COURSE DATA

Data Subject	
Code	34195
Name	Physical Chemistry III
Cycle	Grade
ECTS Credits	6.0
Academic year	2021 - 2022

Study (s)

Degree	Center	Acad. year	Period
1110 - Degree in Chemistry	Faculty of Chemistry	3	Second term

Subject-matter

Degree	Subject-matter	Character
1110 - Degree in Chemistry	7 - Physical Chemistry	Obligatory

Coordination

Name	Department
GRACIA EDO, LOURDES	315 - Physical Chemistry

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 stude nt.In the subjects of Physical Chemistry I and II, the student has acquired knowledge of the macroscopicv iews (mainly thermodynamics) and microscopic (quantum mechanics) matter. This course aims to start on thecomplementary nature of both views, showing how statistical thermodynamics allows calculation of themacroscopic properties of matter from the microscopic properties of its constituents. In addition to thisfundamental purpose, it is aimed to train students in other physical chemical knowledge no t yet acquired, suchas surface phenomena and polymers.

PREVIOUS KNOWLEDGE

Relationship to other subjects of the same degree

1110 - Degree in Chemistry :

1108 - Degree in Chemistry :

1934 - Double Degree Program in Chemistry-Chemical Engineering :

R4-OBLIGATION TO HAVE SUCCESSFULLY COMPLETED THE COURSE

34183 - General Chemistry I

34184 - General Chemistry II

R5-OBLIGATION TO PURSUE THE COURSE SIMULTANEOUSLY

34194 - Physical Chemistry II

R4-OBLIGATION TO HAVE SUCCESSFULLY COMPLETED THE COURSE

34183 - General Chemistry I

34184 - General Chemistry II

R5-OBLIGATION TO PURSUE THE COURSE SIMULTANEOUSLY

34194 - Physical Chemistry II

R4-OBLIGATION TO HAVE SUCCESSFULLY COMPLETED THE COURSE

34183 - General Chemistry I

34184 - General Chemistry II

R5-OBLIGATION TO PURSUE THE COURSE SIMULTANEOUSLY

34194 - 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...)
Basic calculation of deri

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

1110 - Degree in Chemistry

- Develop capacity for analysis, synthesis and critical thinking.
- Show inductive and deductive reasoning ability.
- Solve problems effectively.
- Demonstrate ability to communicate information, ideas, problems and solutions to both specialist and non-specialist audiences and using information technology, as appropriate.
- Demonstrate knowledge of the characteristics and behaviour of the different states of matter and the theories used to describe them.
- 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.
- 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.
- 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.
- 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 subject addresses part of the learning results of the matter Physical Chemistry contained in the document VERIFICA that allow to acquire specific knowledge of chemistry, cognitive skills and general skills recommended by the EUROPEAN CHEMISTRY THEMATIC NETWORK (ECTN) for the Chemistry Eurobachelor® Label. The following table lists the learning outcomes acquired in the subject Phyical Chemistry III related to the competences of the degree in Chemistry.

SPECIFIC KNOWLEDGE OF CHEMISTRY

The learning process should allow the degree graduates to demonstrate:

	Competences of the subject Physical Chemistry III that contemplate the learning outcomes EUROBACHELOR®
The characteristics of the different states of matter and the theories used to describe them.	Demonstrate knowledge of the characteristics and behaviour of the different states of matter and the theories used to describe them..(CE3).
The principles of thermodynamics and their applications to chemistry	Demonstrate knowledge of the principles of thermodynamics and kinetics and their applications in chemistry..(CE6).
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 quantum mechanics and their application to the description of the structure and properties of atoms and molecules..(CE5).
The kinetics of chemical change, including catalysis; the mechanistic interpretation of chemical reactions	Demonstrate knowledge of the principles of thermodynamics and kinetics and their applications in chemistry..(CE6).
The relation between bulk properties and the properties of individual atoms and molecules, including macromolecules (both natural and man-made), polymers and other related materials.	Relate the macroscopic properties and the properties of individual atoms and molecules, including macromolecules (natural and synthetic), polymers, colloids and other materials.CE11).

