COURSE DATA

DATA SUBJECT

Code: 36596
Name: Elements of Physical Chemistry
Cycle: Undergraduate Studies
ECTS Credits: 7.5
Academic year: 2026-27

STUDY (S)

Degree	Center	Acad. year	Period
1929 - Double Degree Program in Physics and Chemistry	Facultat de Física	4	Second quarter

SUBJECT-MATTER

Degree	Subject-matter	Character
1929 - Double Degree Program in Physics and Chemistry	Cuarto Curso (Obligatorio)	COMPULSORY

COORDINATION

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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

COMPETENCES / LEARNING OUTCOMES

1929 - Double Degree Program in Physics and Chemistry

Demonstrate ability to communicate information, ideas, problems and solutions to both specialist and non-specialist audiences and using information technology, as appropriate.

Demonstrate knowledge and understanding of essential facts, concepts, principles and theories related to the areas of chemistry.

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.

Develop capacity for analysis, synthesis and critical thinking.

Evaluate, interpret and synthesise chemical data and information.

Have basic skills in the use of information and communication technology and properly manage the information obtained.

Interpret data from observations and measurements in the laboratory in terms of their significance and the theories that underpin them.

Recognise and analyse new problems and plan strategies to solve them.

Recognise and evaluate chemical processes in daily life.

Relate the macroscopic properties and the properties of individual atoms and molecules, including macromolecules (natural and synthetic), polymers, colloids and other materials.

Relate theory and experimentation.

Show inductive and deductive reasoning ability.

Solve problems effectively.

Solve qualitative and quantitative problems following previously developed models.

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.

Understand the qualitative and quantitative aspects of chemical problems.

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. 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

PRESENCIAL ACTIVITIES

Activity	Hours
Tutorials	11,00
Theory	64,00

Total hours	**75,00**

NON PRESENCIAL ACTIVITIES

Activity	Hours
Attendance at other activities	0,00
Individual or group project	20,00
Independent study and work	50,00
Preparation of lessons	35,00
Preparation for assessment activities	7,00
Resolution of case studies	0,00
Total hours	**112,00**

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

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 continues assessment). The same percentages defined for the first call will remain.

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

- 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
- 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.
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- REQUENA, A. y ZUÑIGA, J., Espectroscopia, Pearson Prentice Hall, 2003.