COURSE GUIDE 2022/23

Faculty 215 - Faculty of Chemistry

Cycle Not Applicable

Degree GQUIMI20 - Bachelor's Degree in Chemistry

Year Third year

COURSE

26138 - Spectroscopic Identification of Organic Compounds

Credits, ECTS: 6

COURSE DESCRIPTION

The subject "Spectrophotometric Identification of Organic Compounds" corresponds to the third year of the Chemistry Degree. It is one of the electives offered in the Advanced Module.The subject prepares the student to go into the determination of the chemical structure of organic compounds by means of the application of the different spectrometric and spectroscopic techniques. In principal, the students should deepen in the routine interpretation and other more special applications of some of the spectroscopic instrumentation, as Fourier transform Infrared Spectroscopy (FTIR), NMR, Raman and Mass Spectrometry. The information provided by these techniques will allow the student to interpret and elucidate the structure of unknow compounds and/or chemical reactions products.

COMPETENCIES/LEARNING RESULTS FOR THE SUBJECT

This subject is one of the optional ones offered in the Advanced Module and therefore, shares the cross skills assigned to it, and more specifically, the competences of [M03CM06], [M03CM11] y [M03CM13].

M03CM06: Ser capaz de comprender la naturaleza de un problema analítico, investigar sobre el mismo en la bibliografía e identificar, valorar y presentar soluciones analíticas para resolverlo.
M03CM11:Capacidad de diseñar, programar y llevar a cabo procesos experimentales, así como de utilizar técnicas instrumentales adecuadas a distintos tipos de problemas de índole química.
M03CM13: Transmitir fenómenos y procesos relacionados con la química y materias afines, en exposiciones orales y/o informes escritos y de manera comprensible, empleando para ello alguna de las dos

The Grade Coordination Committee is the responsible for the coordination of this subject with the rest of the especiality subjects.

CONTENIDOS TEÓRICO-PRÁCTICOS

Fourier transform Infrared Spectroscopy. Spectra resolution. Instrumentation and sample preparation.
Mass spectrosmetry. Basics and intrumentation. Fragmentation proccesses. Main organic compounds mass spectra.
NMR spectroscopy. Fundamentals of the technique and instrumentation. Chemical shift in proton and carbon NMR. Spectra analysis.
UV/Visible spectroscopy: Fundamentals, chomophore compounds. Use of tables in the determination of absorption peaks. Exercises.

TEACHING METHODS

Lectures (M, clases magistrales) focus on providing basic knowledge of the subject.
Practical Classroom Work hours (GA, prácticas de aula) are directed to the application of the acquired theoretical knowledge to solve problems posed by the professor.
Individual assignments will be part of the self-study hours of the students, and consist of the resolution of three problem sets, one of them delivered in the first quarter and two sets delivered in the second quarter.
Practical Lab Work (GL, prácticas de laboratorio) is held individually in the first quarter, and consists of registering two infrared spectra (carried out during the lab hours) and their interpretation (carried out as self-study task).

TYPES OF TEACHING

Types of teaching	M	S	GA	GL	GO	GCL	TA	TI	GCA
Hours of face-to-face teaching	40		15	5					
Horas de Actividad No Presencial del Alumno/a	60		22,5	7,5					

Legend:
M: Lecture-based
S: Seminar
GA: Applied classroom-based groups
GL: Applied laboratory-based groups
GO: Applied computer-based groups
GCL: Applied clinical-based groups
TA: Workshop
TI: Industrial workshop
GCA: Applied fieldwork groups

Evaluation methods

- Continuous evaluation
- End-of-course evaluation

Evaluation tools and percentages of final mark

- Written test, open questions 70%
- Exercises, cases or problem sets 6%
- Individual assignments 24%

ORDINARY EXAMINATION PERIOD: GUIDELINES AND OPTING OUT

The written exam will account for 70% of the final mark and it will be divided into two separate tests each having the same value. The student must obtain a minimum mark of 4.0 in each of them and the final average value has to be at least 5.0 in order to promediate with those marks obtained in the rest of activities. If the student gets in the first test a mark of 4.0 or higher, he/she could have the option, in the second one, of being tested just of the second part or of the whole course syllabus. Lab work and individual work will account for 6 and 24% of the final mark respectively.
Criteria for continuous assessment waiver are those established in Chapter 2, Articles 8 and 12 of the Student Assessment Regulation for Bachelor’s Degrees of the UPV/EHU.
Criteria for final evaluation request are those established in Chapter 2, Article 8 of the Student Assessment Regulation for Bachelor’s Degrees of the UPV/EHU.

"No presentado" grade is given if the student does not take part in the final exam, as established in Chapter 2, Article 12 of the Student Assessment Regulation for Bachelor’s Degrees of the UPV/EHU.

EXTRAORDINARY EXAMINATION PERIOD: GUIDELINES AND OPTING OUT

In the 2nd convocation (July) the student will be evaluated exclusively by means of the mark obtained in a written exam.

MANDATORY MATERIALS

They will be described each year in the student guide.

BIBLIOGRAFÍA

Basic bibliography

G. Sócrates. Infrared Characteristic Group Frequencies. 2nd edition. Wiley & Sons Ltd., 1994.
E. Prestch, P. Bühlmann, C. Affolter, M. Baderstcher. Structural Determination of Organic Compounds. Springer-Verlag, 2007.
E. Prestch, T. Clerk, J. Seibl, W. Simon. Tablas para la elucidación estructural de compuestos orgánicos por métodos espectroscópicos, 2ª Edición. Alhambra, 1989.
R. M. Silverstein, G. Bassler, T. Morrill. Spectrometric Identification of Organic Compounds. 5th Edition, Wiley & Sons, Inc., 2005.
S. Wartewig. IR and Raman Spectroscopy: Fundamental Processing. Wiley, 2003.

Detailed bibliography

J.M. Chalmers, P.R. Griffiths. Handbook of Vibrational Spectroscopy. Wiley, 2002.
J. Simpson. Organic Structure Determination using 2D-NMR Spectroscopy. Academic Press, 2008.
N.J. Harrick. Internal Reflection Spectroscopy. Review and Supplement. Harrick Sci. Corp., 1985

Journals

Vibrational Spectroscopy

Web sites of interest

http://www.spectroscopynow.com
http://www.dq.fct.unl.pt/qoa/jas/ir.html

OBSERVATIONS