UAB
Universitat Autònoma de Barcelona

Experimentation and Computer Resources

Code: 105034
ECTS Credits: 8

2025/2026

Degree	Type	Year
Chemistry	FB	1

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Teaching groups languages

You can view this information at the end of this document.

Prerequisites

Since it is a first-year course, there are no academic prerequisites to enrol.

In any case, it must be taken into account that the subject contains a large part of laboratory sessions and requires a specific regulation. The behavior in the laboratory must follow the Safety Standards in the Teaching Laboratories published by the Chemistry Department.

Before starting the course, students have to fill in the security test that appears on the "Campus Virtual" and, once passed, print and sign the sheet that accredits it. This sheet must be delivered the first day of the laboratory. Without this document you cannot do the practices.

The rules can be found at the following address: http://www.uab.cat/doc/DOC_Normativa_Segur_Lab_Docent

During practices, students must wear the lab coat and approved safety glasses. In addition to the usual writing tools, they have to carry (and know how it works) a scientific calculator that can perform regression calculations. It is advisable that they go in the laboratory with a laptop to do calculations with Excel

Objectives and Contextualisation

The final objective of the subject is that the student reaches the indicated competences.

The part of Experimentation in the laboratory has some general objectives:

- Know and apply safety and work regulations in the laboratory.
- Know the waste disposal system in the laboratory.
- Know the basic material of the chemical laboratory.
- Know the basic operations of the chemical laboratory:
    - weigh out
    - Cleaning the glass material
    - Measurement and transfer of liquids
    - Preparation of solutions
    - Heating of substances
    - Agitation
    - Evaporation
    - Crystallization
    - Filtering and washing substances
    - Simple Extraction
    - Thin layer chromatography
    - Distillation
    - Use of the laboratory notebook
    - Graphic, numerical and computer treatment of laboratory data

As specific objectives of each practice:

Practice 1: Data processing

- Take contact with the concepts of experimental error, accuracy and precision.
- Understand that the glass material for measuring volumes can have two different functions: contain an exact volume and transfer an exac volume.
- Basic statistics calculations.
- Evaluate the precision and accuracy of some results.

- Introduction to the use of a spreadsheet as a tool to represent results.
- Learn to weigh with the following scales: analytical, precision and granetari.
- Learn volumetric techniques and verify their accuracy.

Practice 2: Densities

- Prepare different solutions of known concentration of a salt using different scales: molarity, molality and both weight percent.
- Extract information from the graph of concentration and density of the solution.
- Use the regression byleast squares and determine the concentration of a problem solution from the reading of the graph.
- Relate molarity (M), molality (m) and percentage by weight (%).
- Work with different scales of concentration.

Practice 3: Precipitation reactions. Limiting reagent concept

- Learn the filtration technique for the separation of heterogeneous phases (solid-liquid).
- Observe the concept of limiting reagent with a practical case, adding variable amounts of a soluble salt in the same amount of another soluble salt (which will act as a limiting reagent).
- Observe the insolubility of some salts from the mixture of soluble salts.
- Learn a technique for purifying precipitates.

Practice 4: Redox reactions. Reaction stoichiometry in aqueous solution

- Use the concept of oxidant and reducer by studying simple redox reactions.
- Remember the rules of equalization of redox reactions.
- Demonstrate the differentiated behavior of some reagents in redox reactions depending on whether you work in an acid medium or in a basic medium.
- Basically analyze the solubility of substances in different solvents.
- Make liquid-liquid extractions of substances from one solvent to another of different polarity.
- Determine the concentration of a test solution using a redox reaction.

Practice 5: Determination of atomic and molecular masses

- Learn to manipulate and make calculations with gases.
- Apply the law of ideal gases and Dalton's law of partial pressures.
- Determine the equivalent mass and the atomic mass of a metal from a chemical reaction.
- Determine the molecular mass of a gas from its density.
- Calculate the average molecular mass of the air.
- Work with the vapor pressure of the water in the air and with the concept of relative humidity.

