UNIVERSIDAD DE CASTILLA - LA MANCHA

GUÍA DOCENTE

1. General information

Course: PHYSICAL-CHEMISTRY IV: KINETICS IN CHEMISTRY
Code: 57324
Type: CORE COURSE
ECTS credits: 6
Degree: 398 - UNDERGRADUATE DEGREE PROGRAMME IN CHEMISTRY
Academic year: 2020-21
Center: 1 - FACULTY OF SCIENCE AND CHEMICAL TECHNOLOGY
Group(s): 20 23
Year: 3
Duration: C2
Main language: Spanish
Second language: English
Use of additional languages:
English Friendly: Y
Web site:
Bilingual: N

Lecturer: **ELENA JIMENEZ MARTINEZ** - Group(s): **20 23**

Building/Office	Department	Phone number	Email	Office hours
EDIFICIO MARIE CURIE, 2ª PLANTA	QUÍMICA FÍSICA	926052129	elena.jimenez@uclm.es	Monday, Tuesday and Wednesday: 13:00-14.00 and 16:00-17:00

Lecturer: **FRANCISCO JAVIER POBLETE MARTIN** - Group(s): **20 23**

Building/Office	Department	Phone number	Email	Office hours
EDIFICIO MARIE CURIE 2ª PLANTA, DESPACHOS 2.03	QUÍMICA FÍSICA	926052177	fcojavier.poblete@uclm.es	Wednesday and Thursday: 9:00h-11:00h and 12:30h-13:30h

Lecturer: **MARIA SAGRARIO SALGADO MUÑOZ** - Group(s): **20 23**

Building/Office	Department	Phone number	Email	Office hours
EDIFICIO MARIE CURIE	QUÍMICA FÍSICA	3450	sagrario.salgado@uclm.es	Monday from 9:30 a.m. to 12:30 a.m. and from 4:00 p.m to 5:00 p.m. Tuesday from 9:30 to 11:30

2. Pre-Requisites

It is recommended to take this subject once the subjects of Physical Chemistry I and II of the second course have been passed. It is also important to have completed the subject of Physical Chemistry III, since the results of Statistical Thermodynamics will be used. Lil

3. Justification in the curriculum, relation to other subjects and to the profession

Physical Chemistry IV is part of the Physical Chemistry Matter and is dedicated to the study of Chemical Kinetics. Chemical Kinetics is a branch of Physical Chemistry that studies the rate and mechanisms of chemical reactions. The kinetic approach in the study of ch

The fundamentals of chemical kinetics studied in this subject will be applied to the study of Electrochemical Kinetics and Heterogeneous Catalysis in Physical Chemistry V. On the other hand, the concepts of Statistical Thermodynamics learnt in Physical Chemistry II

4. Degree competences achieved in this course

Course competences

Code	Description
CB01	Prove that they have acquired and understood knowledge in a subject area that derives from general secondary education and is appropriate to a level based on advanced course books, and includes updated and cutting-edge aspects of their field of knowledge.
CB02	Apply their knowledge to their job or vocation in a professional manner and show that they have the competences to construct and justify arguments and solve problems within their subject area.
E09	Know the kinetics of chemical change, including catalysis and reaction mechanisms
E14	Know and know how to apply the metrology of chemical processes, including quality management
E15	Know how to handle the standard chemical instrumentation and be able to elaborate and manage standardized procedures of work in the laboratory and chemical industry
E16	Plan, design and develop projects and experiments
E17	Develop the ability to relate to each other the different specialties of Chemistry, as well as this one with other disciplines (interdisciplinary character)
G01	Know the principles and theories of Chemistry, as well as the methodologies and applications characteristic of analytical chemistry, physical chemistry, inorganic chemistry and organic chemistry, understanding the physical and mathematical bases that require
G02	Be able to gather and interpret data, information and relevant results, obtain conclusions and issue reasoned reports on scientific, technological or other problems that require the use of chemical tools
G04	Know how to communicate, orally and in writing, the knowledge, procedures and results of chemistry, both specialized and non-specialized
T03	Proper oral and written communication
T07	Ability to work as a team and, where appropriate, exercise leadership functions, fostering the entrepreneurial character
T09	Motivation for quality, job security and awareness of environmental issues, with knowledge of internationally recognized systems for the correct management of these aspects
T11	Ability to obtain bibliographic information, including Internet resources

