Universidad Zaragoza

Academic Year/course: 2021/22

27219 - Structure Determination

Syllabus Information

Academic Year: 2021/22
Subject: 27219 - Determinación estructural
Faculty / School: 100 - Facultad de Ciencias
Degree: 452 - Degree in Chemistry
ECTS: 6.0
Year: 4
Semester: First semester
Subject Type: Compulsory
Module:

1. General information

2. Learning goals

2.1. Competences

- Know the basic principles and fundamental aspects of the techniques studied for the structural determination of organic or inorganic compounds.
- Analyze and interpret spectroscopic information in order to reasonably propose the structure of a certain compound.
- Describe the spectroscopic properties of an organic or inorganic compound knowing its structure.
- Apply theoretical and practical knowledge to solve problems in Chemistry and select the most appropriate method to solve them.
- Understand and interpret the spectroscopic and structural information that is collected in the scientific literature.
- Develop skills for critical and autonomous learning in specialized areas of Chemistry and in multidisciplinary areas.

2.2. Learning goals

- Learn about the physical foundations and the information provided by the different spectroscopic techniques (mass spectroscopy, IR, NMR and v-uv) for the structural determination of organic and inorganic compounds.
- Calculate, deduce and compare the values of the main parameters of each spectroscopic technique.
- Determine the structure of the molecules from the interpretation of the experimental spectroscopic data.
- Reasonably predict the spectroscopic characteristics of a certain molecule knowing its structure.
- Select and list the most appropriate techniques for obtaining experimental data that allow the structural determination of a compound.
- Recognize the importance of the different structural determination techniques and that the information provided by each one of them can be complemented with the others.
- Understand, interpret and use the spectroscopic information that is collected in the bibliography.

2.3. Importance of learning goals

3. Assessment (1st and 2nd call)

4. Methodology, learning tasks, syllabus and resources

4.1. Methodological overview

The methodology followed in this course is oriented towards the achievement of the learning objectives. A wide range of teaching and learning tasks are implemented, such as:

- 1. Lectures, in which the teacher will explain the theoretical foundations of the different techniques and how they are applied for the structural determination.
- 2. Resolution and discussion of problems and cases. Typical problems include those in which students will be asked to use the concepts learned in order to deduce the structure compatible with the spectroscopic data given or to propose the expected spectrum for a known molecule.
- 3. Demonstrations, related to the preparation of samples and the measurement of the spectroscopic properties of selected compounds.

Students are encouraged to participate and discuss different aspects of the subject in order to develop critical thinking and inquiry-based learning.

4.2. Learning tasks

The course includes the following learning tasks:

1. Lectures (30 sessions of 1 h, 3 ECTS).
2. Problem resolution, case studies and demonstrations (30 sessions of 1 h, 3 ECTS).

4.3. Syllabus

The course will address the following topics:

- Characterization of chemical compounds: general aspects.
- Infrared spectroscopy. Bases and applications. Types of vibrations. Regions of the IR spectrum. Study of the functional groups. Interpretation of spectra. Problems and case studies. Instrumentation. Sample preparation.
- Mass spectrometry. Bases and applications. Ionization methods and ions analysis. Molecular ion. Isotopic peaks. Mass exact. Fragmentations. Problems and case studies. Instrumentation. Sample preparation.
- Nuclear magnetic resonance: proton. Bases and applications. Instrumentation. Chemical shift and shielding. Chemical equivalence. Integration. Spin-spin coupling. Study of the functional groups. Handling of the data tables. Problems and case studies. Sample preparation.
- Nuclear magnetic resonance: carbono. Bases and applications. Study of the functional groups. Handling of the data tables. Two-dimensional NMR. Problems and case studies.
- Strategies for the assignment of the structure of a compound from the corresponding spectra.
- Nuclear magnetic resonance of other nuclei. Nuclei with different nuclear spin and different isotopic abundance. Satellites. Spin systems. Problems and case studies.
- Nuclear magnetic resonance spectra of first and second order. Chemical and magnetic inequivalence. Simplification of spectra. Fluxionality in chemical compounds. Problems and case studies.
- UV-visible spectroscopy. Chromophores of general interest. Electronic spectra: types of transitions. Transitions in the free ion and in complex ions. Splitting of the d orbitals: strong-field and weak field approximations. Correlation diagrams. Tanabe-Sugano diagrams. Selection rules. Jahn-Teller effect. Problems and case studies.
- Magnetic susceptibilities in transition metal complexes. Effective magnetic moment. Orbital contribution. Problems and case studies.

4.4. Course planning and calendar

Further information concerning the timetable, classroom, office hours, assessment dates and other details regarding this course, will be provided on the first day of class or please refer to the Facultad de Ciencias web (https://ciencias.unizar.es/grado-en-quimica-0). The schedule of sessions is published in the bulletin board and web page of the Faculty of Science (http://ciencias.unizar.es/web/horarios.do)

There will be two partial examinations, whose exact dates will be communicated well in advance on the bulletin board and through the ADD. As a guide, the examinations will take place in early December and in mid-January.

4.5. Bibliography and recommended resources