

**1. General information**

Course: STRUCTURAL ANALYSIS
Type: CORE COURSE
Degree: 409 - CHEMISTRY
Center: 1 - FACULTY OF SCIENCE AND CHEMICAL TECHNOLOGY
Year: 3

Main language: Spanish
Use of additional languages:
Web site:

Code: 57320
ECTS credits: 6
Academic year: 2023-24
Group(s): 20 23
Duration: First semester
Second language: English
English Friendly: Y
Bilingual: N

Lecturer: MARIA ANTONIA HERRERO CHAMORRO - Group(s): 20 23				
Building/Office	Department	Phone number	Email	Office hours
Irica	QUÍMICA INORG., ORG., Y BIOQ.	926052556	mariaantonia.herrero@uclm.es	Tuesday, Wednesday and Thursday from 4:30 p.m. to 6:30 p.m.
Lecturer: BLANCA ROSA LOURDES MANZANO MANRIQUE - Group(s): 20 23				
Building/Office	Department	Phone number	Email	Office hours
San Alberto Magno/first floor	QUÍMICA INORG., ORG., Y BIOQ.	926052050	blanca.manzano@uclm.es	Tuesday, Wednesday and Thursday from 4:30 p.m. to 6:30 p.m.

2. Pre-Requisites

Not established

3. Justification in the curriculum, relation to other subjects and to the profession

Not established

4. Degree competences achieved in this course**Course competences**

Code	Description
CB02	Apply their knowledge to their job or vocation in a professional manner and show that they have the competences to construct and justify arguments and solve problems within their subject area.
E01	Understand and use chemical terminology, nomenclature, conventions and units
E05	Know the chemical elements and their compounds, their forms of obtaining, structure, properties and reactivity, as well as the main techniques for their analysis
E06	Know the structural properties of chemical compounds, including stereochemistry, as well as the main structural research techniques
E17	Develop the ability to relate to each other the different specialties of Chemistry, as well as this one with other disciplines (interdisciplinary character)
G01	Know the principles and theories of Chemistry, as well as the methodologies and applications characteristic of analytical chemistry, physical chemistry, inorganic chemistry and organic chemistry, understanding the physical and mathematical bases that require
G02	Be able to gather and interpret data, information and relevant results, obtain conclusions and issue reasoned reports on scientific, technological or other problems that require the use of chemical tools
G03	Know how to apply the theoretical-practical knowledge acquired in the different professional contexts of Chemistry
G04	Know how to communicate, orally and in writing, the knowledge, procedures and results of chemistry, both specialized and non-specialized
G05	Acquire and adapt new knowledge and techniques of any scientific-technical discipline with incidence in the chemical field
T10	Ability to use specific software for chemistry at user level
T11	Ability to obtain bibliographic information, including Internet resources

5. Objectives or Learning Outcomes**Course learning outcomes**

Description

Know the structure of the main organic functional groups
Know the basic principles of the main methods of structural determination, Ultraviolet-Visible spectroscopy, Infrared, RAMAN, Nuclear Magnetic Resonance and Mass Spectrometry
Apply the concepts of symmetry in the resolution of structural problems
Ability to obtain information from tables and graphs to solve a problem of structural determination
Know the application of these techniques in the analysis and resolution of everyday problems and in related scientific fields
Know the stereochemistry of the compounds
Know the main applications of the methods of structural determination, so that the student is capable of: From spectroscopic data deduce structures of organic and inorganic compounds and, from a determined structure, predict the most significant characteristics of the corresponding spectra
Acquire skill in oral and written exposition
Encourage and promote in the student all those values and attitudes inherent to scientific activity.
Jointly use the techniques of structural determination showing their complementarity
Know the main aspects of the terminology and nomenclature in Inorganic and Organic Chemistry.
The student must be able to discern and select the most appropriate techniques for solving a specific problem

Be able to search and select information in the field of Inorganic and Organic Chemistry, and present it adequately both orally and in writing, developing its capacity for synthesis, being critical and objective

