COURSE DATA

Data Subject	
Code	36469
Name	Determinación Estructural en Química Orgánica
Cycle	Grade
ECTS Credits	6.0
Academic year	2018 - 2019

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
PARRA ALVAREZ, MARGARITA	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 resonance.

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

- To know how to acquire, use and transmit bibliographic information related to organic compounds.

- To know and be able to use the most usual techniques for the structural determination of organic compounds.

- Knowing how to find and use spectroscopic data of organic compounds.

- Understanding the relationship between spectroscopic characteristics and structural properties of the compounds and organic functional groups, applying it to the solution of structural problems.

DESCRIPTION OF CONTENTS

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

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

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. Population of energy levels. Description of the phenomenon of nuclear magnetic resonance: conditions for resonance. Macroscopic magnetization. Relaxation processes. Pulsed NMR spectroscopy and Fourier transform. Instrumentation. Sample preparation for NMR. The NMR spectrum: resolution.

4. Proton Nuclear Magnetic Resonance

Resonance frequencies for different types of nucleus. Chemical shift. Scale. Shielding and deshielding. NMR spectral analysis. NMR proton types. Chemically and magnetically equivalent nuclei. The integration ratio of signals. Splitting of signals: spin-spin coupling. Types of spin-spin coupling. Multiplicity. First order coupling. Factors affecting the proton-proton coupling. Influence of structural and intermolecular factors in the chemical shift: empirical correlations. Tables for estimating the chemical shift.

5. Analysis of proton NMR spectra

Complex spin-spin coupling systems. Second order approximation. Examples of various coupling systems. Chemical exchange processes (intermolecular, with the solvent, intramolecular): applications. Spin-spin decoupling techniques: double resonance. NOE experiments. Bidimensional: COSY and H-C correlation

6. 13-Carbon Nuclear Magnetic Resonance

Analysis of a 13C NMR spectrum. 13C-1H couplings. Decouplings: Broadband (BB), DEPT (Distortionless Enhancement by Polarization Transfer). Chemical shifts of the 13C nuclei. Factors influencing the chemical shift. Empirical correlations.

7. Mass Spectrometry

Fundamentals. Electron impact ionization. Molecular ion fragmentation. Interpretation of MS spectra. Analytical information. Molecular ion and isotopic satellites. Elemental analysis. Exact mass. Instrumentation and types of analyzers. Other ionization methods used in the analysis of organic and bioorganic molecules. Sample introduction systems and coupling to the different chromatographic separation techniques.

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**.

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 8 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.

• **Seminars**.Six seminars of 1 hour each will be held throughout the semester. In some of them, aspects related to the different techniques explained in the course will be developed. As part of the course activities, each group of students will have to elucidate the structure of an unknown sample that will be delivered by the teacher at the beginning of the course. The process developed to carry out the elucidation will be exposed through an oral presentation. For this work, students will be organized in work subgroups as well as in the case of tutoring.

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.- Seminars and tutorials (globally 2 points). In the final grade of each student the following aspects will be considered:

• In-person assistance.

• The contents and both oral and written exercises proposed by the professor in each team-work. The final grade will be global for the whole team-work and will compute the same for each member of the team.

To receive qualification in this paragraph, the student must have attended a minimum of 4 seminars and 6 tutorials.

3. Exams (70 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.

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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

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