

**COURSE DATA****Data Subject**

Code	44604
Name	Advanced physical chemistry
Cycle	Master's degree
ECTS Credits	5.0
Academic year	2021 - 2022

Study (s)

Degree	Center	Acad. Period
2218 - M.U. en Química	Faculty of Chemistry	1 First term

Subject-matter

Degree	Subject-matter	Character
2218 - M.U. en Química	1 - Advanced chemistry	Obligatory

Coordination

Name	Department
PEREZ PLA, FRANCISCO	315 - Physical Chemistry

SUMMARY

The Advanced Physical Chemistry is part of the Advanced Chemistry matter, which aims to expand and complement the Physical Chemistry knowledge acquired in the Grade. Specifically, the course provides a deep insight into Molecular Spectroscopy introducing the basics of photochemistry. The subject also deepens in the thermodynamic study of real systems allowing a better understanding of these systems by reinforcing the knowledge of Statistical Thermodynamics of systems having intermolecular interactions. In this line, the basics of Chemical Kinetics seen in the Grade are extended to complex reactions, and the basic concepts of homogeneous and heterogeneous catalysis and biocatalysis are studied. Finally, the basics of electrochemistry are extended by means of the description of processes taking place on electrodes, in particular the kinetics of the processes that occur on them. The acquired skills are applied to study the problem of electrochemical corrosion.



PREVIOUS KNOWLEDGE

Relationship to other subjects of the same degree

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

Other requirements

Previous knowledge of chemistry is required, at the level attained in the profiles recommended for admission of candidates to the Master Degree.

OUTCOMES

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- Students should apply acquired knowledge to solve problems in unfamiliar contexts within their field of study, including multidisciplinary scenarios.
- Students should be able to integrate knowledge and address the complexity of making informed judgments based on incomplete or limited information, including reflections on the social and ethical responsibilities associated with the application of their knowledge and judgments.
- Students should communicate conclusions and underlying knowledge clearly and unambiguously to both specialized and non-specialized audiences.
- Be able to solve complex chemistry problems, whether in the academic, research or industrial application areas at a specialization or masters-level.
- Promote, in academic and professional contexts in the field of economic policy, ... technological, social or cultural progress within a society based on knowledge and respect for: a) fundamental rights and equal opportunities between men and women, b) the principles of equal opportunities and universal accessibility for people with disabilities and c) the values of a culture of peace and of democratic values.
- Be able to design, perform, analyse and interpret experiences and complex data in the environment of chemistry at a specialization level.
- Acquire advanced knowledge to assess the importance of chemistry in health, the environment, new materials and energy.

LEARNING OUTCOMES

- (1) To know the physical bases of the different types of molecular spectroscopy and of the techniques derived from them, and the photophysical and photochemical processes.
- (2) To Know how to relate intermolecular interactions and description of the different models of real systems (gases, liquids, electrolyte solutions and non-electrolytes), and use the concepts of transience and activity, radial distribution functions, partial molar properties and functions excess.
- (3) To know the concepts of statistical thermodynamics, to systems and independent particles taking into account the intermolecular interactions and their application to obtaining state functions of real gases, liquids and solids behavior.



(4) To be able to obtain the relevant kinetic data of chemical reactions, from proposed mechanisms and know the basics of the homogeneous, heterogeneous catalysis and biocatalysis.

(5) To know the fundamentals of the electrode kinetics and its application to the study and corrosion inhibition.

DESCRIPTION OF CONTENTS

1. Molecular spectroscopy and photochemistry

General aspects of the interaction between light and matter. Models of electromagnetic radiation. Radiation and matter: absorption, emission, dispersion, diffusion and related spectroscopic techniques. Selection rules. The spectroscopic signal: position, width, intensity. Laser emission. Absorption coefficients.

Nuclear magnetic resonance spectroscopy. Basics of NMR technique in chemistry. Factors that determine the position of the NMR bands. Pulse techniques (NMR-TF). Free induction decay ("FID"). Spin Relaxation Time: longitudinal and transverse relaxation.

Electronic spectroscopy absorption and emission. Basics of the structure of the electronic spectra in diatomic molecules. Vibrational structure and the Franck-Condon principle. Different types of polyatomic molecule transitions. Photophysics and photochemistry: radiative and non-radiative transitions. Emission spectroscopy: fluorescence and phosphorescence.

2. Statistical thermodynamics of interacting systems

Intermolecular interactions. Multipolar moments, attractive forces, repulsive forces, models for intermolecular interactions and their limitations.

Statistical thermodynamics of real systems and condensed phases. Partition function of real systems and thermodynamic properties. Application of statistical thermodynamics to real gases. Heat capacity of crystalline solids. Radial distribution function and structure in liquids.

Simulation methods: Force fields, Strategies for simulations of realistic systems, Molecular Dynamics, Monte Carlo method.

3. Chemical Kinetics of complex reactions

Mechanism and rate law: Review of basic concepts. Complex reactions. Mechanism and rate law. Simplification of the rate law. Stationary linear equations.