COMPETENCES AND COGNITIVE SKILLS

The learning process should allow the degree graduates to demonstrate:

	Competences of the subject Physical Chemistry III that contemplate the learning outcomes EUROBACHELOR®
Ability to demonstrate knowledge and understanding of the facts, concepts, principles and fundamental theories related to the topics mentioned above.	Demonstrate knowledge and understanding of essential facts, concepts, principles and theories related to the areas of chemistry..(CE13).
	Solve qualitative and quantitative problems following previously developed models..(CE14).
Ability to apply this knowledge and understanding to the solution of common qualitative and quantitative problems.	Recognise and analyse new problems and plan strategies to solve them..(CE15).
	Understand the qualitative and quantitative aspects of chemical problems..(CE24).
Ability to calculate and process data, related to information and chemistry data.	Solve qualitative and quantitative problems following previously developed models..(CE14). Recognise and analyse new problems and plan strategies to solve them..(CE15).

GENERAL COMPETENCES

The learning process should allow the degree graduates to demonstrate:

	Competences of the subject Physical Chemistry III that contemplate the learning outcomes EUROBACHELOR®
Ability to apply practical knowledge to solve problems related to	Solve problems

qualitative and quantitative information.	effectively..(CG4). Solve qualitative and quantitative problems following previously developed models..(CE14). Relate theory and experimentation..(CE22). Recognise and evaluate chemical processes in daily life..(CE23). Understand the qualitative and quantitative aspects of chemical problems..(CE24). Develop capacity for analysis, synthesis and critical thinking.. (CG1).
Calculation and arithmetic capabilities, including aspects such as analysis error, estimates of orders of magnitude, and correct use of the units.	Show inductive and deductive reasoning ability..(CG2). Solve problems effectively..CG4).
Competences in information management, in relation to primary and secondary sources, including information retrieval through on-line searches.	Demonstrate ability to communicate information, ideas, problems and solutions to both specialist and non-specialist audiences and using information technology, as appropriate..(CG6).

	Have basic skills in the use of information and communication technology and properly manage the information obtained.(CT2).
	Develop capacity for analysis, synthesis and critical thinking.. (CG1).
	Show inductive and deductive reasoning ability..(CG2).
Ability to analyse materials and synthesize concepts.	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..(CB3).
	Demonstrate the ability to adapt to new situations..(CG9).
	Recognise and analyse new problems and plan strategies to solve them..(CE15).
Ability to adapt to new situations and make decisions.	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..(CB3).

Skills related to information technology such as word processing, spreadsheet, recording and storage of data, internet use related to the subjects.	Demonstrate ability to communicate information, ideas, problems and solutions to both specialist and non-specialist audiences and using information technology, as appropriate..(CG6). Have basic skills in the use of information and communication technology and properly manage the information obtained.(CT2). Demonstrate leadership and management skills, entrepreneurship, initiative, creativity, organization, planning, control, leadership, decision making and negotiation..(CG3). Demonstrate ability to work in teams both in interdisciplinary teams and in an international context..(CG5).
Study skills necessary for professional development. These will include the ability to work autonomously.	Learn autonomously.(CG8). Demonstrate the ability to adapt to new situations..(CG9). Students must have developed the learning skills needed to undertake further study

	with a high degree of autonomy.(CB5).
	Acquire a permanent sensitivity to quality, the environment, sustainable development and the prevention of occupational hazards.(CG10).
Ethical commitment to the European Code of Conduct: http://ec.europa.eu/research/participants/data/ref/h2020/other/hi/h2020-ethics_code-of-conduct_en.pdf	Demonstrate a commitment to ethics, equality values and social responsibility as a citizen and as a professional. (CG7).
	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. (CB3).

These learning outcomes, once the subject Physical Chemistry has been completed, should allow the student to:

Unit 1

-Calculation of occupation probabilities of states from the energy and temperature.

-Calculation of occupation probabilities of energy levels from the energy and temperature. Application to spin magnetic resonance

-Calculate molecular partition functions as well as explicit sums under the most common approaches.

-Interpret the meaning of the partition function

-
Calculate, from microscopic properties, the internal energy, heat capacity, entropy and free energy of idea lgas composed of simple molecules (mono, di and triatomic).

