Universidad Zaragoza

Academic Year/course: 2023/24

27219 - Structure Determination

Syllabus Information

Academic year: 2023/24
Subject: 27219 - Structure Determination
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

This subject provides the student with the knowledge and tools to determine the molecular structure, from spectroscopic data, of chemical compounds. Structural determination techniques are used in all areas of chemistry and related disciplines such as biochemistry, geology, materials science, medical and pharmaceutical research, etc. The identification of compounds, the monitoring of chemical reactions, the determination of the degree of purity of a substance or the design of new materials, whose properties are related to their structure, are fields where the knowledge and skills acquired in this subject are applied.

These approaches and objectives are aligned with the following Sustainable Development Goals (SDGs) of the United Nations 2030 Agenda (https://www.un.org/sustainabledevelopment/es/):

- Goal 4: Quality education
- Goal 7: Affordable and non-polluting energy
- Goal 9: Industry, Innovation and Infrastructure

2. Learning results

To know the physical fundamentals 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.

To calculate, deduce and compare the values of the main parameters of each technique.

To determine the structure of molecules from the interpretation of experimental spectroscopic data.

To reasonably predict the spectroscopic characteristics of a given molecule knowing its structure.

To select and relate the most appropriate techniques to obtain experimental data for the structural determination of a compound.

To recognize the importance of the different techniques of structural determination and that the information provided by each one can be complemented by the others.

To understand, interpret and use the spectroscopic information provided in the literature.

3. Syllabus

General analysis and characterization of chemical compounds.

Infrared spectroscopy. Fundamentals and applications. Types of vibrations. Zones of the infrared spectrum. Study of functional groups of interest. Interpretation of spectra. Instrumentation. Sample preparation.

Mass spectrometry. Fundamentals and applications. Ionization methods and ion analysis. Molecular ion. Isotopic peaks. Exact mass. Fragmentations. Instrumentation. Sample preparation.

Proton nuclear magnetic resonance. Fundamentals and applications. Instrumentation. Chemical displacement and shielding. Chemical equivalence. Integration. Spin-spin coupling. Study of functional groups of interest. Handling of tables. Spectrum simulation. Sample preparation.

Carbon nuclear magnetic resonance. Fundamentals and applications. Study of functional groups of interest. Handling of tables. Two-dimensional NMR and most common two-dimensional techniques.

Strategies for assigning the structure of a compound from the corresponding spectra.

Nuclear magnetic resonance of other nuclei. Nuclei with different spin values and isotopic abundances.

Second order spectra. Chemical and magnetic inequivalence. Fluxionality.

Ultraviolet-visible spectroscopy. Types of transitions. D-orbital splitting: strong field and weak field.

Tanabe-Sugano diagrams. Selection rules.

Magnetic susceptibilities. Effective magnetic moment. Orbital contribution.

4. Academic activities

1.- Lectures, in which the theoretical foundations of the different techniques and how they are applied to the structural determination will be presented (3 credits)

2.- Problem solving and applied issues. Collective discussion of the resolution of problems and questions, of increasing complexity (3 credits).

There will be 4 sessions per week, of 1 hour duration. The problem solving classes will be interspersed between the master classes, so that, after presenting the fundamentals and characteristics of each technique, we will move on to solving related problems and cases.

5. Assessment system

Continuous assessment. There will be two midterm written tests of theoretical and practical content. The final grade of the subject will be obtained as the arithmetic mean of the grades of each of the midterm tests. The subject will be considered passed if a minimum grade of 5 points (out of 10) is obtained in the average of the two midterm exams . A minimum of 4 points (out of 10) must be obtained in each of the midterm exams in order to obtain an average.

Global test. Students who do not use the continuous evaluation system or who do not pass the subject by this procedure , will take a global test consisting of a single written exam of theoretical and practical content. A minimum grade of 5 points (out of 10) is required to pass.

The student's final grade will be the best of the grades obtained between the continuous evaluation and the global test.

The evaluation regulations can be consulted at: http://wzar.unizar.es/servicios/coord/norma/evalu/evalu.html