Universitat Autònoma de Barcelona

2019/2020

Analysis and Determination of Properties

Code: 102533
ECTS Credits: 6

Degree	Type	Year	Semester
2502444 Chemistry	OB	3	2

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

Having studied or being currently enrolled in Physical Chemistry, Spectroscopic Analysis Methods and Separation Techniques. Have passed the security test (virtual campus)

During practices, students must wear the approved lab coat and safety goggles. In addition to the usual tools to write, they should bring a scientific calculator, a laboratory book and a spatula.

Objectives and Contextualisation

The main objective of the subject is that the student reaches the competences indicated in the corresponding section.

The general objectives are:

1. Apply the fundamental laws and the theoretical principles acquired by the student in the courses of the subjects referenced in Prerequisites section.

2. Familiarize the student with the use of specific instrumentation, the acquisition of data in the laboratory and its interpretation, the introduction to the methods of analysis of data ...

3. To develop in the student a critical mentality that refers to the level of confidence of their measures, calculations and the interpretation of results.

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.
- Communicate orally and in writing in ones own language.
- Develop synthesis and analyses studies in chemistry from previously established procedures.

- Evaluate the health risks and environmental and socioeconomic impact associated to chemical substances and the chemistry industry.
- Handle chemical products safely.
- Handle standard instruments and material in analytic and synthetic chemical laboratories.
- Have numerical calculation skills.
- Learn autonomously.
- Manage the organisation and planning of tasks.
- Manage, analyse and synthesise information.
- Operate with a certain degree of autonomy and integrate quickly in the work setting.
- Propose creative ideas and solutions.
- Reason in a critical manner
- Recognise and analyse chemical problems and propose suitable answers or studies to resolve them.
- Show an understanding of the basic concepts, principles, theories and facts of the different areas of chemistry.
- Show initiative and an enterprising spirit.
- Show motivation for quality.
- Show sensitivity for environmental issues.
- Use IT to treat and present information.
- Use the English language properly in the field of chemistry.
- Work in a team and show concern for interpersonal relations at work.

Learning Outcomes

1. Adapt to new situations.
2. Apply statistical methods to treat data.
3. Apply suitable calibration methods in each case studied.
4. Apply the acquired theoretical contents to the explanation of experimental phenomena.
5. Be ethically committed.
6. Communicate clearly in English.
7. Communicate in English in the laboratory.
8. Communicate orally and in writing in ones own language.
9. Critically evaluate experimental results and deduce their meaning.
10. Describe basic safety regulations.
11. Design simple experiments for the study of simple chemical and physical systems.
12. Develop the habits and skills of a laboratory.
13. Draft a laboratory logbook containing descriptions of the developed procedures, the observations made, the results obtained, the interpretation of the same and the conclusions.
14. Evaluate risks in the use of chemicals and laboratory procedures.
15. Evaluate the influences of variable parameters in measurement, such as concentration, temperature, pressure, dissolvent, etc.
16. Follow safety procedures in the chemistry laboratory.
17. Follow standard laboratory procedures described in English.
18. Follow standard laboratory procedures.
19. Handle instruments to record different types of spectrums.
20. Handle laboratory instruments and materials for the determination of chemical and physical properties and the analysis of products and reagents.
21. Handle standard instruments and material in chemical laboratories for analysis and synthesis in the field of organic chemistry.
22. Handle the instruments and material used in different separation techniques.
23. Have numerical calculation skills.
24. Identify the main reagents in a laboratory and their commercial presentation.
25. Identify the risks of synthetic reagents.
26. Interpret experimental data obtained from separation processes in the laboratory.
27. Interpret the data from observations and measurements in the laboratory in terms of their meaning and of the theories sustaining the same.
28. Interpret the data on chromatographic separation processes obtained using computer tools (simulation programs).
29. Interpret the safety notes on chemistry products.