Practice 6: Using the calorimeter to study phase change and dissolution processes

- Determine the calorific capacity of the calorimeter using the method of mixtures, since it is a data that we need to know to complete this practice and the following ones.
- Determine the latent heat of ice melting.
- Determine the enthalpy of dissolution of two liquid substances.

Practice 7: Determination of heat of reaction and dissolution

- Determine the heats of reaction (enthalpies of reaction) of different chemical processes (acid / base and redox) in solution by using a calorimeter at constant pressure
- Analyze the factors on which the measured enthalpy changes depend. Study the stoichiometry of acid-base neutralization reactions.
- Compare the reaction enthalpies of the acid-base and redox reactions.

Practice 8: Determination of the enthalpy and entropy variation of the urea solution

- The objective of the experimentis to determine ΔH^o and Keq for the dissolution of urea, NH_2CONH_2, in water. From this information, ΔG^o and ΔS^o will be calculated.

Practice 9: Liquid-liquid extraction and separation of mixtures

- Learn the simple extraction technique.
- Separation of three known substances dissolved in an organic solvent from a simple extraction process taking advantage of the different acid-base character of the substances to be separated.
- Checking the efficiency of the separation using the thin layer chromatography technique.
- Separation of an unknown binary mixture. A problem sample will be assigned and information will be given to the student about the compound title it contains. Recognize the separated substances.

Practice 10: Kinetics of the reaction of methyl violet in basic medium

- Determine the pseudo-constant velocity k' for the reaction of methyl violet in basic medium in excess of hydroxyl ion and at room temperature.
- Determine the order of the reaction with respect to hydroxyl and methyl violet.
- Determine the rate constant k for the reaction of methyl violet in basic medium.

Practice 11: Measurement of pH. Relative strength of acids and bases

- Learn to use a pH meter.
- Measure the pH of a set of aqueous solutions of acids and bases and sort them according to their relative strength.
- Observe the influence of dilution on balance.
- Observe the different behavior between buffer solutions and undamped systems from the observation of pH changes when a strong acid or base is added.

Practice 12: Acid-base volumes. Indicators

- Achieve the basic methodology to carry out volumetries, which in this case are based on acid-base equilibria.
- Experimental study of the importance of choosing the indicator correctly.
- Know how to build an experimental valuation curve, check that it has the theoretically predicted form, and see that the indicators change in the predicted area.

Practice 13: Determination of the acidity constant of acetic acid

- In general terms, the objective of this experiment is the quantitative study of the chemical equilibrium by analyzing an acid-base equilibrium in aqueous medium.
- Determine the acidity constant of the acidic and observe that the equilibrium constants correspond to a "palpable" reality experimentally.
- Learn to obtain quantitative data from a series of experimental results that follow a physical law.

Practice 14: Solubility and Kps of salts poorly soluble in water. Effect of the common ion

- Learn to prepare a saturated solution of a poorly soluble salt in a controlled manner.
- Determine the solubility of a poorly soluble salt.
- Learn the practical concept of ion exchange.
- Determine the solubility product of a poorly soluble salt.
- Observe and reflect on the effect of the common ion.

Practice 15: Electrochemical Cells

- Construction of a Table of Potential Standards
- Construction of simple electrochemical galvanic cells to obtain electricity from chemical reactions.

Practice 16: Synthesis of acetylsalicylic acid

- Synthesize a certain amount of acetylsalicylic acid (ASA) from commercial salicylic acid (AS).

- Purify the reaction product (AAS).
- Determine the performance of the reaction.
- Discuss, qualitatively, the purity of the product obtained.

Computer Resources

The general objective of this part of the subject is to provide a basis for students in transversal computer skills in science and specific to the field of chemistry.

It is intended for students to acquire skills in the management and analysis of experimental data, in the visualization and manipulation of three-dimensional and electronic structures and finally in programming.

