



## 1. General information

**Course:** ADVANCED TECHNIQUES OF STRUCTURAL CHARACTERIZATION**Type:** CORE COURSE**Degree:** 2366 - MASTER DEGREE PROGRAMME IN CHEMICAL**Center:** 1 - FACULTY OF SCIENCE AND CHEMICAL TECHNOLOGY**Year:** 1**Main language:** Spanish**Use of additional languages:****Web site:****Code:** 311123**ECTS credits:** 6**Academic year:** 2023-24**Group(s):** 20**Duration:** First semester**Second language:** English**English Friendly:** Y**Bilingual:** N

Lecturer: <b>ANTONIO DE LA HOZ AYUSO</b> - Group(s): <b>20</b>				
Building/Office	Department	Phone number	Email	Office hours
San Alberto Magno	QUÍMICA INORG., ORG., Y BIOQ.	926295411	antonio.hoz@uclm.es	Monday, Tuesday and Wednesday from 17 to 19 h
Lecturer: <b>BLANCA ROSA LOURDES MANZANO MANRIQUE</b> - Group(s): <b>20</b>				
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## 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
CB08	Students are able to integrate knowledge and deal with the complexity of making judgements on the basis of incomplete or limited information, including reflections on the social and ethical responsibilities linked to the application of their knowledge and judgements.
CB09	Students are able to communicate their conclusions and the ultimate knowledge and rationale behind them to specialist and non-specialist audiences in a clear and unambiguous way.
CB10	Students possess the learning skills that will enable them to continue studying in a largely self-directed or autonomous way.
CE04	Evaluate the usefulness of separation, analysis and structural determination techniques for joint application in problem solving, and be skilled in the use of such techniques in both research and routine laboratories applying methods of organic and inorganic analysis and/or synthesis.
CE09	To develop experiments that serve as a basis for R+D+I activities in the field of chemistry, facilitating their transfer to the productive world by means of new standardised work procedures validated for routine and/or control laboratories.
CG02	To achieve advanced training in the fundamentals and potential of the instrumental techniques available in chemistry for the development of scientific research and/or application in specialised control laboratories.
CG03	To achieve advanced training in the management and handling of experimental techniques and procedures in the chemical laboratory.

## 5. Objectives or Learning Outcomes

## Course learning outcomes

## Description

To understand the effect of radiofrequency pulses in NMR.

To know the phenomenon of X-ray diffraction applied to the determination of structures from single crystals or microcrystalline powder.

To know the basis and information provided by RAMAN and IR spectroscopy techniques, especially applied to the study of surfaces.

To understand the rationale and information provided by X-ray spectroscopy techniques (XRF, XANES, EXAFS) and electron spectroscopy (XPS, Auger).

To know the basis and information provided by scanning electron microscopy (SEM), transmission electron microscopy (TEM) and local probe electron microscopy (AFM and STM) techniques. Use of electron microscopy for quantitative analysis (SEM-EDX).

To know the origin of the information conveyed in one- and two-dimensional techniques.

To know the applications of the main one- and two-dimensional pulse sequences.

Handling processing and simulation software for different techniques.

To be able to analyse the information provided by a given technique in order to deduce the structure of the product under study and to know how to select and apply the most appropriate characterisation technique for each type of structural analysis.

To know the main methods of sensitivity transfer

To learn the most advanced NMR techniques, solid resonance, gradients, inverse resonance, imaging, diffusion...

