COURSE DATA

DATA SUBJECT

Code: 36451
Name: Physical Chemistry II
Cycle: Undergraduate Studies
ECTS Credits: 6
Academic year: 2026-27

STUDY (S)

Degree	Center	Acad. year	Period
1110 - Degree in Chemistry	Facultat de Química	3	First quarter
1934 - Double Degree Program in Chemistry-Chemical Engineering	Facultat de Química	3	First quarter

SUBJECT-MATTER

Degree	Subject-matter	Character
1110 - Degree in Chemistry	Physical Chemistry	COMPULSORY
1934 - Double Degree Program in Chemistry-Chemical Engineering	Tercer curso	COMPULSORY

COORDINATION

GIMENEZ ROMERO DAVID

SUMMARY

With the subject ***Physical Chemistry II***, it is intended essentially that students acquire basic knowledge of two fundamental parts of Physical Chemistry, such as Quantum Chemistry and Spectroscopy. Quantum Chemistry is the application of quantum physics to the study of atomic and molecular structure. Spectroscopy can be defined as the study of the interaction of electromagnetic radiation with matter and uses primarily quantum chemistry knowledge. Both subjects are increasingly interdisciplinary, as they are commonly used in other branches of chemistry.

Therefore, this subject will set the foundations for the student to successfully address subsequently the study of different parts of Chemistry and Physical Chemistry itself, usually using the concepts of Quantum Chemistry and Spectroscopy.

PREVIOUS KNOWLEDGE

RELATIONSHIP TO OTHER SUBJECTS OF THE SAME DEGREE

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

OTHER REQUIREMENTS

This course has no enrolment requirements with other Degree¿s courses. In any case, in order to successfully address the subject, it is essential that the student has a prior knowledge, according to the level required in the first year of the Degree in Chemistry. This knowledge comprises:

- Basic knowledge of Mechanics and Electromagnetism (Physics I and II).
- Basic concepts of Atomic and Molecular Structure (Chemistry I).
- Basic concepts of Mathematics, such as: logarithms, exponentials, complex numbers, derivatives and simple integrals, ordinary differential equations and fundamentals of statistics.

COMPETENCES / LEARNING OUTCOMES

1110 - Degree in Chemistry

Act autonomously in learning, making informed decisions in different contexts, forming judgements based on experimentation and analysis, and transferring knowledge to new situations.

At the end of the course, the student will be able to address new problems and develop strategies to solve them.

At the end of the course, the student will be able to describe the characteristics and behaviour of the different states of matter and the theories used to explain them.

At the end of the course, the student will be able to distinguish between qualitative and quantitative aspects of chemical problems.

At the end of the course, the student will be able to identify chemical processes in everyday life.

At the end of the course, the student will be able to identify the main types of chemical reactions and their key characteristics.

At the end of the course, the student will be able to implement sustainable and environmentally friendly methodologies.

At the end of the course, the student will be able to relate theory and experimentation.

At the end of the course, the student will be able to solve problems effectively.

At the end of the course, the student will be able to state the principles of quantum mechanics and apply them to the description of the structure and properties of atoms and molecules.

At the end of the course, the student will be able to state the principles of thermodynamics and kinetics and apply them in chemistry.

At the end of the course, the student will correctly use chemical terminology, nomenclature, conventions and units.

At the end of the course, the student will demonstrate inductive and deductive reasoning skills.

At the end of the course, the student will demonstrate the ability to analyse, synthesise and apply critical reasoning.

At the end of the course, the student will interpret the relationship between the variation of the characteristic properties of chemical elements and the periodic table.

At the end of the course, the student will relate chemistry to other disciplines.

Collaborate effectively in teams, assuming responsibilities and leadership roles and contributing to collective improvement and development.

Communicate effectively, both orally and in writing, adapting to the characteristics of the situation and the audience.

Contribute to the design, development and implementation of solutions that address social needs, taking the Sustainable Development Goals as a reference.

Demonstrate critical and self-critical reasoning within the field of study, considering aspects such as professional ethics, moral values and the social implications of the different activities undertaken.

Express oneself correctly, both orally and in writing, in any of the official languages of the Valencian Community.

Propose creative and innovative solutions to complex situations or problems within the field of study, in order to respond to diverse professional and social needs.

Understand and recognise, from within the discipline, inequalities based on sex and gender in society; integrate different needs and preferences related to sex and gender into problem-solving and solution design.

DESCRIPTION OF CONTENTS

1. Basic concepts. Principles of Quantum Mechanics

Development of quantum theory. Wave-particle duality. Schrödinger equation. Mathematical formalism. Postulates of Quantum Mechanics. Stationary states. Uncertainty Principle.

2. Model Systems

Translational motion: particle in a one-dimensional box. Particle in a two-dimensional box. Separation of variables technique. Finite tunneling barriers. Vibrational motion: Harmonic Oscillator.