5. Objectives or Learning Outcomes

Course learning outcomes

Description
Ability to solve chemical problems applying the proper methodologies of physical chemistry
Dexterity in the handling of the main instrumental techniques used in physical chemistry and in the experimental determination of the structural, thermodynamic and kinetic properties of chemical systems

Additional outcomes

6. Units / Contents

Unit 1: KINETIC THEORY OF GASES. Molecular model of an ideal gas. Pressure of an ideal gas. Temperature. Maxwell speed distribution. Distribution of energies. Molecular collisions with a wall. Effusion speed. Intermolecular collisions. Mean free path.

Unit 2: TRANSPORT PHENOMENA. Transport properties of an ideal gas. Phenomenological equations for viscosity, diffusion and thermal conductivity. Transport coefficients according to the kinetic theory of gases. Transport in condensed phases in the absence of applied electric fields. Fick's laws for diffusion. Statistical vision of the diffusion.

Unit 3: INTRODUCTION TO FORMAL KINETICS. Elementary and complex reactions: Molecularity. Reaction rate. Rate equation. Empirical kinetic equations: order of reaction and rate constant. Obtaining kinetic data: Experimental methods in chemical kinetics. Kinetic data analysis: Differential method and integration method. Half-life period. Influence of temperature on the reaction rate.

Unit 4: KINETICS OF COMPLEX REACTIONS. Kinetic equations of complex reactions. Reversible, parallel and consecutive reactions. Approximate methods to solve the rate equation. Steady state approximation. Approximation of the rate limiting step. Influence of temperature on the rate of a complex reaction. Chain reactions. Polymerization reactions.

Unit 5: THEORIES OF REACTION RATES. Collision theory. Collision cross section and reaction cross section. Potential energy surfaces and reaction path. Molecular dynamics of the reaction. Transition state theory (TST). Trimolecular and unimolecular reactions.

Unit 6: KINETICS AND CATALYSIS IN LIQUID PHASE. Effect of the solvent. Collisions in liquid phase. Reactions controlled by diffusion. Application of TST to reactions in solution: Brønsted-Bjerrum equation. Primary salt effect. Influence of solvation. General mechanism of catalysis. Acid-base catalysis. Enzymatic catalysis. Autocatalysis and oscillating reactions.

Unit 7: PHOTOCHEMISTRY. Principles of photochemistry. Primary photophysical and photochemical processes. Diagrams of Jablonski. Secondary photochemical processes. Quantum yields. Kinetics of photophysical and photochemical processes. Quenching: Stern-Volmer equation. Intermolecular energy transfer processes.

Unit 8: EXPERIMENT 1. KINETICS OF THE REACTION OF HI WITH H2O2 IN ACID MEDIUM FOLLOWED BY VOLUMETRY. The partial order of reaction with respect to each reagent is determined. The time evolution of the reaction is followed by volumetry, assessing the iodine formed with sodium thiosulfate in the presence of starch. By varying the initial concentration of I-, the pseudo-first order rate constants are determine from the slope of the appropriate graphical representation. From them and knowing the concentration of I- the bimolecular rate constant is determined.

Unit 9: EXPERIMENT 2. DETERMINATION OF THE ORDER OF REACTION AND THE RATE CONSTANT OF THE REACTION OF S2O82- + 2 I- BY THE METHODS OF THE INITIAL RATES. The partial reaction orders and the rate constant of the reaction between persulfate ions and iodide ions in aqueous solution will be determined at room temperature by the method of initial rates. The formation of I2 in this reaction is followed in the presence of sodium thiosulfate. The partial reaction order with respect to persulfate is determined by keeping the iodide in excess and vice versa.

Unit 10: EXPERIMENT 3. KINETICS OF HYDROLYSIS OF TERT-BUTYL YODIDE BY CONDUCTIMETRY. Taking advantage that a significant variation of the conductivity of the solution occurs in the course of the reaction, the conductimetry is used to monitor the temporal evolution of the reaction. The reaction kinetics is performed at three temperatures, the Arrhenius parameters are then determined. The thermodynamic formulation of the TST is used to determine the activation enthalpy and entropy.