-Calculate the equilibrium constant for reactions between ideal gas formed by single molecules.

-
Predict the sense of balance and its change with temperature from the fundamental energies ofreactants an d products and the accessibility of energy states in them.

Unit 2

-Calculate characteristics rates of a gas sample at equilibrium.

-Calculate the frequency of collision of gas molecules with each other and the container walls.

-Calculate the mean free path of gas molecules.

-Calculate the rate constant for a reaction between gas from the collision theory.

-Interpret the potential energy surface of a reactive system. Find the stationary points and classify them as stable species (reactants, products, intermediates) or not (state transition). Drawing on these surfaces the reaction pathways of minimum energy.

-Calculate the rate constant for a reaction from the transition state theory.

-
Being able to use the thermodynamic formulation of transition state theory to interpret the dependence of therate constant with temperature. Calculate the enthalpy, entropy and free energy of activation.

Unit 3

-
Define the concept of transport process from the standpoint of identifying macroscopicphenomenolog ical and turn when a system is or not far from its thermodynamic state of balance.

-
Explain and differentiate between different types of transport processes, based on the thermodynamic qua ntitywhich is transported.

-Explain, derive and apply general and specific laws of such transport phenomena for the corresponding systems.

-Explain Kohlrausch's law and the law of independent migration of ions in solution.

-Describe and explain the evolution of a system on a non-stationary.

-Derive and reason Fick's second law of diffusion.

-
Apply the solutions of the diffusion equation to problems of environmental pollution and to assess itspred ictive power.

-Relate the ion mobility to the conductivity of ions in solution, minus the Nernst-
Einstein equation the diffusionof ions in solution.

Unit 4

- Define surface tension.

-
Determine the effect of surface tension at interfaces curves: influence of the radius of curvature, vaporpr essure by varying the curvature, up / down by a capillary.

- Explain the variation of surface tension with concentration.
- Distinguish between chemisorption and physisorption.
- Define and classify adsorption isotherms.
- Deduce the Langmuir isotherm and determine the characteristic parameters.
- Explain the influence of temperature on adsorption.
- Explain the variation of the fraction of coating with pressure by varying the temperature.
- Determine and interpret the characteristic parameters of the BET isotherm.

- Interpret the electrocapillary curves.

- Assess the change in surface tension of the surface charge density and capacity with the applied potential.

Unit 5

- Explain the general mechanism of heterogeneous catalysis.

- Apply knowledge of formal kinetics to the deduction of the kinetic law of some processes inheterogeneous catalysis: Mechanisms of Langmuir-Hishelwood and Rideal-Eley.

- Give an overview of the use of solid catalysts.

- Explain the differences between electrode processes (faradaic and non-faradaic).

-Calculate the current-current function for some processes: electron transfer and diffusion-controlledreversible processes.

- Give an electric vision of electrode processes.

Unit 6

- Define polymer or macromolecule.

- Define and determine the average molecular masses characteristic of macromolecular systems.

- Define the size of a polymer.

- Define the characteristic temperatures of a polymer.

- Explain the change in the state of a polymer as a function of temperature.

- Explain the thermodynamic aspects of a polymer in a solvent. Determine the free energy change of mixing.

- Define of colloidal systems.

- Classify colloidal systems.

- Determine the structure and stability of colloidal systems.

- Explain the kinetic aspects of colloidal systems.

- Explain the thermodynamic aspects of colloidal systems.

Cite practical applications of colloidal systems.

Finally,

Demonstrate an ethical and responsible conduct in the exercise of their professional work, values that are transmitted by teachers and researchers of the University, as a generator and transmitter of scientific knowledge.

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, . 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. Kohlrauschs 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

ACTIVITY	Hours	% To be attended
Theory classes	51,00	100
Tutorials	9,00	100
Development of group work	7,00	0
Development of individual work	7,00	0
Study and independent work	41,00	0
Preparing lectures	14,00	0
Preparation of practical classes and problem	14,00	0
Resolution of online questionnaires	7,00	0
TOTAL	**150,00**	

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

The evaluation of the course can be done through two different systems: presential and non-presential. In principle, all the students are assigned to the presential system. The students can ask for a change of the evaluation system by means of a written request to the teacher during the first 3 weeks of the course. In the non-presetial system the final grade correspond to the mark obtained in the exam.

