Teaching Guide				
Identifying Data				2022/23
Subject (*)	Advanced Physical Chemistry		Code	610G01020
Study programme	Grao en Química			
Descriptors				
Cycle	Period	Year	Type	Credits
Graduate	1st four-month period	Fourth	Obligatory	6
Language	SpanishEnglish			
Teaching method	Hybrid			
Prerequisites				
Department	Química			
Coordinador	Iglesias Martinez, Emilia		E-mail	emilia.iglesias@udc.es
Lecturers	Canle López, Moisés Iglesias Martinez, Emilia Santaballa Lopez, Juan Arturo		E-mail	moises.canle@udc.es emilia.iglesias@udc.es arturo.santaballa@udc.es
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General description	KEY WORDS: ionic interactions and molecular transport phenomena. Rate equation and reaction mechanisms. Chemical Kinetic Theories. Homogeneous catalysis. Introduction to electrochemical kinetics. Macromolecules and colloids. Advanced Physical Chemistry addresses the phenomenological study of the interactions between ions and molecules, which allow us to understand the configuration of macromolecules of chemical and biological interest. Transport phenomena in solution makes possible the characterization of macromolecules and are central to the application of certain techniques to kinetic study of reactions. Chemical kinetics introduces the time variable in the study of a chemical reaction, analyzing the factors that modify reaction rate in order to determine the rate equation, and finally to propose a reaction mechanism at the molecular level to interpret the observed macroscopic reaction.			

Study programme competences / results	
Code	Study programme competences / results
A1	Ability to use chemistry terminology, nomenclature, conventions and units
A3	Knowledge of characteristics of the different states of matter and theories used to describe them
A4	Knowledge of main types of chemical reaction and characteristics of each
A10	Knowledge of chemical kinetics, catalysis and reaction mechanisms
A14	Ability to demonstrate knowledge and understanding of concepts, principles and theories in chemistry
A19	Ability to follow standard procedures and handle scientific equipment
A20	Ability to interpret data resulting from laboratory observation and measurement
A22	Ability to plan, design and develop projects and experiments
A23	Critical standards of excellence in experimental technique and analysis
A25	Ability to recognise and analyse link between chemistry and other disciplines, and presence of chemical processes in everyday life
A27	Ability to teach chemistry and related subjects at different academic levels
B1	Learning to learn
B3	Application of logical, critical, creative thinking
B4	Working independently on own initiative
C3	Ability to use basic information and communications technology (ICT) tools for professional purposes and learning throughout life
C6	Ability to assess critically the knowledge, technology and information available for problem solving

Learning outcomes	
Learning outcomes	Study programme competences / results

Methodology: · Be able to plan, design, and perform experiments related to the transport of matter and charge transport. · Be able to propose and design a kinetic study of a chemical reaction. · Simple software application to the quantitative analysis of kinetic data. · Interpretation of kinetic results on the basis of reaction mechanisms. · Simulation / prediction of unpublished data from the rate equation	A3 A4 A10 A19 A20 A22 A23 A27	B1 B3 B4	C3
Conceptual: · Knowledge of interionic interactions and inter-or intramolecular interactions and their relationship with association phenomena, self-aggregation or molecular conformation. · Mastering the own methods of chemical kinetics. Interpretation at molecular level (mechanistic) of chemical reactions. Understand and know the factors that can change the rate of a chemical reaction. · Understand the catalysis process and its relation to chemical-, photochemical- or electrochemical-activation	A1 A4 A10 A14	B3	
Attitudinal: · Provide appropriate reports of an experimental study · Analyze and critique published kinetic studies of low difficulty.	A22 A23 A25 A27	B1 B3 B4	C3 C6