30. Learn autonomously.
31. Manage the organisation and planning of tasks.
32. Manage, analyse and synthesise information.
33. Manipulate the main reagents and dissolvents in a chemistry laboratory.
34. Memorise the scientific terms used in English in the field of experimental chemistry / physical chemistry.
35. Observe the physical and chemical properties of different substances.
36. Observe the reactivity and behaviour of representative compounds in the laboratory.
37. Operate with a certain degree of autonomy and integrate quickly in the work setting.
38. Perform a synthetic and analytic study to determine chemical and physical properties using instructions supplied for a detailed procedure.
39. Perform correct evaluations of the health risks and environmental impact of magnetic fields.
40. Perform standard tests on which the results obtained are based.
41. Properly use the necessary computer tools to calculate, graphically represent and interpret the data obtained, as well as its quality.
42. Propose creative ideas and solutions.
43. Reason in a critical manner
44. Recognise and interpret the stages of an analytical procedure.
45. Recognise potential risks in the laboratory before they are produced.
46. Recognise potentially dangerous reagents and dissolvents.
47. Recognise some of the different instruments and equipment used in spectrophotometric methods and analytical chromatography.
48. Recognise the use of each reagent in the laboratory and take appropriate safety precautions in each case (special goggles and/or gloves, extractor hood, gas mask, etc.).
49. Relate experimental data with the physical and chemical properties and/or analysis of the systems that are the object of study.
50. Relate the acquired knowledge with the use of the corresponding analytical techniques in the laboratory.
51. Relate the characteristics of compounds with their elemental physical and chemical properties.
52. Relate the fundamental principles, theories and facts of chemistry with experimental data obtained in the laboratory during the study of different physical and chemical systems.
53. Relate the result obtained with the original information, including the correct interpretation of the errors associated to the value obtained.
54. Resolve qualitative and/or quantitative problems in accordance with previously developed models.
55. Safely dispose of waste from chemical reactions.
56. Safely handle inflammable, toxic and/or corrosive reagents.
57. Safely handle the different radiations involved in each spectroscopic technique.
58. Safely handle the electrical circuits that form part of different spectrometers.
59. Selectively distinguish the rejection of reagents and chemical products.
60. Show initiative and an enterprising spirit.
61. Show motivation for quality.
62. Show sensitivity for environmental issues.
63. Understand the labelling of chemical reagents in English.
64. Use IT to treat and present information.
65. Use data processors to produce reports.
66. Use graphic design programs to draw chemical formulas and their reactions.
67. Use safety equipment properly.
68. Use spectroscopy devices to confirm experimental results.
69. Use standard instruments and material in chemical laboratories for analysis and synthesis in the field of inorganic chemistry.
70. Use statistical methods to treat the results of analyses and obtain quality information.
71. Use suitable strategies for the safe elimination of reagents.
72. Use the basic materials of a chemical laboratory.
73. Use the most common English chemistry terms.
74. Work in a team and show concern for interpersonal relations at work.
75. Work safely in the laboratory while following the adequate procedure.
76. Write simple laboratory reports in English

Content

The development of the contents will begin with four hours of lectures (two sessions of 2 hours each). In these lectures, the content and methodology needed for the realization of the four blocks of this subject will be presented. There will be 24 laboratory sessions of 4 hours each, with the contents indicated below.

Spectroscopic methods (5/6 days)

- AAS (Atomic absorption spectroscopy). Determination of Cu in alcoholic beverages

- AAS (Atomic emission spectroscopy). Determination of K in water

- UV-Visible Spectrophotometry. Determination of Fe (II) in a vitamin complex

- UV-Visible Spectrophotometry. Multicomponents Simultaneous determination of Co and Ni by formation of a colored complex with PAR

- UV-Visible Spectrophotometry. Determination of the pKa of a synthetic indicator

Chromatographic methods (6/7 days)

- Liquid chromatography. Determination of caffeine in coffee beverages and / or cola by HPLC-UV-Vis

- Liquid chromatography. Identification of sulfonamides in veterinary medicine by HPLC-UV-Vis

- Gas chromatography. Separation and identification of alcohol mixtures by GC-FID and / or GC-TCDy)

- Gas chromatography. Quantitative determination of pool water THM (SAF) by HS-GC-ECD (SAQ)

- Liquid chromatography. Computer simulation of a chromatographic process by HPLC.

. Determination of the methanol content in a alcoholic beverage by gas chromatography (GC-FID))

KINETICS (8 days)

- Kinetics by polarimetry. Sucrose inversion reaction.

- Kinetics by conductimetry. Basic hydrolysis of ethyl acetate

- Iodization of cyclohexanone in acid medium: kinetic study.

- Study of the effect of ionic strength on the speed of the oxidation reaction of iodide with the anion peroxodisulfat.

- Solvatochromism as a tool to characterize the properties of a solvent

CHEMICAL SURFACES AND ELECTROCHEMISTRY(4 days)

- Adsorption isotherm

- Conductivity of ionic solutions

- Determination of the critical micelle concentration by measures of condutivitat.

- Wastewater treatment through electrochemical processes

- Surface tension. wettability

Methodology

This subject consists of 4 parts distributed according to the methodology and the theoretical knowledge employed. Before beginning the laboratory sessions there will be two sessions in the theory classroom about

the rules that appear in this Teaching Guide, the latest information and the methodology and contents of the blogs.

