PERSONA CIÈNCIA EMPRESA
UNIVERSITAT RAMON LLULL

COURSE: ORGANIC CHEMISTRY

SUBJECT MATTER: Materials Science and Technology
MODULE: Core Topics of Industrial Engineering
PROGRAM: Degree in Chemical Engineering

GENERAL FEATURES

Type: ☐ Basic Formation, ☑ Compulsory, ☐ Elective

☐ Final Degree Project, ☐ Internship

Duration: Annual
Semester/s: 5 and 6
Number of ECTS credits: 12
Language/s: Spanish, Catalan, English

DESCRIPTION

SHORT DESCRIPTION AND JUSTIFICATION

Annual subject corresponding to the third year of the Degree in Chemistry and Chemical Engineering of the Universitat Ramon Llull.

The introductory chapters cover the nomenclature in organic chemistry (Chapter 1), bonding in organic chemistry (Chapter 2, covalent bonding, resonance, etc.), stereochemistry (Chapter 3), acids and bases (Chapter 4), introduction to organic reaction (Chapter 5; introduction to the theory of mechanisms, transition state, reaction intermediate, etc.).

Description of functional groups: Chapter 6 (alkanes), Chapter 7 (alkenes), Chapter 8 (alkynes), Chapter 9 (aromatic compounds), Chapter 11 (alkyl halides), Chapter 13 (alcohols and ethers), Chapters 14 to 17 (carbonyl compounds), Chapter 18 (amines).

Chapter 10 consists on an introduction to structure determination covering the basics of Infrared Spectroscopy, Proton NMR and Mass Spectrometry.

Chapter 11 covers the theory of substitution and elimination reactions (SN1, SN2, E1, E2, ...)

COMPETENCES

- Be able to understand and apply knowledge of organic chemistry on the practice of Chemical Engineering. (**CB1, E2**)
- Be able to identify, formulate and solve typical problems of Organic Chemistry (reaction mechanisms, prediction of reaction products, synthetic problems, etc.) and Structural Determination (IR, NMR, UV-Vis, MS) (**CB2, E7**).
- Be able to assess the impact of organic chemistry in the sustainable development of society. (**T3**)
- Knowledge of the fundamentals of science, technology and chemistry of materials. Understand the relationship between microstructure, synthesis or processing and material properties. (**CRI3**)

PREREQUISITES

According to the program planning and academic regulations.

CONTENTS

1. **Introduction. Classification and nomenclature of organic functional groups.**
   1.1. Introduction. 1.2. IUPAC nomenclature. 1.3. Nomenclature of hydrocarbons. 1.4. Nomenclature of functional groups.
2. **Bonding in organic molecules.**
   2.1 The nature of atoms, atomic orbitals. 2.2. Covalent bonding: Valence Bond Theory (VB Theory) and Molecular Orbital Theory (MO Theory). 2.3. Localized covalent bonding: inductive effect. 2.4. Delocalized covalent bonding: Method of Resonance. 2.5. Hydrogen bonding.
3. **The three dimensional shape of molecules.**
   3.1. Stereoisomerism: types of stereoisomers. 3.2. Cis-Trans Isomerism in Alkenes. 3.3. Optical activity and chirality. 3.4. Homochiral compounds: Resolution and asymmetric synthesis. 3.5. Conformational analysis.
4. **Acids and bases.**
   4.1. Brönsted-Lowry ccid-base theory . 4.2. Lewis acid-base theory. 4.3. Tautomerism.
5. **Introduction to organic reaction**
   5.1. Types of organic reactions. 5.2. How reactions occur: reaction mechanisms. 5.3. Polar reactions: nucleophile, electrophile. 5.4. Description of a reaction: rate, equilibrium constant, energy diagrams, transition state, reaction intermediate.
6. **Saturated hydrocarbons (alkanes or paraffins)**
   6.1. Introduction. 6.2. Synthesis of alkanes. 6.3. Reactivity of alkanes. 6.4. Applications of methane.
7. **Alkenes**
   7.1. Introduction. 7.2. Synthesis of alkenes. 7.3. Reactivity of alkenes. 7.4. Diene systems: Diels-Alder reaction.
8. **Alkynes**
   8.1. Introduction. 8.2. Synthesis of alkynes. 8.3. Reactivity of alkynes. 8.4. Reactions of acetylene.
9. **Aromatic Compounds: Benzene**
   9.1. Introduction. 9.2. Benzene: Determination of structure. 9.3. Benzene: Description of aromaticity. 9.4. Other aromatic systems. 9.5. Synthesis of enzene. 9.6. Benzene Reactivity. 9.7. Aromatic Amines. 9.8. Phenols. 9.9. Alkylbenzenes. 9.10. Naphthalene: Properties and reactivity.
10. **Structural determination: Infrared spectroscopy (IR), Proton Nuclear Magnetic Resonance (1H NMR) and Mass Spectrometry (MS)**
    10.1. Introduction. 10.2. The electromagnetic spectrum: Infrared spectroscopy (IR). 10.3. Origin of absorptions in the IR: stretching and bending. 10.4. Interpretation of IR spectra: spectral regions. 10.5. Spectroscopy of hydrocarbon compounds. 10.6. Proton nuclear

