Universidad Zaragoza

Year : 2020/21

27221 - Spectroscopy and Molecular Properties

Syllabus Information

Academic Year: 2020/21
Subject: 27221 - Spectroscopy and Molecular Properties
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

1.1.Aims of the course

1.2.Context and importance of this course in the degree

1.3.Recommendations to take this course

2.Learning goals

2.1.Competences

2.2.Learning goals

2.3.Importance of learning goals

3.Assessment (1st and 2nd call)

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

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: Lecture classes (3.1 ECTS), problem?solving sessions (1.5 ECTS)and laboratory sessions (1.4 ECTS)

Students are expected to participate actively in the class throughout the semester. In laboratory sessions, special attention will be paid to the understanding of the instrumental part and to the development of the skills and attitudes needed for the work in the laboratory.

Classroom materials will be available via Moodle. Further information regarding the course will be provided on the first day of class.

4.2.Learning tasks

The course includes 6 ECTS organized according to:

- Molecular symmetry (0.9 ECTS): 9 hours (6 h theory; 3 h problems).
- Photochemistry (0.5 ECTS): 5 hours (3 h theory; 2 h problems).
- Molecular spectroscopy (3.5 ECTS): 25 hours (17 h theory; 8 h problems) + 10 hours of laboratory (3 sessions).
- Polymers (1.1 ECTS): 7 hours (5 h theory; 2 h problems) + 4 hours of laboratory (1 session).

4.3.Syllabus

The course will address the following topic:

- Topic 1. Molecular symmetry:
  - Introduction to molecular symmetry and group theory.
  - Symmetry operations and symmetry elements. Symmetry classification of molecules in point groups.
  - Irreducible representations and symmetry species. Character tables. Direct products of irreducible representations. Selection rules in spectroscopy.
  - Application of symmetry concepts to the study of normal modes of vibration and molecular orbitals.
- Topic 2. Photochemistry:
  - Introduction to photochemistry.
  - Properties of molecules in excited electronic states. Overview of deactivation processes. Jablonski diagrams.
  - Basic photochemical reactions.
- Topic 3. Molecular spectroscopy:
  - Basic principles in spectroscopy; interaction between electromagnetic radiation and matter. Transition moment. Selection rules. Width of spectroscopic signals.
  - Rotational spectroscopy. Energy levels of molecules considered as rigid rotors. Centrifugal distortion constants. Stark effect in rotational spectroscopy.
  - Vibration in diatomic molecules; anharmonicity. Normal modes of vibration in polyatomic molecules. Characteristic group frequency in IR spectroscopy.
  - Raman effect. Vibrational and rotational Raman spectra. Light polarization in Raman effect. Application of IR and Raman spectra to the structure determination of molecules.
  - Electronic spectroscopy of diatomic molecules. Frank-Condon principle. Electronic spectroscopy of polyatomic molecules. Characteristics and applications of transitions in UV-vis.
  - Fluorescence spectroscopy: basic principles and applications.
  - Fundamentals of photoelectron spectroscopy. Interpretation of UPS and XPS spectra.
  - Resonance spin spectroscopy; Larmor precession. 1H-NMR spectroscopy. Chemical shift and coupling constant. Analysis of NMR spectra of nuclei other than 1H; nuclear cuadruple relaxation.
  - Fundamentals of electron spin resonance spectroscopy ESR. Analysis of hyperfine structure in some examples.
- Topic 4. Polymers:
  - Physicochemical properties and characterization of polymers.
  - Kinetics and mechanisms of polymerization.
  - Degradation and stability.
  - Solubility of polymers.

4.4.Course planning and calendar

For further details concerning the timetable, classroom and further information regarding this course please refer to the Faculty website (http://ciencias.unizar.es/web/horarios.do).

4.5.Bibliography and recommended resources

http://biblos.unizar.es/br/br_citas.php?codigo=27221&year=2019