COURSE DATA

Data Subject	
Code	36469
Name	Structural Determination in Organic Chemistry
Cycle	Grade
ECTS Credits	6.0
Academic year	2023 - 2024

Study (s)

Degree	Center	Acad. year	Period
1110 - Degree in Chemistry	Faculty of Chemistry	4	First term

Subject-matter

Degree	Subject-matter	Character
1110 - Degree in Chemistry	17 - Organic Chemistry Applied	Optional

Coordination

Name	Department
GAVIÑA COSTERO, PABLO	325 - Organic Chemistry

SUMMARY

The course "Structure Determination in Organic Chemistry" is part of the subject "Applied Organic Chemistry" of 22.5 ECTS that is part of the Chemistry, Industry and Society Module. This is an optional subject of 6.0 ECTS credits taught in the 7th semester of fourth grade.

The basic objective of this course is to deepen and broaden the knowledge acquired in the Organic Chemistry courses. Its approach is fundamentally practical and its aim is to provide students with an overview of the main currently available spectroscopic techniques (UV-visible, infrared and nuclear magnetic resonance) as well as mass spectrometry, and its practical application to obtain information and structure determination of organic compounds. In addition, it is aimed for the students to acquire sufficient knowledge to design the best way to approach a given structure determination problem from the information provided by each type of spectrum, as well as be familiar with the applications and limitations of each of the spectroscopic techniques.

Today most of the structural elucidation problems, both in the research and industrial fields, are solved in an easy, fast and secure way with the use of the techniques that are studied in this course. It provides students and future chemists with sufficient resources for the application of spectroscopic methods to the resolution of the less complex structural problems.

PREVIOUS KNOWLEDGE

Relationship to other subjects of the same degree

There are no specified enrollment restrictions with other subjects of the curriculum.

Other requirements

Although the subject has a basic training character, it is essential that the student possesses a solid background in terminology, nomenclature and structural properties of the functional groups of organic molecules. The student should get acquainted with the previously gained concepts of stereochemistry and spectroscopy of organic molecules as well as the theoretical fundamentals required to understand the physical and chemical principles related to absorption spectroscopy and spin nuclear magnetic resona

OUTCOMES

1110 - Degree in Chemistry

- Show inductive and deductive reasoning ability.
- Solve problems effectively.
- Demonstrate ability to work in teams both in interdisciplinary teams and in an international context.
- Ability to recognise chemical elements and their compounds: preparation, structure, reactivity, properties and applications.
- Relate the macroscopic properties and the properties of individual atoms and molecules, including macromolecules (natural and synthetic), polymers, colloids and other materials.
- Recognise and analyse new problems and plan strategies to solve them.
- Evaluate, interpret and synthesise chemical data and information.
- Carry out standard experimental procedures involved in synthetic and analytical work, in relation to organic and inorganic systems.
- Relate theory and experimentation.
- Students must be able to apply their knowledge to their work or vocation in a professional manner and have acquired the competences required for the preparation and defence of arguments and for problem solving in their field of study.

- Students must have developed the learning skills needed to undertake further study with a high degree of autonomy.
- Express oneself correctly, both orally and in writing, in any of the official languages of the Valencian Community.
- Have basic skills in the use of information and communication technology and properly manage the information obtained.

LEARNING OUTCOMES

The previous section includes the competences contained in the document VERIFICA. This subject addresses part of the learning results of the matter Applied Organic Chemistry that allow to acquire specific knowledge of chemistry, cognitive skills and general skills recommended by the EUROPEAN CHEMISTRY THEMATIC NETWORK (ECTN) for the Chemistry Eurobachelor® Label. The following table lists the learning outcomes acquired in the subject Structural Determination in Organic Chemistry related to the competences of the degree in Chemistry.

SPECIFIC KNOWLEDGE OF CHEMISTRY	
The learning process should allow the degree graduates to demonstrate:	
	Competences of the subject Structural Determination in Organic Chemistry **that contemplate the learning outcomes EUROBACHELOR®**
The principles and procedures used in chemical analysis and the characterisation of chemical compounds.	Demonstrate knowledge of the principles, procedures and techniques for the determination, separation, identification and characterisation of chemical compounds.(CE8) Understand the qualitative and quantitative aspects of chemical problems..(CE24).
The principal techniques of structural investigations, including spectroscopy	Ability to recognise chemical elements and their compounds: preparation, structure, reactivity, properties and applications..(CE7). Demonstrate knowledge of the principles, procedures and techniques for the determination, separation, identification and characterisation of chemical compounds.(CE8)

The structural features of chemical elements and their compounds, including stereochemistry.	Ability to recognise chemical elements and their compounds: preparation, structure, reactivity, properties and applications..(CE7). Relate the macroscopic properties and the properties of individual atoms and molecules, including macromolecules (natural and synthetic), polymers, colloids and other materials.CE11).

