Molecular Spectroscopy

Code: 106811
ECTS Credits: 6

2025/2026

Degree	Type	Year
Nanoscience and Nanotechnology	OB	3

Contact

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Teaching groups languages

You can view this information at the end of this document.

Prerequisites

There is no compulsory pre-requisite but it is highly advisable to have passed and keep in mind the subjects of "Chemical Bonding and Structure of Matter", "Basics of Mathematics", "Calculus", "General Physics", "Chemistry of elements", "Organic Chemistry", "Quantum Phenomena I" and "Mathematic Tools I".

Objectives and Contextualisation

This subject is focused on the study and understanding of the interaction between electromagnetic radiation and matter, and how this interaction can be used in the structural characterization of molecules and materials. The subject includes some theoretical foundations involved in radiation / matter interaction and some of the most common spectroscopic techniques. For each type of spectroscopic technique, it is intended to establish a connection between the spectrum and the structural information that can be extracted. Special weight is given to molecular symmetry and group theory as a tool to explain certain spectra.

The specific objectives of the subject are the following:

- Understand the basics of the interaction between electromagnetic radiation and matter.

- Understand the rules that determine the frequencies and intensities of a transition.

- Know how to apply this knowledge to solve quantitatively and qualitatively chemical problems with the help of molecular spectroscopy.

Learning Outcomes

1. CM13 (Competence) Apply chemical knowledge to solve quantitative and qualitative problems, using bibliographic sources when necessary.
2. CM14 (Competence) Work collaboratively to plan and organise the basic tasks carried out in a physicochemical analysis laboratory.
3. CM15 (Competence) Handle chemical products and wastes while taking their impact on safety and the environment into account.

4. KM24 (Knowledge) Describe the interaction of electromagnetic radiation with matter as the basis for characterising molecule and material structures.
5. SM21 (Skill) Apply the main techniques used in to identify and characterise the structure and composition of the material.

Content

1. Introduction to spectroscopy

Populations of energy levels: Boltzmann's distribution law. Electromagnetic radiation. Stimulated absorption and emission. Selection rule. Spectrophotometer. Bandwidth. Radiation sources. Lasers. Fourier transform spectroscopy.

2. Rotation and vibration spectra of diatomic molecules

Nuclear motion in a diatomic molecule. Born-Oppenheimer approach. Rigid rotor. Rotational levels and rotation spectrum. Harmonic oscillator and vibrational levels. Fine structure of vibrational bands. Centrifugal distortion and anharmonicity. Vibration-rotation coupling. Dissociation energy

3. Molecular symmetry

Symmetry operations and elements. Axes of rotation. Symmetry planes and axes of improper rotation. Product of symmetry operations. Symmetry point groups. Consequences of symmetry: polarity and chirality

4. Group theory.

Symmetry operations and matrices. Characters of matrices. Symmetry classes. Character tables. Symmetry of atomic orbitals. Reducible and irreducible representations. Linear combinations adapted to symmetry. Integrals throughout the space and selection rules.

5. Vibration spectra of polyatomic molecules

Motion of nuclei in a polyatomic molecule: rotation and vibration. Normal vibration modes. Selection rules in IR spectra. Symmetry and selection rules. Determination of normal modes from symmetry. IR spectra and molecular interactions. Raman spectroscopy. Rotational Raman spectroscopy. Vibrational Raman spectroscopy. Rules of selection and symmetry.

6. Electronic spectra.

Atomic spectra. Spectral terms in polyelectronic atoms. Spectral terms, levels and states. Spectral terms in diatomic molecules. Vibrational structure of electronic bands. Franck-Condon principles. Fluorescence and phosphorescence. Dissociation and predissociation. Electronic spectra of polyatomic molecules.

7. Magnetic resonance spectra

Introduction to nuclear magnetic resonance. Selection rules in NMR spectra. Vector model. Chemical shielding and displacement. Spin-spin coupling. Chemical equivalence and magnetic equivalence. NMR and chemical processes. Fourier transform NMR. Longitudinal and transverse relaxation. NMR spectra of nuclei with $I \geq 1$. NMR spectra in solids. Electronic spin resonance spectra. Hyperfine coupling.

