Bachelor´s Degree in Chemistry

# Subject Guide

## 1. Information about the subject

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| **SUBJECT** | Experimentation in Physical Chemistry II | **CODE** | GQUIMI01-4-002 |
| **EDUCATIONAL OFFER** | Bachelor´s Degree in Chemistry | **CENTER** | Facultad de Química |
| **TYPE** | Compulsory | **N° TOTAL CREDITS** | 6.0 |
| **PERIOD** | First Semester | **LANGUAGE** | Spanish |

| **COORDINATORS/ES** | **EMAIL** |
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## 2. Context

This subject belongs to the "Fundamental" module and to the "Physical Chemistry" speciality of the Curriculum of the Degree in Chemistry of the University of Oviedo (BOE of July 15, 2010, pp. 62634-62638). It is a compulsory subject delivered during the first semester of the fourth year of the degree.

This subject is deeply related to the other subjects belonging to the same speciality in the degree. It relates in particular to the second course "Experimentation in Physical Chemistry I" in the sense that it deepens and expands many aspects of laboratory work initiated there, such as, for

example, handling of scientific instrumentation for measuring physico-chemical magnitudes, preparation of laboratory notebooks, calculations based on data obtained from measurements, improvement in the use of hygiene and safety standards, etc. In addition, this subject addresses several practical components developed from a theoretical point of view in the other subjects of the same speciality: "Physical Chemistry I" (Thermodynamics of the electrolytic and non-electrolytic real solutions), "Physical Chemistry II" (Quantum Chemistry and Molecular Spectroscopy), and "Physical Chemistry III" (Chemical Kinetics, and Transport and Surface Phenomena). The practical treatment of some of the concepts studied in these theoretical subjects allows to deepen and to consolidate the knowledge acquired in them.

## 3. Requirements

To take this course, it is compulsory for the student to have passed the "Experimentation in Physical Chemistry I" subject, of the second year of the Degree.

On the other hand, although it is not obligatory, it is highly recommended for the students to have also passed the subjects "Physical Chemistry I" (2nd year), "Physical Chemistry II" (3rd year), and "Physical Chemistry III" (3rd year). As mentioned in the previous section, in these subjects several theoretical contents closely related to those of the course are explained. That is the case for the thermodynamics of the non-electrolytic and electrolytic real solutions (equilibrium constants of ionic dissociations, strong and weak electrolytes, etc.), chemical kinetics (formal kinetics of first-order reactions, global and partial reaction orders, Arrhenius equation, methods for the determination of reaction orders, etc.), transport phenomena (transport of electric charge in electrolytic solutions, Kohlrausch laws, Ostwald law, etc.), surface phenomena (adsorption of liquids on solids, Langmuir and Freundlich adsorption isotherms, etc.), quantum chemistry (Born-Oppenheimer approximation, electronic structure of polyatomic molecules, etc.), and molecular spectroscopy (V-UV spectroscopy, HOMO-LUMO transitions, etc.).

## 4. Competencies and learning results

1. General Competences

At the end of the course, students must have attained the following general competences, selected from the total of those to be acquired in

the Chemistry Degree:

GC-3: knowing computer science related to the field of Chemistry:

In particular, student will be able to:

Using commercial spreadsheets to make graphs and numerical fittings, as well as performing calculations pre-programmed in them.

Using non-standard computer programs where data and results are collected in files that must be edited and handled on non-Windows operating systems (such as Linux).

GC-8: Expressing him/herself correctly (both oral and written) within the scientific field.

GC-18: Working in group.

B) Specific competences.

Likewise, we will work to achieve the following specific competences:

EC-2: relating the macroscopic properties of the matter with those of the individual atoms and molecules.

EC-7: Mastering the principles of thermodynamics and its applications in chemistry.

EC-12: Applying the principles of Quantum Mechanics to the description of the structure and properties of atoms and molecules.

EC-22: Acquiring ability to evaluate, interpret and synthesize chemical information.

C) Learning outcomes.

The competences associated with this subject imply the following learning outcomes:

- Preparing and correctly presenting an oral and written laboratory report. In particular, a laboratory notebook should be kept up to date, since it will be the main source of information for the preparation of the report.