Learning Outcomes

1. CM01 (Competence) Interpret data obtained from experiments or models to propose solutions to problems in the field of general chemistry.
2. CM02 (Competence) Work together as a team during practical sessions in general chemistry laboratories.
3. CM03 (Competence) Work autonomously in the field of chemistry, integrating knowledge and skills for problem solving, preparing laboratory protocols and delivering exercises and reports.
4. CM03 (Competence) Work autonomously in the field of chemistry, integrating knowledge and skills for problem solving, preparing laboratory protocols and delivering exercises and reports.
5. KM01 (Knowledge) Relate the structure of the atom, chemical bonding, intermolecular forces, and states of aggregation to the properties of matter.
6. KM02 (Knowledge) Identify concepts, principles and theories in the field of thermochemistry, homogeneous and heterogeneous equilibria, chemical kinetics and electrochemistry.
7. SM01 (Skill) Accurately use the terminology of chemical compounds, chemical equations and magnitudes of chemistry.
8. SM02 (Skill) Determine the properties of elements and simple molecules by applying Lewis' theories, valence bond theory, and molecular orbital theory.
9. SM03 (Skill) Correctly perform calculations on simple chemical reactions from a thermodynamic and perspective to predict their evolution.
10. SM04 (Skill) Properly handle the typical instruments and materials of a general chemistry laboratory.

Content

The subject consists of two differentiated parts:

- Experimentation in the laboratory (5 ECTS), and
- Computer Resources (3 ECTS).

Each of the parties has a specific content.

The Experimentation part is structured in 3 blocks, and each consists of several practices in the laboratory.

The Computer Resources part consists of 20 sessions divided in 4 blocks.

The following is a likely list of practices as an example, even if the professors in each academic year can modify them or select others.

PRACTICES OF EXPERIMENTATION IN CHEMISTRY

BLOCK 1: Introduction to experimentation in Chemistry

Practice 1: Data processing. Measurement of volumes. Experimental errors. Use of Excel to make graphs and calculations.
Practice 2: Densities. Determination of the concentration of a solution from its density. Use of excel to make graphs and linear regressions.
Practice 3: Precipitation reactions. Limiting reagent concept. Performance of precipitation reactions of $CaCO_3$.
Practice 4: Redox reactions. Stoichiometry of the reactions in aqueous solution. Redox reactions in test tube. Determination of the concentration of a test solution by means of a redox reaction.
Practice 5: Determination of atomic and molecular masses. Determination of the molecular mass of a gas. Determination of the equivalent mass and the atomic mass of a metal.

BLOCK 2: Thermodynamics and kinetics

Practice 6: Use of the calorimeter to study phase change processes. Calibration of a digital thermometer. Calculation of the calorific capacity of the calorimeter. Determination of hot melting ice.
Practice 7: Determination of heat of reaction. Determination of neutralization enthalpies in acid-base reactions and dissolution enthalpies.
Practice 8: Determination of the enthalpy and entropy variation of the urea solution. Calculation of the Gibbs free energy and the reaction constant of the urea solution in water.
Practice 9: Liquid-liquid extraction and separation of mixtures. Separations of known and unknown mixtures of two and three components. Identification by thin layer chromatography.
Practice 10: Kinetics. Kinetics of the reaction of methyl violet in basic medium. Study of reaction kinetics following spectrophotometrically the concentration of methyl violet. Calculation of the order of the reaction and the speed constant.

