UAB
Universitat Autònoma de Barcelona

Spectroscopy

Code: 102531
ECTS Credits: 6

2025/2026

Degree	Type	Year
Chemistry	OB	2

Contact

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Teachers

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Teaching groups languages

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

Prerequisites

- Only students that have passed the basic topics of "Fonaments de Química I" can do the course of "Espectroscòpia".
- The course assumes that the student has working knowledge of quantum chemistry; it is thus very advisable to have taken (and preferably passed) the "Química Quàntica" subject.

Objectives and Contextualisation

In the topic of Spectroscopy the focus is the study of the interaction of electromagnetic radiation and matter, and how this interaction can be used to determine details on the structure of the latter. The theoretical foundations that explain the interaction of radiation and matter, and predict the structured form of spectra are laid out first, relying on a working knowledge of quantum chemistry. Laser radiation is discussed, as its use is ubiquitous in current spectroscopic techniques. A specific focus is made on molecular symmetry and the application of the Group Theory applied to symmetry as a powerful tool to explain characteristics of certain spectra in polyatomic molecules. Different spectroscopic techniques based on absorption, emission and Raman dispersion (i.e., rotational, vibrational and electronic) as well as those based on spin magnetic ressonance (i.e., nuclear magnetic resonance) are discussed. For each kind, the structure of the corresponding spectrum is connected to the structural parameters of the molecules using quantitative relations derived from quantum mechanics.

Specific goals of the topic:

- Understand the basics of the interaction between the electromagnetic radiation and matter.
- Understand the rules that determine the frequency and intensity of a transition.

- Know how to apply this knowledge to be able to solve problems both in qualitative and quantitative aspects.

Competences

- Adapt to new situations.
- Apply knowledge of chemistry to problem solving of a quantitative or qualitative nature in familiar and professional fields.
- Be ethically committed.
- Have numerical calculation skills.
- "Interpret data obtained by means of experimental measures, including the use of IT tools; identify their meaning and relate the data with appropriate chemistry, physics or biology theories."
- Learn autonomously.
- Manage, analyse and synthesise information.
- Manage the organisation and planning of tasks.
- Obtain information, including by digital means.
- Propose creative ideas and solutions.
- Reason in a critical manner
- Resolve problems and make decisions.
- Show an understanding of the basic concepts, principles, theories and facts of the different areas of chemistry.
- Show motivation for quality.
- Use IT to treat and present information.
- Use the English language properly in the field of chemistry.

Learning Outcomes

1. Adapt to new situations.
2. Apply the physical principles of matter-radiation interactions to the qualitative and quantitative interpretation of spectrums.
3. Be ethically committed.
4. Employ and generalise the relationships between structure and spectroscopic methods.
5. Establish spectroscopic response in different structural characteristics.
6. Handle computer programs, including simulators, to support the previous interpretation.
7. Have numerical calculation skills.
8. Identify the physical principles that govern matter-radiation interactions.
9. Learn autonomously.
10. Manage, analyse and synthesise information.
11. Manage the organisation and planning of tasks.
12. Obtain information, including by digital means.
13. Propose creative ideas and solutions.
14. Reason in a critical manner
15. Recognise spectroscopic terminology in the English language.
16. Recognise the English terms used to describe chemical structure.
17. Resolve problems and make decisions.
18. Show motivation for quality.
19. Use IT to treat and present information.
20. Use the physical principles of matter-radiation interactions to relate the signals of different spectrums with the possible species present in a certain chemical system.

Content

Theory and Problems:

1. Introduction to Spectroscopy.

   Nature of the electromagnetic radiation. Electromagnetic spectrum. Spectroscopic techniques. FT Spectroscopy. Spectral line width. Intensity of spectral lines. Selection rules. Raman Spectroscopy. Lasers. Example of spectroscopy of absorption/emission: Rotational spectroscopy.

2. Molecular Symmetry.

   Symmetry elements and operations. Symmetry Point Groups (SPG). Systematic determination of a SPG of a molecule. Group Representations. Reducible and irreducible representations. Character Tables.