Contents	
Topic	**Sub-topic**
Ionic and molecular interactions	· Ionic interactions in the liquid phase: activity coefficient. Debye-Hucke's law. Ionic strength. · Molecular interactions. Dipole moment. Polarizability: equation of Clausius-Mossotti. Dipolar interactions. Hydrophobic interaction: self-aggregation and molecular conformation. ·Colloids: direct and reverse micelles, biological membranes. · Macromolecules
Transport phenomena	· Flux. Diffusion. Fick's first law. Stokes-Einstein equation. · Thermal conductivity · Electrical conductivity: the Debye-Huckel-Onsager theory. · Viscosity
Rate equation and reaction mechanism	· Integrated rate equation. Initial rates. Order of reaction. The method of flooding. Physical properties in kinetic studies. Experimental techniques. · Complex reaction schemes: parallel and concurrent reactions, reversible reactions, consecutive reactions. · The steady-state approximation. · Reaction mechanisms: elementary reactions. Deduction of reaction mechanisms.
Kinetic Theories and their applications	· Collisions theory: the frequency factor · Transition state theory. The activated complex. Statistical thermodynamics approach. Activation parameters. Potential energy surfaces. · Reactions in the gas phase: Lindeman mechanism · Reactions is solution. Diffusion controlled reactions · Photochemical reactions

Catalysis	· Homogeneous, heterogeneous and microheterogeneous catalysis · General mechanism of catalysis: rate equations. · Homogeneous catalysis: nucleophilic catalysis, acid-base catalysis, ... · Linear free energy relations: the Swain-Scott equation, the Bronsted law, the Hammett correlation, the Taft equation. · Microheterogeneous catalysis; micellar catalysis, enzyme catalysis. · Heterogeneous catalysis: Langmuir isoterm. Rate equations.
Introduction to electrochemical kinetics	· Electrochemical reactions: special topics · Interface electrode-solution: the Gouy-Chapman model · Rate of charge transfer. The Butler-Volmer equation · Voltametry
Lab experiments	· Laboratory experiments relative to transport phenomena, determination of reaction rate equations and catalytic processes.

Planning				
Methodologies / tests	Competencies / Results	Teaching hours (in-person & virtual)	Student?s personal work hours	Total hours
Guest lecture / keynote speech	A4 A10 A25 A27 B3	21	50	71
Seminar	A1 A4 A10 A14 B1 B3 C6	7	28	35
Laboratory practice	A19 A20 A22 A23 A25 A27 B1 B3 B4 C3 C6	20	20	40
Mixed objective/subjective test	A1 A3 A4 A10 A14 A20	4	0	4
Personalized attention		0	0	0
(*)The information in the planning table is for guidance only and does not take into account the heterogeneity of the students.				

Methodologies	
Methodologies	Description
Guest lecture / keynote speech	In the lectures the teacher introduces all concepts, models, methodologies and theories of the fundamental contents of the discipline program. It could be also possible to use case studies, project-based learning (PBL) & flipped classroom.
Seminar	This activity will be carried out in interactive way. Concepts will be emphasized through the detailed development of standard exercises, and doubts raised by students will be solved.
Laboratory practice	Experiments related to the concepts addressed in the course are carried out. It consists of two stages: The first includes the understanding of the experiment/s to be carried out in the lab (its theoretical basis and related techniques) and the development of the experimental work (planning, execution and critical analysis of the obtained the results. The second stage involves the delivery of the corresponding e-report. Presentation (including oral exposition), methodological justification and critical interpretation, as well as the comparison with bibliographic data, will be assessed.
Mixed objective/subjective test	Proposal of questions, exercises and/or simulations, related with lectures, seminars and lab experiments. The student alone will demonstrate, during a fixed time interval, the acquired knowledge and his capacity for solving exercises and/or developing conceptual questions.

Personalized attention	
Methodologies	Description

Seminar Laboratory practice	It recommends to the students the use of tutorials to solve all kind of doubts, questions and concepts that have not remained sufficiently clear, and that refer, either to the development of material concepts or to find the answers to problems introduced in the seminars, laboratory practices or in the preparation of the final test. The teachers will be available to solve any question about the contents of the subject at the established timetable. Students with a waiver for academic assistance will have both face-to-face and e-mail tutorials or Teams, whenever necessary. Before carrying out the experimental laboratory work, the student must demonstrate an understanding of the scientific article that describes the experience to be reproduced. During the development of the experiment, the student is advised on the complications that may arise. After it, the teachers will guide each student in the interpretation of the results, based on the theoretical models developed in the classroom for the quantitative treatment of the results.