Computer classroom practices

1. Vibrational spectroscopy

2. Electronic Spectroscopy

Activities and Methodology

Title	Hours	ECTS	Learning Outcomes
Type: Directed			
Classroom practices	4	0.16	CM13, CM14, CM13
Problems sessions	16	0.64	CM13, CM13
Theoretical sessions	30	1.2	
Type: Autonomous			
Performance of excercices	10	0.4	CM13, CM14, CM13
Personal study	80	3.2	CM13, CM14, CM13

The subject will consist of three types of teaching activities:

1. Theoretical classes

The teacher will develop the contents of the program in-person or virtually, according to the instructions of the academic authorities. The contents of the theoretical classes will be available in advance on the Virtual Campus.

2. Problem classes

Several problems will be proposed for each topic, which will be solved by the students under the supervision of the teacher. Problem classes will be devoted to the discussion of the results of the problems in relation with the contents of the subject.

3. Computer classroom practices

Simulation of spectra of some molecules using quantum chemistry methods.

Annotation: Within the schedule set by the centre or degree programme, 15 minutes of one class will be reserved for students to evaluate their lecturers and their courses or modules through questionnaires.

Assessment

Continous Assessment Activities

Title	Weighting	Hours	ECTS	Learning Outcomes
Classroom practices	15	4	0.16	KM24, SM21
Exams	70	5	0.2	KM24, SM21
Exercises	15	1	0.04	CM13, CM14, CM15, KM24, SM21

Written exams

Throughout the course there will be two partial exams. The weights of these exams in the final mark will be 40% and 30%, respectivelly, so that the whole of the two partial exams will represent 70% of the final mark.

The minimum mark of a partial exam that allows to calculate the average of the course is 4. If these marks can not be reached, at the end of the course one or both partial exams can be retrieved. The mark obtained in the recovery will replace the one obtained in the first attempt. It is also possible to come up with the recoveries to improve marks. In this case, the last mark obtained in each partial exam is the one that prevails. In order to be entitled to a recovery, it is compulsory to have submitted to both partial exams.

Trace work

Throughout the course, a certain number of student tracking tests (problems solved individually or in groups, short classroom tests, etc.) will be collected. The average grade of these tests will represent 15% of the final mark

Classroom practices

During the course, two obligatory classroom practices will be carried out. The result of these practices will be evaluated through a specific test that will represent 15% of the final mark

The requirements to pass the subject are:

1. The mark of each partial exam must be equal to or greater than 4

2. The average mark of the subject must be equal or superior 5

3.The completion of classroom practices is mandatory

The subject will be considered non-evaluable if neither of the two partial exams has been made. To qualify for the "Matrícula d'Honor" qualification, the marks obtained in the partial exams will be taken intoaccount preferably.

Students who have opted for single assessment will have to take a final test that will consist of an examination of the entire theoretical syllabus and problems of the subject. This test will be carried out on the day on which the students of the continuous evaluation do the second partial exam. The student's grade will be:

Course grade = (Final test grade · 85 + Laboratory grade · 15)/100

If the final grade does not reach 5, the student has another opportunity to pass the subject through the recovery exam that will be held on the date set by the coordination of the degree. In this test 85% of the mark corresponding to the theory and problems part can be recovered. The practical part is not recoverable.

The realization and evaluation of the practices will be done in the same terms as for continuous assessment students.

Bibliography

Basic Texts:

- P. Atkins, J. de Paula, *Atkins. Química Física*, 8a Ed., Ed. Panamericana , 2008. Electronic version available.

- C. N. Banwell, E. M. McCash, *Fundamentals of Molecular Spectroscopy*, 4th Ed., McGraw Hill, 1994.

- J. M. Hollas, *Basic Atomic and Molecular Spectroscopy*, Royal Society of Chemistry, 2002. Electronic version available.

Specialized texts:

- P. Atkins, R. Friedman, Molecular Quantum Mechanics, 5th Ed., Oxford University Press, 2011.

Software

GaussView 6.0 and Gaussian-16

Groups and Languages

Please note that this information is provisional until 30 November 2025. You can check it through this link. To consult the language you will need to enter the CODE of the subject.

Name	Group	Language	Semester	Turn
(PAUL) Classroom practices	1	Catalan	first semester	afternoon
(PLAB) Practical laboratories	1	Catalan	first semester	morning-mixed
(PLAB) Practical laboratories	2	Catalan	first semester	morning-mixed
(TE) Theory	1	Catalan	first semester	afternoon