UNIVERSIDAD DE CASTILLA - LA MANCHA

GUÍA DOCENTE

1. General information

Course: ADVANCED TECHNIQUES OF STRUCTURAL DETERMINATION
Code: 310590
Type: ELECTIVE
ECTS credits: 6
Degree: 2326 - MASTER DEGREE PROGRAMME IN CHEMICAL RESEARCH
Academic year: 2019-20
Center: 1 - FACULTY OF SCIENCE AND CHEMICAL TECHNOLOGY
Group(s): 20
Year: 1
Duration: C2
Main language: Spanish
Second language: English
Use of additional languages:
English Friendly: Y
Web site:
Bilingual: N

Lecturer: **ANTONIO DE LA HOZ AYUSO** - Group(s): **20**

Building/Office	Department	Phone number	Email	Office hours
San Alberto Magno	QUÍMICA INORG., ORG., Y BIOQ.	926295411	antonio.hoz@uclm.es	Lunes,Martes y Jueves 10 a 12 h

Lecturer: **BLANCA ROSA LOURDES MANZANO MANRIQUE** - Group(s): **20**

Building/Office	Department	Phone number	Email	Office hours
San Alberto Magno/first floor	QUÍMICA INORG., ORG., Y BIOQ.	926052050	blanca.manzano@uclm.es	Monday,wednesday 16.30 to 18.30 h tuesday and thurday 19:00-20:00

Lecturer: **ANA MARIA RODRIGUEZ FERNANDEZ-PACHECO** - Group(s): **20**

Building/Office	Department	Phone number	Email	Office hours
Politécnico/A23	QUÍMICA INORG., ORG., Y BIOQ.	926051961	anamaria.rfdez@uclm.es	Se anunciará a través del Moodle a principio de curso

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
E05	Knowing the usefulness of separation techniques, analysis and structural determination, their joint application in the resolution of research problems, as well as possessing skills in the use of such techniques.
E06	Knowing the main concepts and applications of coordination and organometallic chemistry.
E07	Knowing the principles of sustainable chemistry and safety standards for handling known chemicals
E08	Knowing the kinetics of chemical processes, including catalysis, reaction mechanisms and the methods and techniques used to determine them.
E10	Being able to address synthesis problems, including planning and development of preparation of compounds with new properties, methods of control of selectivity, especially the stereoselective methods.
G01	Knowing the precision of the experimental data and its use for the planning of experimental research work.
T02	Ability to work in a team and to exercise leadership functions, fostering the entrepreneurial character
T04	Ability to use specific software for research in chemistry.
T05	Ability to obtain bibliographic information at the research level, including Internet resources (databases, specialized scientific bibliography, social networks, etc ...), as well as carry out a selection and classification of it.
T06	Being able to develop professionally through continuous training.

5. Objectives or Learning Outcomes

Course learning outcomes

Description

Knowing the effect of radio frequency pulses in NMR.

Knowing the phenomenon of X-ray diffraction applied to the determination of structures from monocrystals.

Knowing the foundation and the information they provide different techniques, both electron microscopy and spectroscopic characterization of surfaces and coordination compounds.

Knowing the main methods of transfer sensitivity.

Knowing the most advanced techniques of NMR resonance solid, gradients, reverse resonance image, diffusion.

Manage software for processing and simulation of NMR.

Knowing how to handle crystallographic data bases and data processing programs structures determined by X-ray diffraction.

Knowing how to use the appropriate techniques and obtain information for the characterization of catalysts and precatalysts.

Being able to analyze the information provided by a particular technique in order to deduce the structure of the derivative under study and know how to select and apply the technique most suitable for each type of structural analysis characterization.

Knowing the origin of the information transmitted in mono and two-dimensional techniques.

Knowing the major applications monkey sequences and two dimensional pulses.

