Universitat Autònoma de Barcelona

2020/2021

Molecular Spectroscopy

Code: 103283
ECTS Credits: 5

Degree	Type	Year	Semester
2501922 Nanoscience and Nanotechnology	OB	3	1

The proposed teaching and assessment methodology that appear in the guide may be subject to changes as a result of the restrictions to face-to-face class attendance imposed by the health authorities.

Contact

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Use of Languages

Principal working language: catalan (cat)
Some groups entirely in English: No
Some groups entirely in Catalan: Yes
Some groups entirely in Spanish: No

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 ones 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 ones 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

Nature of electromagnetic radiation. Energy and type of radiation. Electromagnetic spectrum and spectroscopic techniques. Intensity of spectral lines.
Dipolar moment of the transition. Selection rules Spectral line width. Principle of uncertainty. Lasers

2. Rotation and vibration spectroscopy of diatomic molecules

Approach to Born-Oppenheimer and Equation of nuclear Schrödinger. Models of the rigid rotor and of the harmonic oscillator.
Selection rules. Anharmonicity. Dissociation energies.

3. Molecular symmetry

Elements and symmetry operations. Timely symmetry groups. Classification Systematic determination of the specific group of a molecule. Applications of symmetry. Optical isomery. Dipole moment

4. Theory of groups

Group properties. Classes of symmetry elements. Reduced and irreducible representations. Species of symmetry. Character tables. Decomposition of reductible representations in their irreducible components.

5. Vibrational spectroscopy of polyatomic molecules

Vibration of polyatomic molecules. Normal vibration modes. Types of vibrations: voltage and deformation. Symmetry of normal vibration modes. Selection rules Raman effect. Polarizability Selection rules. Application of group theory to vibrational analysis. Ruleof mutual exclusion.

6. Electronic spectroscopy

Atomic Spectroscopy. Spectral Terms. Interaction Spin Orbit. Permitted Transitions. Electronic state of diatomic molecules. Electronic transitions in diatomic molecules. Vibrational structure of electronic bands. Principle of Franck-Condon. Electronic transitions Selection rules Symmetry considerations. Fluorescence and phosphorescence. Photoelectron spectroscopy

7. Magnetic resonance spectroscopy

Nuclear spin Interaction with a magnetic field. Nuclear Magnetic Resonance (NMR). Nuclear energy levels. Selection rules. Nuclear shielding and chemical shift. Spin-spin coupling. Equivalent nuclei. First-order systems. Chemical and magnetic equivalences. Applications .Electron Spin Resonance.

Computer classroom practices

1. Vibrational spectroscopy

2. Electronic Spectroscopy

Methodology

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.

Activities

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 excercices	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	

Assessment

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 minimum ones can not be reached, at the end of the course one or both partial exams can be retrieved. The note obtained in the recovery will replace the note obtained in the first attempt. It is also possible to come up with the recoveries to improve note. In this case, the last note obtained in each partial 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 note 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.

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

Bibliography

Basic Texts:

- P. Atkins, J. de Paula, Atkins' Physical Chemistry, 8th Ed., Oxford University Press, 2005.

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

Specialized texts:

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