UNIVERSIDADE DA CORUÑA

Teaching Guide				
Identifying Data				2020/21
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	Brandariz Lendoiro, Maria Isabel Iglesias Martinez, Emilia	E-mail	i.brandariz@udc.es emilia.iglesias@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.			
Contingency plan	1. Modifications to the contents -No changes will be made 2. Methodologies *Teaching methodologies that are maintained: -Guest lecture -Seminar -Lab practices (the parts of interpreting the original paper of the lab experiment and the results report of simulated data) -Mixed/objective probes -Personal attendance *Teaching methodologies that are modified -The Lab development of experiments 3. Mechanisms for personalized attention to students -e-mail ; -Moodle forums -Teams 4. Modifications in the evaluation -The mark of lab experiments is added to the others two parts. *Evaluation observations: 5. Modifications to the bibliography or webgraphy -No changes			

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 lay. Stokes-Einstein equation. · Thermal conductivity · Electric conductivity: the Deby-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 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
Glossary	A1 A14 B1	0	5	5
Seminar	A1 A4 A10 A14 B1 B3	7	21	28
Long answer / essay questions	A14 B3 C6	0	2	2
Laboratory practice	A19 A20 A22 A23 A25 A27 B1 B3 B4 C3	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 exposition classes the teacher introduces all concepts, models, methodologies and theories of the fundamental contents of the discipline program.
Glossary	Elaboration of a list of key concepts (terms, authors, typical equations, ...), with their explanation, that arise in each topic. It is a Moodle activity in which the number of concepts per student is limited, seeking maximum participation.

Seminar	This activity will be carried out in a small groups. Certain concepts will be emphasized through the detailed development of standard exercises and doubts raised by the student will be resolved.
Long answer / essay questions	Periodically at the end of each thematic unit, including the corresponding seminar/s, a test/essay will be proposed during the seminar classes, so that the student can demonstrate the use and participation in these sessions. It is contemplated that it be done through Moodle on specific dates and in a certain time. The aim is not only to monitor the evolution of the students, but also to promote the continuous evaluation system.
Laboratory practice	Experiments related to the concepts addressed during the course will be carried out. It will consist of three phases: The first refers to completing a questionnaire through Moodle related to the experiment/s that corresponds to develop in the Laboratory. The second includes the work of the student in the Laboratory: planning of the experiment, its development and analysis of results. The third consists of preparing the Results Report, which will assess the presentation, methodological justification and interpretation, as well as the comparison with bibliographic results.
Mixed objective/subjective test	Proposal of questions and exercises, related with the concepts introduced in the classes of theory, seminar or in Lab experiments, to solve. 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**
Glossary 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 work, the student will summarize the scientific article that reflects the experiment that will be reproduced. During its development the student is advised on the complications that may arise. After ending the Lab work, the instructor will help the 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**
Glossary	A1 A14 B1	Preparation of a glossary of terms / concepts, ..., that arise in each topic. To obtain the maximum score, each student must propose a maximum of ten terms that cover all the topics of the content.	10
Laboratory practice	A19 A20 A22 A23 A25 A27 B1 B3 B4 C3	The evaluation of this activity takes into account the Moodle questionnaire, the laboratory work and the results report (written or as an oral presentation): -Understanding the script of the experiment (s) through a questionnaire in Moodle previously to the development of the experiment in the Laboratory. -Development of the experiment in the Laboratory: planning, data collection and analysis. -Laboratory report that reflects the presentation and the quantitative treatment of the experimental results and their explanation based on theoretical models.	15

Mixed objective/subjective test	A1 A3 A4 A10 A14 A20	Performance of written examination about theoretical and practical questions, regarding the contents treated in all parts of the course. It is required to surpass each of the activities 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 and essay tests are not passed, even if the average with the qualification of all the activities is higher than 5, the numerical qualification that appears in the ACTA will be the score obtained in both mixed and essay tests. The student will obtain the qualification of No Presented when he do not take part in the laboratory practice program and, therefore, do not present to the mixed test.	50
Long answer / essay questions	A14 B3 C6	Throughout the course there will be four / five short tests lasting less than 30 min, each one related to the thematic units of the content. Development through Moodle will be preferred whenever possible.	25

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. If it is not possible to participate in the essay test, the qualification will be added to the mixed text.-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. For those students who have not obtain a 5.0 out of 10 on the essay test, its grade will be added to the mixed text.

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). Modern Electrochemistry 1. Ionics. 2nd ed.. Plenum Press, New York
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
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).