## 6. Units / Contents

**Unit 1:****Unit 2:****Unit 3:****Unit 4:**

Unit 5:  
Unit 6:  
Unit 7:  
Unit 8:  
Unit 9:  
Unit 10:  
Unit 11:

#### 7. Activities, Units/Modules and Methodology

Training Activity	Methodology	Related Competences (only degrees before RD 822/2021)	ECTS	Hours	As	Com	Description
Writing of reports or projects [OFF-SITE]	Reading and Analysis of Reviews and Articles	CB08 CB09	1.44	36	Y	Y	
Class Attendance (theory) [ON-SITE]	Lectures	CB08 CB09 CB10 CE04 CE09 CG02 CG03	1.2	30	Y	Y	
Study and Exam Preparation [OFF-SITE]	Self-study	CB08 CB10 CE04 CG02	1.44	36	Y	N	
Analysis of articles and reviews [OFF-SITE]	Self-study	CB08 CB09	1.2	30	Y	Y	
Project or Topic Presentations [ON-SITE]	Project/Problem Based Learning (PBL)	CB08 CB09 CB10	0.12	3	Y	N	
On-line debates and forums [OFF-SITE]	Cooperative / Collaborative Learning	CB09 CB10 CE04	0.28	7	Y	N	
Final test [ON-SITE]	Assessment tests	CB09 CG02	0.08	2	Y	Y	
Problem solving and/or case studies [ON-SITE]	Guided or supervised work	CB08 CB09 CB10 CE04 CE09 CG02	0.24	6	Y	Y	
<b>Total:</b>			<b>6</b>	<b>150</b>			
<b>Total credits of in-class work: 1.64</b>			<b>Total class time hours: 41</b>				
<b>Total credits of out of class work: 4.36</b>			<b>Total hours of out of class work: 109</b>				

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

Evaluation System	Continuous assessment	Non-continuous evaluation*	Description
Projects	20.00%	20.00%	
Test	40.00%	60.00%	
Assessment of problem solving and/or case studies	30.00%	15.00%	
Other methods of assessment	5.00%	5.00%	
Assessment of active participation	5.00%	0.00%	
<b>Total:</b>	<b>100.00%</b>	<b>100.00%</b>	

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).

#### 9. Assignments, course calendar and important dates

Not related to the syllabus/contents	
Hours	hours
<b>Unit 1 (de 11):</b>	
<b>Activities</b>	<b>Hours</b>
Writing of reports or projects [AUTÓNOMA][Reading and Analysis of Reviews and Articles]	2
Class Attendance (theory) [PRESENCIAL][Lectures]	2.5
Study and Exam Preparation [AUTÓNOMA][Self-study]	3
Analysis of articles and reviews [AUTÓNOMA][Self-study]	3
On-line debates and forums [AUTÓNOMA][Cooperative / Collaborative Learning]	.5
Final test [PRESENCIAL][Assessment tests]	.15
<b>Unit 2 (de 11):</b>	
<b>Activities</b>	<b>Hours</b>
Writing of reports or projects [AUTÓNOMA][Reading and Analysis of Reviews and Articles]	1
Class Attendance (theory) [PRESENCIAL][Lectures]	1.5
Study and Exam Preparation [AUTÓNOMA][Self-study]	2
Analysis of articles and reviews [AUTÓNOMA][Self-study]	2
Final test [PRESENCIAL][Assessment tests]	.15
<b>Unit 3 (de 11):</b>	
<b>Activities</b>	<b>Hours</b>
Writing of reports or projects [AUTÓNOMA][Reading and Analysis of Reviews and Articles]	4
Class Attendance (theory) [PRESENCIAL][Lectures]	2.5

