COURSE DATA

Data Subject

Code	36596
Name	Elements of Physical Chemistry
Cycle	Grade
ECTS Credits	7.5
Academic year	2023 - 2024

Study (s)

Degree	Center	Acad. year	Period
1929 - D.D. in Physics-Chemistry	Double Degree Program Physics and Chemistry	4	Second term

Subject-matter

Degree	Subject-matter	Character
1929 - D.D. in Physics-Chemistry	4 - Cuarto Curso (Obligatorio)	Obligatory

Coordination

Name	Department
ROCA SANJUAN, DANIEL	315 - Physical Chemistry
RUIZ PERNIA, JOSE JAVIER	315 - Physical Chemistry

SUMMARY

The syllabus of the Double Degree in Physics and Chemistry contains only one compulsory subject that deals with the theoretical contents of Physical Chemistry: "Elements of Physical Chemistry", located in the eighth four-month period. This is a specific module of this double degree, in which both macroscopic and microscopic contents of the three subjects of the Degree in Chemistry that correspond to this specialty (Physical Chemistry I, II and III) are studied, and which are not included in subjects such as Thermodynamics, Quantum Physics I and II, Statistical Physics, etc. Thus, the two most important content blocks are spectroscopy and chemical kinetics, to which specific topics related to chemical thermodynamics, thermostatistics and electrochemistry have been added. The learning outcomes acquired in this module will be complemented later, in the fifth year, with those of the practical subject "Physical Chemistry Laboratory".

PREVIOUS KNOWLEDGE

Relationship to other subjects of the same degree

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

Other requirements

Requirements R4-OBLIGATION TO HAVE PREVIOUSLY PASSED THE COURSE34183 - General Chemistry I34184 - General Chemistry II34233 - General Physics I34234 - General Physics II34235 - General Physics IIIR5-OBLIGATION TO TAKE THE SUBJECT SIMULTANEOUSLY34246 - Statistical Physics

OUTCOMES

1929 - D.D. in Physics-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

At the end of the course, the student must be able to:

Formulate the Hamiltonian operator for a polyatomic molecule.

Describe the Born-Oppenheimer approximation and the concept of the potential energy surface.

Analyse the exact solutions of the hydrogen ion molecule and those obtained with the approximate OM-CLOA method.

Describe the application of the OM-CLOA method on the hydrogen molecule.

Discuss the electronic structure of diatomic molecules using the qualitative OMs and SCF-HF models.

Apply Hückel's method to conjugated and aromatic systems.

Correctly describe the spectroscopic phenomenon and the types of spectroscopy.

Describe the semiclassical approach to radiation-matter interaction.

Define the transition dipole moment and differentiate between generic and specific selection rules.

Describe the different factors on which the intensity and width of a spectroscopic signal depend.

Formulate Boltzmann's law of distribution and relate the intensity of a signal

spectroscopic with the population of energy levels and the transition probability.

Define the experimental measurement of the intensity of a spectroscopic signal.

To formulate the separation of the different types of nuclear motion.

Plot the rotational energy levels of diatomic and linear rotors, and interpret the shape of the pure rotational spectrum using the selection rules.

Plot the vibrational energy levels for a diatomic molecule using the

harmonic and anharmonic approaches.

Diagram the transitions that make up a spectrum of pure vibration and interpret the effect of anharmonicity on these transitions.

Explain the characteristics of the rotation-vibrational spectra of diatomic molecules and extract structural information from the P, Q and R branches.

State the properties of the vibrational motion of a polyatomic molecule and the concept of normal modes of vibration.

To analyse in a simple way the vibrational spectrum of a polyatomic molecule.

Describe the characteristics of rotational and vibrational Raman spectroscopy.

Analyse the electronic spectrum of a diatomic molecule and explain its vibrational structure using the Franck-Condon principle.

Define the concept of a chromophore group and differentiate the types of transitions that occur in the electronic spectrum of polyatomic molecules.

Describe the phenomena of fluorescence and phosphorescence and their properties.

Outline the different photophysical and photochemical processes.

Calculate equilibrium constants in ideal and non-ideal systems from the variation of free energy.