3. Vibrational Spectroscopy.

   Vibration of diatomic molecules: harmonic oscillator model; anharmonicity; dissociation energy. Vibration of polyatomic molecules: vibrational normal modes; types of normal modes; symmetry of the normal modes; selection rules for polyatomic molecules and mutual exclusion rule.

4. Electronic Spectroscopy.

   Atomic spectroscopy: atomic spectral terms; selection rules. Electronic spectroscopy of diatomic molecules: spectral terms; selection rules; vibrational structure and vibronic spectra; Franck-Condon Principle. Electronic spectroscopy of polyatomic molecules: molecular orbitals adapted to symmetry; molecular spectral terms; selection rules. Fluorescence and phosphorescence. Photoelectron spectroscopy: UPS and XPS.

5. Magnetic Resonance Spectroscopy.

   Nuclear spin. Interaction with a magnetic field. Nuclear magnetic resonance (NMR) spectroscopy. Energy levels and selection rules. Nuclear shielding. Chemical shift. Spin-spin coupling and coupling patterns.

Lab Sessions:

There will be a total of 3 sessions of 4 hours each, the contents of which will be:

Session 1: Simulation of vibrational spectra

Session 2: Simulation of electronic spectra

Session 3: Simulation of NMR spectra

Throughout the sessions, calculations and simulations of the spectra of molecules must be carried out, and the results obtained must be understood and analyzed, relating them to the material seen in the theory sessions. The final objective of the lab sessions is to analyze a case molecule according to its spectroscopic properties, following a problem-based learning (PBL) methdology through cases.

The development is as follows. The first two hours are devoted to calculations related to the simulation of spectra corresponding to each session (vibrational, electronic, 1H-NMR) for specific molecules following the instructions in the lab guides. Students will be given a report that they will have to fill in and answer, and that will help them assess the level of understanding of the tasks performed and the quality of the work. The last two hours are devoted to the case molecule, where the spectroscopy properties corresponding to the session will be simulated, based on what has been done and learned previously. They will also be used to discuss, organize the information and prepare the presentation, taking advantage of the fact that the teachers will be in the laboratory to help them with any questions.

Activities and Methodology

Title	Hours	ECTS	Learning Outcomes
Type: Directed			
Lab Sessions	12	0.48	1, 2, 18, 4, 5, 10, 6, 3, 12, 13, 14, 16, 15, 17, 7, 20, 19
Problem Solving Sessions	12	0.48	2, 9, 18, 4, 5, 11, 8, 6, 14, 16, 15, 17, 7, 20
Seminars	8	0.32	1, 2, 18, 4, 5, 10, 6, 3, 12, 13, 14, 17, 7, 20, 19
Theory Lectures	27	1.08	2, 9, 4, 5, 10, 8, 6, 12, 14, 16, 15, 20
Type: Supervised			
Case Preparation	10	0.4	1, 2, 9, 18, 4, 5, 10, 11, 8, 6, 3, 12, 13, 14, 17, 7, 20, 19
Type: Autonomous			
Personal Study	50	2	2, 9, 4, 5, 10, 11, 8, 6, 12, 14, 17, 7, 20
Problem Solving	18	0.72	2, 9, 4, 5, 10, 11, 8, 6, 12, 13, 14, 17, 7, 20
Quizz Preparation	5	0.2	1, 2, 9, 18, 4, 5, 10, 11, 8, 6, 12, 13, 14, 17, 20, 19

The activities belong to four different categories:

Theory Lectures:

The lecturer will explain the syllabus to the classroom using blackboard and multimedia material, which will be made available to the students in the "Moodle Classroom". These expositive sessions will conform most of the theory lecturing of the syllabus.

Problem-solving Sessions:

A list of graded exercises, classified according to the units of the syllabus, will be made available to all students in the "Moodle Classroom" at the beginning of the term. On appointed days, announced in the theory lectures, or whenever it is adequate in terms of covered material, selected problems will be solved in the lecture room, linking with the theoretical foundations seen in the theory lectures necessary to solve the exercise and in the process strengthen the concepts explained in the theory lectures. No compromise is taken to solve all problems in the collection explicitly, to leave room for individual initiative and encourage individual work by the student.

