PRESENCIAL][]	3
Global activity	
Activities	**hours**
Workshops or seminars [PRESENCIAL][Problem solving and exercises]	18
Class Attendance (theory) [PRESENCIAL][Lectures]	27
Class Attendance (practical) [PRESENCIAL][Practical or hands-on activities]	40
Group tutoring sessions [PRESENCIAL][Group tutoring sessions]	1
Study and Exam Preparation [AUTÓNOMA][Self-study]	134
Progress test [PRESENCIAL][]	2
Final test [PRESENCIAL][]	3
	Total horas: 225

10. Bibliography and Sources

Author(s)	Title/Link	Publishing house	Citv	ISBN	Year	Description
Bruice, Paula Yurkanis	Organic Chemistry	Pearson Education		978-84-8322-979-8	2017	
	https://www.pearson.com/us/higher-education/product/Bruice-Organic-Chemistry-8th-Edition/9780134042282.html					
Carey, Francis A.	Organic Chemistry	McGraw Hill		978-0-07-351121-4	2017	
	https://www.mheducation.com/highered/product/organic-chemistry-carey-giuliano/M9780073511214.html					
García Calvo-Flores, Francisco	Problemas resueltos de química orgánica	Paraninfo		978-84-9732-458-8	2015	
	https://www.paraninfo.es/catalogo/9788497324588/problemas-resueltos-de-quimica-organica					

McMurry, John	Organic Chemistry	Cengage learning	978-1-305-08048-51-3	2016
	https://www.cengagebrain.co.uk/shop/isbn/9781305080485			
Quiñoá Cabana, Emilio	Cuestiones y ejercicios de química orgánica : una guía de estudio	McGraw-Hill	9788448607128	2015
	https://www.mheducation.es/9788448607128-spain-bl-cuestiones-y-ejercicios-de-quimica-organica-una-guia-de-autoevaluacion-libro-digital			
Quiñoá Cabana, Emilio	Nomenclatura y representación de los compuestos orgánicos :	McGraw-Hill	978-84-481-4363-3	2010
	https://www.mheducation.es/9788448143633-spain-nomenclatura-y-representacion-de-los-compuestos-organicos			
Solomons, T. W. Graham	Organic Chemistry	Limusa Wiley	978-1-118-87576-6	2016
	https://www.wiley.com/en-us/Organic+Chemistry%2C+12th+Edition-p-9781118875766			
Vollhardt, K. Peter C.	Organic Chemistry. Structure and Function	Omega	978-1-4641-2027-51-4	2018
	https://macmillanlearning.com/Catalog/product/organicchemistry-eighthedition-vollhardt			
Wade, L. G. , Jr.	Organic Chemistry	Pearson/Prentice Hall	978-607-32-3847-2	2017
	https://www.pearson.com/us/higher-education/program/Wade-Organic-Chemistry-Plus-Mastering-Chemistry-with-Pearson-e-Text-Access-Card-Package-9th-Edition/PGM203813.html			
Straumanis, Andrei	Organic chemistry: a guided inquiry	Houghton Mifflin	0-618-30852-0	2004
Brown, W. Howard.	Organic chemistry /	Cengage Learning,	978-1-305-58035-0	2016
Ege, Seyhan	Organic chemistry: structure and reactivity	Hougton Mifflin Company	0-618-31809-7	2004