COMPETENCES AND COGNITIVE SKILLS	
The learning process should allow the degree graduates to demonstrate:	
	Competences of the subject Structural Determination in Organic Chemistry **that contemplate the learning outcomes EUROBACHELOR®**
Ability to demonstrate knowledge and understanding of the facts, concepts, principles and fundamental theories related to the topics mentioned above.	Demonstrate knowledge and understanding of essential facts, concepts, principles and theories related to the areas of chemistry..(CE13).
Ability to apply this knowledge and understanding to the solution of common qualitative and quantitative problems.	Solve qualitative and quantitative problems following previously developed models..(CE14). Recognise and analyse new problems and plan strategies to solve them..(CE15). Understand the qualitative and quantitative aspects of chemical problems..(CE24).
Competences for the evaluation, interpretation and synthesis of information and chemical data.	Interpret data from observations and measurements in the laboratory in terms of their significance and the theories that underpin them..(CE20).

GENERAL COMPETENCES	
The learning process should allow the degree graduates to demonstrate:	
	Competences of the subject Structural Determination in Organic Chemistry **that contemplate the learning outcomes EUROBACHELOR®**
ility to apply practical knowledge to solve problems related to qualitative and quantitative information.	Solve problems effectively..(CG4). Solve qualitative and quantitative problems following previously developed models..(CE14). Relate theory and experimentation..(CE22). Recognise and evaluate chemical processes in daily life..(CE23). Understand the qualitative and quantitative aspects of chemical problems..(CE24).
Study skills necessary for professional development. These will include the ability to work autonomously.	Demonstrate leadership and management skills, entrepreneurship, initiative, creativity, organization, planning, control, leadership, decision making and negotiation..(CG3). Demonstrate ability to work in teams both in interdisciplinary teams and in an international context..(CG5). Learn autonomously.(CG8). Demonstrate the ability to adapt to new situations..(CG9). Students must have developed the learning skills needed to undertake further study with a high degree of autonomy.(CB5).

DESCRIPTION OF CONTENTS

1. Physical methods of structural determination. UV-visible spectroscopy (UV-Vis).

The electromagnetic spectrum. Types of radiation/matter interactions. Absorption spectroscopy: transitions between energy levels. Ultraviolet (UV) -visible spectroscopy. Electronic transitions. Fundamental concepts. The UV-VIS spectrophotometer. Sample preparation. Characteristic absorptions of organic molecules. Chromophores: olefins, polyenes, benzene and derivatives, carbonyl compounds. Effects of solvent and pH.

2. Infrared Spectroscopy (IR)

The Fundamentals of Infrared Spectroscopy. Molecular Vibrations. Hooke's law. Types of vibrations. Factors that influence the position and shape of the bands: bands coupling, hydrogen bonding, conjugation, electronic effects and ring strain. The infrared spectrophotometer. Sample preparation. Characteristic absorptions of the functional groups of organic molecules. IR spectra interpretation.

3. Fundamentals of Nuclear Magnetic Resonance spectroscopy

Nuclear spins. Nuclei in an external magnetic field. Energy levels population. Description of the phenomenon of nuclear magnetic resonance: resonance conditions. Macroscopic magnetization. The relaxation processes. Simplification of the analysis of the resonance process. Shielding. The NMR spectrum: Resolution. Continuous Wave NMR Spectrometers. Pulse method and Fourier transform. Angle of a pulse Width of a pulse. Induction Free Decay (FID). Fourier transform. Spectra accumulation. Pulse spectrometer and Fourier transform.

4. Proton Nuclear Magnetic Resonance

Resonance frequencies for the different nuclei. Chemical shift. The scale. Shielding and decoupling. Sample preparation for NMR. NMR spectra analysis. Types of protons in NMR. Integration of the signals area. Signal splitting: spin-spin coupling. Types of spin-spin coupling. Multiplicity. First order couplings. More complex couplings. Chemical shift values. Factors that affect chemical displacement: Inductive effect, Magnetic anisotropy, Van der Waals repulsions, Existence of hydrogen bonds, Conjugative effects. Tables for estimating the chemical shift.

5. Analysis of proton NMR spectra

Complex spin-spin coupling systems. Second-order approximation. Examples of coupling systems. Special effects in NMR: Chemical exchange processes (intermolecular, with the solvent, Intramolecular). Spin-spin decoupling: double resonance. Introduction to the Nuclear Overhauser Effect (NOE). Two-dimensional experiments 1H 1H (COSY).

6. 13-Carbon Nuclear Magnetic Resonance

Analysis of a 13C NMR spectrum. 13C- 1H Couplings. Decoupling: Broad Band BB, Off-resonance, DEPT (Distortionless Enhancement by Polarization Transfer). Chemical shifts of 13C nuclei. Number of signals. Solvent signals. Factors influencing the displacement (). Empirical correlations. Two-dimensional experiments 1H 13C: HETCOR and HSQC.

7. Mass Spectrometry

Introduction. The mass spectrometer. Types of mass spectrometers. Most relevant ionization methods. Electron impact mass spectrometry. The molecular ion and isotopic peaks. Recognition of the molecular ion. Deduction of the molecular formula. Factors that control the modes of fragmentation. Main types of fragmentation. Fragmentation in . Benzyl fragmentation. Allylic fragmentation. Fragmentation of not activated bonds. Fragmentation of mono-halogenated derivatives. Retro Diels-Alderreaction. McLafferty transpositions. Onium reactions. Loss of CO. Elimination of water. Fragmentations into bi- and poly-functionalized compounds. Other ionization methods for analysis of bioorganic molecules. MALDI-TOF-MS.