Assessment			
Methodologies	Competencies / Results	Description	Qualification
Laboratory practice	A19 A20 A22 A23 A25 A27 B1 B3 B4 C3 C6	In the evaluation of this activity, the laboratory work and the Results Report are taken into account: -Interview in the Laboratory, prior to the development of the experiment, which reflects the understanding of the chemical system, the methodology to be applied, the technique used and the necessary safety. -Development of the experiment in the Laboratory: planning, data collection and their analysis. -Report of results that will be evaluated in terms of presentation, quantitative treatment and explanation of the results based on theoretical models	20
Mixed objective/subjective test	A1 A3 A4 A10 A14 A20	Written examination to answer theoretical questions and solve exercises related to the contents of the lectures, seminars and Lab experiments. It is required to carry out the Lab practices and pass the mixed test to pass the course. The qualification of a surpassed activity will be kept in the remaining opportunities of the current academic year (second opportunity). If the mixed probe is not passed, even if the average qualification of all activities is higher than 5, the numerical mark that appears in the "Acta" will be score obtained in the mixed test. The student will obtain the qualification of Not Presented when he/she does not carry out the Laboratory classes and, therefore, does not appear for the final examination either. Students who request an early call for December will be governed by the present teaching guide.	80

Assessment comments
-Attendance to all laboratory practices and delivery of the corresponding report are required, either for partial-time student or for full-time student. -Attendance to seminars is not mandatory for students with academic exemption. -To pass the course it will be necessary to obtain a mark not lower than 5.0 out of 10 in all valuable activities and achieve a minimum qualification of 5.0 in the proportional sum of all the activities. -The qualification of "Matricula" is preferably granted at the first opportunity. -Second Opportunity: repetition of the exam upon contents of seminars, lab practical and theory clases.

Sources of information

Basic	- P. W. Atkins, J. de Paula (2008). Química Física, 8ª Ed. . Panamericana - Espenson J. H. (1995). Chemical kinetics and reaction mechanisms 2ª ed.. McGraw-Hill, New York. - Laidler K. J. (1994). Chemical Kinetics . Harper and Row, New York. - Bockris, J.O.M., Reddy, A K.N. (1998). Electroquímica Moderna. . Reverté. 1980 - P. W. Atkins, J. de Paula (2010). Physical Chemistry, 9th Ed. . Oxford University Press
Complementary	- P. L. Brezonik (1994). Chemical Kinetics and Process Dynamic in Aquatic Systems.. Lewis Publishers - P. Sanz Pedredo (1992). Físicoquímica para Farmacia y Biología.. Masson-Salvat Medicina - R. A. Jackson (2004). Mechanism in Organic Reactions.. Royal Society of Chemistry (RSC) - LEVINE I. N. (2004). Fisicoquímica 5ª ed.. McGraw-Hill, Madrid - KORITA, J, DVORAK, J., KAVAN, L. (1987). Principles of Electrochemistry. 2nd ed.. Wiley, Chichester - BERRY R. S., RICE S. A., ROSS J. (2000). Physical Chemistry. 2ª ed.. Oxford University Press, New York - J. BERTRAN-RUSCA, J. NUÑEZ-DELGADO Eds , (2002). Química Física, vol. II. Ariel Ciencia - S. R. Logan (2000). Fundamentos de Cinética Química. Addison Wesley - BOCKRIS, J.O.M., REDDY, A.K.N., GAMBOA-ADELCO, M.E. (2000). Modern Electrochemistry 2A. Fundamentals of Electrodics.. Kluwer Academic/Plenum Press: New York

Recommendations
Subjects that it is recommended to have taken before
General Chemistry 1/610G01007 General Chemistry 2/610G01008 General Chemistry 3/610G01009 Chemistry Laboratory 1/610G01010 Physical Chemistry 1/610G01016 Physical Chemistry 2/610G01017 Physical Chemistry 3/610G01018 Experimental Physical Chemistry/610G01019
Subjects that are recommended to be taken simultaneously
Subjects that continue the syllabus
Other comments
Prerequisites: -They are necessary the knowledges of Chemistry and Physical Chemistry materias -To know draft,synthesize and correctly present a work. -To dominate the graphic representation, linear regression with basic knowledges of statistics. -To use at basic level tools of computing, such as Excel, Word, Power Point. -It recommends to know English of intermediate level (reading).