6. Units / Contents

Unit 1: NMR basic concepts: ^1H and ^{13}C NMR

Unit 1.1 Basic concepts of NMR spectroscopy

Unit 1.2 ^1H and ^{13}C NMR. Chemical Shift

Unit 1.3 Spin spin coupling: Double resonance

Unit 1.4 Applications of ^1H and ^{13}C NMR

Unit 1.5 Relaxation processes

Unit 1.6 Introduction of the multipulses resonance

Unit 2: NMR of other nuclei different from ^1H and ^{13}C

Unit 2.1 Other nuclei of interest in NMR

Unit 2.2 Spin spin coupling

Unit 2.3 Satellites of spin spin coupling

Unit 2.4 Dynamic resonance

Unit 2.5 Metodology for spectra simplification

Unit 2.6 NMR of important nuclei in Inorganic Chemistry

Unit 3: Vibrational spectroscopy

Unit 3.1 Basic concepts of IR and Raman spectroscopy

Unit 3.2 Normal modes of vibration. Use of symmetry

Unit 3.3 Applications of the IR and Raman spectroscopy in Inorganic Chemistry

Unit 4: Vibrational spectroscopy

Unit 4.1 Applications of the IR in Organic Chemistry

Unit 5: Mass spectrometry

Unit 5.1 Basic concepts of mass spectrometry

Unit 5.2 Applications of the mass spectrometry

Unit 5.3 Introduction to the techniques of chemical ionization

7. Activities, Units/Modules and Methodology

Training Activity	Methodology	Related Competences (only degrees before RD 822/2021)	ECTS	Hours	As	Com	Description
Class Attendance (theory) [ON-SITE]	Lectures	E01 E05 E06 G01 G05 T10	1.28	32	Y	N	The face-to-face classes will be dedicated to the transmission of knowledge to the students with the support of computer media and the blackboard. Simultaneously, an interaction with the student is favored by means of questions and programs such as Socrative.
Workshops or seminars [ON-SITE]	Problem solving and exercises	E01 E05 E17 G02 G03 G04 T10 T11	0.8	20	Y	N	A list of problems that students must have previously worked on is presented. In class, they are corrected and students are asked to participate by asking questions or solving them on the blackboard.
Problem solving and/or case studies [ON-SITE]	Group tutoring sessions	E01 E05 E17 G02 G03 G04	0.08	2	Y	N	Cases or problems are presented directly in class. The students have time to think about it and a debate is held on the solution.
Study and Exam Preparation [OFF-SITE]	Self-study	E06 E17 G01 G05 T10 T11	3.6	90	N	-	The student body prepares both theoretical and practical material.
Mid-term test [ON-SITE]	Assessment tests	E17 G02 G03 G04	0.16	4	Y	N	Test that allows partial elimination of the subject. A 4 is required to eliminate the subject and it will be averaged with other evaluation methods.
Final test [ON-SITE]	Assessment tests	E17 G02 G03 G04	0.08	2	Y	Y	Final exam to which the student can take the whole subject if he/she has not eliminated in the partial tests, with part of the subject if he/she has eliminated the subject, or not take the final exam if he/she has eliminated the whole subject.
Total:				6	150		
Total credits of in-class work: 2.4				Total class time hours: 60			
Total credits of out of class work: 3.6				Total hours of out of class work: 90			

As: Assessable training activity

Com: Training activity of compulsory overcoming (It will be essential to overcome both continuous and non-continuous assessment).

8. Evaluation criteria and Grading System

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Evaluation System	Continuous assessment	continuous evaluation*	Description
Assessment of problem solving and/or case studies	10.00%	0.00%	It will be taken into account the participation in the lessons and the solving and proposal of problems.
Mid-term tests	90.00%	0.00%	Two short test will be done during the semester to follow the concept adquisition of the student.
Final test	0.00%	100.00%	This must be done by those who have not passed the course through progress tests.
Total:	100.00%	100.00%	

According to art. 4 of the UCLM Student Evaluation Regulations, it must be provided to students who cannot regularly attend face-to-face training activities the passing of the subject, having the right (art. 12.2) to be globally graded, in 2 annual calls per subject, an ordinary and an extraordinary one (evaluating 100% of the competences).

Evaluation criteria for the final exam:

Continuous assessment:

Continuous evaluation following the adquisition of theoretical concepts (90%) and the resolution of problems and real examples (10%). These evaluations show the adquisition of the competences.

