COURSE DATA

Data Subject	
Code	42933
Name	Structural determination by RMN
Cycle	Master's degree
ECTS Credits	2.0
Academic year	2021 - 2022

Study (s)

Degree	Center	Acad. year	Period
2109 - Master's Degree in Experimental Techniques in Chemistry	Faculty of Chemistry	1	First term

Subject-matter

Degree	Subject-matter	Character
2109 - Master's Degree in Experimental Techniques in Chemistry	1 - Advanced laboratory of experimental techniques in chemistry	Obligatory

Coordination

Name	Department
ESTEVAN ESTEVAN, FRANCISCO	320 - Inorganic Chemistry

SUMMARY

Laboratory Subject dedicated to the learning of advanced work methodologies used in the structural determination, based on the use of nuclear magnetic resonance and the interpretation of spectra

PREVIOUS KNOWLEDGE

Relationship to other subjects of the same degree

There are no specified enrollment restrictions with other subjects of the curriculum.

Other requirements

Prior knowledge of chemistry and experimental work in the laboratory of chemistry taught in the degrees indicated in the recommended income profile for the student of the master's degree are required.

COMPETENCES (RD 1393/2007) // LEARNING OUTCOMES (RD 822/2021)

2109 - Master's Degree in Experimental Techniques in Chemistry

- To acquire basic skills to develop laboratory work in biomedical research.
- Be able to access the information required (databases, scientific articles, etc.) and to interpret and use it sensibly.
- Ser capaces de seleccionar y optimizar las variables instrumentales para obtener los mejores parámetros analíticos en las técnicas experimentales estudiadas.
- Ser capaces de emplear las herramientas básicas para el tratamiento de datos experimentales en el laboratorio.
- Realizar estudios realacionados con el análisis y/o la caracterización de sustancias químicas tales como: control de calidad, diseño de protocolos de trabajo para laboratorios, diseño e implementación de procesos de acreditación y validación, diseño y desarrollo de proyectos I+D+I, emisión de informes, certificaciones y/o dictámenes, etc.
- Ser capaces de planificar y gestionar los recursos disponibles de un laboratorio químico, teniendo en cuenta los principios básicos de la calidad, prevención de riesgos, seguridad y sostenibilidad.
- Seleccionar la instrumentación química comercializada apropiada para el estudio a arealizar y de aplicar sus conocimientos para utilizarla de manera correcta.
- To prepare a clear and concise memory of the results of your work and the conclusions obtained.

LEARNING OUTCOMES (RD 1393/2007) // NO CONTENT (RD 822/2021)

At the end of the teaching-learning process, the student should be able to:
1.- Calculate coupling constants in a spectrum.
2- Explain the need for various pulses.
3- Calculate the duration of a pulse of 90 degrees.
4 -Calculate relaxation times.
5.- Interpret a monodimensional spectrum.
6.- Interpret two-dimensional spectra.
7.- Interpret the mechanisms of fluxionality of molecules.
8.- Establish the thermodynamic parameters of these processes.

DESCRIPTION OF CONTENTS

1. Experimental aspects of NMR

Choice of solvent (s) and working conditions.

2. Acquisition and interpretation of spectra

Obtainment of monodimensional spectra of samples, covering different centres of interest (1H, 13C, 19F, 31P).

Obtainment of two-dimensional homonuclear spectra (COSY).Obtaining of heteronuclear two-dimensional spectra (HSQC, HMBC).

Obtainment of spectra at different temperatures.

Obtainment of spectra of solid samples (as 11B, 27, 29Si nuclei).

Interpretation of the obtained spectra.

WORKLOAD

ACTIVITY	Hours	% To be attended
Laboratory practices	20,00	100
Development of individual work	5,00	0
Study and independent work	10,00	0
Readings supplementary material	4,00	0
Preparation of evaluation activities	5,00	0
Resolution of case studies	6,00	0
TOTAL	**50,00**	

TEACHING METHODOLOGY

Presential Activities

Laboratory classes will begin with seminars in which Professor will perform a brief introduction of the objective, fundamentals and experimental practices methodology to perform.

The teacher will held in the laboratory the necessary explanations on operation of the instruments to be used in each practice prior to their use by students and will supervise its use during practices, to enhance knowledge on the techniques used.

Students will carry out the practice following the corresponding protocols or manual of practices.