magnetic resonance: nature of the absorptions in NMR. 10.7. Chemical shift in 1H-NMR: Regions of the spectrum, equivalent protons. 10.8. Integration and spin-spin coupling.10.9. Spectroscopy of hydrocarbon compounds. 10.9. Mass Spectrometry: Basics and instrumentation. Ionization. 10.10. Determination of the molecular formula, types of ions and isotopes.

11. **Alkyl halides. Organometallic compounds**
    11.1. Introduction. 11.2. Synthesis of alkyl halides. 11.3. Reactivity of alkyl halides. 11.4. Organometallics: Grignard compounds, organolithium, Gilman reagents, organozinc, organocadmium. 11.5. Spectroscopy of halogenated compounds.
12. **Nucleophilic substitution and elimination reactions**
    12.1. Introduction. 12.2. Bimolecular nucleophilic substitution reaction (SN2). 12.3. Unimolecular nucleophilic substitution reaction (SN1). 12.4. Allylic transpositions (SN1', SN2'). 12.5. Bimolecular elimination reaction (E2). 12.6. Unimolecular elimination reaction (E1). 12.7. Nucleophilic aromatic substitution. 12.8. Phase transfer catalysis (PTC).
13. **Alcohols and ethers**
    13.1. Introduction. 13.2. Synthesis of alcohols. 13.3. Reactivity of alcohols. 13.4. Synthesis of ethers. 13.5. Reactivity of ethers. 13.6. Spectroscopy of alcohols and ethers.
14. **Aldehydes and ketones. Nucleophilic addition reactions**
    14.1 . Structure and reactivity of carbonyl compounds. 14.2. Synthesis of aldehydes and ketones. 14.3. Nucleophilic addition reactions. 14.5. Spectroscopy of aldehydes and ketones.
15. **Carboxylic acids and derivatives. Acyl nucleophilic substitution reactions.**
    15.1. Introduction. 15.2. Synthesis of carboxylic acids. 15.3. Reactivity of carboxylic acids. 15.4. Structure and reactivity of carboxylic acid derivatives. 15.5. Acyl nucleophilic substitution reactions. 15.6. Spectroscopy of carboxylic acids and derivatives.
16. **Substitution reactions at α-carbonyl**
    16.1. Reactivity of enols: General mechanism of α-carbonyl substitutions. 16.2. α-carbonyl substitution reactions.
17. **Carbonyl condensation reactions**
    17.1. General mechanism of carbonyl condensation reactions. 17.2. Carbonyl condensation reactions.
18. **Amines**
    18.1. Introduction. 18.2. Synthesis of amines. 18.3. Reactivity of amines. 18.4. Spectroscopy of amines.

METHODOLOGY

LEARNING ACTIVITIES

Learning activities	Hours	ECTS Credits	Competences
Lectures	76	2,8	CB1, E2, CB2, E7, T3, CRI3
Case and Problem-Solving Sessions	19	0,7	CB1, E2, CB2, E7, T3, CRI3
Seminars	19	0,7	CB1, E2, CB2, E7, T3, CRI3
Personal study	200	7,4	CB1, E2, CB2, E7, T3, CRI3
Assessment Tasks (Exams, Continuous Assessment...)	11	0,4	CB1, E2, CB2, E7, T3, CRI3
TOTAL	**325**	**12,0**	

TEACHING METHODOLOGY

Theoretical Sessions: Concepts are exposed through presentations or explanations (possibly including demonstrations).

Sessions of solving exercises, problems and cases: Resolution of exercises, approach and resolution of problems, and presentation and discussion of cases by the professor with the active participation of students.

Seminars: It is conducted by a professor in order to review, discuss and answer questions about the issues presented in the theoretical sessions, and sessions for solving exercises, problems and cases.