8. Application of spectroscopic techniques to the determination of structures of organic compounds

Solution of problems by the combined application of the different techniques discussed in previous themes in order to determine the structure of simple organic compounds. Use of software as aid to structural assignment based on spectroscopic techniques.

WORKLOAD

ACTIVITY	Hours	% To be attended
Theory classes	51,00	100
Tutorials	9,00	100
Development of group work	10,00	0
Study and independent work	30,00	0
Preparation of practical classes and problem	50,00	0
TOTAL	**150,00**	

TEACHING METHODOLOGY

The subject has been conceived to give to the student the role of principal actor of its own learning and is organized in the following manner:

• **In-person theoretical classes.**

These classes will be dedicated to the exposition to the students of the fundamental aspects of the subject. Thus, the different topics found in the program will be discussed in detail in an orally form. In this way, the student will obtain a global and comprehensive view of the subject. Both, the blackboard and power point presentations will be used during this time. Previously to the classes, the educational material needed for an easy follow-up of the subject will be introduced in the "Virtual Lecture Room". These classes will be complemented with the personal work of the student.

• **Practical classes and seminars**.

In these classes, the application of the concepts introduced in the theoretical classes will be performed for the students. Previously to the attendance of the practical classes, the students must have worked the problems proposed by the professor. The resolution of these problems will be carried out either by the professor or by the students, in an individual form or in a team-work.

• **Tutorial classes.** There in all will be 9 sessions uniformly distributed along the course. Each session will last for one hour. During these sessions, the professor will evaluate the learning process of the students, who will be previously organized in small work-groups. Homework previously settled by the professor will be collected in the tutorials. In the same token, the tutorial classes will be used to solve the questions that could have come up along the course, together with the guidance about the selection of the most appropriate methods for the resolution of possible future problems.

EVALUATION

The academic achievement of the student and the final grade of the course will be due, in a weighted manner, according to the percentages shown in each section to be evaluated. All grades will be based in an absolute score over 10 points, according to the established scale in RD 1125/2003. These criteria will be kept in each exam.

The following parts will be considered and evaluated:

1. Direct assessment of the Professor (1 point):

In this assessment will be considered several aspects. Among them, we can highlight the following:

• In-person assistance to the classes with an active participation.

• Progression in the use of the proper language of organic chemistry.

• Problem resolution and questions.

• Critical turn of mind.

2.-**Tutorials, Questionnaires and Tasks** (globally 2 points): The mark of each student in this section will take into consideration:

• Assistance.

• Qualifications of the questionnaires.

• Content and written presentation of the tasks entrusted by the teacher to each work subgroup. The rating of the tasks will be an overall mark for the subgroup and be counted equally to each member..

To receive a mark in this section, the student must complete all the questionnaires and have attended a minimum of 7 tutorial classes.

3. Exams (7 points): The exam will take place in the date established by the Chemistry Faculty and it will be the same for all the subgroups of the subject. The exam will consist of several questions and exercises which allow the professor to evaluate of the aforementioned competences acquired by the students.

The exam will consist of two parts, according to the dual purpose of the course: i) issues that should be developed and / or explain certain spectroscopic characteristics of known organic compounds and ii) the reasoned determination of the structure of two organic compounds by analyzing as a whole their spectra.

To pass the subject, obtaining 3.3 points over 7 in the exam will be mandatory in order to aspects 1 and 2 be considered. In the second examination session, the qualification obtained in parts 1 and 2 will be maintained and the third part will be evaluated again as a new exam.

In the second examination session, the qualification obtained in parts 1 **(Direct assessment of the Professor)** and 2 **(Tutorials, Questionnaires and Tasks)** will be maintained and the third part will be evaluated again as a new exam.

Final warning

Copying or plagiarism of any assignment that is part of the evaluation will make it impossible to pass the course, and the student will be subject to the appropriate disciplinary procedures.

Please note that, according to Article 13 d) of the University Student Statute (RD 1791/2010, December 30), "*it is the duty of a student to refrain from using or cooperating in fraudulent procedures in evaluation tests, in the work performed or in official University documents*".

REFERENCES

Basic

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- HESSE, M.; MEIER, H.; ZEEH, B. Métodos espectroscópicos en Química Orgánica, 2ª edición, Madrid: Editorial Síntesis, 2005.
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- ChemBioOffice Ultra, PerkinElmer (CambridgeSoft) Amplia selección de aplicaciones y funcionalidades que permite a químicos y biólogos dibujar, formular, modelar y editar estructuras moleculares químicas y biológicas así como simular espectros de RMN de protón y carbono.

Additional

- PRETSCH, E.; BÜHLMANN, P.; AFFOLTER, C.; HERRERA, A.; MARTINEZ, R. Determinación estructural de compuestos orgánicos, Amsterdam: Elsevier-Masson. 2005.
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