COURSE INFORMATION

Structural Elucidation of Organic Compounds

Course number: 757509210
Degree in Chemistry
Chemistry Department
Academic Year: 2018-2019
Compulsory course. 3rd year
First semester: 6.0 credits

Course schedule:

Classes: Tue 9.00-10.00. Thu 11.30-12-30
See http://www.uhu.es/fexp/archivos/curso1819/quimica/horarios/01_teoria_quimica_18_19_v7.pdf
Problem sessions: Thu 12.30-13.30. Same place.
Check final dates and any changes on the Moodle site for the course.

TEACHING STAFF

Prof.: Jesús Fernández Arteaga
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Office hours:

First-Second Semester: Mon, Tue, Thu 9.00-11-00.

Students are welcomed to come to my office to discuss homework problems or any aspect of the course during office hours or at other times by email appointment.

SYLLABUS

1. DESCRIPTION

Integration in the Study Plan:
In the previous subjects taught belonging to the Organic Chemistry Area, it has been studied the different functionalization of the organic molecules, as well as their reactivity and synthesis. In the field of Organic Chemistry the elucidation of the structure of organic molecules holds a vital place since it is used both for the identification of compounds isolated from natural sources, and in the field of the synthesis to check whether the obtained product has the desired structure.

Impact on the professional profile:
The theoretical and practical knowledge of the different techniques used for the characterization of structures is essential for the accurate professional performance of a Chemist..

2. PREREQUISITES

Having studied previously the courses "Basic Concepts of Organic Chemistry" and "Organic Chemistry" (second year).

3. OBJECTIVES/LEARNING OUTCOMES

The main objective of the course is that the student were able to determine the structure of an unknown compound, based on the spectroscopic information obtained from the UV-Vis, IR, NMR and HR-MS spectra. The student must understand the physical principles on which each technique is based, the experimental and instrumental aspects, the structural information provided by each methodology, and finally, the student should make use of the structural information provided by each method, to propose the structure of the compound.

4. TEACHING METHODOLOGY

Theory lectures:
Meant to structure the contents and to clarify concepts. They are realized in the classroom and serve to treat the contents from a communicative perspective, encouraging the participation of the students and the realization of exercises as instruments for improving the significance of the transmitted knowledge. The activities that are realized in the classroom will be supported with diverse educative resources such as presentations in PowerPoint, molecular models, etc.

Tutorial sessions:
Here the student proposes and clarifies doubts related to any aspect of the taught matter.

5. CONTENTS

Block I. Mass spectrometry. (5 hours)
- Topic 1. Introduction to the determination of structures: (2 hours).
Chemical methods and physical methods. Spectroscopic methods.
- Topic 2. Mass spectrometry: (3 hours)
Introduction. Instrumentation. Ionization methods. Types of ions. Determination of molecular masses. Fragmentation of positive ions. General rules of fragmentation of organic molecules. Analysis of the mass spectrum. Representative examples.

Block II. UV and IR spectroscopy. (7 hours)
- Topic 3. Ultraviolet Spectroscopy: (3 hours)
The electromagnetic spectrum. Absorption of light: Beer-Lambert Law. UV-Visible spectroscopy.
- Topic 4. Infrared Spectroscopy: (4 hours)
Introduction. Types of vibrations. Hydrogen bond. Polyatomic molecules. Characteristic absorption of different functional groups. FTIR spectrophotometer. Preparation of the sample. Interpretation of IR spectra.

Block III. Nuclear Magnetic Resonance. (24 hours)
- Topic 5. Nuclear Magnetism, NMR: (4 hours)
Basic principles of nuclear magnetic resonance. Spectrophotometers. Effects of chemical shift that influence NMR. Intensities of the bands. Reference substances. Solvents.
- Topic 6. 1H Nuclear Magnetic Resonance Spectroscopy: (8 hours)
Spin-spin coupling. The coupling constant. Relation between chemical shift-molecular structure. Complex spectra. Homotopic, enantiotopic and diastereotopic groups. Stereoisomery and NMR. Proton couplings with other nuclei. Double resonance experiments. Spin decoupling. NOE effect (Nuclear Overhouser Effect): Proximity in the 1H-1H space.
- Topic 7. 13C Nuclear Magnetic Resonance Spectroscopy: (6 hours)

Magnetic resonance of 13C. Decoupling techniques. 13C quantitative analysis. DEPT experiments. Spectral correlations.
- Topic 8. 2D Nuclear Magnetic Resonance Spectroscopy: (5 hours)
COSY, HETCOR, TOCSY, NOESY and HMBC. Magnetic resonance image.
- Topic 9. NMR with other important nuclei: (1 hour)
31P, 15N, 19F.

Block IV. Solving exercises of high complexity. (9 hours)

6. BIBLIOGRAPHY

Basic:

- "Spectrometric identification of organic compounds" R.M. Silverstein, F.X. Webster, D.J. Kiemle. (Wiley, 7th Edition). .

Specific:

- "Nuclear Magnetic Resonance and Spectroscopy" J. B. Lambert, E. P. Mazzola (Pearson)
- "Spin Dynamics, Basics of Nuclear Magnetic Resonance" M. H. Levitt (Wiley, 2nd Edition 2008).
- "Organic Structures from Spectra" L.D. Field, S. Sternhell, J.R. Kalman (Wiley).
- "Tablas para la elucidación estructural de compuestos orgánicos por métodos espectroscópicos", E. Pretsch, T. Clerc, J. Seibl, W. Simon (Ed. Springer-Verlag).
- "Basic One- and Two-Dimensional NMR Spectroscopy", H. Friebolin (Ed. Wiley-VCH).

7. ASSESSMENT/GRADING

For the final qualification the basic norms of behavior and working, which should be respected by the University community of the Faculty of Experimental Sciences and which were approved by the Faculty Council, will be taken into account.

The competences acquired in each thematic unit will be evaluated jointly by taking into account the different activities of the course; i.e., exam, laboratory report, guided activities.

- Final exam/quiz: The mark obtained in the final exam counts 70% of the final assessment of the course. The exam/quiz will consist of theoretical and practical questions.

- 30% of the final assessment will be obtained by continuous evaluation: through the control of attendance at theoretical classes, attendance at programmed tutoring, periodic delivery of directed activities, together with the elaboration and / or exhibition of works carried out (bibliographic, problems, issues), individually or as a team and other.

In order to approve the course a minimum mark of 5.0 in the final exam/quiz is required. Furthermore, the global mark (consisting of the weighted contributions of exam and continuous evaluation) has to be 5.0 or higher (on a scale from 0 to 10) in order to receive approval..