Universidad Zaragoza

Academic Year/course: 2023/24

60453 - Structural characterization techniques

Syllabus Information

Academic year: 2023/24
Subject: 60453 - Structural characterization techniques
Faculty / School: 100 - Facultad de Ciencias
Degree: 543 - Master's in Molecular Chemistry and Homogeneous Catalysis
ECTS: 6.0
Year: 1
Semester: First semester
Subject type: Compulsory
Module:

1. General information

The main objective is to provide the student with a variety of tools for structural characterization and measurement of physical and chemical properties, essential for research in chemical synthesis and catalysis in academia and industry. It focuses on four techniques: nuclear magnetic resonance spectroscopy, mass spectrometry, visible-ultraviolet and fluorescence spectrophotometry and electrochemical techniques. The aim is to provide the student with an overview (specific equipment and data interpretation) and knowledge of how to combine the information obtained from each of the techniques, with a view to structural characterization. These objectives pursue "Quality Education", goal 4 of the Sustainable Development Goals (SDGs) (https://www.un.org/sustainabledevelopment/es/).

2. Learning results

To know the physical foundations on which all the techniques presented throughout the subject are based and the type of information provided by each technique.

To interpret the information provided by the spectra or diagrams generated by each technique and relate it directly to the structure of the compound.

To know and identify for each technique the instrumentation used, its most relevant components and its specific functions.

To conduct sample preparation, perform programmed experiments and design new ones (provided the software and technique allow it) and manipulate the most relevant parameters of each experiment to achieve a given information.

To acquire an integrated vision of the different techniques, selecting that particular technique or combination of them that are most appropriate for the resolution of specific problems.

3. Syllabus

Block 1. MRI

Topic 1. Physical fundamentals.

Topic 2. 1D experiments.

Topic 3. The NOE effect.

Topic 4. 2D experiments.

Topic 5. Instrumentation.

Topic 6. Dynamic processes

Block 2. UV-Vis Spectroscopy and Luminescence

Topic 7. UV-Vis, principles.

Topic 8. UV-Vis, applications. Colorants. Vapochromism and solvochromism.

Topic 9. Luminescence, principles.

Topic 10. Luminescence, applications. Light emitting devices and sensors.

Block 3. Mass Spectrometry and coupled Techniques

Topic 11. Fundamentals of mass spectrometry.

Topic 12. Tandem mass spectrometry.

Topic 13. Chromatographic techniques coupled to mass spectrometry.

Block 4. Electrochemical techniques

Topic 14. Basic concepts.

Topic 15. Cyclic voltammetry and other electrochemical techniques.

4. Academic activities

Methodology based on:

1. Expository participative classes (3 ECTS).

2. Problem classes and seminars in which real problems are analysed. In them, it is also discussed how the results of the different techniques are interpreted in scientific publications (2 ECTS).

3. Practical sessions, of compulsory attendance, in which the parts of the instrumental equipment and its operation are analysed (1 ECTS).

4. Completion of a guided work of a practical nature.

Other activities:

-Group or individualized tutoring.

-Students may attend the practical sessions or take the postgraduate course of the Consejo Superior de Investigaciones Científicas (CSIC) "Practical course on structural determination techniques".

5. Assessment system

Type of tests, assessment criteria and levels of demand

The continuous assessment of this subject is based on the following activities with the weighting shown below:

1. A written test to be taken during the global assessment period consisting of the solving of problems as well as theoretical and theoretical-practical questions (50 %).

2. Preparation and oral presentation, individually or in groups, of a guided work of a practical nature (25 %).

3. Problem solving exams and theoretical-practical questions of each technique or analysis of publications related to the topic (25 %).

The final grade will be the better of GRADE 1 or GRADE 2:

GRADE 1 = 0.25 x grade for exams + 0.25 x grade for the work submitted + 0.50 x grade for global written test

GRADE 2 = global written test grade.

Students will be graded in the second annual call by means of a single written test that will include all the theory, problems and practice topics defined as programmed learning activities.