Calculate equilibrium molalities in electrolyte equilibria using the Davies equation to estimate activity coefficients.

Calculate the standard potential of the battery reaction using its relation to the free energy, as well as from the table of normal electrode potentials.

Calculate the potential of a reversible galvanic cell using the Nernst equation.

Calculate thermodynamic properties of a battery reaction from the variation of the potential with temperature.

Calculate equilibrium constants from standard potential data.

Calculate electrolyte activity coefficients from battery potential data using the electrochemical equilibrium condition at the electrodes.

Calculate molecular partition functions both as explicit sums and under the most common approximations.

Calculate, from microscopic properties, the internal energy, heat capacity, entropy and free energy of ideal gases consisting of single molecules (mono-, di- and triatomic).

Calculate the equilibrium constant for reactions between ideal gases formed by simple molecules.

Predict the direction of equilibrium and its change with temperature from the fundamental energies of reactants and products and the accessibility of the energy states in them.

Obtain the order and rate constant of complex chemical reactions from experimental data and use different methods for their determination.

Use the limiting-stage and steady-state approaches to establish whether a proposed mechanism for a chemical reaction is compatible with the available kinetic data.

Describe some mechanisms of complex reactions and explain the phenomenon of catalysis.

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

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

Use the thermodynamic formulation of the transition state theory to interpret the dependence of the rate constant on temperature. Calculate enthalpy, entropy and activation free energy.

Distinguish between chemisorption and physisorption.

Define and classify adsorption isotherms.

Derive the Langmuir isotherm and determine the characteristic parameters.

Explain the influence of temperature on adsorption.

Calculate the variation of the coating fraction with pressure as the temperature varies.

Determine and interpret the characteristic parameters of the BET isotherm.

Interpret electrocapillary curves.

Determine the variation of surface tension, surface charge density and capacitance with applied potential.

Explain the general mechanism of heterogeneous catalysis.

Apply the knowledge of Formal Kinetics to the deduction of the kinetic law of some processes with heterogeneous catalysis: Langmuir-Hinshelwood and Eley-Rideal mechanisms.

Explain in general terms the use of solid catalysts.

List the differences between electrospray processes (faradaic and non-faradaic).

Deduce the current-current function for some processes: electron transfer and reversible diffusion-controlled processes.

To give an electrical view of electrostatic processes.

Define polymer or macromolecule.

Determine the characteristic molecular mass averages of macromolecular systems.

Define the size of a polymer.

Define the characteristic temperatures of a polymer.

Explain the variation of the state of a polymer as a function of temperature.

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

DESCRIPTION OF CONTENTS

1. Molecular structure

Polyelectronic molecules: general approach. Born-Oppenheimer approximation. The hydrogen ion molecule (OM-CLOA method). The hydrogen molecule Diatomic molecules (homonuclear and heteronuclear). Polyatomic molecules Pi-electronic systems Hückel's method.

2. Fundamentals of spectroscopy

Spectroscopy: types of spectra. Radiation-matter interaction: semiclassical approach. Boltzmann's law of distribution. The spectroscopic signal: position, intensity and width. Lambert-Beer law. Laser emission.

3. Rotation and vibration spectroscopies

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

4. Electronic spectroscopy and introduction to photochemistry

Quantum interpretation of electronic spectra. Types of electronic spectroscopy. Atomic spectra. Molecular absorption spectra (diatomic). Vibrational structure: Franck-Condon principle. Chromophores. Molecular emission spectra: fluorescence and phosphorescence. Photophysical and photochemical processes.

5. Chemical and electrochemical equilibrium

Introduction. Thermodynamic condition of chemical equilibrium. Chemical equilibrium in a mixture of ideal gases. Equilibrium constants. Chemical equilibrium in real gases. Chemical equilibrium in non-electrolytic ideal solutions. Chemical equilibrium in non-electrolytic real solutions. Chemical equilibrium in electrolyte solutions. Electrode potential Properties of the electrochemical potential Thermodynamics of a battery Measurement of thermodynamic quantities from the potential difference between the electrodes of a battery. Liquid junction potential Applications of the measurement of the electromotive force: activity coefficient, pK, solubility product, and prediction of the spontaneity of redox reactions and metallic

corrosion.