Classroom activities performed in the laboratory, presentations and exhibitions of works will be part of the ongoing evaluation of the student (formative activities AF2 of verifica and teaching methodology MD1 of verifica)

Written examinations of the subject will be carried out on the date specified in the programming of the assessment tests (formative activities AF4 of verifica and teaching methdology MD1 of verifica).

The competences to acquire from the presential activities will be:

- Generals: CG1 and CG3
- Specific: CE2, CE3, CE4, CE5 y CE6

Non-presential activities

Students will conduct the non-presential activities requested by the teacher (memoirs, reports of practices, etc.) and they will deliver them on the specified date.

The competences to acquire from the presential activities will be:

- Specific: CE7

EVALUATION

1. -Continuous evaluation of the student in classes and seminars (participatory assistance, material handling and equipment, organization of work, understanding and use of the screenplay of practices, performing calculations, team work, etc.)

Along the sessions, focus in the resolution of practical assays, the assistance and participation of the students will be evaluated individually (by oral answers or by writing questions planned by the professor, by planning questions which its answer will be relevant for all the group). Also, these questions will include the design of working protocols, the selection of variables and the tools for the data treatment (verifica competences CE2, CE3, CE5 and CE6). The competences to evaluate: specifics: CE2, CE3, CE4, CE5 and CE6

WEIGHT 40

2.- An assessment of non-classroom-based activities (memories and/or reports of practices delivered)

The reports performed by the students will include the main conclusions extracted from the laboratory work (working protocols, variable selection and data treatment; verifica competences CE2, CE5, CE6 and CE7) and it will be done by couples to improve the group working (consensus decision making: verifica competences CG1 and CE7)

WEIGHT 30

3. -Written examinations (Based on the results of learning the content and on the specific objectives of each subject)

The exam will consist in the resolution of questions and practical examples related to the studied techniques (verifica competences: CE2, CE4, CE5 and CE6).

WEIGHT 30

REFERENCES

Basic

- Bakhmutov V.I.. Practical NMR relaxation for chemists, Wiley, 2004.

Duer, M.J., Introduction to solid state NMR spectroscopy, Wiley 2004.4

Hore P. J., Nuclear Magnetic Resonance. Oxford Science Publication, 1995.

Hennel, J. W. y Klinowski, J. Fundamentals of Nuclear Magnetic Resonance Longman.

Keeler J., Understanding NMR Spectroscopy, Wiley, 2005.

Morris, G. y Emsley, J. Multidimensional NMR methods for the solution state, Wiley 2010.

Günther, H., NMR spectroscopy: Basic principles, concepts and applications in chemistry, 3rd ed. Wiley-VCH, 2013

Pregosin, P. S., NMR in Organometallic Chemistry, Wiley-VCH, Weinheim, 2012.

Mitchell, T. N., Costisella, B., NMR- from spectra to structures, Heidelberg, Springer-Verlag, 2007.

ADDENDUM COVID-19

This addendum will only be activated if the health situation requires so and with the prior agreement of the Governing Council

Contents

The contents initially indicated in the teaching guide are maintained.

Workload and temporary teaching planning

Regarding the workload:

The different activities described in the Teaching Guide are maintained with the intended dedication.

Regarding the temporary teaching planning:

No variation with respect to what was initially planned in the teaching guide has been considered.

Teaching Methodology

With regard to laboratory courses, the maximum face-to-face teaching will be lying in compliance with the rules of distance and occupation of spaces fixed by the academic authorities. In this sense, the teaching type "L" will be 100% face-to-face, and the teaching type "U" will be non-face-to-face and will be taught through the tools offered by the virtual classroom. [Indicate if there is any variation with respect to the teaching guide (individual work ...)]

The methodology used for non-face-to-face classes shall be:

1. Synchronously using virtual classroom tools (Teams, Blackboard ...)

2. Asynchronously using locut power-point presentations or other virtual classroom tools

3. Resolution of exercises and questionnaires

If there is a closure of the facilities for health reasons that totally or partially affects the classes of the course, they will be replaced by non-face-to-face sessions following the established schedules and using the tools of the virtual classroom.

Evaluation

The evaluation system described in the Teaching Guide of the subject in which the various evaluable activities have been specified as well as their contribution to the final grade of the subject is maintained.

If there is a closure of the facilities for health reasons affecting the development of any face-to-face evaluable activity of the subject, it will be replaced by a test of a similar nature that will be carried out in virtual mode using the computer tools licensed by the University of Valencia. The contribution of each evaluable activity to the final grade of the subject will remain unchanged, as set out in this guide.

References

The literature recommended in the Teaching Guide is maintained since it is accessible.