COURSE DATA

Data Subject	
Code	34197
Name	Physical chemistry laboratory II
Cycle	Grade
ECTS Credits	6.0
Academic year	2017 - 2018

Study (s)

Degree	Center	Acad. year	Period
1108 - Degree in Chemistry	Faculty of Chemistry	3	Second term

Subject-matter

Degree	Subject-matter	Character
1108 - Degree in Chemistry	7 - Physical chemistry	Obligatory

Coordination

Name	Department
GARCIA CUESTA, INMACULADA	315 - Physical Chemistry

SUMMARY

Physical Chemistry Laboratory II is a compulsory subject that is taught in the sixth semester, during the 3rd year of the Degree in Chemistry.

It focuses on experimentation in chemical thermodynamics of interfaces, spectroscopy, electrochemistry, photochemistry, quantum chemistry, and chemical kinetics. In the laboratory, different instrumental techniques are applied to the study of systems of physicochemical interest and computers are used for the study of atoms and molecules.

PREVIOUS KNOWLEDGE

Relationship to other subjects of the same degree

There are no specified enrollment restrictions with other subjects of the curriculum.

Other requirements

It is recommended that the student has prior knowledge taught in the subjects Physical Chemistry I, II and III, Physical Chemistry Laboratory I, Chemical Informatics, and Mathematics I and II.

Basic knowledge of physical chemistry related to:
   Formal kinetics
   Spectroscopy
   Electrochemistry
   Kinetic theory of gases
   Thermodynamics of two-phase systems
   Quantum chemistry of molecular systems
And general knowledge of:
   Chemical nomenclature and stoichiometric calculations
   Preparation of

COMPETENCES (RD 1393/2007) // LEARNING OUTCOMES (RD 822/2021)

1108 - Degree in Chemistry

- Develop capacity for analysis, synthesis and critical thinking.
- Show inductive and deductive reasoning ability.
- Demonstrate leadership and management skills, entrepreneurship, initiative, creativity, organization, planning, control, leadership, decision making and negotiation.
- Solve problems effectively.
- Demonstrate ability to work in teams both in interdisciplinary teams and in an international context.
- Demonstrate ability to communicate information, ideas, problems and solutions to both specialist and non-specialist audiences and using information technology, as appropriate.
- Demonstrate a commitment to ethics, equality values and social responsibility as a citizen and as a professional.
- Learn autonomously.
- Demonstrate the ability to adapt to new situations.
- Acquire a permanent sensitivity to quality, the environment, sustainable development and the prevention of occupational hazards.
- Demonstrate knowledge of the main aspects of chemical terminology, nomenclature, conventions and units.

- Interpret the variation of the characteristic properties of chemical elements according to the periodic table.
- Demonstrate knowledge of the characteristics and behaviour of the different states of matter and the theories used to describe them.
- Demonstrate knowledge of the main types of chemical reaction and their main characteristics.
- Demonstrate knowledge of the principles of quantum mechanics and their application to the description of the structure and properties of atoms and molecules.
- Demonstrate knowledge of the principles of thermodynamics and kinetics and their applications in chemistry.
- Relate the macroscopic properties and the properties of individual atoms and molecules, including macromolecules (natural and synthetic), polymers, colloids and other materials.
- Demonstrate knowledge and understanding of essential facts, concepts, principles and theories related to the areas of chemistry.
- Solve qualitative and quantitative problems following previously developed models.
- Recognise and analyse new problems and plan strategies to solve them.
- Evaluate, interpret and synthesise chemical data and information.
- Handle chemicals safely.
- Handle the instrumentation used in the different areas of chemistry.
- Interpret data from observations and measurements in the laboratory in terms of their significance and the theories that underpin them.
- Relate theory and experimentation.
- Recognise and evaluate chemical processes in daily life.
- Understand the qualitative and quantitative aspects of chemical problems.
- Develop sustainable and environmentally friendly methods.
- Relate chemistry with other disciplines.
- Students must be able to apply their knowledge to their work or vocation in a professional manner and have acquired the competences required for the preparation and defence of arguments and for problem solving in their field of study.
- Students must have the ability to gather and interpret relevant data (usually in their field of study) to make judgements that take relevant social, scientific or ethical issues into consideration.
- Students must be able to communicate information, ideas, problems and solutions to both expert and lay audiences.
- Students must have developed the learning skills needed to undertake further study with a high degree of autonomy.
- Express oneself correctly, both orally and in writing, in any of the official languages of the Valencian Community.