6. Statistical thermodynamics

Introduction. Partition function in non-interacting particle systems. Molecular partition function. Thermodynamic properties of the ideal gas. The equilibrium constant between ideal gases.

7. Formal Kinetics

Introduction. Complex reactions: reversible reactions, competitive reactions, consecutive reactions. Reaction mechanisms. Limiting-stage approximation Steady state approximation Variation of the rate constant with temperature. Catalysis.

8. Molecular kinetics

Introduction. Molecular velocities. Potential energy surfaces. Transition state theory (TST): Basic hypotheses and development. Thermodynamic formulation of TST. Limitations of TST.

9. Solid and electrified interfaces

Solid interface. Physisorption and chemisorption. Adsorption isotherms Langmuir isotherm. Brunauer, Emmet and Teller (BET) isotherm. Other isotherms. Electrified interface. Structure of the electrified interface. Helmholtz-Perrin, Gouy-Chapman and Stern models.

10. Heterogeneous catalysis and electrode kinetics

Introduction. General mechanism of catalysis. Characteristics and stages of heterogeneous catalysis. Examples and applications. General mechanism of electrode kinetics. Rate law of electron transfer. Relationship between current and reaction rate: Butler-Volmer equation. Approximate forms of this relationship

11. Macromolecules

Introduction to macromolecular systems. Classification and types of polymers. Molecular mass distribution. Physical properties of polymers. Thermodynamics of polymers in solution.

WORKLOAD

ACTIVITY	Hours	% To be attended
Theory classes	64,00	100
Tutorials	11,00	100
Development of group work	10,00	0
Development of individual work	10,00	0
Study and independent work	50,00	0
Preparing lectures	17,00	0
Preparation of practical classes and problem	18,00	0
Resolution of online questionnaires	7,00	0
TOTAL	**187,00**	

TEACHING METHODOLOGY

The course is structured around three main axes: theory sessions, tutorials and seminars.

In the theory classes, the fundamental concepts for each of the subjects included in the syllabus will be explained, indicating the bibliographical sources necessary for the student's further study. In addition, students will be provided with notes made by the teaching staff which can be used as a starting point for the student's work, but never as the only study material. After explaining the theoretical concepts, problems corresponding to the subject will be carried out.

Regarding the tutorial sessions, in addition to the doubts presented by the students, work will be done on questions and problems proposed by the teacher sufficiently in advance so that the student can try to solve them by his or her own means and participate actively.

EVALUATION

The assessment of the course will be carried out in two ways, one face-to-face and one distance learning. In principle, all students are assigned to the face-to-face route. They may request a change to the non-attendance track by writing to the teacher within a period of no more than 3 weeks from the beginning of the course. In the non-attendance track, the final mark corresponds to the exam mark.

The on-site assessment of the course will be carried out through a final exam (written/oral) and continuous assessment activities. The exam will account for 70% of the final grade and will consist of a series of theoretical and practical questions (problems) divided into several sections. The 30% of the grade will come from continuous assessment activities (deliverables or questionnaires) and face-to-face activities (participation in tutorials and seminars). In order to pass the course, a total mark equal to or higher than 5 must be obtained. In addition, a minimum mark of 40% of the total of the corresponding section must be obtained in each of the sections considered in the total assessment.

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

Final warning

Copying or plagiarism of any assignment that is part of the evaluation will make it impossible to pass the course, and the student will be subject to the appropriate disciplinary procedures.

Please note that, according to Article 13 d) of the University Student Statute (RD 1791/2010, December 30), "*it is the duty of a student to refrain from using or cooperating in fraudulent procedures in evaluation tests, in the work performed or in official University documents*".

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.
- HOLLAS, J. M., Modern Spectroscopy, 2ª ed., John Wiley & Sons, 1992.
- LEVINE, I.N., Química Cuántica, 5ª ed., Prentice Hall, 2001.
- REQUENA, A. y ZUÑIGA, J., Espectroscopia, Pearson Prentice Hall, 2003.