

**COURSE DATA****DATA SUBJECT**

Code: 34195
Name: Physical Chemistry III
Cycle: Undergraduate Studies
ECTS Credits: 6
Academic year: 2025-26

STUDY (S)

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

GRACIA EDO LOURDES

SUMMARY

Physical Chemistry III is a compulsory subject taught in the sixth semester. In the current curriculum it consists of a total of 6.0 ECTS credits.

This course aims, essentially, the completion and integration of the physicochemical training of the student

In the subjects of Physical Chemistry I and II, the student has acquired knowledge of the macroscopic views (mainly thermodynamics) and microscopic (quantum mechanics) matter. This course aims to start on the complementary nature of both views, showing how statistical thermodynamics allows calculation of the macroscopic properties of matter from the microscopic properties of its constituents. In addition to this fundamental purpose, it is aimed to train students in other physical chemical knowledge not yet acquired, such as surface phenomena and polymers.

PREVIOUS KNOWLEDGE**RELATIONSHIP TO OTHER SUBJECTS OF THE SAME DEGREE**

**1110 - Degree in Chemistry**

Obligation to have previously passed the subject(s)

34183 - General Chemistry I

34184 - General Chemistry II

Obligation to take the subject(s) simultaneously

36451 - Physical Chemistry II

1934 - Double Degree Program in Chemistry-Chemical Engineering

Obligation to have previously passed the subject(s)

34183 - General Chemistry I

34184 - General Chemistry II

Obligation to take the subject(s) simultaneously

36451 - Physical Chemistry II

OTHER REQUIREMENTS

In order to successfully address the subject, it is essential that the student possesses a number of previous concepts. These skills include:

Management of thermodynamic concepts (internal energy, entropy and free energy, spontaneity and balance) and basic kinetics (mechanism, slow step, reaction order, integrated equations).

Management of quantum concepts such as wave function states and levels. Knowledge of the solutions of model systems (particle in the box, rigid rotor...)

COMPETENCES / LEARNING OUTCOMES

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Act autonomously in learning, making well-founded decisions in various contexts, forming judgements based on experimentation and analysis, and applying knowledge to new situations.

Address new problems and propose strategies to solve them.

Collaborate effectively in work teams, assume responsibilities and leadership roles, and contribute to collective improvement and development.

Communicate effectively both orally and in writing, adapting to the context and audience.

Contribute to the design, development and implementation of solutions that respond to social demands, using the Sustainable Development Goals as a reference.

Demonstrate both inductive and deductive reasoning skills.

Demonstrate critical and self-critical thinking, considering professional ethics, moral values and social implications of the different activities carried out throughout the degree.

Demonstrate the ability to analyse, synthesise and reason critically.

Describe the characteristics and behaviour of the different states of matter and the theories used to explain them.

Distinguish between the qualitative and quantitative aspects of chemical problems.



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

Identify chemical processes in everyday life.

Identify the main types of chemical reactions and their associated key characteristics.

Implement sustainable and environmentally friendly methodologies.

Interpret the relationship between the variation in the characteristic properties of chemical elements and the Periodic Table.

List the principles of quantum mechanics and apply them to the description of the structure and properties of atoms and molecules.

Propose creative and innovative solutions to complex situations or problems in the field, addressing diverse professional and social needs.

Relate chemistry to other disciplines.

Relate theory to experimentation.

Solve problems effectively.

State the principles of thermodynamics and kinetics and their application in chemistry.

Understand and analyse, from the perspective of the degree programme, social inequalities based on sex and gender; integrate gender-sensitive approaches into problem-solving and solution design.

Use chemical terminology, nomenclature, conventions and units correctly.

DESCRIPTION OF CONTENTS

1. Statistical Thermodynamics: Fundamentals and Independent Particle Systems

1. - Introduction to Statistical Thermodynamics

1.1. Origin of Statistical Thermodynamics

1.2. States of a system. Relationship between macroscopic and microscopic properties of a system

2. - How do you calculate thermodynamic properties? The concept of ensemble

2.1. Probability of a microstate in the canonical ensemble

2.2. Thermodynamic functions in the canonical ensemble

2.3. Properties and interpretation of the canonical partition function 3.- Partition function in non-interacting particle systems

4. - Molecular partition function

5. - Ideal gas thermodynamic properties

6. - The equilibrium constant between ideal gases



2. Molecular Kinetics

1. Introduction
2. Collision theory
 - 2.1. Molecular rates
 - 2.1.1. Velocity Distribution functions
 - 2.1.2. Obtaining the velocity distribution functions
 - 2.2. Characteristic rates
 - 2.3. Energy distribution
 - 2.4. Collisions with the walls. Effusion
 - 2.5. Intermolecular collisions and mean free path
 - 2.6. Collisions and chemical reactivity
3. Potential energy surfaces
4. Transition state theory (TST)
 - 4.1. Basic assumptions and development
 - 4.2. Thermodynamic formulation of TST
 - 4.3. Limitations of TST