Detection of reaction intermediates: Intermediate products and reaction centers. Techniques for the detection and characterization of intermediates. The technique of stopped-flow. Other techniques (SF-EXAFS, MS-ESI).

Data analysis Chemical Kinetics I: Monitoring of physical properties. Analysis of simple irreversible reactions. General analysis of simple reactions.

Data analysis Chemical Kinetics II: The response Model. Two-dimensional responses. Factorization of multi-channel responses. The chemical model. Systems of differential and algebraic-differential equations. The integration of model. Stiff systems. The least-squares technique. Objective functions. Minimization of the objective function.

**4. Corrosion and electrodic processes**

Electrochemistry of Molecules and Materials.

Overview of Electrochemistry. Types of electrodes. Disturbance and electrical response in cells. Electrode processes. The interfacial region electrode / solution. Scales and units Electrochemical potential magnitudes.

Irreversibility Electrochemical Cells.

Faradaic and non-faradaic electrode processes. Transport in electrochemical cells. Nernst diffusion controlled processes. The electron transfer coefficient and the symmetry parameter.

Simulation and Data Processing in electrode Processes.

Current-potential curves. Voltammetry of electroactive films. Electro-synthesis and characterization of conductive polymers. Metal electro-deposits and electro-solutions. Equivalent electrical circuits. Simulation and multiparameter fitting of the electrode response.

Metallic Corrosion and Inhibition.

The phenomenon of corrosion. Corrosion types. Experimental techniques for measuring the corrosion rate. Predicting corrosion of technological materials. Methods for corrosion inhibition.

5. Catalysis

Basics. Interaction catalyst/substrate. Sabatiers principle. Catalyst deactivation: sintering and thermal degradation.

Homogeneous catalysis. Catalysis by metal complexes. Acid-base catalysis. Organocatalysis. Recovery and recycling of the homogeneous catalyst. hybrid catalysis. "Click Chemistry". Biocatalysis.

Heterogeneous catalysis. Stages of the catalytic process. Langmuir-Hinshelwood kinetics. Solid-gas catalysis. Solid catalyst types. Catalyst characterization. Catalytic solid / liquid and liquid / liquid systems. Phase-transfer catalysts.

WORKLOAD

ACTIVITY	Hours	% To be attended
Theory classes	40,00	100
Tutorials	5,00	100
Seminars	5,00	100
Development of individual work	15,00	0
Study and independent work	30,00	0
Readings supplementary material	10,00	0
Preparation of evaluation activities	20,00	0
TOTAL	125,00	



TEACHING METHODOLOGY

The subject will be taught through participatory lectures, seminars will be held where, among other training activities, applied practical problems, and tutored classes designed to assess understanding of the subject by students.

EVALUATION

First call:

The rating of the subject, on first call, will be obtained from the marks obtained in the final exam, continuous assessment activities conducted and the papers presented throughout the course. Exam, work and activities will be averaged according to the following percentages:

- (A) Final exam: 60%.
- (B) continuous assessment activities (b.1 + b.2): 40%.
 - (B.1) activities throughout the year: 20%.
 - (B.2) Work performed during the course: 20%.

Second call:

The rating of the subject, on second call, will be obtained from the exam grades obtained second call and the work presented throughout the course. Examination and averaged works according to the following percentages:

- (A) Final exam: 80%.
- (B) Work performed during the course: 20%.

REFERENCES

Basic

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Additional

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- HARRIS, R. K. Nuclear Magnetic Resonance Spectroscopy. A Physico-chemical view, Pitman. Londres. 1983. ISBN 0273016849
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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**

The contents initially indicated in the teaching guide are maintained.

Workload and temporary teaching planning

Regarding the workload:

The different activities described in the Teaching Guide are maintained but the hours of dedication to each activity are changed, as shown in the following table:

ACTIVITY	Hours	% To be attended
Theory classes	40.00	70-100
Tutorials	5.00	70-100
Seminars	5.00	70-100
Study and independent work	75.00	0
TOTAL	125.00	

Regarding the temporary teaching planning:

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.

Teaching Methodology

Theory courses: Theory classes and classroom tutoring will tend to the maximum possible face-to-face teaching, always respecting the health restrictions that limit the capacity of the classrooms to 50% of their usual occupation. Depending on the capacity of the classroom and the number of students enrolled, some of the students may need to follow the classes synchronously in an auxiliary classroom. If this situation arises, students will attend the main classroom or auxiliary classroom for weekly rotary shifts (preferably in alphabetical order). However, the rotation system will be fixed once the actual enrollment data is known, guaranteeing, in any case, that the percentage of face-to-face teaching of all students enrolled in the subject is the same.



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

1. Synchronously using virtual classroom tools (Teams, Blackboard ...)
2. Asynchronously using locut power-point presentations or other virtual classroom tools
3. Resolution of exercises and questionnaires

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.

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.

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

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.