Universitat Autònoma de Barcelona

2019/2020

Methods of Spectroscopic Analysis

Code: 102488
ECTS Credits: 6

Degree	Type	Year	Semester
2502444 Chemistry	OB	3	1

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: Yes

Teachers

Manuel Valiente Malmagro

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 subject 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.

The laboratory practices related to the contents of this subject will be developed in the course Analysis and Determination of Properties.

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 line diode 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.

Methodology

Theory lectures and seminars:

The exhibition model (masterclass) will be combined with audiovisual support and training activities that can be carried out in groups or individually. In the master classes, the teacher will offer a global vision of the treated topic emphasizing on the associated key concepts for its adequate comprehension and will answer to the eventual doubts or questions.

In order to favour the achievement of the proposed learning objectives, training activities will be introduced aimed at promoting cooperative learning and student participation. For the individual study and preparation of topics in depth, a basic and complementary bibliography will be indicated. The activities are designed to acquire specific competences as well as to develop transversal competences.

Throughout the four-month period there will also be different seminars dedicated to the presentation of works on selected applications of the instrumental techniques studied. The aim of these seminars is to deepen the aspects dealt with in the theory classes. The works will be elaborated in group and will be exposed in oral form to the whole of the class.

Exercises sessions

The knowledge acquired in theory classes will be applied by solving questions and numerical problems. They will be developed following two different strategies: (a) The teacher will solve some selected problems or typical problems before the whole 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 helped by the teacher, will face similar problems and questions or problems that demand novel approaches.

Activities

Title	Hours	ECTS	Learning Outcomes
Type: Directed			

Lectures and seminars	40	1.6	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	38	1.52	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

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, evidences, etc.) and individual activities carried out inside and outside the classroom. They will have a weight of 30% of the final mark

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

It will be considered a "not presented" in the subject if the student does not show any of the two controls, regardless of whether or not you have done cooperative and / or collaborative activities.

To pass the course a minimum of 5 points (out of 10) is requested in the average of the controls and the cooperative and collaborative activities.

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	0	0	8, 1, 4, 3, 2, 5, 9, 6, 7, 10, 11, 12, 13, 15, 14, 17, 16

Bibliography

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.

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

Frame, Eileen M. Skelly; Frame, George M.; Robinson, James W. Undergraduate Instrumental Analysis. Seventh edition. 2014. CRC Press. ISBN: 9781420061352

Gary D. Christian, Purnendu K. Dasgupta, Kevin A. Schug. Analytical Chemistry. Seventh edition. 2013. John Wiley & Sons. ISBN: 9780470887578

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