Lab Sessions:

The practical sessions will present the students the possibility to compute spectroscopic properties of certain molecules using a quantum chemistry program or other software to simulate spectra and use the detailed results to weave theoretical aspects with the outcome of spectrum recording. It is a goal of the lab sessions to bring up the benefits of a synergy between theoretical and experimental approaches in modern chemistry.

Logistically, the students of all enrollment groups will be divided in four groups, the composition of which will be known beforehand, in order to make an efficient use of the lab and computer facilities available. Practical sessions for each subgroup will take place at the appointed dates in different labs and under supervision of qualified instructors. For all lab sessions, the lab protocol will be made available in the "Moodle Classroom", and the students have to bring their own copy (hard or electronic) and read it before the lab session. It is advisable to bring also a personal notebook to write down the results obtained and other annotations.

On appointed days, the students will be summoned to the computer room. At the end of each practical session the students will be given an answer sheet and questionnaire, to be completed and turned in before leaving the lab, which will serve the purpose of self-assessing the level of comprehension of the task just completed and the quality of the results obtained.

For each session, students will do, in groups, a final practice, where the previously developed techniques will be applied to a specific molecule (case) and make an analysis of its spectroscopic properties, this way following a problem-based learning (PBL) methodology by means of solving cases. The groups will make an exhibition of this final work in front of the professors, which will be the grade corresponding to the practical part.

Personal Work:

Personal work by the student is a very important, almost indispensible aspect of the students' attitude towards passing the topic. Besides the most obvious areas (like readying and studying notes and books, preparing exercises, etc.) specific, well delimited areas of the theory syllabus will be left to the students to work out by themselves. In these cases, personal consultation hours will be made available to help coalescing the knowledge gained by the students.

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
Final Exam	60%	3	0.12	2, 9, 4, 5, 8, 3, 13, 14, 17, 7, 20
Lab sessions	25%	0	0	1, 2, 9, 18, 4, 5, 10, 11, 6, 3, 12, 13, 16, 15, 17, 7, 20, 19
Partial Exams	60%	3	0.12	2, 9, 4, 5, 8, 3, 13, 14, 17, 7, 20
Short Quizzes	15%	2	0.08	2, 18, 4, 5, 8, 3, 13, 14, 17, 7, 20

The assessment can be based on a continuous assessment modality or, for those students who have taken it, on a single assessment modality.

The continuous assessment modality includes the following elements:

1. Midterm exams: Two written midterm exams will be administered. Given the distribution of teaching hours for the assessable content covered in the midterms, the first midterm will account for 60% of the midterm grade, and the second midterm will account for 40%. In order to average the midterm grade with the rest of the course assessment activities, the following is required: i) a minimum score of 4/10 on each midterm, and ii) a minimum average score of 5/10 across both midterms according to the mentioned weighting.

2. Laboratory sessions: A certain "case-molecule" will be solved, in groups of 4 people. Students will have to work and analyze, using quantum chemistry software and spectroscopic databases, the spectroscopic properties of a proposed molecule. Students will have to present the case-molecule in a short oral presentation and answer questions from the teachers. The mark will reflect both the quality of the results and the presentation and the individual answers of the students. A minimum grade of 4/10 is required to average with the rest of the subject's assessment activities (25%).

3. Short quizzes: Test-type quizzes will be proposed, which will be done in the classroom and will be carried out throughout the course (15%).

A second chance exam will be scheduled for those students who have not obtained a minimum grade of 4/10 in the partial exams. It will only be necessary to recover the partial (or partials) with a grade lower than 4/10. Students who wish to improve their grade may take the second chance exam, but by doing so they will forfeit the grade obtained in the partial exams and assume the grade of the final exam. Furthermore, the second chance exam will not be a valid assessment way for obtaining the Distinction with Honours.