The presential evaluation of the course is done through a final and continuous assessment activities. 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 tests) and attendance (participation in tutorials and seminars). To pass the course 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 40% 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.

REFERENCES

Basic

- LEVINE,I. N., Fisicoquímica. 5ºedición. McGraw Hill, 2004. ISBN 9788448137861 (v. 1) ISBN 9788448137878 (v. 2)

- ATKINS, P., DE PAULA, J. Química Física. 8ª edición. Editorial Médica Panamericana, 2008. ISBN 9789500612487
- ENGEL, T., REID, P. Química Física. Pearson Addison Wesley 2006. ISBN 9788478290772

Additional

- McQUARRIE, D.A., SIMONS, J.D., Physical Chemistry. A Molecular Approach. University Science Books, Sausalito. ISBN 9780935702996
- TUÑÓN, I., SILLA, E., Termodinámica Estadística para Químicos y Bioquímicos, Síntesis, 2008. ISBN 9788497566899

ADDENDUM COVID-19

This addendum will only be activated if the health situation requires so and with the prior agreement of the Governing Council

Contents

1.- The contents initially indicated in the teaching guide are maintained.

Workload and temporary teaching planning

Regarding the workload:

1.- The different activities described in the Teaching Guide are maintained with the intended dedication.

Regarding the temporary teaching planning:

2.- The material to follow the theory/tutoring/classroom-seminar classes allows to continue the temporary teaching planning both in days and schedule, whether the teaching is face-to-face in the classroom or not, although in some of the activities the student has the freedom to follow the non-face-to-face sessions according to his own planning.

Teaching Methodology

Theory subjects:

Situation of minimal attendance: In theory classes and tutorials the occupation will be, at most, 30% of their usual occupation. Teaching will be online. Students who have a laboratory session before or after theory classes, and the time to travel is longer than the time established in the schedules, will be able to follow the class in person in the classroom assigned in the schedules. When there are students in this situation, classes will be taught by synchronous videoconference in the group classroom.

Maximum face-to-face situation: In theory classes and tutorials, the occupation will respect the sanitary restrictions that limit the capacity of the classrooms. Depending on the capacity of the classroom and the number of students enrolled, it may be necessary that part of the students have to follow the classes synchronously. If this situation arises, the students will attend the group classroom in weekly rotating shifts (preferably in alphabetical order), so as to ensure that the percentage of attendance of all the students enrolled in the subject is the same.

Confinement situation: If for health reasons it is not possible to continue with hybrid teaching, totally or partially affecting the classes of the subject, these will be replaced by synchronous non-face-to-face sessions following the established schedules and using the virtual classroom tools.

The methodology used for non-face-to-face classes shall be:

1. Synchronously using virtual classroom tools (preferably Teams)

2. Asynchronously using presentations with audio narration or other virtual classroom tools

3. Resolution of exercises and questionnaires

In all subjects

If there is a closure of the facilities for health reasons that totally or partially affects the classes of the course, they will be replaced by non-face-to-face sessions following the established schedules and using the tools of the virtual classroom.

In the case of students confined to home due to COVID, they will be ensured on-line teaching through Teams.

Evaluation

The evaluation system described in the Teaching Guide of the subject in which the various evaluable activities have been specified as well as their contribution to the final grade of the subject is maintained.

Only in duly justified exceptional cases will the examination be considered as the sole evaluation method.

If there is a closure of the facilities for health reasons affecting the development of any face-to-face evaluable activity of the subject, it will be replaced by a test of a similar nature that will be carried out in virtual mode using the computer tools licensed by the University of Valencia. The contribution of each evaluable activity to the final grade of the subject will remain unchanged, as set out in this guide.

References

2.- The literature recommended in the Teaching Guide is maintained since it is accessible, and it is complemented by notes, slides and problems uploaded to the Virtual Classroom as material of the course.