BLOCK 3: Chemical equilibrium, electrochemistry and organic functional groups

Practice 11: Measurement of pH. Relative strength of acids and bases. Calibration and use of a pH meter. Study of buffer concept. Calculation of the degree of dissociation of a weak acid.
Practice 12: Acid-base volumes. Indicators. Performance of acid-base titrations with indicators and potentiometric monitoring. How to choose the right indicator for a valuation.
Practice 13: Determination of the acidity constant of acetic acid. Application of the method of solutions. Using a graphical method and the least-squares adjustment to find a dissociation constant.
Practice 14: Solubility and Kps of salts poorly soluble in water. Effect of the common ion. Determination of the solubility of $PbCl_2$ in water. Preparation and use of ion exchange resins. Determination of the Kps of $PbCl_2$. Effect of the common ion.
Practice 15: Electrochemical Cells. Construction of galvanic cells. Calculation of potential tables.
Practice 16: Synthesis of acetylsalicylic acid. Obtention and purification of the product from commercial salicylic acid.

The content of the Computer Resource part includes the following practices:

Block A. Basic Excel

- Practice 1. Introduction to Excel, data organization, open-import-export data, software overview, elementary calculations, format and conditional formatting, adjust decimals, sort, apply sort filters.
- Practice 2. Statistical formulas (variability in software language function), logical formulas.
- Practice 3. Graphs, histograms, bars, x-y, line / trend curve adjustments.
- Practice 4. Templates and forms.

Block B. Structures and databases

- Practice 5. Safety data sheets.
- Practice 6. Introduction 2D molecular drawing.
- Practice 7. 3D molecular geometry, exploration of conformations, perspectives.
- Practice 8. Atomic and molecular orbitals.
- Practice 9. Analysis of solids structures.

- Practice 10. SciFinder.

Block C. Advanced Excel

- Practice 11. PivotTables.
- Practice 12. Data analysis.
- Practice 13. Advanced regressions.
- Practice 14. Iterative calculations and "Goal Search".
- Practice 15. Advanced calculations using Solver

Block D. Programming in the field of Chemistry

- Practice 16. Introduction to Python programming and language
- Practice 17. First steps in Python programming.
- Practice 18. Deepening in Python programming.
- Practice 19. Learning to integrate Python codes in chemical fields
- Practice 20. Presentationand evaluation of codes

Activities and Methodology

Title	Hours	ECTS	Learning Outcomes
Type: Directed			
Computer classrom sessions/online mentoring (depending on pandemic situation)	40	1.6	
Laboratory Practices (depending on the pandemic situation)	74	2.96	
Theory lesson	1	0.04	
Type: Autonomous			
Reading guides and preparation of laboratory practices (experimental part)	18	0.72	
Solving problems related to learning of the Computational Resources part	39	1.56	

The subject "Experimentation and Computer Resources" has two main parts. One of experimentation that focuses on the work of chemical laboratories. The other of computer resources that is oriented to the acquisition of knowledge and skills of fundamental computer tools to perform data analysis, carry out searches for bibliographic holdings, introduce advanced concepts of security and generation of supporting materials. chemical field (molecular drawing, models).

Experimentation.

The subject "Experimentation and Computer Resources" (8 ECTS), together with the subject "Fundamentals of Chemistry I" and "Fundamentals of Chemistry II (16 ECTS), is part of the" Chemistry "subject of the Chemistry degree, which has a total of 24 ECTS of a basic nature and located in the first year of the Degree. The subjects are totally independent with respect to the evaluation, but they are coordinated, so that the evaluation of the part of the subjects "Fundamentals of Chemistry I and II "which is related to the practices, is done after finishing the corresponding block of practices, so the practices benefit from having the theoretical explanations close to time and serve to finish understanding the theory.

The laboratory practices consist of 3 blocks, after which the specific subject is dealt with in the theory subject.

Each laboratory block has several practices, of 4 hours each, which are carried out in the laboratories of the Chemistry Department or in the Computer Room of the Faculty. The last session of the block is devoted to the correction and commentary of the practices carried out. Before starting the practices there will be a joint session in a classroom where the rules that appear in this Teaching Guide and the last minute information will be remembered.

The laboratory practices are done in pairs and each block of practices change the partners of the couples. For each block of practices, the lists of pairs are published on the virtual campus. The evaluations are individual.

