60458 - Advanced structural characterization techniques

Información del Plan Docente

Academic Year	2017/18
Faculty / School	100 - Facultad de Ciencias
Degree	543 - Master's in Molecular Chemistry and Homogeneous Catalysis
ECTS	4.0
Year	1
Semester	Second semester
Subject Type	Optional
Module	---

1.General information

1.1.Introduction

The subject includes the study of specific techniques for the characterization of materials. These techniques are considered complementary to the basic techniques of structural characterization of organic or organometallic compounds. It is intended that students acquire sufficient knowledge to address the structural, morphological and functional characterization of new compounds and materials, using the most appropriate techniques selected in a reasoned way.

1.2.Recommendations to take this course

Prior knowledge of instrumental and spectroscopic methods is recommended. Text comprehension in scientific English is also desirable. Class attendance and continuous study facilitates passing the subject.

1.3.Context and importance of this course in the degree

The subject *Techniques of advanced structural characterization* is an optional subject of 4 ECTS taught in the second quarter of the school year. The characterization of a molecule or material is essential to know its chemical composition and structure as well as its thermal, optical, magnetic and electrical properties. The subject is included within the *Structural Characterization* module. In this module, it is compulsory for the student to address a subject on the structural characterization techniques that allow carrying out an initial identification of the chemical composition and structure of the molecules prepared.

In this course, students will receive information on more advanced or specific instrumental techniques that are being used today to determine the structure of molecules and materials from the nanoscale to the macroscopic scale. The knowledge that students acquire in the compulsory subject *Structural characterization techniques*, as well as in other optional subjects, as *Crystallography and Diffraction Techniques*, constitute undoubtedly a solid base to assimilate the contents of this subject. Also, this subject is essential to the issues addressed in several of the optional subjects of the module *Horizons in Molecular Chemistry and Catalysis*.

The Institute of Chemical Synthesis and Homogeneous Catalysis and the Institute of Materials Science of Aragon make available to master students art equipment, and this allows students to approach in a practical way this type of advanced instrumental techniques.

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1.4.Activities and key dates

The programmed activities will take place during the second term in four-hour sessions per week. The information about schedules, calendars and exams is available at the websites of the Sciences Faculty, https://ciencias.unizar.es/calendario-y-horarios, and the Master, http://masterqmch.unizar.es.

The presentation of works will be done according to the schedule to be announced well in advance.

2.Learning goals

2.1.Learning goals

Knowledge of advanced concepts on spectroscopic and instrumental techniques and their application in the characterization (structural, thermal, optical, magnetic, electrical) of compounds and organic, inorganic and organometallic materials.

Knowledge of the scope of each technique and its various forms, and their interrelation and complementarity.

To select the appropriate techniques, design experiments and evaluate methods of characterization in each case, depending on the problem to solve.

2.2.Importance of learning goals

The knowledge gained in this course will allow students to address the structural characterization and evaluation of properties of molecules and materials prepared using advanced instrumental techniques specific for the problem to solve. Students will be able to select the technique(s) more suitable for the material to study, from its molecular and / or supramolecular structure and dimensions (from the nanoscale to the macroscale) to its most characteristic properties (thermal, optical, magnetic, electrical).

3.Aims of the course and competences

3.1.Aims of the course

The subject is focused on the study of specific techniques for the characterization of materials, which are considered complementary to the basic techniques of structural characterization of organic or organometallic compounds. It is intended that students acquire sufficient knowledge to address the structural, morphological and functional characterization of new compounds and materials, using the most appropriate techniques, selected in a reasoned manner.

3.2.Competences

To know the basis of different instrumental techniques for the structural characterization and the evaluation of properties (thermal, optical, magnetic, electrical) of molecules and materials.

To know the type of molecule or material that can be studied with the techniques learned, and which is the most adequate procedure for sample preparation in each case.

To be able to elect the most appropriate technique(s) to resolve a particular problem knowing the fundaments of the techniques learned and their complementarity.

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To validate and interpret the results of each technique.

To integrate the data obtained from the different techniques selected to solve a particular problem.
Capacity to present adequately the results obtained from the different techniques.

