Spectroscopy

2015/2016

Code: 102531
ECTS Credits: 6

Degree	Type	Year	Semester
2502444 Chemistry	OB	2	2

Contact

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Use of languages

Principal working language: english (eng)

Teachers

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Prerequisites

- Teaching, including teaching materials handed over to students, will be in English, hence good communication skills in English 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 ("Fonaments de Química") and Experimentation and Documentation ("Experimentació i Documentació") can take 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 symmetry as a powerful tool to explain characteristics of certain spectra in polyatomic molecules. From there on, different spectroscopic techniques 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.

Skills

- 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.
- "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. 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, analyse and synthesise information.
13. Manage the organisation and planning of tasks.
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. Systematic determination of molecular point group. 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. Mutual exclusion rule.

4. Electronic Spectroscopy.

   Atomic spectroscopy. Spectral terms. Selection Rules. Electronic spectroscopy of diatomic molecules. Vibrational structure: vibronic spectra. Franck-Condon principle. Electronic spectroscopy of polyatomic molecules. Symmetry considerations. Fluorescence and phosphorescence. Photoelectron spectroscopy.

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:

A total of five sessions (4 hours each), plus a sixth session of evaluation (order to be determined). The contents willbe:

1. Basic experimental techniques in spectroscopy (I): IR of gas and liquid samples.
2. Basic experimental techniques in spectroscopy (II): UV-VIS and NMR
3. Simulation of Vibrational Spectra
4. Simulation of Electronic Spectra
5. Simulation of NMR Spectra
6. A Project/Case, worked out in the simulation sessions (3 to 5 above).

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 with the possibility to (1) 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, and also (2) be introduced to basic spectroscopic techniques in a real chemistry lab. 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 assessing the level of comprehension of the task just completed and the qualityof the results obtained, and from which the lab grade will be drawn.

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.

Activities

Title	Hours	ECTS	Learning outcomes
Type: Directed			
Lab Sessions	16	0.64	1, 2, 5, 4, 20, 6, 7, 12, 22, 8, 3, 14, 15, 16, 18, 17, 19, 9, 23, 21
Problem Solving Sessions	8	0.32	2, 11, 5, 4, 20, 6, 7, 13, 10, 22, 8, 16, 18, 17, 19, 9, 23
Theory Lectures	26	1.04	2, 11, 4, 6, 7, 12, 10, 22, 8, 14, 16, 18, 17, 23
Type: Supervised			
Case Preparation	6	0.24	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	70	2.8	2, 11, 6, 7, 12, 13, 10, 22, 8, 14, 16, 18, 17, 19, 9, 23
Problem Solving	10	0.4	2, 11, 4, 6, 7, 12, 13, 10, 22, 8, 14, 15, 16, 18, 17, 19, 9, 23

Evaluation

The evaluation is based on a "continuous evaluation" scheme, comprising the following items:

1. **Lab reports**, turned in at the end of each practical session **10%**

2. **Solve a given "Case"**: working in groups of 4 people, the students will have to work out, using quantum chemistry software and spectroscopic databases as needed, detailed spectroscopic properties of proposed molecules, present their case in a short oral presentation, and answer questions from the evaluators. The grade will reflect both the quality of the results and presentation (same for all members), and the individual responses of each student **15%**

3. **A certain number of short exercises** will be proposed, spread out along the semester, some to be returned on the spot, some to be done at home **15%**

4. **Two partial written exams**, covering approximately one-half of the syllabus each and to be held on dates and times known at the time of enrollment. A minimum score of 4/10 is required in each for them to count towards the final grade. Each of these tests will count towards 30% of the final grade. **2x30%=60%.**

   A final exam which will only be compulsory for students who have not scored 4/10 in any or both of the partial exams above. This exam will be divided in two halves matching the contents of the first set of tests. The student is required to take at least the part where s/he did not attain 4/10. Students wishing to improve their score can take this exam too, whole or piecewise, but in doing so they give up the grade in the partial exam and take instead the grade of the final. Note that it is possible to lower the grade in this way **60%**

To pass the subject, students need to attain sufficient proficiency in the **practical** and **theoretical** aspects of the topic. The final grade is obtained by adding the following three contributions, (a), (b), and (c):

(a) Practical aspects: items (1)+(2)

(b) Theoretical aspects: Item (4)

(c) Personal work: item (3)

However, it is necessary that grades of the Practical (a) and Theoretical (b) parts of the topic are **each at least** 4/10. The topic od Spectroscopy is passed with a total grade of 5/10. Note that lab attendance is compulsory. For grading purposes, a student will be considered as non-evaluable ("no presentat"), if any of the following applies:

1. has not attended any lab session without motive. This includes showing up without goggles and/or apron when required, as the student will not be accepted in the lab on safety grounds.

2. cannot achieve a grade of 5/10 with his/her own evaluation items, and could not achieve it with the same items even if s/he had achieved in those the highest grade.

Evaluation activities

Title	Weighting	Hours	ECTS	Learning outcomes
Case Presentation	15%	1	0.04	1, 5, 4, 20, 12, 13, 22, 14, 15, 16, 18, 17, 19, 9, 21
Final Exam	60%	3	0.12	2, 11, 6, 7, 10, 22, 3, 15, 16, 18, 17, 19, 9, 23
Lab Reports	10%	1	0.04	2, 5, 20, 6, 7, 12, 22, 8, 3, 15, 16, 18, 17, 9, 23
Partial Exams	60%	6	0.24	2, 11, 6, 7, 10, 22, 3, 15, 16, 18, 17, 19, 9, 23
Turned-in Exercises	15%	3	0.12	2, 20, 6, 7, 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.