- Managing computer software in the field of Physical Chemistry.

- Demonstrating knowledge and understanding of facts, concepts, principles and theories related to the contents of the subject.

More specifically, at the end of the course, and in relation to the contents specified in the following section, the student should be able to:

1. Distinguishing strong and weak electrolytes by conductivity measurements.

2. Determining the equilibrium dissociation constant of a weak acid or base from conductivity measurements.

3. Using the conductivity measurements of an electrolyte to determine its concentration.

4. Obtaining the molar conductivity at infinite dilution of an strong and weak electrolyte.

5. Calculating electronic properties of planar conjugated molecules using the Hückel method (HMO) and spectroscopic information.

6. Obtaining structural information on molecules with long conjugated chains using the FEMO method and spectroscopic information.

7. Using semi-empirical calculation methods to derive structural properties of compounds lacking spectroscopic information.

8. Deriving kinetic equations to determine partial reaction orders by applying the initial rate-of-reaction method.

9. Determining the initial concentrations of reagents necessary to apply the kinetic equations for obtaining partial reaction orders.

10. Obtaining, from experimental measurements of reaction times, the rate constant of a reaction, the partial reaction orders and its activation energy.

11. Determining the influence of the ionic strength, and control its effect, on the speed of an ionic reaction.

12. Distinguishing a process of physical adsorption from one of chemical adsorption.

13. Determining the type of empirical adsorption isotherm best suited to a process.

14. Obtaining the parameters of the Langmuir and Freundlich adsorption isotherms.

15. Determining the adsorption capacity of a solid adsorbate.

**5. Contents**

1. Transport Phenomena (electrical conductivity): Determination of the dissociation degree, the average ionic activity coefficient and the dissociation equilibrium constants (Ka and Kc) of a weak acid by electrical conductivity measurements. (12 lab hours).

2. Molecular Spectroscopy: Determination of structural properties of aromatic compounds and conjugated polyenes by V-UV spectroscopy and molecular electronic structure semi-empirical calculations. (12 lab hours).

3. Chemical Kinetics: Obtaining the partial orders of reaction, the global order, the rate constant and the activation energy of an ionic reaction. (12 lab hours).

4. Surface Phenomena (Adsorption): construction of the adsorption isotherm of acetic acid by activated charcoal. (12 lab hours).

**6. Methodology and working plan**

The main work is done in the lab in groups of two or three students. Each one should bring the script of the experiment studied before the beginning of each practice. The teacher briefly explains the operating procedure at the beginning of each experiment and makes a personalized monitoring of the work of each group. At the seminars (PA), the lecturer discusses: (1) techniques for calculating experimental errors, (2) procedures for the preparation of laboratory reports, (3) strategies for oral presentation of research results, (4) the optimal procedure for the preparation of a laboratory notebook, (5) the specific hygiene and safety standards of the subject, and (6) a brief synopsis of the theoretical foundations of the experiments. During the development of the experiments, in the lab, each student must write a laboratory notebook, which

can be completed in non-teaching time. The notebook is periodically reviewed throughout the lab period and must be submitted on the day of the practical exam, which is individual, as well as the theoretical exam. In addition, also in non-teaching time, each group should prepare a report of one of the experiments, following the guidelines that are given in the seminar, whose script will be the basis of the oral presentation. This presentation is done by the group on the same day of the theoretical exam. The written report is submitted two weeks after the end of the lab period.

| MODALITIES | | Hours | % | Total |
|---|---|---|---|---|
| Lab classes | Lectures | | | 60 |
| | Classroom practices / Seminars / Workshops | 6 | 10,00 | |
| | Lab practices / Field / informatics / languages | 51 | 85,00 | |
| | Hospital clinical practices | | | |
| | Group Tutorials | | | |
| | External practicees | | | |
| | Assessment sessions | 3 | 5,00 | |
| Non-contact classes | Group work | 30 | 33,33 | 90 |
| | Individual Work | 60 | 66,67 | |
| | Total | 150 | | |