Study and Exam Preparation [AUTÓNOMA][Self-study]	3
Analysis of articles and reviews [AUTÓNOMA][Self-study]	3
Project or Topic Presentations [PRESENCIAL][Project/Problem Based Learning (PBL)]	1
On-line debates and forums [AUTÓNOMA][Cooperative / Collaborative Learning]	.5
Final test [PRESENCIAL][Assessment tests]	.15
Problem solving and/or case studies [PRESENCIAL][Guided or supervised work]	1
<b>Unit 4 (de 11):</b>	
<b>Activities</b>	<b>Hours</b>
Writing of reports or projects [AUTÓNOMA][Reading and Analysis of Reviews and Articles]	5
Class Attendance (theory) [PRESENCIAL][Lectures]	3.5
Study and Exam Preparation [AUTÓNOMA][Self-study]	4
Analysis of articles and reviews [AUTÓNOMA][Self-study]	4
Project or Topic Presentations [PRESENCIAL][Project/Problem Based Learning (PBL)]	1
On-line debates and forums [AUTÓNOMA][Cooperative / Collaborative Learning]	1
Final test [PRESENCIAL][Assessment tests]	.15
Problem solving and/or case studies [PRESENCIAL][Guided or supervised work]	1
<b>Unit 5 (de 11):</b>	
<b>Activities</b>	<b>Hours</b>
Writing of reports or projects [AUTÓNOMA][Reading and Analysis of Reviews and Articles]	2
Class Attendance (theory) [PRESENCIAL][Lectures]	1
Study and Exam Preparation [AUTÓNOMA][Self-study]	1.5
Analysis of articles and reviews [AUTÓNOMA][Self-study]	1
Project or Topic Presentations [PRESENCIAL][Project/Problem Based Learning (PBL)]	1
On-line debates and forums [AUTÓNOMA][Cooperative / Collaborative Learning]	.5
Final test [PRESENCIAL][Assessment tests]	.15
<b>Unit 6 (de 11):</b>	
<b>Activities</b>	<b>Hours</b>
Writing of reports or projects [AUTÓNOMA][Reading and Analysis of Reviews and Articles]	4
Class Attendance (theory) [PRESENCIAL][Lectures]	4
Study and Exam Preparation [AUTÓNOMA][Self-study]	4.5
Analysis of articles and reviews [AUTÓNOMA][Self-study]	2
On-line debates and forums [AUTÓNOMA][Cooperative / Collaborative Learning]	.5
Final test [PRESENCIAL][Assessment tests]	.15
Problem solving and/or case studies [PRESENCIAL][Guided or supervised work]	.7
<b>Unit 7 (de 11):</b>	
<b>Activities</b>	<b>Hours</b>
Writing of reports or projects [AUTÓNOMA][Reading and Analysis of Reviews and Articles]	2.4
Class Attendance (theory) [PRESENCIAL][Lectures]	2
Study and Exam Preparation [AUTÓNOMA][Self-study]	2.4
Analysis of articles and reviews [AUTÓNOMA][Self-study]	2
On-line debates and forums [AUTÓNOMA][Cooperative / Collaborative Learning]	.5
Final test [PRESENCIAL][Assessment tests]	.2
Problem solving and/or case studies [PRESENCIAL][Guided or supervised work]	.2
<b>Unit 8 (de 11):</b>	
<b>Activities</b>	<b>Hours</b>
Writing of reports or projects [AUTÓNOMA][Reading and Analysis of Reviews and Articles]	3.6
Class Attendance (theory) [PRESENCIAL][Lectures]	3
Study and Exam Preparation [AUTÓNOMA][Self-study]	3.6
Analysis of articles and reviews [AUTÓNOMA][Self-study]	3
On-line debates and forums [AUTÓNOMA][Cooperative / Collaborative Learning]	.8
Final test [PRESENCIAL][Assessment tests]	.2
Problem solving and/or case studies [PRESENCIAL][Guided or supervised work]	.7
<b>Unit 9 (de 11):</b>	
<b>Activities</b>	<b>Hours</b>
Writing of reports or projects [AUTÓNOMA][Reading and Analysis of Reviews and Articles]	3.6
Class Attendance (theory) [PRESENCIAL][Lectures]	3
Study and Exam Preparation [AUTÓNOMA][Self-study]	3.6
Analysis of articles and reviews [AUTÓNOMA][Self-study]	3
On-line debates and forums [AUTÓNOMA][Cooperative / Collaborative Learning]	.8
Final test [PRESENCIAL][Assessment tests]	.2
Problem solving and/or case studies [PRESENCIAL][Guided or supervised work]	.7
<b>Unit 10 (de 11):</b>	
<b>Activities</b>	<b>Hours</b>
Writing of reports or projects [AUTÓNOMA][Reading and Analysis of Reviews and Articles]	1.2
Class Attendance (theory) [PRESENCIAL][Lectures]	1
Study and Exam Preparation [AUTÓNOMA][Self-study]	1.2
Analysis of articles and reviews [AUTÓNOMA][Self-study]	1
On-line debates and forums [AUTÓNOMA][Cooperative / Collaborative Learning]	.4
Final test [PRESENCIAL][Assessment tests]	.1
Problem solving and/or case studies [PRESENCIAL][Guided or supervised work]	.2
<b>Unit 11 (de 11):</b>	