Non-continuous evaluation:

An exam will be 90% of the grade and the resolution or practical cases will be evaluated with a 10% adapted to students who cannot attend classes

Specifications for the resit/retake exam:

The qualification will be the 100% of the final exam mark

9. Assignments, course calendar and important dates	
Not related to the syllabus/contents	
Hours	hours
Study and Exam Preparation [AUTÓNOMA][Self-study]	90
Mid-term test [PRESENCIAL][Assessment tests]	4
Final test [PRESENCIAL][Assessment tests]	2
Unit 1 (de 5): NMR basic concepts: 1H and 13C NMR	
Activities	Hours
Class Attendance (theory) [PRESENCIAL][Lectures]	10
Workshops or seminars [PRESENCIAL][Problem solving and exercises]	5
Problem solving and/or case studies [PRESENCIAL][Group tutoring sessions]	1
Unit 2 (de 5): NMR of other nuclei different from 1H and 13C	
Activities	Hours
Class Attendance (theory) [PRESENCIAL][Lectures]	9
Workshops or seminars [PRESENCIAL][Problem solving and exercises]	6
Unit 3 (de 5): Vibrational spectroscopy	
Activities	Hours
Class Attendance (theory) [PRESENCIAL][Lectures]	7
Workshops or seminars [PRESENCIAL][Problem solving and exercises]	4
Problem solving and/or case studies [PRESENCIAL][Group tutoring sessions]	1
Unit 4 (de 5): Vibrational spectroscopy	
Activities	Hours
Class Attendance (theory) [PRESENCIAL][Lectures]	3
Workshops or seminars [PRESENCIAL][Problem solving and exercises]	2
Unit 5 (de 5): Mass spectrometry	
Activities	Hours
Class Attendance (theory) [PRESENCIAL][Lectures]	3
Workshops or seminars [PRESENCIAL][Problem solving and exercises]	3
Global activity	
Activities	hours
Class Attendance (theory) [PRESENCIAL][Lectures]	32
Workshops or seminars [PRESENCIAL][Problem solving and exercises]	20
Problem solving and/or case studies [PRESENCIAL][Group tutoring sessions]	2
Study and Exam Preparation [AUTÓNOMA][Self-study]	90
Mid-term test [PRESENCIAL][Assessment tests]	4
Final test [PRESENCIAL][Assessment tests]	2
Total horas: 150	

10. Bibliography and Sources						
Author(s)	Title/Link	Publishing house	Citv	ISBN	Year	Description
Akitt, J. W.	NMR and chemistry : an introduction to modern NMR spectroscopy	Taylor & Francis			2000	RMN
D. C. Harris, M. D. Bertolucci	Symmetry and Spectroscopy					Espectroscopia vibracional
D.W. Brown, A.J. Floyd y M. Sainsbury	Organic Spectroscopy	John Wiley & sons; W. B. Saunders			1988	Parte de organica

Drago, R. S.	Physical Methods in Chemistry	Company	1997	libro general
E. Pretch, P. Bühlmann, C. Affolter, A. Herrera y R. Martínez	Determinación estructural de compuestos orgánicos.	Determinación estructural de compuestos orgánicos. Springer-Verlag Ibérica, barcelona	2001	RMN, Parte de organica
E. Pretch, T. Clerc, J. Seibl y W. Simon	Tablas para la elucidación estructural por métodos espectroscópicos. 3ª Edición.	Elsevier	1998	RMN, Parte de organica
F.A. Cotton	La Teoría de Grupos aplicada a la Química	Limusa	1983	Espectroscopia vibracional
J. A. Iggo	NMR Spectroscopy in Inorganic Chemistry,	Oxford Science Publications	1999	RMN
J.B. Lambert, H.F. Shurvell, D. Lighter y R.G. Cooks;	Introduction to Organic Spectroscopy	MacMillan,	1987	Parte de organica
K. Nakamoto	Infrared and Raman Spectra of Inorganic and Coordination Compounds	John Wiley and Sons	1997	Espectroscopia vibracional
Kemp, W	NMR in Chemistry. A Multinuclear Introduction	Mac Millan	1986	RMN
A. García, E. Teso	Análisis Orgánico	UNED	1992	Parte de organica
M. Hesse, H. Meier, B. Zeeh;	Métodos espectroscópicos en Química Orgánica	Ed. Síntesis, 2ª edición	1999	Parte de organica
Sandström, J.	Dynamic NMR Spectroscopy	Academic Press	1982	
Verkade, J. G.; Quin L. D.	Phosphorus-31 NMR Spectroscopy in Stereochemical Analysis	VCH	1987	RMN
W. Kemp	Organic Spectroscopy	MacMillan	1991	Parte de organica
¿ Ebsworth E. A. V. Rankin, D. W. H., Cradock S.	Structural Methods in Inorganic Chemistry	Blackwell Scientific Publications	1987	libro general
A. K. Brisdon	Inorganic Spectroscopic Methods	Oxford Science Publications	1998	RMN