In the continuous assessment modality, in order to pass the subject, students must achieve sufficient competence in the practical and theoretical aspects of the subject. The final grade will be obtained from the weighted average of the grades of the partial exams, the practices and the evidence. The Spectroscopy subject is passed with a total grade of 5/10.

The single assessment modality (only for those students who have taken part in it) will consist of:

1. Final written exam, equivalent to the first and second partial exams, which will take place on the same day as the second partial exam in the continuous assessment mode. A minimum grade of 5/10 is required to average with laboratory practices (75%).

2. Laboratory sessions, which will be identical to those of the continuous assessment, that is to say, carrying out the practices according to the established calendar, and presenting the molecule case on the appropriate day (25%).

A second chance exam will be scheduled for those students who did not obtain a minimum grade of 5/10 in the final exam, which will take place on the same day as the second chance exam in the continuous assessment mode. A minimum grade of 5/10 must be obtained to average the laboratory practices.

In the single assessment modality, to pass the subject, students must achieve sufficient competence in the practical and theoretical aspects of the subject. The final grade will be obtained from the weighted average of the grades of the final exam and the laboratory practices. The Spectroscopy subject is passed with a total grade of 5/10.

NON-ASSESSMENT STUDENTS:

Students who do not attend at least 25% of the proposed assessment items, the final grade will be NON-ASSESSMENT

IMPORTANT WARNING ABOUT LABORATORY PRACTICES:

Attendance at laboratory sessions is mandatory and those students who do not attend any of these sessions without reason will not pass the subject.

Any student who is involved in an incident that could have serious consequences in terms of safety maybeexpelled from the laboratory andsuspended from the subject.

Bibliography

Basic Texts:

- C. N. Banwell, E. M. McCash, *Fundamentals of Molecular Spectroscopy*, 4th Ed., McGraw Hill, 1994. (An old Spanish translation exists: C. N. Banwell, *Fundamentos de Espectroscopía Molecular*, Ed. del Castillo, Madrid, 1977, ISBN 9788421901526).
- J. M. Hollas, *Modern Spectroscopy*, 4th Ed., John Wiley & Sons, 2004 *(Does not cover magnetic resonance).*
- P. Atkins, J. de Paula, *Atkins' Physical Chemistry*, 8th Ed., Oxford University Press, 2005

Specialized Texts and Monographies:

- P. Atkins, R. Friedman, *Molecular Quantum Mechanics*, 5th Ed., Oxford University Press, 2011.
- D. J. Willock, *Molecular Symmetry*, Wiley, 2009.
- P. J. Hore, *Nuclear Magnetic Resonance*, Oxford Chemistry Primers, Oxford University Press, 1995.

Software

Laboratory practices will be carried out with the Gaussian16 program for calculations and Gausview6 for the construction and visualization of molecules.

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	second semester	morning-mixed
(PAUL) Classroom practices	2	Catalan	second semester	morning-mixed
(PLAB) Practical laboratories	1	Catalan	second semester	morning-mixed
(PLAB) Practical laboratories	2	Catalan	second semester	morning-mixed
(PLAB) Practical laboratories	3	Catalan	second semester	morning-mixed
(PLAB) Practical laboratories	4	Catalan	second semester	morning-mixed
(PLAB) Practical laboratories	5	Catalan	second semester	afternoon
(PLAB) Practical laboratories	6	Catalan	second semester	afternoon
(PLAB) Practical laboratories	7	Catalan	second semester	afternoon
(PLAB) Practical laboratories	8	Catalan	second semester	afternoon
(SEM) Seminars	1	Catalan	second semester	morning-mixed
(SEM) Seminars	2	Catalan	second semester	morning-mixed

(SEM) Seminars	3	Catalan	second semester	afternoon
(SEM) Seminars	4	Catalan	second semester	afternoon
(SEM) Seminars	5	Catalan	second semester	morning-mixed
(SEM) Seminars	6	Catalan	second semester	morning-mixed
(SEM) Seminars	7	Catalan	second semester	morning-mixed
(TE) Theory	1	Catalan	second semester	morning-mixed
(TE) Theory	2	Catalan	second semester	morning-mixed