UAB
Universitat Autònoma de Barcelona

2021/2022

Experimentation and Computer Resources

Code: 105034
ECTS Credits: 8

Degree	Type	Year	Semester
2502444 Chemistry	FB	1	A

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

Teachers

Maria Mercè Capdevila Vidal

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Montserrat López Mesas

Albert Rimola Gibert

Eva Monteagudo Soldevilla

José Emilio Sánchez Aparicio

Prerequisites

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

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 can not 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 do 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 materia
    - 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 by least 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 redoxreactions.
- 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 studyphase change and dissolution processes

- Determinethe 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 experiment is to determine ΔH^o and K_{eq} 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 basicmedium 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.
- Observethe 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 constantscorrespond 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 obtainelectricity 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.

For the part of Computer Resources, the general objective is to provide a solid basis for students in cross-cutting and specific skills in computer tools. It is intended that the students acquire strong notions, both structural and analytical in database management and algorithm.

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 orally and in writing in ones own language.
- 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.
- Obtain information, including by digital means.
- Propose creative ideas and solutions.
- 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.
- 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.

Learning Outcomes

1. Adapt to new situations.
2. Be ethically committed.
3. Communicate orally and in writing in ones own language.
4. Determine concentrations of acid and bases from acid-base estimations.
5. Have numerical calculation skills.
6. Identify safety measures in a chemistry laboratory.
7. Identify the main bibliographic sources in the field of chemistry.
8. Learn autonomously.
9. Manage the organisation and planning of tasks.
10. Manage, analyse and synthesise information.
11. Name and formulate the organic and inorganic chemical compounds.
12. Obtain information, including by digital means.
13. Perform basic synthesis, separation and analyses procedures in a chemistry laboratory.
14. Perform bibliographic inquiries in the field of chemistry using sources of information in English and recognise the basic chemistry terms in this language.
15. Perform bibliographic research of chemical documentation.
16. Properly use glass materials in a chemistry laboratory.
17. Properly use the protocols for handling reagents and chemical waste taking into account their physical and chemical properties.
18. Propose creative ideas and solutions.
19. Rationalise the results obtained in the laboratory in processes of synthesis, separation and analysis of chemical compounds on the basis of knowledge of their structure and properties.
20. Reason in a critical manner
21. Resolve problems and make decisions.
22. Show initiative and an enterprising spirit.
23. Show motivation for quality.
24. Show sensitivity for environmental issues.
25. Use IT to treat and present information.
26. Use computer programs for the statistical treatment of data.
27. Work properly with chemical equations and the main magnitudes of matter.

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 ....

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: Useof 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 reactionconstant 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 methylviolet. 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. Obtantion 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, general presentation of the software, elementary calculations, format and conditional format, adjust decimals, sort order, apply sort filters.
Practice 2. Statistical formulas (variability in software language function), logical formulas.
Practice 3. Graphs, histograms, bars, x-y, line adjustments / trend curve.
Practice 4. Templates and forms.

Block B Structures and databases

Practice 5. Safety files.

Practice 6. Introduction 2D molecular drawing.
Practice 7. 3D geometry, exploration of conformations, perspectives, etc...

Practice 8. Atomic and molecular orbitals.
Practice 9. Structures of solids.
Practice 10. Scifinder.

Block C. Advanced Excel

Practice 11. Dynamic tables.
Practice 12. Data analysis.
Practice 13. Multiple regression. Iterative calculations and "Goal Search".
Practice 14. Advanced calculations using Solver.

Block D. Programming in the molecular field

Practice 15. Introduction to Linux.Introduction to Python.

Practice 16. Python Programming 1.
Practice 17. Python Programming 2.
Practice 18. Python integration in chemical fields 1- Scientific modules and resolution of chemical problems.
Practice 19. Python integration in chemical fields 2- Scientific modules and resolution of chemical problems.
Practice 20. Python integration in chemical fields 3- molecular visualization and UCSF Chimera.

Methodology

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 "Experimentationand 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 can not 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.

The Computer Resources part consists of 20 practices with a scheme that follows this model:

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 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.

The delivery of the works is mandatory and can be done individually or in groups depending on the activity. An unjustified foul implies a zero in practice. There may be additional assessment tests to those scheduled for each session.

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.

Activities

Title	Hours	ECTS	Learning Outcomes

Type: Directed			
Computer classrom sessions/online mentoring (depending on pandemic situation)	40	1.6	1, 11, 8, 3, 22, 23, 4, 13, 9, 10, 7, 12, 19, 20, 14, 15, 21, 5, 27, 17, 25, 26
Laboratory Practices (depending on the pandemic situation)	74	2.96	1, 11, 8, 3, 22, 23, 4, 13, 9, 6, 16, 12, 18, 19, 20, 21, 5, 27, 17, 26
Theory lesson	1	0.04	11, 9, 6, 27
Type: Autonomous			
Reading guides and preparation of laboratory practices (experimental part)	18	0.72	11, 8, 9, 10, 20, 5, 27
Resolució of problems related to learning of the Computational Resources part	28	1.12	8, 3, 22, 23, 9, 10, 12, 18, 20, 14, 21, 5, 25, 26

Assessment

Evaluation of all ERI

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 thesubject.

Regarding the part of Computer Resources: RI consists only of online sessions for each one of the 20 practices. The grades for each practice will have an identical weight on the final grade of RI. A non-submitted one without valid justification will be scored with a 0. Failure to exceed a minimum of 5/10 implies suspension. The non-delivery of 5 or more works of the 20 implies not passing of this part and therefore of all the matter.

Assessment Activities

Title	Weighting	Hours	ECTS	Learning Outcomes
Practice Report (part Experimentation)	80%	15	0.6	1, 11, 8, 3, 23, 4, 13, 9, 10, 6, 16, 2, 24, 19, 20, 21, 5, 27, 17, 26

Preparation of practices. Pre-laboratory exercise (Experimentation part)	20%	3	0.12	11, 3, 6, 5, 27	
assessment in the form of tests (Computational Resuorces part)	100%	21	0.84	8, 22, 10, 7, 12, 18, 20, 14, 15, 21, 5, 25, 26	

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 Prentrice 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://www-ingebook-com.are.uab.cat/ib/NPcd/IB_BooksVis?cod_primaria=1000187&codigo_libro=6751)

- 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.

Another 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. 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.Sscientific database manager.