Universidad Zaragoza

Academic Year/course: 2024/25

60456 - Crystallography and diffraction techniques

Syllabus Information

Academic year: 2024/25
Subject: 60456 - Crystallography and diffraction techniques
Faculty / School: 100 - Facultad de Ciencias
Degree: 543 - Master's in Molecular Chemistry and Homogeneous Catalysis
ECTS: 2.0
Year: 1
Semester: Second semester
Subject type: Optional
Module:

1. General information

The objective of this subject is to enable students to recognize the potential of the different diffraction techniques in the framework of any research, basic or applied, in the field of chemistry. It will also help them to learn how to follow the process of measurement and subsequent treatment of the data until the structural information is obtained.

The understanding of the fundamental concepts associated with diffraction techniques should contribute to the training of students so that they have the autonomous criteria to use these methodologies when faced with certain problems of identification or characterization of samples in the academic or business environment. The structural information obtained through experimental diffraction studies is essential in the establishment of very powerful structure-activity relationships, which allow to progress in the rationalization of very diverse chemical processes.

2. Learning results

To assimilate the fundamental concepts of spatial symmetry, showing an adequate understanding of its nomenclature and its application to crystallography.

To manage, using a criterion, the concepts involved in the diffraction process and, especially, in the interrelation between the experimental results of the diffraction processes and the internal structure of the crystals.

To know the most common experimental methods for the realization of diffraction diagrams, both for powder and for single crystal samples. To understand the fundamental requirements of samples that make them eligible for X-ray diffraction studies.

To know the appropriate procedures for the determination of molecular structures from diffraction data.

To interpret the main characteristics of diffraction diagrams and assess the quality of the data obtained.

To process the diffraction data to obtain the required structural information, either at the crystalline or molecular level.

To interpret the structural results obtained from the experiments.

To know the existence and basic experimental requirements for other structural determination processes based on diffraction of radiation other than X-rays.

3. Syllabus

1. Structure/Property: paradigm of modern science. What is structural crystallography? Diffraction experiments.

2. Spatial symmetry. Space groups. Nomenclature. International tables.

3. X-rays and other radiation. Scientific equipment for diffraction.

4. Crystal structure and diffraction. Reflections and intensities. Bragg's law, reciprocal network and structure factor.

5. Diffraction data processing. The refinement of three-dimensional structures. Absolute structures.

6. Presentation and validation of results. Contextualization of structural data.

7. Diffraction experiments on polycrystalline samples. Applications and methodologies.

8. Steps in a conventional process of structural determination. Programs used (monocrystalline samples).

9. Seminars for presentation and discussion of articles in the area of molecular chemistry and catalysis.

4. Academic activities

The learning process will use in-class presentations, previously made available, that the teachers will explain by raising various questions and stimulating students' participation in the description and understanding of the concepts. In some classes, short reading texts will be provided to introduce the concepts to be explained in class and to serve as a preliminary motivation for the student.

In addition to the interactive classes with the students, at the beginning of the term we will include the reading of curricular adaptation texts for those students who require it, as well as the analysis, study and subsequent commentary of complementary

texts to the concepts developed in class.

In addition, practical exercises on spatial symmetry, evaluation of systematic absences, or reciprocal network, will be proposed. These will be worked on in groups, The teacher will perform a step-by-step solving of a molecular structure in class, based on the students' indications.

Master Classes: 1 ECTS

Problem solving and seminars. Computer practice : 1 ECTS

5. Assessment system

The assessment of the student, in relation to the expected learning results, will be carried out **continuously** based on the following activities:

1.- Exams on the solving of problems, practical questions, exercises and other similar activities covered in the subject. At the end of each topic, a questionnaire with a reduced number of basic questions will be distributed for students to elaborate as personal work outside the class; these documents will be a key element in the assessment (40 %).

2.- Presentation of the structural results published in a recent scientific work of interest to the student. The student must demonstrate knowledge, correct and precise use of the concepts covered in the subject (20 %).

3.- Written or oral test (to be decided by the students), to be taken at the end of the subject, consisting of the solving of problems and questions on the contents taught (40 %).

Those students who do not pass the subject, or wish to improve their grade, may opt for a global test consisting of a commentary on the structural part of a current publication related to the topics covered by the master's degree (40%) and the answer to a series of theoretical questions on the concepts taught throughout the term (60%).

The enrolment in the subject entitles the student to 2 official exam calls per enrolment. The performance of the exams and the number of official calls will be in accordance with the Rules of Permanence in Master Studies and the Rules of Learning Assessment Standards of the Faculty of Sciences (https://ciencias.unizar.es/normativas-asuntos-academicos).

6. Sustainable Development Goals

7 - Affordable and Clean Energy
9 - Industry, Innovation and Infrastructure
12 - Responsible Production and Consumption