UAB
Universitat Autònoma de Barcelona

Methods of Spectroscopic Analysis

Code: 102488
ECTS Credits: 6

2025/2026

Degree	Type	Year
Chemistry	OB	3

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

You must have passed the subject Fundamentals of Chemistry. It is recommended to have acquired the knowledge and skills taught in the subject Analytical Chemistry and Electroanalysis

Objectives and Contextualisation

The course aims to complement the students' basic knowledge of instrumental analysis techniques within Analytical Chemistry and, in particular, spectroscopic methods of analysis.

The knowledge acquired in this course is fundamental in order to understand and approach the learning of subjects from other areas of knowledge, taking advantage of the multidisciplinary nature of the subject Analytical Chemistry.

The main objectives of the course are:

1. To describe the fundamental principles and associated instrumentation of the main optical analysis techniques.

2. To apply this knowledge to the resolution of chemical analysis problems.

Laboratory practices related to the contents of this subject will be developed in the Laboratory of Chromatographic and Spectroscopic Analysis.

Competences

- Apply knowledge of chemistry to problem solving of a quantitative or qualitative nature in familiar and professional fields.
- Learn autonomously.
- Manage the organisation and planning of tasks.
- Obtain information, including by digital means.
- Reason in a critical manner
- Recognise and analyse chemical problems and propose suitable answers or studies to resolve them.
- Resolve problems and make decisions.
- Show an understanding of the basic concepts, principles, theories and facts of the different areas of chemistry.
- Use IT to treat and present information.
- Work in a team and show concern for interpersonal relations at work.

Learning Outcomes

1. Classify electroanalytical and optical analysis methods, and how they are used.
2. Describe the principles involved in electrochemical and optical analysis methods.
3. Employ information and communication technology in the documentation of cases and problems.
4. Employ the principles of electrochemistry and (optical) spectrophotometry to solve analytical problems.
5. Explain the basic operations of electroanalytical and optical equipment.
6. Identify the statistical methods for the treatment of the results of analyses to obtain information on their quality.
7. Interpret the results obtained from analytical problems, as well as their quality parameters.
8. Learn autonomously.
9. Manage the organisation and planning of tasks.
10. Obtain information, including by digital means.
11. Plan the right strategy in the different stages of the analytical procedure to solve the problems being addressed.
12. Reason in a critical manner
13. Recognise the stages of the analytical procedure in chemical analysis.
14. Resolve a collection of instrumental analysis problems.
15. Resolve problems and make decisions.
16. Use IT to treat and present information.
17. Work in a team and show concern for interpersonal relations at work.

Content

PART I: INTRODUCTION

1. Introduction to instrumental analysis techniques. Approach to the problems that Analytical Chemistry must currently solve. Definition of instrument. Basic characteristics of the instruments. Analytical properties. Quantitative analysis: Calibration.

2. Introduction to optical methods of analysis. Properties of light. Principles of radiation-matter interaction: reflection, dispersion, refraction, diffraction, polarization. The electromagnetic spectrum. Absorption and emission of energy by atoms and molecules. Classification of optical analysis techniques. Molecular and atomic techniques. Absorption and emission techniques.

PART II: MOLECULAR SPECTROSCOPY

3. UV-visible molecular absorption spectrophotometry. Basis of the technique. Transmittance and absorbance. Deduction Lambert-Beer's Law. Limitations of law. Basic components of analytical instrumentation. Radiation sources. Selection of wavelength. Detectors. Single beam, double beam and diode-array spectrophotometers. Quantitative analysis applications. Photometric evaluations. Resolution of mixtures. Spectroscopy of derivatives.

4. Molecular absorption spectrophotometry IR. Fundamentals: vibration spectra. Basic components of analytical instrumentation. Fourier transform IR spectroscopy (FTIR). Sample preparation. Qualitative analysis. Quantitative analysis: Gas analysis. NIR.

5. Molecular Luminescence. Fundamentals of luminescence: fluorimetry and phosphorimetry. Excitation and emission spectra. Variables affecting luminescence. Quantitative relationships. Quenching techniques: Stern-Volmer Law. Instrumentation. Chemoluminescence. Applications: FRET and fluorescent markers.

PART III: ATOMIC SPECTROSCOPY

6. Atomic absorption spectroscopy. Fundamentals of atomic absorption. Atomic spectra. Atomization: effect of temperature. Instrumentation. Flame atomic absorption spectroscopy. Background radiation. Atomic absorption spectroscopy with graphite furnace. Generation of hydrides and cold steam. Correction of the background signal. Spectral and chemical interference. Quantitative analysis applications.

7. Atomic emission techniques. Fundamentals of atomic emission. Atomization systems: flame and plasma. Instrumentation. Flame photometry. Induction coupled plasma spectroscopy (ICP): Fundamentals. Sequential and multichannel instrumentation. Spectral and chemical interference. Applications.

PART IV: OTHER ANALYTICAL TECHNIQUES

8. Mass spectrometry. Fundamentals. Characteristics of the mass spectrum. Mass spectrometers. Sample introduction systems. Ion sources: Inductive coupling plasma, electronic impact, chemical ionization, ionization and field desorption. Maldi and electrospray. Mass analyzers: quadrupole, time of flight, magnetic sector and double focus. Detectors. Qualitative and quantitative applications. Atomic mass spectrometry. Ionization systems: induction coupled plasma. Characteristics and applications. Molecular mass spectrometry. Ionization source: electron impact, chemical ionization, electrospray and MALDI. Qualitative and quantitative applications. Hybrid and tandem systems.