- Have basic skills in the use of information and communication technology and properly manage the information obtained.

LEARNING OUTCOMES (RD 1393/2007) // NO CONTENT (RD 822/2021)

This course pursues the learning outcomes contained in the degree explanatory report within the Physical Chemistry subject area. These learning outcomes imply that, at the end of the course, the student is able to:

1. Demonstrate ability to define the state of a chemical system according to its macroscopic properties, and analyse its spontaneous evolution.

2. Demonstrate ability to understand and predict the behaviour and reactivity of atoms and molecules based on an analysis of their structure, which can be determined from spectroscopic data.

3. Understand and make effective use of bibliographic and technical information concerning physicochemical phenomena.

4. Complete the tasks assigned as a member of a team and from a gender perspective.

5. Solve problems with rigour.

6. Demonstrate adaptation to new situations.

7. Demonstrate capacity for analysis and synthesis.

8. Demonstrate ability for inductive and deductive analysis.

9. Demonstrate capacity for organisation and planning.

10. Demonstrate leadership and gender perspective.

11. Demonstrate skill in the management of the main instrumental techniques used in chemistry and be able to determine, through experimental work, the thermodynamic and structural properties and the kinetic behaviour of chemical systems.

12. Demonstrate skill in the treatment and spread of errors of the quantities measured in the laboratory and skill to handle software to carry out the processing of experimental data.

13. Demonstrate skill in handling computer software for calculating the microscopic properties of matter and for simulating those techniques not available in the laboratory because of their high cost.

14. Demonstrate ability to prepare a report on an experiment conducted in the laboratory and a laboratory notebook for all practical sessions.

15. Write and make oral presentations using native languages correctly.

16. Manage information rigorously.

17. Show gender perspective and ethical commitment.

DESCRIPTION OF CONTENTS

1. Study of an oscillating reaction: the Belousov-Zhabotinskii reaction

The existence of oscillations in the concentration of some intermediate species involved in the reaction is shown by means of electromotive force measurements. In the experiment, the formation of spatio-temporal figures can also be observed. A model of reaction mechanism to accurately reproduce the oscillations is discussed.

2. Voltammetry of potassium ferricyanide in aqueous potassium chloride solution

The experiment focuses on the electrochemical behaviour of anion ferricyanide in aqueous potassium chloride solution using cyclic voltammetry and potentiometry.

3. Fluorescence spectroscopy. Study of the effect of the molecular structure in the capacity of fluorescent dyes and the transfer of energy of excited molecules of riboflavin

In the first part of the experiment, we obtain the fluorescence, absorption and excitation spectra of a series of dyes from the same family; the intensity of fluorescence will be related to the molecular structure. In the second part, the energy transfer from an excited molecule (riboflavin) to another non-excited (IK) will be analysed.

4. Determination of the surface tension of hydro-alcoholic mixtures

The experiment focuses on the measurement of the surface tension of binary mixtures of an alcohol and water. An equation relating the surface tension with the concentration of alcohol in aqueous solution is established and used for the determination of the surface excess concentration of alcohol.

5. Kinetic study of the triphenylphosphine photochemical oxidation

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A kinetic study of the photochemical oxidation of triphenylphosphine in organic medium is performed by measuring the remaining fraction of triphenylphosphine using reverse phase HPLC chromatography.

6. Kinetic theory of gases. Measurement of the viscosity of a gas, estimate of the molecular diameter and determination of the molecular mass

The diameter and the molecular mass of two gases are estimated from the viscosity and the mass by applying the kinetic theory of gases.

7. Quantum chemical calculations I. Geometric and electronic structures

The main methods for semi-empirical calculations are introduced. The methods are applied to a set of molecules of the family of alkanes, alkenes, and aromatic systems.

8. Quantum chemical calculations II. Electronic spectra

The geometric and electronic structures of the molecule of lumiflavin are determined and the absorption and emission spectra are computed.

9. Study of electronic systems with the Hückel method

The aim of the study is to familiarise students with the method of molecular orbitals constructed as a linear combination of atomic orbitals (MO-LCAO). To achieve such goal the Hückel method is used because of its simplicity.