**7. Evaluation of the student's learning results**

| Aspect | Criteria | Instrument | Weight |
|---|---|---|---|
| Concepts and calculations | Mastery of the theoretical knowledge and of the methods of calculation proper to the subject | Written classroom exam* | 40% |
| Experimental Methodology | Mastering of experimental methods and techniques of the subject | Lab exam* | 30% |
| Elaboration of technical reports and oral presentations | The following aspects will be evaluated:<br><br>- General adequacy of the written report and oral presentation of an experiment to the scheme explained in the corresponding seminars.<br><br>- Bibliographic search.<br><br>- Oral and written expression | oral and written report | 20% |
| Preparation of laboratory | The following aspects will be | Lab notebook | 5% |

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| notebooks | evaluated:<br><br>- Keeping the notebook up to date.<br><br>- Originality.<br><br>- Answering the questions and solving the problems raised in the scripts and by the teacher. | | |
| Lab work | The following aspects will be evaluated:<br><br>- Compliance with the measures of hygiene and security, punctuality and attendance (Attitude).<br><br>- Adequate development of data acquisition and analysis processes (Aptitude).<br><br>- Results of the experiments (skill). | Teacher observation and notes | 5% |

* To pass the subject it is mandatory to obtain at least four points out of ten (4/10) in each of the two exams (theoretical and practical), regardless of the remaining qualifications.

The following cases are considered for the evaluation results:

A) The weighted sum of all grades in the regular exam is equal to or greater than (5/10) and in both exams (theoretical and practical) you get a grade equal to or higher than (4/10). In this case the subject is passed.

B) The weighted sum of all grades in the regular exam is equal to or greater than (5/10), but in one or other of the exams (or both) a grade lower than (4/10) is obtained. In this case the subject is not passed and the student must go to the extraordinary call for the part (or parts) with a grade lower than four points. In this call the marks of all the remaining concepts are maintained.

C) The weighted sum of all grades in the regular exam is less than (5/10), and in one or other of the exams (or both) a grade lower than (5/10) is obtained. In this case the subject is not passed and the student must go to the extraordinary exam of the part (or parts) with a grade lower than five points. In this call the marks of all the remaining concepts are maintained.

D) The weighted sum of all grades in the ordinary examination is less than (5/10), but in both exams a grade of 5/10 or higher is obtained. In this case the subject is not passed and the student must present a new version of the laboratory notebook and the written report in the extraordinary call. In this call the marks of all the remaining concepts are maintained.

## 8. Resources, bibliography and complementary documentation

1. Basic bibliography.

1. I. Levine, Physical Chemistry, (6th edition), McGraw-Hill, 2008

2. P. W. Atkins and J. de Paula, Physical Chemistry, (9th edition), Oxford University Press, 2009.

1. Complementary bibliography.

1. S. Senent Pérez, A. Hernanz Gismero, M. C. Izquierdo Sañudo, R. Navarro Delgado, F. Peral Fernández y M. D. Troitiño Núñez, Técnicas instrumentales fisicoquímicas, UNED, 1990.

2. R. J. Sime, Physical Chemistry: methods, techniques, and experiments, Saunders College Publishing, 1990.

3. R. J. Sime, Physical Chemistry calculations, Prentice Hall, 2005.

4. A. Horta Zubiaga, S. Esteban Santos, R. Navarro Delgado, P. Cornago Ramírez y C. Barthelemy González, Técnicas experimentales de Química, UNED, 1991.

5. A. M. Halpern y G. McBane, Experimental Physical Chemistry: A laboratory textbook, Prentice Hall, 2006.

6. J. Guilleme, J. Casanueva, E. Díez, P. Herrasti, J. Juan, R. López, P. Ocón, J. M. L. Poyato, J. San Fabián, A. Sánchez, J. M. G. de la Vega y J. Zuluaga, Experimentación en Química Física, Universidad Autónoma de Madrid, 2003.

7. C. W. Garland, J. W. Nibler y D. P. Shoemaker, Experiments in Physical Chemistry, McGraw-Hill, 2008.

Practice scripts, as well as other supplementary material (seminar notes, instrument management videos, self-test on the content of each experiment, test models, etc.) will be available to students through the Virtual Campus.