3. Hydrogen Atom

Introduction. Orbital angular momentum. Rigid rotor. Hydrogen Atom: approach to the formal solution of the Schrödinger equation. Energy and functions of the bound states. Spin angular momentum.

4. Many-electron atoms

Many-electron atoms: general approach. Approximate methods. Helium Atom. Orbital approach. Anti-symmetry principle. Self-consistent field (SCF) orbitals. Electronic states.

5. Molecular structure

Many-electron molecules: general approach. Born-Oppenheimer approximation. The hydrogen ion-molecule (MO-LCAO method). The hydrogen molecule. Diatomic molecules. Polyatomic molecules. pi-electronic systems. Hückel method.

6. Foundations of Spectroscopy

Electromagnetic radiation. Spectroscopy: types of spectra. Radiation-matter interaction: semi-classical approximation. Boltzmann distribution law. The spectroscopic signal: position, intensity and width. Spectroscopic signal intensity. Lambert-Beer Law. Laser emission.

7. Rotation and Vibration Spectroscopies

Collective nuclear motion spectroscopies. Rotational energy levels of diatomic and linear molecules. Pure rotational spectra. Microwave spectroscopy. Vibrational energy levels. Vibration spectra of diatomic molecules. Rotation-vibration spectra. Vibration spectra of polyatomic molecules: vibration normal modes. IR spectroscopy. Raman spectroscopy.

8. Electronic Spectroscopy

Quantum interpretation of the electronic spectra: diatomic molecules. Vibrational structure: Franck-Condon principle. Selection rules. Electronic spectroscopy of polyatomic molecules. Fluorescence and phosphorescence.

WORKLOAD

PRESENCIAL ACTIVITIES

Activity	Hours

Tutorials	9,00
Theory	51,00
Total hours	**60,00**

NON PRESENCIAL ACTIVITIES

Activity	**Hours**
Attendance at other activities	0,00
Individual or group project	0,00
Independent study and work	90,00
Preparation of lessons	0,00
Preparation for assessment activities	0,00
Resolution of case studies	0,00
Total hours	**90,00**

TEACHING METHODOLOGY

The development of the course is structured around the following axis:

- lectures
- tutorials

With respect to the former, they will give an overview of the main topics and they will make emphasis on those key concepts necessary for their understanding. The most recommended resources for further preparation in depth of the subject will be indicated.

Tutorials will be devoted to the approach and resolution of problems and questions, which will allow for identifying the essential elements and concepts of each subject. For these sessions, a list of questions and problems will be provided that will serve for reinforcing the knowledge of the student and to exercise themselves in each subject discussed. The student must deliver the solved problems and questions as indicated by the teacher.

EVALUATION

The following assessment systems will be used:

• Tests consisting of Written, Oral and/or Practical Exams.

• Evaluation of group tutorial sessions, seminars, preparation of assignments and/or oral presentations.

• Continuous assessment of each student based on face-to-face activities, participation and degree of involvement in the teaching-learning process.

The assessment of student learning will take into account all the aspects set out in the methodology section of this teaching guide.

Modality A

FIRST CALL

The final grade will consist of:

The exam (75%), which will consist of a series of theoretical questions and numerical problems, which will deal with the basic concepts taught in class. The exam will be the same for all groups. Continuous assessment (25%), which includes assessment tests carried out throughout the course in the form of multiple or brief choice tests, the evaluation of group tutorial sessions, through the completion and/or delivery of exercises and questions, and the continuous assessment of each student based on participation and degree of involvement in the teaching-learning process. **Only in exceptional cases and within the period established by the professors, may modality A be waived.**

The minimum grade of the written exam must be equal to or greater than 4.5 out of 10 in order to average with the grade of the continuous assessment. The minimum overall grade to pass the subject is 5.0 out of 10.

SECOND CALL

In the second call, students will take an exam consisting of a series of theoretical questions and numerical problems, which will deal with the basic concepts taught in class. The exam will be the same for all groups. The final grade, including the continuous assessment, will be carried out using the same weighting as in the first call. The minimum overall grade to pass the subject is 5.0 out of 10.

Modality B

This modality will only be accepted in those very exceptional cases in which the teacher has accepted the student's application.

FIRST AND SECOND CALLS

The final grade will consist of the exam (90%) and the continuous assessment activities (10%). The minimum grade of the written exam must be equal to or greater than 4.5 out of 10 in order to average with the grade of the continuous assessment. The minimum overall grade to pass the subject is 5.0 out of 10.

The default modality will be A. Accessing modality B will require a justification of the non-possibility of attending face-to-face activities and approval by the professor who teaches the subject.

Final Warning

The copying or manifest plagiarism of any task that is part of the evaluation will make it impossible to pass the subject, then submit to the appropriate disciplinary procedures.

It should be noted that, in accordance with article 13 d) of the University Student Statute (RD 1791/2010, of December 30th), "*it is the duty of a student to refrain from using or cooperating in fraudulent procedures in assessment tests, in the work carried out or in official documents of the University*".

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