10. Molecular modeling: structure and reactivity

The study aims to familiarise students with the following concepts: potential energy surface, local minimum, global minimum, saddle point, barrier of potential, optimisation of the geometry, internal coordinates, field of forces, and molecular mechanics.

11. Parker actinometer

The experiment involves the assembly and calibration of the Parker actinometer.

WORKLOAD

ACTIVITY	Hours	% To be attended
Laboratory practices	48,00	100
Tutorials	12,00	100
Development of group work	6,00	0
Development of individual work	20,00	0
Study and independent work	24,00	0
Readings supplementary material	6,00	0
Preparation of evaluation activities	20,00	0
Preparation of practical classes and problem	14,00	0
TOTAL	**150,00**	

TEACHING METHODOLOGY

The following methodologies will be applied during the course:

- Lectures
- Practical classes
- Data processing, calculations, and resolution of questions
- Information search

In advance, the students will have at their disposal an explanatory text for each experiment or computational study, which they may download from the Department of Physical Chemistry webpage (section “laboratoris docents”). There they will find general information about how to work in the laboratory, educational materials, and links of interest that may be consulted at any time.

Each student must attend 60 classroom hours on the dates and times laid down in the academic course catalogue (OCA). During this time, the following educational activities will be carried out: 6 experimental/computational assignments, 2 seminars devoted to activities related to the acquisition of transferable skills, and 1 session for evaluation, all distributed in 15 sessions of 4 hours each.

The experiments or computational studies are organised in groups of two with 4 sessions devoted to each of the groups as follows:

Session 1: Explanation of the two experiments.

Session 2: Conduct of the first experiment.

Session 3: Conduct of the second experiment.

Session 4: Calculations and questions about both experiments in the computer room.

The six experiences scheduled will be carried out in twelve sessions. Two more sessions will be devoted to seminars and the last one will be used for assessment.

The course is organised into the following items:

1. Preparatory session

Each experiment has a few specific objectives which are described in the corresponding explanatory text, as well as the recommended literature to use for its preparation. Before the practical session, students must carefully read the text, prepare an outline of the experimental procedure, answer the questions proposed, and do the calculations necessary to make the experiment.

2. Practical work

The practical work will be carried out in pairs and in some cases the results will be shared by all the students, which can help to enhance teamwork.

Students should write all the experimental data and measurements in their notebooks while they are working in the laboratory.

3. Calculations and discussion of results

Students will start to do the calculations in the laboratory. Furthermore, they should analyse the experimental results obtained in the laboratory as well as previous calculations, and express the results with appropriate units and significant figures. Therefore, this stage aims to develop the student's capacity for analysis.

4. Laboratory notebook

Students should keep the laboratory notebook up to date. The teacher will periodically review the notebook, and the student will submit it at the end of the course within the deadline set by the teacher.

5. Report on the experiments or computational studies

One goal of this course is that students become familiar with the writing of a scientific piece of work. To achieve such goal, each student must submit a report on one of the experiments or computational studies carried out during the course, as assigned by the lecturer. This work will be prepared individually and submitted by the deadline set.

6. Seminars

Students will be instructed about searching bibliographic information and the use of databases. The results, experimental techniques, and computational methods used in the course will be discussed.

EVALUATION

Attendance to all sessions is compulsory. To pass the course the student must attend at least 90% of the seminars and laboratory sessions. The learning assessment applies to individual work and will be based on the following criteria:

1. Continuous assessment, based on classroom activities, participation and involvement of the student in the teaching-learning process during the laboratory sessions: attitude, skills acquired, and laboratory notebook: 30% of the overall mark.

2. Theoretical and practical tests consisting of oral and/or written examinations which shall include both theoretical and practical questions and problems: 40% of the overall mark.

3. Presentation of results: reports, and/or oral communication: 30% of the overall mark.

FIRST EXAMINATION SITTING

The final mark will be calculated as the average of the three sections indicated above. To pass the course, students must obtain a minimum mark of 5.0; in addition, each of the sections must achieve a minimum mark of 4.0 out of 10.

SECOND EXAMINATION SITTING

In the second attempt, students will be able to re-sit the theoretical and practical tests and the presentation of results, namely the examination and the report.

Assessment will take place following the same weighting criteria as in the first sitting.

NOTE: This course is excluded from the regulations on advance calls for completing graduate studies (Degree Committee agreement of 26/03/2015).

REFERENCES

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