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	R	Description
Class Attendance (theory) [ON-SITE]	Lectures	E05 E06 E08 E10 G01 T06	0.92	23	Y	Y	Y	
Workshops or seminars [ON-SITE]	Guided or supervised work	E05 E06 E08 E10 G01 T02 T05 T06	0.64	16	Y	Y	Y	
Group tutoring sessions [ON-SITE]	Group tutoring sessions	E05 E08 E10 G01 T06	0.16	4	Y	N	Y	
Writing of reports or projects [OFF-SITE]	Self-study	E05 E08 E10 G01 T02 T05 T06	3.8	95	Y	N	Y	
Study and Exam Preparation [OFF-SITE]	Self-study	E05 E08 E10 G01 T05 T06	0.4	10	Y	N	Y	
Progress test [ON-SITE]	Assessment tests	E05 E08 E10 G01 T05 T06	0.08	2	Y	N	Y	
		Total:	**6**	**150**				
Total credits of in-class work: 1.8								**Total class time hours: 45**
Total credits of out of class work: 4.2								**Total hours of out of class work: 105**

As: Assessable training activity
Com: Training activity of compulsory overcoming
R: Rescheduling training activity

8. Evaluation criteria and Grading System

	Grading System		
Evaluation System	**Face-to-Face**	**Self-Study Student**	**Description**
Assessment of active participation	10.00%	0.00%	
Assessment of problem solving and/or case studies	30.00%	20.00%	
Theoretical papers assessment	25.00%	20.00%	
Oral presentations assessment	20.00%	10.00%	
Final test	15.00%	50.00%	
Total:	**100.00%**	**100.00%**	

9. Assignments, course calendar and important dates

Not related to the syllabus/contents

Hours	**hours**
Unit 1 (de 11):	
Activities	**Hours**
Class Attendance (theory) [PRESENCIAL][Lectures]	2
Writing of reports or projects [AUTÓNOMA][Self-study]	3.1
Study and Exam Preparation [AUTÓNOMA][Self-study]	.46
Unit 2 (de 11):	
Activities	**Hours**
Class Attendance (theory) [PRESENCIAL][Lectures]	4
Writing of reports or projects [AUTÓNOMA][Self-study]	6.2
Study and Exam Preparation [AUTÓNOMA][Self-study]	.92
Unit 3 (de 11):	
Activities	**Hours**
Class Attendance (theory) [PRESENCIAL][Lectures]	5
Writing of reports or projects [AUTÓNOMA][Self-study]	7.75
Study and Exam Preparation [AUTÓNOMA][Self-study]	1.15
Unit 4 (de 11):	
Activities	**Hours**
Class Attendance (theory) [PRESENCIAL][Lectures]	1
Writing of reports or projects [AUTÓNOMA][Self-study]	1.55
Study and Exam Preparation [AUTÓNOMA][Self-study]	.23