Assistance is mandatory. An unjustified fault implies a zero of the practice. Students must enter the laboratory with the guide of the practice read and the calculations requested by the preparation of solutions prepared. They may have to do a short test (less than 10 minutes) to verify that they have actually read the guide.

Before each practice, the teacher will explain the most important points and the details to take into account.

Once the practice is finished and the material is ordered, the students fill out, individually, the practice report and answer the questions that are asked for their evaluation. In some specific cases, the students may take the report home so they can make the calculations more calmly and hand it over the next day.

The space of the subject in the "Campus Virtual" will be the place where the students will be able to find all the necessary documentation for the practices. Before starting the first block of practices will be published: safety standards in the laboratory and the book of practices, which contains a first part explaining the usual techniques in the laboratory and the scripts of all practices.

Before starting the course, students must take the security test that appears on the virtual campus and, once passed, print and sign the sheet that states it. This sheet will be delivered the first day in the laboratory. Without this document you cannot do the practices.

Punctually, before each block, the specific calendar and list of pairs of the block will be published. Subsequently, the ratings of the block will be published.

Computer Resources.

Due to the different levels of complexity of the topics covered in each block, teaching will be given in various ways.

The standard procedure for most practices in blocks A, B and C will be:

1. A few days before class, students receive introductory material to the theoretical and practical knowledge of the practice. (Introductory videos by teachers, study documents, internet links, etc.). It can include some basic exercises to solve.

2. On the scheduled day of the classes, the teachers briefly recapitulate the fundamental concepts and develop practical cases.

3. At the end of the class, students will have to solve an online test in person and lasting between 10 and 20 minutes. It is not allowed to take the test from any other classroom or place other than the one assigned by the face-to-face class.

For block D (programming), introductory videos will also be offered but the face-to-face class will propose an extensive presentation and cases to be developed together with the teacher for a better homogeneity in overcoming the contents and competences. Occasional work, face-to-face or non-face-to-face, must be solved and submitted. Depending on the degree of comprehension or progress, the student may have the option of more or less complex statements. Finally, a group work will be requested with its presentation on the last day of the blog.

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
Assessment in the form of tests and project	100%	10	0.4	CM01, CM02, CM03, KM01, SM02
Practice Report (part Experimentation)	80%	15	0.6	CM01, CM02, CM03, KM02, SM01, SM03, SM04
Preparation of practices. Pre-laboratory exercise (Experimentation part)	20%	3	0.12	KM02, SM03, SM04

All the activities that are carried out count for the evaluation.

Both parts of the course have an individual and independent assessment. The final grade is the average of the marks of the two parts of the subject, weighted by the number of credits of each part. A grade of "not presented" will only be possible for cases where the student has not submitted the assessments of more than 4 practices (approximately 20%). It is necessary to pass both parts to pass the course. The pass is obtained with a 5/10.

Regarding the part of Experimentation in the laboratory: A system of continuous evaluation is followed, without the possibility of re-evaluation with a special work or examination. The minimum grade to pass it is 5 points (out of 10). In this note the most important weight are the reports that are delivered at the end of each practice (weight 80%). The report must put the experimental results obtained into practice and answer the questions asked, leaving a record of the necessary graphs and calculations. The methodology followed for the answers, the way in which the answers are communicated and the goodness of the experimental data found are assessed. Preliminary tests will also be taken into account (before starting each practice) to show that the reports and the work attitude in the laboratory have been read (weight 20%). Failure to attend the correction and comment session of the blog practices has a penalty of 1 point (out of 10) on the blog note. The final grade for this part will be the average of the grades for all blocks.

Attendance is mandatory. An unjustified misconduct implies a zero of practice.

Laboratory Safety Warning: A student who is involved in an incident that may have serious safety consequences may be expelled from the laboratory and suspended from the subject.