Attendance at the classroom and in the laboratory is mandatory. An unjustified lack involves a zero of the practice. The students, in groups of 2 students, will perform 24 laboratory sessions of 4 hours, during which there will be 19-20 different practices. Students will previously have the scripts of the practices for their preparation. They have to enter the laboratory with the script of the practice read and with the calculations that ask for the preparation of dissolutions raised from home

Students must write in the laboratory booknote all the experimental results and the teacher's explanations. Once the practice is finished, and the material has been completed, students fill out and / or write the report of the practice (introduction and objectives, results and discussion, conclusions, bibliography and an annex showing the expressions amputated for evaluation of the uncertainties). All the results obtained in the laboratory must be presented in tables with the uncertainties and the corresponding units. The graphs must be presented with a title, the magnitudes represented, the corresponding units, the bars of uncertainties and the results of the adjustments if applicable

In some cases, the students will report to the house in order to make the calculations more time

Activities

Title	Hours	ECTS	Learning Outcomes
Type: Directed			
Development of the laboratory practices	96	3.84	1, 4, 3, 2, 9, 7, 6, 8, 60, 61, 12, 55, 11, 59, 63, 39, 32, 24, 25, 28, 26, 27, 29, 22, 20, 21, 19, 58, 57, 56, 33, 5, 62, 36, 35, 37, 42, 43, 40, 38, 47, 46, 44, 48, 45, 13, 53, 50, 51, 49, 54, 16, 18, 17, 23, 75, 74, 68, 72, 70, 69, 71, 67, 65, 14, 15
Lectures in a classroom	4	0.16	10, 52, 71
Type: Autonomous			
Reading and study of guidelines, preparation of laboratory practices, writting of reports	44	1.76	4, 30, 9, 11, 76, 32, 28, 26, 27, 73, 34, 43, 53, 49, 41, 64

Assessment

The evaluation process follows the principle of continuous evaluation. The overall score will be constituted by the weighted sum of 3 sections: QF laboratory (30%); QA laboratory (30%) and written exam (40%)

The laboratory score will consist mainly of the qualification of the reports, but may include, with different weights, other concepts such as: prelab tests (short written test to verify that the student has adequately prepared the practice that he/she is going to perform); laboratory notebook; behavior and attitude. The concepts to be evaluated and the corresponding weighting factors will be explained in the presentation of the laboratory. If a student obtains a score <3.5 in one laboratory, the subject will be considered suspended and the score of the suspended laboratory will be the global grade of the subject.

The written examination will consist of two parts, each corresponding to one of the two laboratories. Its score will be the average of the scores of the two parts. In order to compute the average, the score of each part must be equal or higher than 4.0; if this minimum score of 4.0 is not obtained in one (or both parts), a recovery exam will be available. If the recovery does not reach 4.0, the subject will be considered suspended and the grade of the subject will be the score of the suspended exam.

To participate in the recovery, students must have been previously evaluated in a set of activities the weight of which equals a minimum of two thirds of the total grade of the subject and have reached a global grade equal or higher than 3.5

In the case of non-compliance with safety regulations, a student may be expelled from the laboratory and suspend the practice of that day. In the case of serious or repetitive breach of safety regulations may be expulsion from the laboratory and suspend the subject.

Assessment Activities

Title	Weighting	Hours	ECTS	Learning Outcomes
Personal work	10%	0	0	1, 3, 2, 30, 9, 7, 6, 8, 60, 61, 12, 55, 11, 59, 63, 39, 31, 32, 24, 25, 28, 26, 27, 29, 22, 20, 21, 19, 58, 57, 56, 33, 5, 62, 36, 35, 37, 42, 43, 40, 38, 47, 46, 48, 45, 13, 53, 51, 49, 16, 18, 17, 75, 74, 68, 72, 69, 71, 67, 14, 15
Report of results	30%	0	0	1, 4, 30, 9, 6, 8, 60, 61, 11, 76, 32, 28, 26, 27, 73, 42, 43, 40, 44, 13, 53, 50, 52, 51, 49, 54, 23, 41, 70, 64, 66, 65, 15
Results of the laboratory practice	20%	0	0	61, 12, 11, 32, 28, 26, 22, 20, 21, 19, 36, 35, 37, 43, 40, 38, 13, 53, 49, 54, 18, 23, 72, 69, 15
Written exam	40%	6	0.24	4, 2, 9, 10, 26, 27, 29, 73, 34, 43, 44, 53, 50, 52, 49, 54, 23, 70

Bibliography

P.W. ATKINS.; J. DE PAULA,

Atkins' Physical Chemistry.

9ª ed. Oxford University Press, 2009.

(Traducción de la 8ª ed., Ed. Pananmericana, 2008)

J. Guiteras, R. Rubio, G. Fonrodona,

Curso experimental de Química Analítica.

Ed. Sintesis 2003

D.A. Skoog, F.J.Holler, T.A. Nieman,

Principios de Análisis Instrumental,

5ª ed Mc Graw Hil, 2001

D.C.Harris, C.A. Lucy

Quantitative Chemical Analysis, 9th ed.

Mac Millan Eduction, 2016

J.N. Miller, J.C. Miller Statistics and Chemometrics for Analytical Chemistry 6th ed.

Pearson2010

The practices guideline contains specific bibliographic information for each of the practices