Activities	Hours
Writing of reports or projects [AUTÓNOMA][Reading and Analysis of Reviews and Articles]	7.2
Class Attendance (theory) [PRESENCIAL][Lectures]	6
Study and Exam Preparation [AUTÓNOMA][Self-study]	7.2
Analysis of articles and reviews [AUTÓNOMA][Self-study]	6
On-line debates and forums [AUTÓNOMA][Cooperative / Collaborative Learning]	1.5
Final test [PRESENCIAL][Assessment tests]	.4
Problem solving and/or case studies [PRESENCIAL][Guided or supervised work]	1.5
<b>Global activity</b>	
Activities	hours
Class Attendance (theory) [PRESENCIAL][Lectures]	30
Analysis of articles and reviews [AUTÓNOMA][Self-study]	30
On-line debates and forums [AUTÓNOMA][Cooperative / Collaborative Learning]	7
Writing of reports or projects [AUTÓNOMA][Reading and Analysis of Reviews and Articles]	36
Project or Topic Presentations [PRESENCIAL][Project/Problem Based Learning (PBL)]	3
Study and Exam Preparation [AUTÓNOMA][Self-study]	36
Final test [PRESENCIAL][Assessment tests]	2
Problem solving and/or case studies [PRESENCIAL][Guided or supervised work]	6
<b>Total horas: 150</b>	