Activities and Methodology

Title	Hours	ECTS	Learning Outcomes
Type: Directed			
Lectures and seminars	37	1.48	8, 1, 4, 3, 2, 5, 9, 10, 11, 12, 13, 17, 16
Problems and exercices	12	0.48	8, 4, 3, 6, 7, 11, 12, 15, 14, 17
Type: Supervised			
Tutorials	5	0.2	4, 5, 9, 6, 7, 10, 11, 12, 13, 14, 17

Type: Autonomous			
Exercices solving and seminar preparation	33	1.32	8, 4, 3, 9, 6, 7, 10, 11, 12, 15, 14, 17, 16
Study	49	1.96	8, 1, 3, 2, 5, 9, 7, 10, 11, 12, 17, 16

Theory Classes and Seminars:
The lecture model will be combined with audiovisual support and training activities that can be completed in groups or individually. In the lectures, the instructor will provide an overview of the topic covered, emphasize key concepts for understanding, and answer any questions or concerns. To facilitate the achievement of the learning objectives, training activities aimed at promoting cooperative learning and student participation will be introduced. For individual study and in-depth preparation of the topics, a basic and complementary bibliography will be provided. The activities are designed to acquire specific skills as well as develop transversal skills.
During the semester, seminars will be held dedicated to the presentation of group projects on selected applications of the instrumental techniques studied. The aim of these seminars is to delve deeper into aspects covered in the theory classes. The projects will be presented orally by the group members to the entire class. Optionally, a seminar led by specialists in the field of analytical instrumentation studied in the course could also be held. These invited seminars would not only serve to expand the course syllabus but also to introduce students to specialists with a wide range of experience and provide other forms of communication that will enrich their career placement.
Problem Classes
The knowledge acquired in the lectures will be applied by solving questions and problems. These will be developed following two different strategies: (a) The professor will solve selected problems or standard problems in front of the entire group, allowing the student to learn to identify the essential elements of the approach and how to approach its resolution; and (b) the students, in small groups, guided and assisted by the professor, will address similar problems and questions or problems that require novel approaches.
Additionally, and if possible, visits will be made to companies that manufacture analytical instrumentation based on optical measurements and/or large research facilities where optical analysis techniques are applied.

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 Term	50	4	0.16	8, 1, 4, 3, 2, 5, 9, 6, 7, 10, 11, 12, 13, 15, 14, 17, 16
Middle Term	20	2	0.08	8, 1, 4, 3, 2, 5, 9, 6, 7, 10, 11, 12, 13, 15, 14, 17, 16
Training activities and seminars	30	8	0.32	8, 1, 4, 3, 2, 5, 9, 6, 7, 10, 11, 12, 13, 15, 14, 17, 16

Continuous Assessment

The competences of this course will be evaluated by means of:

a) Middle term test (individual assessment), including the 1st part of the subject. 20% of the final mark.

b) Final term test (individual assessment), including the whole subject. 50% of the final mark.

c) Cooperative and collaborative activities (seminars, problems, evidence, etc.) and individual (evidence) carried out inside and outside the classroom. They will have a weight of 30% in the final grade, adding both cooperative and individual contributions.

To participate in the second chance exam, the students must have been previously evaluated in a set of activities whose weight must be equivalente to a minimum of two thirds of the total grade of the subject.

It will be considered that the student is not assessable when the activities carried out are not equivalente to 51% of those that are evaluated to obtain the total qualification of the subject.

Single Assessment

The students who have taken the single evaluation modality must take a final test which will consist of a final term test, including the whole subject, to be taken on the day that the students of the continuous evaluation take the second partial exam. The student's final grade will be the grade of this test.

If the final grade does not reach 5, the student has another opportunity to pass the subject by means of the second chance exam that will be held on the date set by the degree coordinator. The final student's grade will be the grade of this second test.

The same non-assessable criterion will be applied as in the continuous evaluation.

Bibliography

1. F. James Holler, Douglas A Skoog, Stanley R. Crouch. Principios de Analisis Instrumental. 6.ª Edición. 2008. ISBN-10: 9706868291. Cengage Learning Editores. ISBN-13: 9789706868299.
2. Skoog, Douglas A., Donald M. West, F. James Holler y Stanley R. Crouch. Fundamentos de química analítica. Novena edición. 2015. Cengage Learning Editores. ISBN: 978-607-519-937-6
3. Frame, Eileen M. Skelly; Frame, George M.; Robinson, James W. Undergraduate Instrumental Analysis. Seventh edition. 2014. CRC Press. ISBN: 9781420061352
4. Gary D. Christian, Purnendu K. Dasgupta, Kevin A. Schug. Analytical Chemistry. Seventh edition. 2013. John Wiley & Sons. ISBN: 9780470887578
5. Kellner, R., Mermett, M., Otto, M., Widmer, H.M. (Eds.); Analytical Chemistry. Wiley-VCH, Weinheim, 1998
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Software

Microsoft Office

Acrobat Reader

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	first semester	morning-mixed

(PAUL) Classroom practices	2	Catalan	first semester	afternoon
(TE) Theory	1	Spanish	first semester	morning-mixed
(TE) Theory	2	Catalan	first semester	morning-mixed