

Molecular Spectroscopy

Code: 103283
ECTS Credits: 5

2024/2025

Degree	Type	Year
2501922 Nanoscience and Nanotechnology	OB	3

Contact

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Teaching groups languages

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Prerequisites

There is no compulsory pre-requisite but it is highly advisable to have passed and keep in mind the subjects of "Chemical Link and Structure of Matter", "Mathematical Foundations", "Mechanics and Waves", Classical Physics, "Element Chemistry" and "Organic Chemistry". It is recommended to take simultaneously the subject "Quantum Phenomena 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.

Competences

- Apply the concepts, principles, theories and fundamental facts of nanoscience and nanotechnology to solve problems of a quantitative or qualitative nature in the field of nanoscience and nanotechnology.
- Be ethically committed.
- Communicate orally and in writing in one's own language.
- Demonstrate knowledge of the concepts, principles, theories and fundamental facts related with nanoscience and nanotechnology.

- Interpret the data obtained by means of experimental measures, including the use of computer tools, identify and understand their meanings in relation to appropriate chemical, physical or biological theories.
- Learn autonomously.
- Manage the organisation and planning of tasks.
- Obtain, manage, analyse, synthesise and present information, including the use of digital and computerised media.
- Propose creative ideas and solutions.
- Reason in a critical manner
- Recognise and analyse physical, chemical and biological problems in the field of nanoscience and nanotechnology and propose answers or suitable studies for their resolution, including when necessary the use of bibliographic sources.
- Resolve problems and make decisions.
- Show sensitivity for environmental issues.
- Work correctly with the formulas, chemical equations and magnitudes used in chemistry.

Learning Outcomes

1. Analyse situations and problems in the field of physics and chemistry, and propose experimental responses or studies using bibliographic sources.
2. Apply the acquired theoretical contents to the explanation of experimental phenomena.
3. Apply the physical principles of matter-radiation interactions to the interpretation of spectrums.
4. Be ethically committed.
5. Communicate orally and in writing in one's own language.
6. Correctly use computer tools to calculate, graphically represent and interpret the data obtained, as well as its quality.
7. Critically evaluate experimental results and deduce their meaning.
8. Describe the basics of the most significant molecular spectroscopies (ANAR, UV-visible, NMR, masses).
9. Design simple experiments for the study of simple chemical and physical systems.
10. Employ information and communication technology in the documentation of cases and problems.
11. Evaluate the best spectroscopic methodology to solve a structural problem.
12. Identify the physical principles that govern matter-radiation interactions.
13. Interpret the data obtained from experimental measurements to characterise a chemical compound or a material.
14. Learn autonomously.
15. Manage the organisation and planning of tasks.
16. Obtain, manage, analyse, synthesise and present information, including the use of digital and computerised media.
17. Propose creative ideas and solutions.
18. Reason in a critical manner
19. Recognise and analyse physical and chemical problems related with the structure of organic and inorganic compounds
20. Relate experimental data with the physical and chemical properties and/or analysis of the systems that are the object of study.
21. Relate the physical principles of matter-radiation interactions with the signals of the different spectrums.
22. Resolve problems and make decisions.
23. Show sensitivity for environmental issues.
24. Understand group theory and tables of characters with the symmetry of molecules.
25. Use graphic design programs to draw chemical formulas and their reactions.
26. Work correctly with the formulas, chemical equations and magnitudes used in chemistry.

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	1, 2, 3, 14, 7, 5, 8, 9, 10, 15, 12, 4, 23, 16, 17, 18, 19, 21, 24, 22, 26, 6, 25
Problems sessions	15	0.6	1, 2, 3, 14, 7, 11, 5, 9, 10, 15, 12, 13, 4, 23, 17, 18, 19, 21, 24, 20, 22, 26

Theoretical sessions	26	1.04	1, 2, 3, 14, 7, 11, 5, 8, 9, 10, 15, 12, 13, 4, 23, 18, 19, 21, 24, 20, 22
Type: Autonomous			
Performance of exercises	5	0.2	1, 2, 3, 14, 7, 11, 5, 8, 10, 15, 12, 13, 4, 23, 16, 17, 18, 19, 21, 24, 20, 22, 26
Personal study	65	2.6	

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

Continuous Assessment Activities

Title	Weighting	Hours	ECTS	Learning Outcomes
Classroom practices	15	4	0.16	1, 2, 3, 14, 7, 11, 5, 10, 12, 13, 4, 16, 17, 18, 19, 21, 24, 20, 22
Exams	70	5	0.2	2, 3, 14, 7, 11, 5, 8, 12, 13, 4, 17, 18, 19, 21, 24, 20, 22
Exercises	15	1	0.04	1, 2, 14, 7, 11, 5, 8, 9, 10, 15, 12, 13, 4, 23, 16, 17, 18, 19, 21, 24, 20, 22, 26, 6, 25

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%, respectively, 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 into account 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:

$$\text{Course grade} = (\text{Final test grade} \cdot 85 + \text{Laboratory grade} \cdot 15)/100$$

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

Language list

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