10. Bibliography and Sources						
Author(s)	Title/Link	Publishing house	Citv	ISBN	Year	Description
S. L. Flegler, J. W. Heckman, Jr., Klomparens, K. L.	Scanning and Transmission Electron Microscopy. An Introduction	Oxford University Press			1993	Libro que profundiza en las técnicas de SEM y TEM y en mic. electrónica par análisis
J. M. Albella, A. M. Cintas, T. Miranda, J. M. Serratosa	Introducción a la Ciencia de materiales. Técnicas de preparación y caracterización	CSIC	Madrid	84-00-07343-6	1993	Libro de ciencia de materiales. Incluye técnicas de rayos X, de microscopia electrónica y esp. vibracional.
J. C. Vickerman, I. S. Gimore, Eds.	Surface Analysis. The Principal Techniques	Wiley	Chichester	9780470017630	2009	Libro sobre diferentes técnicas de caracterización de superficies. Muy bueno el capítulo de XPS
	<a href="https://www.wiley.com/en-us/Surface+Analysis%3A+The+Principal+Techniques%2C+2nd+Edition-p-9780470017630">https://www.wiley.com/en-us/Surface+Analysis%3A+The+Principal+Techniques%2C+2nd+Edition-p-9780470017630</a>					
A. R. West	Basic Solid State Chemistry	WILEY		0-471-91798-2	1984	Libro básico de Química del estado sólido pero que incluye también técnicas de caracterización
	<a href="https://onlinelibrary.wiley.com/doi/abs/10.1002/%28SiCl%291099-0739%28200004%2914%3A4%3C227%3A%3AAID-AOC949%3E3.0.CO%3B2-F">https://onlinelibrary.wiley.com/doi/abs/10.1002/%28SiCl%291099-0739%28200004%2914%3A4%3C227%3A%3AAID-AOC949%3E3.0.CO%3B2-F</a>					
G. Ertl	Reaction at Solid Surfaces	Wiley	Hoboken	9780470535295	2009	Estudio detallado de las superficies de sólidos y reacciones sobre ellas
	<a href="https://onlinelibrary.wiley.com/doi/book/10.1002/9780470535295">https://onlinelibrary.wiley.com/doi/book/10.1002/9780470535295</a>					
J. M. Thomas, W. J. Thomas	Principles and Practice of Heterogeneous Catalysis	VCH	Weinheim	3-527-29239-X	1997	Libro sobre catálisis heterogénea. Incluye un capítulo de caracterización de las superficies de catalizadores, con muchas técnicas a un nivel relativamente básico.
	<a href="https://onlinelibrary.wiley.com/doi/abs/10.1002/bbpc.199700023">https://onlinelibrary.wiley.com/doi/abs/10.1002/bbpc.199700023</a>					
H. Günther	NMR Spectroscopy	WILEY	Weinheim	978-3-527-33004-1	2013	Libro avanzado de RMN con bastantes aspectos teóricos
	<a href="https://www.wiley.com/en-us/NMR+Spectroscopy%3A+Basic+Principles%2C+Concepts+and+Applications+in+Chemistry%2C+3rd+Edition-p-9783527330003">https://www.wiley.com/en-us/NMR+Spectroscopy%3A+Basic+Principles%2C+Concepts+and+Applications+in+Chemistry%2C+3rd+Edition-p-9783527330003</a>					
H. Friebolin	Basic One- and Two Dimensional NMR Spectroscopy	WILEY	Manheim	978-3-527-32782-9	2010	Texto básico y muy didaction sobre RMN en una y dos dimensiones
	<a href="https://www.wiley.com/en-us/Basic+One+and+Two+Dimensional+NMR+Spectroscopy%2C+5th%2C+Completely+Revised+and+Updated+Edition-p-9783527327829">https://www.wiley.com/en-us/Basic+One+and+Two+Dimensional+NMR+Spectroscopy%2C+5th%2C+Completely+Revised+and+Updated+Edition-p-9783527327829</a>					
R. Freeman	Magnetic Resonance in Chemistry and Medicine	Oxford University Press	Oxford	0-19-926225-X	2005	libro práctico y didáctico que enlaza la RMN clásica y la imagen por RMN
	<a href="https://global.oup.com/academic/product/magnetic-resonance-in-chemistry-and-medicine-9780199262250?cc=es&amp;lang=en&amp;">https://global.oup.com/academic/product/magnetic-resonance-in-chemistry-and-medicine-9780199262250?cc=es&amp;lang=en&amp;</a>					
S. Berger, S. Braun	200 and More NMR Experiments: A Practical Course	VCH	Weinheim	978-3-527-31067-8	2004	Libro práctico sobre secuencias de pulso mono y bidimensionales
	<a href="https://www.wiley.com/en-us/200+and+More+NMR+Experiments%3A+A+Practical+Course-p-9783527310678">https://www.wiley.com/en-us/200+and+More+NMR+Experiments%3A+A+Practical+Course-p-9783527310678</a>					
A. K. Cheetham, P. Day	Solid State Chemistry. Thecniques	Oxford University Press	Oxford	0-19-855165-7	1991	Incluye la mayoría de las técnicas vistas en la asignatura, en algunos caos a un nivel más elevado
	<a href="https://onlinelibrary.wiley.com/doi/10.1002/qua.560340110">https://onlinelibrary.wiley.com/doi/10.1002/qua.560340110</a>					
Jenny P. Glusker; Mitchell Lewis and Miriam Rossi	Crystal Structure Analysis for Chemists and Biologists	VCH		0-89573-273-4	1994	
	<a href="https://onlinelibrary.wiley.com/doi/abs/10.1002/crat.2170310212">https://onlinelibrary.wiley.com/doi/abs/10.1002/crat.2170310212</a>					
M. Martínez-Ripoll, F. Hernández-Cano	Cristalografía	WILEY			2016	Una buena parte de los contenidos se encuentran también en: <a href="http://www.xtal.iqfr.csic.es/Cristalografia/">http://www.xtal.iqfr.csic.es/Cristalografia/</a>

