2023/2024

Spectroscopy

Code: 102531
ECTS Credits: 6

Degree	Type	Year	Semester
2502444 Chemistry	OB	2	2

Contact

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Teaching groups languages

You can check it through this link. To consult the language you will need to enter the CODE of the subject. Please note that this information is provisional until 30 November 2023.

Teachers

Mariona Sodupe Roure

Prerequisites

- Teaching, including teaching materials handed over to students, will be in English, and hence that good skills on English communication and understanding are necessary. Written evaluation materials, including exams and lab reports, can be turned in Catalan and Spanish and, of course, English.
- Only students that have passed the basic topics of Fundamentals of Chemistry I ("Fonaments de Química I") can do the course of Spectroscopy ("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 Quantum Chemistry ("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 interaction of electromagnetic radiation with 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

- "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."
- 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.
- Communicate clearly in English.
- Have numerical calculation skills.
- Learn autonomously.
- Manage the organisation and planning of tasks.
- Manage, analyse and synthesise information.
- 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. Communicate clearly in English.
5. Communicate in English in the laboratory.
6. Employ and generalise the relationships between structure and spectroscopic methods.
7. Establish spectroscopic response in different structural characteristics.
8. Handle computer programs, including simulators, to support the previous interpretation.
9. Have numerical calculation skills.
10. Identify the physical principles that govern matter-radiation interactions.
11. Learn autonomously.
12. Manage the organisation and planning of tasks.
13. Manage, analyse and synthesise information.
14. Obtain information, including by digital means.
15. Propose creative ideas and solutions.
16. Reason in a critical manner
17. Recognise spectroscopic terminology in the English language.
18. Recognise the English terms used to describe chemical structure.
19. Resolve problems and make decisions.
20. Show motivation for quality.
21. Use IT to treat and present information.
22. Use the most common English chemistry terms.

23. 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:

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. Example: Rotational spectroscopy of diatomic molecules. Lasers.

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: Normal modes of vibration; types of normal modes; symmetry of 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: vibrational structure and vibronic spectra; Franck-Condon Principle. Electronic spectroscopy of polyatomic molecules: Symmetry considerations. Fluorescence and phosphorescence. Photoelectron spectroscopy: UPS and XPS.

5. Magnetic Resonance Spectroscopy.

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

Lab Sessions:

There will be a total of 3 sessions of 4 hours each, thecontents 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.

The development is as follows. The approx. 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.

Methodology

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 "Campus Virtual". 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 "Campus Virtual" 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, explaining the theoretical foundations, computational details, etc., 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 quantum chemistry code 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 two groups, the composition of which will be known beforehand, in order to make efficient use of the lab and computer facilities available. Practical sessions for each subgroup will take place at the appoited dates in different labs and under supervision of qualified instructors. For all lab sessions, the lab protocol will be made available in the "Campus Virtual", and the students have to bring their own hard copy 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. Besides, in experimental lab sessions it is compulsory that students show up with apron and protective goggles.

On appointed days, the students will be summoned to the lab/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.

In the last session, the students will carry out, in groups, a final practice that is to apply the techniques developed in the sessions of the previous practices to a specific molecule (the case) and make an analysis of its spectroscopic properties. The groups will make an exhibition of this final work infront 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.

Important Note:

Teaching, including all teaching and evaluation materials (e.g. exams, lab report forms) will be given out in English. However, written answers in evaluation materials will be accepted in Catalan and Spanish.

The proposed teaching methodology may experience some modifications depending on the restrictions to face-to-face activities enforced by health authorities.

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.

Activities

Title	Hours	ECTS	Learning Outcomes
Type: Directed			
Lab Sessions	20	0.8	1, 2, 5, 4, 20, 6, 7, 13, 22, 8, 3, 14, 15, 16, 18, 17, 19, 9, 23, 21
Problem Solving Sessions	12	0.48	2, 11, 5, 4, 20, 6, 7, 12, 10, 22, 8, 16, 18, 17, 19, 9, 23
Theory Lectures	27	1.08	2, 11, 4, 6, 7, 13, 10, 22, 8, 14, 16, 18, 17, 23
Type: Supervised			
Case Preparation	10	0.4	1, 2, 11, 5, 4, 20, 6, 7, 12, 13, 10, 22, 8, 3, 14, 15, 16, 18, 17, 19, 9, 23, 21
Type: Autonomous			
Personal Study	50	2	2, 11, 6, 7, 12, 13, 10, 22, 8, 14, 16, 18, 17, 19, 9, 23
Problem Solving	18	0.72	2, 11, 4, 6, 7, 12, 13, 10, 22, 8, 14, 15, 16, 18, 17, 19, 9, 23
Quizz Preparation	5	0.2	1, 2, 11, 4, 20, 6, 7, 12, 13, 10, 22, 8, 14, 15, 16, 18, 17, 19, 23, 21

Assessment

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. Partial exams: There will be two written partial exams. A minimum average grade of 5/10 (and a minimum grade of 4 in each partial) is required to average with the rest of the subject's assessment activities (60%).

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 (25%).

3. Short quizzes: Test-type quizzes will be proposed, which will be solved online through the Moodle 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.

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. It is necessary that the grades of the theoretical (1) and practical (2) partsbe equal to or higher than 5/10 each. 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. It is necessary that the grades of the theoretical (1) and practical (2) parts be equal to or higher than 5/10 each. The Spectroscopy subject is passed with a total grade of 5/10.

Students will be considered "non-evaluable" if they do not appear in 66% of the proposed evaluation items.

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 may be expelled from the laboratory andsuspended from the subject.

Assessment Activities

Title	Weighting	Hours	ECTS	Learning Outcomes
Final Exam	60%	3	0.12	2, 11, 6, 7, 10, 22, 3, 15, 16, 18, 17, 19, 9, 23
Lab sessions	25%	0	0	1, 2, 11, 5, 4, 20, 6, 7, 12, 13, 22, 8, 3, 14, 15, 18, 17, 19, 9, 23, 21
Partial Exams	60%	3	0.12	2, 11, 6, 7, 10, 22, 3, 15, 16, 18, 17, 19, 9, 23
Short Quizzes	15%	2	0.08	2, 20, 6, 7, 10, 22, 3, 15, 16, 18, 17, 19, 9, 23

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.