4.Assessment (1st and 2nd call)

4.1.Assessment tasks (description of tasks, marking system and assessment criteria)

The student will have to demonstrate the achievement of the intended learning outcomes through continuous assessment, which is based on the following activities; their corresponding weight in the final score is included in brackets:

1.- Classwork based on solving problems and theoretical and practical issues (20%).

2.- Performance of practical work individually or in group (25%).

3.- Written test performed on the overall assessment period consisting on problem solving and theoretical and practical (55%) issues.

The subject is considered passed if the weighted average of the three marks according to the percentages indicated is equal to or greater than 5.

Students who do not opt for continuous assessment or fail the course for this procedure may conduct a comprehensive assessment test, which will represent 100% of the final grade, both the first and second call. This will consist of a written test on all the content addressed in the development of the subject, including seminars test. Students who want to improve their continuous assessment grade may also perform overall test in the first round, keeping the best of the qualifications obtained.

The number of official examination calls per registration and their use will be subjected to the statements of the *Regulation of Permanence in Master Studies* and the *Regulation of the Learning Assessment* (http://www.unizar.es/ice/images/stories/calidad/Reglamento%20Evaluacion.pdf). The latest document will also regulate the general design and scoring criteria of the assessment activities, as well as the exam schedules and timetable for the post-examination review.

5.Methodology, learning tasks, syllabus and resources

5.1.Methodological overview

The learning process designed for the course is essentially based on interactive lectures that are complemented with problem-solving sessions, seminars and tutorials. In lectures, the basics of techniques, their applicability and type of information that can be extracted from each of them will be explained. In problem-solving sessions, practical problems will be raised with the purpose of extracting data of given chemical systems using results from different instrumental techniques, among those revised in the course. Both types of sessions may be eventually complemented by practical seminars with the corresponding equipment.

In addition, the teacher will propose case studies to be performed individually or in groups, focused on the approach of a study protocol of a test sample, or on the interpretation of data obtained from the techniques, which are studied and

accessible in our research Institutes.

5.2.Learning tasks

The course includes the following learning tasks:

- Interactive lectures (2.4 ECTS).
- Problem-solving sessions, seminars and case studies (1 ECTS).
- Practice sessions with technical equipment (0.6 ECTS).
- Tutorials.

5.3.Syllabus

The course will address the following topics:

Topic 1. Structural characterization techniques.

- Solid state and soft matter Nuclear Magnetic Resonance (NMR); surface characterization techniques as X-ray photoelectron spectroscopy (XPS); x-ray absorption spectroscopy; circular dichroism.

Topic 2. Morphological and compositional characterization techniques.

- Advanced microscopies: Electronic microscopies (TEM, SEM), scanning probe microscopies (AFM, STM).

Topic 3. Thermal characterization techniques.

- Differential scanning calorimetry (DSC); thermogravimetric analysis (TGA).

Topic 4. Magnetic characterization techniques.

- Electron paramagnetic resonance (EPR); magnetic properties.

5.4.Course planning and calendar

Further information concerning the timetable, classroom, assessment dates and other details regarding this course, will be provided on the first day of class or please refer to the Faculty of Science website https://ciencias.unizar.es/calendario-y-horarios.

The submission of assignments will be done according to the schedule that will be announced in advance.

Students will be provided with diverse teaching material either at reprography or through the University's virtual platmform https://moodle2.unizar.es/add.

5.5.Bibliography and recommended resources

BB Solid-State NMR Spectroscopic Methods in Chemistry. D. D. Laws, H.-M. L. Bitter, A. Jerschow. En: Angewandte chemie. International edition Weinheim: Wiley-VCH, 1998- [Publicación periódica]. Año 2002, v. 41, pp. 3096-3129

BB X-ray absorption: principles, applications, techniques of EXAFS, SEXAFS, and XANES / edited by D.C. Koningsberger and R. Prins New York: Wiley, cop. 1988

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BC Berova, Nina; Nakanishi, Koji. Circular Dichroism: Principles and Applications. Wiley. 2000

BC Clarke, A.; Eberhardt, C. Microscopy Techniques for Materials Science. CRC Press. 2002

BC Haynes, P. J. Principles of Thermal Analysis and Calorimetry. Royal Society of Chemistry. 2002

BC Levitt, M. H. Spin Dynamics: Basics of Nuclear Magnetic Resonance. 2nd. ed. Wiley. 2008