COURSE DATA

Data Subject	
Code	34195
Name	Physical chemistry III
Cycle	Grade
ECTS Credits	6.0
Academic year	2018 - 2019

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
TUÑON GARCIA DE VICUÑA, IGNACIO NILO	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 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, and to further train them in spectroscopy with a subject dedicated to magnetic resonance.

PREVIOUS KNOWLEDGE

Relationship to other subjects of the same degree

1110 - 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

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 derivatives and integrals.
Management of different systems of units.

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 communicate information, ideas, problems and solutions to both specialist and non-specialist audiences and using information technology, as appropriate.
- Learn autonomously.
- Demonstrate knowledge of the main aspects of chemical terminology, nomenclature, conventions and units.
- 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.
- 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)

Unit 1

-Express the nuclear spin angular momentum from the nuclear spin.

-Identify the number of nuclear states in response to the nuclear spin.

-Establish the relationship between the nuclear spin angular momentum and the nuclear magnetic dipole moment.

-Calculate the energy of the nuclear spin states when the core is immersed in a magnetic field

-Calculate the resonant frequency for a core unshielded.

-Describe the phenomenon of shielding.

-Define the chemical shift.

-Predict the influence of spin-spin coupling in a simple system like the AX.

-Structural determination from NMR spectra using ChemOffice program.

Unit 2

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

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

-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 ideal gas 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 of reactants and products and the accessibility of energy states in them.

Unit 3

-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 the rate constant with temperature. Calculate the enthalpy, entropy and free energy of activation.

Unit 4

-Define the concept of transport process from the standpoint of identifying macroscopic phenomenological 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 quantity which 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 its predictive power.

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

Unit 5

- Define surface tension.

- Determine the effect of surface tension at interfaces curves: influence of the radius of curvature, vapor pressure 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 6

-Explain the general mechanism of heterogeneous catalysis

-Apply knowledge of formal kinetics to the deduction of the kinetic law of some processes in heterogeneous 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-controlled reversible processes.

- Give an electric vision of electrode processes.

Unit 7

- 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. Nuclear Magnetic Resonance

1.1. - Presentation
1.2. - Magnetic properties of atomic nuclei
1.2.1. - Nuclear spin and nuclear spin angular momentum
1.2.2. - Nuclear magnetic dipole moment: nuclear magneton, gyro-magnetic ratio
1.3.- Magnetic field interaction with atomic nuclei
1.3.1. Energy - magnetic field interaction with the nuclear magnetic moment
1.3.2. - Precession and Larmor frequency
1.3.3. - Cleavage of the energy levels of nuclear spin
1.4. - NMR spectroscopy
1.4.1. - Resonance frequency
1.4.2. - Population levels
1.4.3. - Selection rules

1.4.4.- Classical description of the measurement equipment
1.5.- Chemical shift
1.5.1. - Shielding and chemical shift
1.5.2. - Scale of chemical shifts
1.6.- Fine structure of the spectrum
1.6.1. - AX system
1.6.2. - A2 system
1.6.3. - AXN system
1.6.4. - Values of spin-spin coupling
1.6.5. - Origin of spin-spin coupling in solution

2. 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

3. Molecular Kinetics

3.1. Introduction
3.2. Collision theory
3.2.1. Molecular rates
3.2.1.1. Distribution functions of velocity
3.2.1.2. Obtaining the distribution functions of velocity
3.2.2. Characteristic rates
3.2.3. Energy distribution
3.2.4. Collisions with the walls. Effusion
3.2.5. Intermolecular collisions and mean free path
3.2.6. Collisions and chemical reactivity
3.3. Potential energy surfaces
3.4. Transition state theory (TST)
3.4.1. Basic assumptions and development
3.4.2. Thermodynamic formulation of TST
3.4.3. Limitations of TST

4. Transport Phenomena and Electrolytic Conductivity

4.1. - Introduction
4.1.1. - Macroscopic description of non-equilibrium states
4.1.2. - Definition of basic concepts
4.1.3. - Phenomenological laws
4.2. - Types of transport processes and properties transported
4.2.1. - Thermal conduction. Fourier's law
4.2.2. - Viscosity. Newton's law. Poiseuille's law
4.2.3. - Dissemination. Fick's first law
4.2.4. - Ionic conduction: electrical conductivity, . Ohm's law. Migration
4.3. - Microscopic viewpoint. Transport phenomena in hard sphere gas
4.3.1. - Coefficient of thermal conductivity, k
4.3.2. - Coefficient of viscosity,
4.3.3. - Diffusion coefficient, D
4.4. - The general equation of diffusion
4.4.1. - Fick's second law
4.4.2. - Solutions of the diffusion equation
4.4.3. - Diffusion with convection. General diffusion equation
4.4.4. - Molar conductivity. Kohlrauschs law. Ion mobility

5. Surface Phenomena

5.1. - Liquid interface
5.1.1. - Surface tension
5.1.2. - Curve interfaces
5.1.2.1. - Young-Laplace equation
5.1.2.2. - Vapour pressure on curved surfaces
5.1.2.3. - Capillarity
5.1.3. - Multicomponent systems
5.2. - Solid interface
5.2.1. - Physisorption and chemisorption
5.2.2. - Adsorption isotherms
5.2.2.1. - Langmuir isotherm
5.2.2.2. - Extensions to the Langmuir isotherm
5.2.2.3. - Effect of temperature on adsorption equilibrium
5.2.2.4. - Limitations on the Langmuir isotherm
5.2.3. - Other isotherms
5.3. - Electrified interfaces
5.3.1.- Structure of the electrified interface

6. Heterogeneous Catalysis and Electrode Kinetics

6.1.Introduction
6.2.-Introduction to catalysis
6.2.1-Basic principles of catalysis
6.2.1.1. General mechanism of catalysis
6.2.1.2. - Typical mechanisms of heterogeneous catalysis
6.2.1.3. - Examples of catalysis
6.3. Introduction to electrode kinetics
6.3.1. Electron transfer
6.3.2. Reversible electrochemical reaction controlled by diffusion
6.3.3. Reaction with chemical equilibrium prior to electron transfer

7. Introduction to Macromolecular and Colloidal Systems

7.1. Introduction to macromolecular systems
7.1.1. Introduction
7.1.2. Molecular weight distribution
7.1.3. Physical properties of polymers
7.1.4. Thermodynamics of polymers in solution
7.2. Introduction to colloidal systems
7.2.1. Classification and preparation
7.2.2. Structure and stability: thermodynamic and kinetic aspects
7.2.3. 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 will 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