3. Transport Phenomena and Electrolytic Conductivity

- 1.- Introduction
 - 1.1.- Macroscopic description of non-equilibrium states
 - 1.2.- Definition of basic concepts
 - 1.3.- Phenomenological laws
3. - Types of transport processes and properties transported
 - 2.1.- Thermal conduction. Fourier's law
 - 2.2.- Viscosity. Newton's law. Poiseuille's law
 - 2.3.- Dissemination. Fick's first law
 - 2.4.- Ionic conduction: electrical conductivity, χ . Ohm's law. Migration
4. - Microscopic viewpoint. Transport phenomena in hard sphere gas
 - 4.1.- Coefficient of thermal conductivity
 - 4.2.- Coefficient of viscosity
 - 4.3.- Diffusion coefficient, D
5. - The general equation of diffusion
 - 5.1.- Fick's second law
 - 5.2.- Solutions of the diffusion equation
 - 5.3.- Diffusion with convection. General diffusion equation
 - 5.4.- Molar conductivity. Kohlrausch's law. Ion mobility



4. Surface Phenomena

- 1- Liquid interface
 - 1.1.- Surface tension
 - 1.2.- Curve interfaces
 - 1.2.1.- Young-Laplace equation
 - 1.2.2.- Vapour pressure on curved surfaces
 - 1.2.3.- Capillarity
 - 1.3. - Multicomponent systems
- 2.- Solid interface
 - 2.1.- Physisorption and chemisorption
 - 2.2.- Adsorption isotherms
 - 2.2.1- Langmuir isotherm
 - 2.2.1.1.- Extensions to the Langmuir isotherm
 - 2.2.1.2.- Effect of temperature on adsorption equilibrium
 - 2.2.1.3- Limitations on the Langmuir isotherm
 - 2.2.2. - Other isotherms
 - 3. - Electrified interfaces
 - 3.1.- Structure of the electrified interface

5. Heterogeneous Catalysis and Electrode Kinetics

- 1. Introduction
- 2.- Introduction to catalysis
 - 2.1- Basic principles of catalysis
 - 2.1.1. General mechanism of catalysis
 - 2.2.2.- Typical mechanisms of heterogeneous catalysis
 - 2.2.3- Examples of catalysis
- 3. Introduction to electrode kinetics
 - 3.1. Electron transfer
 - 3.2. Reversible electrochemical reaction controlled by diffusion
 - 3.3. Reaction with chemical equilibrium prior to electron transfer

6. Introduction to Macromolecular and Colloidal Systems

- 1. Introduction to macromolecular systems
 - 1.1. Introduction
 - 1.2. Molecular weight distribution
 - 1.3. Physical properties of polymers
 - 1.4. Thermodynamics of polymers in solution
- 2. Introduction to colloidal systems



- 2.1. Classification and preparation
- 2.2. Structure and stability: thermodynamic and kinetic aspects
- 2.3. Applications

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	14,00
Independent study and work	41,00
Preparation of lessons	28,00
Preparation for assessment activities	7,00
Resolution of case studies	0,00
Total hours	90,00

TEACHING METHODOLOGY

The development of the course is structured around three main themes: the theory sessions, tutorials and seminars.

In the lectures will explain the fundamental concepts for each of the themes listed on the agenda, indicating the bibliographic sources necessary for deepening the student. In addition, students have notes made by the team of teachers who can serve as a starting point for student work, not as unique material of study. After presenting the theoretical lectures, problems will be made for the subject.

With respect to the tutoring sessions, in addition to the questions submitted by students, they will work on issues and problems proposed by the teacher in sufficient time so that students can try to resolve them by their means and participate actively.

In addition, we plan to hold seminars for the expansion and deepening of some aspects of the issues highlighted by their interest or currency. Seminars and Conference will focus on complementary aspects of their training in Physical Chemistry. For this task, students attending the event and answer a questionnaire prepared by the instructor.



EVALUATION

First Call

The evaluation of the subject is done through a final exam (with the possibility of doing it orally) and continuous assessment activities. There will be two modalities, A and B. In modality A, the exam will be 70% of the final grade and will consist of a series of theoretical and practical issues (problems) divided into several sections. 30% of the grade will come from continuous assessment activities (deliverables or quizzes or written tests) and attendance (participation in tutorials and seminars). In modality B, the exam will be 90% of the final grade and 10% of the grade will come from assessment activities (deliverables or quizzes).

The default modality will be A. Accessing modality B will require a justification regarding the inability to attend in person and approval by the teacher who teaches the subject.

To pass the subject must obtain a total score equal or higher than 5. It will also be necessary that each of the points considered in the overall evaluation to attain a minimum score of 45% of the corresponding section. Learning will be evaluated by taking into account all aspects outlined in the Methodology section of this course guide. Attendance and reply to a Seminar-Conference will be equivalent to a tutorial.

Second Call

Only the part corresponding to the final exam can be recovered (never the continuous assessment). The same percentages defined for the first call will remain.

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"*.

REFERENCES



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- ATKINS, P., DE PAULA, J. Química Física. 8ª edición. Editorial Médica Panamericana, 2008. ISBN 9789500612487
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- McQUARRIE, D.A., SIMONS, J.D., Physical Chemistry. A Molecular Approach. University Science Books, Sausalito. ISBN 9780935702996
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