Regarding the part of Computer Resources: The quizzes in block A, B and C have the same weighting as 1. For block D, the non-face-to-face assessments will weigh 0.5 and the final group work 2.5. Non-contact assignments will be assessed in proportion to the difficulty of the chosen statement.
The internships are compulsory and can be done individually or in groups as indicated by the teacher. An unjustified lack of attendance implies a zero in practice. The teaching staff reserves the right to carry out additional assessments to those established at the beginning of the course. It is emphasized that face-to-face tests can only be taken in the classroom on the day of the practice (with the exception of indications to the contrary by the teacher). Any attempt to perform the test from another location will be valued at zero. Repetitive attempts of this kind or other types of fraud will lead to the immediate suspension of the subject.

The non-delivery of 4 or more works of the 20 implies not passing of this part and therefore of all the matter.

Bibliography

Main reference textbooks:

- The main document for the laboratory part is the "Book of practices of the subject Experimentation in Chemistry". Chemistry Department. It contains the necessary information to work in the laboratory and the guides of all the practices. Each practice indicates which concepts of the book should review. It is located in the "Campus Virtual" of the UAB.

- The textbook "R. H. Petrucci, F.G. Herring, J. D. Madura, C. Bissonnette, Química General, Pearson Prentice Hall (11ena Ed.) 2017" will provide the theoretical information necessary for each practice. In the guide of each one are indicated the pages of the book that should be read. (online book: https://bibcercador.uab.cat/permalink/34CSUC_UAB/avjcib/alma991010080899706709)

- Book on Python programmingfor the Computer Resources part : Learning Python, 5th Edition: Lutz, Mark; O'Reilly Media, Inc. 2013.

Complementary textbooks:

- A book of laboratory practices that can be found in the library in case one of the experiments is not clear. Manuel Fernández González, Laboratory Operations of Chemistry, Ed. Anaya (2004).

-A textbook that is in the library and that contains explanations about the use of Excel, significant figures and complementary information on block 4 (Chemical Balance). Daniel C. Harris. "Quantitative chemical analysis". Ed. Reverté S.A. Barcelona (2006)

- A book that is in the library and that provides more information about block 3 (Thermodynamics and kinetics) and block 4 (Electrochemistry). R. Chang. General Chemistry, 9th edition, Ed. McGraw-Hill, 2007.

Other resources:

Safety regulations in the teaching laboratories of the Chemistry Department: http://www.uab.cat/doc/DOC_Normativa_Segur_Lab_Docent

Orbital viewer: http://www.orbitals.com/orb/ov.htm

Analysis of properties: EI, AE, density, electrical conductivity: http://www.webelements.com/ and http://www.dayah.com/periodic/

Different resources of visualization of atomic and molecular orbitals: http://www.mpcfaculty.net/ron_rinehart/orbitals.htm

Software

Excel.

Gaussian 16. Electronic structure calculation program.

GaussView 6. Molecular visualization program.

Python. programming language.

UCSF Chimera and ChimeraX. Molecular visualization program with Python integration.

Jupiter Notebook. Python program manager.

Conda. Python package manager.

Marvin Beans. Molecular visualizer. 2D drawings and 3D structures.

SciFinder. Scientific database manager.

Rdkit. Python package for handling chemical structures

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
(PLAB) Practical laboratories	1	Catalan	annual	morning-mixed
(PLAB) Practical laboratories	2	Catalan	annual	morning-mixed
(PLAB) Practical laboratories	3	Catalan	annual	morning-mixed
(PLAB) Practical laboratories	4	Catalan	annual	morning-mixed
(PLAB) Practical laboratories	5	Catalan	annual	afternoon
(PLAB) Practical laboratories	6	Catalan	annual	afternoon
(PLAB) Practical laboratories	7	Catalan	annual	afternoon
(TE) Theory	1	Catalan	annual	morning-mixed
(TE) Theory	2	Catalan	annual	morning-mixed