Personal study activities: Student personal work required to acquire the skills of each subject and assimilate the knowledge outlined in the theoretical sessions and sessions of solving exercises, problems and cases. Whenever it may be necessary, it has to be used the recommended material for consultation.

Evaluation activities (exams, follow-up activities): oral and / or written tests made during the term-time of the course or after it.

ASSESSMENT

ASSESSMENT METHODS

Assessment Methods	Weight (%)	Competences
Final Exam	40	CB1, E2, CB2, E7, CRI3
Midterm Exam/s	30	CB1, E2, CB2, E7, CRI3
Follow-up Activities	30	CB1, E2, CB2, E7, T3, CRI3

LEARNING OUTCOMES

1. **Demonstrate understanding and ability to apply knowledge** of organic chemistry (structure, reactivity, stereochemistry, ...) and Structural Determination (IR, NMR, UV-Vis, MS) in the practice of Chemical Engineering (**CB1**, **E2**, **CRI3**)
2. **Identify, formulate and solve typical problems** of Organic Chemistry (reaction mechanisms, prediction of reaction products, synthetic problems, etc.) and Structural Determination (IR, NMR, UV-Vis, MS) (**CB2, E7**, **CRI3**)
3. **Assess the impact of organic chemistry** in sustainable development of the society (**T3**)

QUALIFICATION

Exams and follow-up activities

December	Nomenclature (N)	Examination in class time
February	First semester examination (P)	
April	Spectroscopy (E)	Examination in class time
June	Final examination (F)	

The final rating is the best among:
(0.1 • N + 0.3 • P + 0.2 • E + 0.4 • F) (requirement of three qualifications greater than 4 and F ≥ 4)
and
(F) (requirement of three qualifications greater than 4).

In the case of having two qualifications less than 4 before the Final Examination (F), the student cannot attend such examination and may, alternatively, request the cancellation of the call or have as qualification in the Act the lowest of the grades obtained in examinations (N, P or E).

In the case of making the Final exam (F) and then breaching the requirement for three qualifications higher than 4 points, the student will be rated in the Act with the lowest of grades in exams (N, P, E or F).

In the second and successive calls, due to the characteristics of this matter, a single exam that includes Nomenclature, Spectroscopy and full contents of the course will take place.

ASSESSMENT OF THE COMPETENCES

E2: Qualification included in the Act
E7: Final Exam Qualification (Extraordinary Exam)
T3: Bologna Mean
CRI3: Qualification included in the Act

BIBLIOGRAPHY

BASIC BIBLIOGRAPHY:

- J. McMurry, *Organic Chemistry* (7th edition), Brooks/Cole Publishing Company, Pacific Grove, California, 2008.

BIBLIOGRAPHY or COMPLEMENTARY MATERIAL:

- http://iqs.moodle.com
- S. Seyhan. Química Orgánica.Tomos 1 y 2. Ed. Reverté, 1997.
- R. T. Morrison, R. N. Boyd, *Organic Chemistry* (6th edition), Prentice Hall International Inc, New Jersey, 1992
- A. Streitwiesser, C. H. Heathcock, E. M. Kosover, *Introduction to Organic Chemistry* (4th edition), MacMillan Publishing Company, New York, 1992
- E. Fernández, F. Fariña, *Nomenclatura de la Química Orgánica (Secciones A, B, C, D, E, F y H)*, CSIC-RSEQ, Madrid, 1987
- A. Messeguer, M. A. Pericás, *Nomenclatura de Química Orgànica (Seccions A, B i C)*, CSIC-Institut d'Estudis Catalans, Barcelona, 1989
- E. Quiñoá, R. Riguera, Cuestiones y Ejercicios de Química Orgánica. Una guía de estudio y autoevaluación. McGraw-Hill, Madrid, 1994.
- E. Quiñoá, R. Riguera, Nomenclatura y representación de los compuestos orgánicos. Una guía de estudio y autoevaluación. McGraw-Hill, Madrid, 1996.
- K. Weissermel, H. J. Arpe, Química Orgánica Industrial. Productos de partida e *intermedios más importantes*, Reverté, 1978.

DOCUMENT HISTORY

PREVIOUS REVISIONS
September 25, 2016, Dr. José I. Borrell
June 20, 2015, Dr. José I. Borrell
June 26, 2014, Dr. José I. Borrell
July 24th, 2012, Dr. José I. Borrell
7th September 2011, Dr. José I. Borrell
14th July 2011, Dr. José I. Borrell

CURRENT REVISION
August 20, 2018, Dr. José I. Borrell