Unit 5 (de 11):	
Activities	**Hours**
Class Attendance (theory) [PRESENCIAL][Lectures]	3
Group tutoring sessions [PRESENCIAL][Group tutoring sessions]	1
Writing of reports or projects [AUTÓNOMA][Self-study]	4.65
Study and Exam Preparation [AUTÓNOMA][Self-study]	.69
Unit 6 (de 11):	
Activities	**Hours**
Workshops or seminars [PRESENCIAL][Guided or supervised work]	12
Group tutoring sessions [PRESENCIAL][Group tutoring sessions]	1
Writing of reports or projects [AUTÓNOMA][Self-study]	18.6
Study and Exam Preparation [AUTÓNOMA][Self-study]	2.76
Progress test [PRESENCIAL][Assessment tests]	3
Unit 7 (de 11):	
Activities	**Hours**
Class Attendance (theory) [PRESENCIAL][Lectures]	2
Workshops or seminars [PRESENCIAL][Guided or supervised work]	2
Writing of reports or projects [AUTÓNOMA][Self-study]	6.2
Study and Exam Preparation [AUTÓNOMA][Self-study]	.92
Unit 8 (de 11):	
Activities	**Hours**
Class Attendance (theory) [PRESENCIAL][Lectures]	3
Workshops or seminars [PRESENCIAL][Guided or supervised work]	4
Group tutoring sessions [PRESENCIAL][Group tutoring sessions]	1
Writing of reports or projects [AUTÓNOMA][Self-study]	9.3
Study and Exam Preparation [AUTÓNOMA][Self-study]	1.38
Unit 9 (de 11):	
Activities	**Hours**
Class Attendance (theory) [PRESENCIAL][Lectures]	2
Workshops or seminars [PRESENCIAL][Guided or supervised work]	2
Group tutoring sessions [PRESENCIAL][Group tutoring sessions]	1
Writing of reports or projects [AUTÓNOMA][Self-study]	7.75
Study and Exam Preparation [AUTÓNOMA][Self-study]	1.15
Unit 10 (de 11):	
Activities	**Hours**
Class Attendance (theory) [PRESENCIAL][Lectures]	2
Workshops or seminars [PRESENCIAL][Guided or supervised work]	2
Writing of reports or projects [AUTÓNOMA][Self-study]	6.2
Study and Exam Preparation [AUTÓNOMA][Self-study]	.92
Unit 11 (de 11):	
Activities	**Hours**
Class Attendance (theory) [PRESENCIAL][Lectures]	1
Workshops or seminars [PRESENCIAL][Guided or supervised work]	3
Group tutoring sessions [PRESENCIAL][Group tutoring sessions]	1
Writing of reports or projects [AUTÓNOMA][Self-study]	6.2
Study and Exam Preparation [AUTÓNOMA][Self-study]	.92
Progress test [PRESENCIAL][Assessment tests]	3
Global activity	
Activities	**hours**
Class Attendance (theory) [PRESENCIAL][Lectures]	25
Workshops or seminars [PRESENCIAL][Guided or supervised work]	25
Group tutoring sessions [PRESENCIAL][Group tutoring sessions]	5
Writing of reports or projects [AUTÓNOMA][Self-study]	77.5
Study and Exam Preparation [AUTÓNOMA][Self-study]	11.5
Progress test [PRESENCIAL][Assessment tests]	6
Total horas:	150

10. Bibliography and Sources

Author(s)	Title/Link	Publishing house	Citv	ISBN	Year	Description
A. K. Cheetham, P. Day	Solid State Chemistry	Oxford University Press		5	1991	
A. R. West	Basic Solid State Chemistry	WILEY		0-471-91798-2	1984	
F. A. Cotton	La teoría de grupos aplicada a la química	Limusa	Mexico	968-18-1047-3		
H. Friebolin	Basic One- and Two Dimensional NMR Spectroscopy https://www.wiley.com/en-us/Basic+One+and+Two+Dimensional+NMR+Spectroscopy%2C+5th%2C+Completely+Revised+and+Updated+Edition-p-9783527327829	WILEY		978-3-527-32782-9	2016	
H. Günther	NMR Spectroscopy https://www.wiley.com/en-	WILEY		978-3-527-33004-1	2013	

	us/NMR+Spectroscopy%3A+Basic+Principles%2C+Concepts+and+Applications+in+Chemistry%2C+3rd+Edition-p-9783527330003			
J. C. Vickerman, I. S. Gimore, Eds.	Surface Analysis. The Principal Techniques	Wiley	Chichester 9780470017630	2009
J. M. Albella, A. M. Cintas, T. Miranda, J. M. Serratosa	Introducción a la Ciencia de materiales. Técnicas de preparación y caracterización	CSIC	84-00-07343-6	1993
J. M. Thomas, W. J. Thomas	Principles and Practice of Heterogeneous Catalysis	VCH	3-527-29239-X	1997
Jenny P. Glusker; Mitchell Lewis and Miriam Rossi	Crystal Structure Analysis for Chemists and Biologists	VCH	0-89573-273-4	1994
M. Martínez-Ripoll, F. Hernández-Cano	Cristalografía			2016
	http://www.xtal.iqfr.csic.es/Cristalografia/index.html			
R. Freeman	Magnetic Resonance in Chemistry and Medicine	Oxford University Press	0-19-926225-X	2005
	https://global.oup.com/academic/product/magnetic-resonance-in-chemistry-and-medicine-9780199262250?cc=es&lang=en&			
S. Berger, S. Braun	200 and More NMR Experiments: A Practical Course	VCH	978-3-527-31067-8	2004
	https://www.wiley.com/en-us/200+and+More+NMR+Experiments%3A+A+Practical+Course-p-9783527310678			