Unit 11: EXPERIMENT 4. ACID CATALYSIS: KINETICS OF THE REACTION OF MUTAROTATION OF ALPHA-D-GLUCOSE BY POLARIMETRY. The mutarotation reaction of alpha-D-glucose to produce beta-D-glucose can be followed by measuring the change in the rotation angle of the polarized light as it passes through the solution. Since alpha-D-glucose is dextrorotatory and beta-D-glucose is levorotatory, a decrease in the total rotation angle will be observed. This mutarotation reaction is catalyzed in acidic medium (HCl). Under pseudo-first order conditions and varying the catalyst concentration, the catalysis rate constant and the mutarotation rate constant can be determined from the proper graphical plot.

7. Activities, Units/Modules and Methodology

Training Activity	Methodology	Related Competences (only degrees before RD 822/2021)	ECTS	Hours	As	Com	Description
Class Attendance (theory) [ON-SITE]	Lectures	CB01 CB02 E09 G01	0.96	24	N	-	
Workshops or seminars [ON-SITE]	Problem solving and exercises	CB01 E17 G02 G04 T03 T11	0.48	12	Y	N	
Group tutoring sessions [ON-SITE]	Group tutoring sessions	E09 G01 G02 G04 T03	0.16	4	N	-	
Class Attendance (practical) [ON-SITE]	Practical or hands-on activities	CB01 CB02 E14 E15 E16 E17 G02 G04 T03 T07 T09 T11	0.64	16	Y	Y	
Practicum and practical activities report writing or preparation [OFF-SITE]	Self-study	G02 G04 T03 T11	0.48	12	Y	N	
Writing of reports or projects [OFF-SITE]	Self-study	E17 G02 G04 T03 T11	0.96	24	N	-	
Study and Exam Preparation [OFF-SITE]	Self-study	E09 E17 G01 T03	2.16	54	N	-	
Progress test [ON-SITE]	Assessment tests	E09 E17 G01 G04 T03	0.08	2	Y	N	
Progress test [ON-SITE]	Assessment tests	E09 E17 G01 G04 T03	0.08	2	Y	N	
		Total:	**6**	**150**			
		Total credits of in-class work: 2.4					**Total class time hours: 60**
		Total credits of out of class work: 3.6					**Total hours of out of class work: 90**

As: Assessable training activity
Com: Training activity of compulsory overcoming (It will be essential to overcome both continuous and non-continuous assessment).

8. Evaluation criteria and Grading System

Evaluation System	Continuous assessment	Non-continuous evaluation*	Description
Assessment of problem solving and/or case studies	20.00%	0.00%	The student will solve in a seminar class (1/2 hour) an exercise proposed by the lecturer. Throughout the semester, the two proposed exercises will be similar o equal to those solved in the class.
Laboratory sessions	20.00%	20.00%	Attendance to all lab sessions is mandatory. The work in the laboratory and the corresponding report presented will be evaluated. To pass the matter it will be mandatory to have performed the experimental work in the laboratory. In the ordinary examination some questions related to the experimental work will be asked (10% value).
Progress Tests	30.00%	0.00%	First partial exam corresponding to topics 1 to 4.
Progress Tests	30.00%	0.00%	Second partial exam corresponding to topics 5 to 7.
Final test	0.00%	80.00%	Final test
Total:	**100.00%**	**100.00%**	

According to art. 4 of the UCLM Student Evaluation Regulations, it must be provided to students who cannot regularly attend face-to-face training activities the passing of the subject, having the right (art. 12.2) to be globally graded, in 2 annual calls per subject , an ordinary and an extraordinary one (evaluating 100% of the competences).

Evaluation criteria for the final exam:

Continuous assessment:

CONTINUOUS EVALUATION SYSTEM
To pass the matter, it is mandatory to:
1) Perform and pass the laboratory work.
2) Obtain an average minimum grade of 5 over 10 with a minimum of 4 in the progress tests and questions about the lab practical work.

In the case of not passing the subject, students have the possibility to recover any of the progress tests not passed in the ordinary call, maintaining the previous evaluation criteria.

In addition, a series of optional tests will be proposed in Microsoft Forms applications. The results of the active participation in these optional teaching activities can raise the final grade, once the subject is passed, up to 0.5 points.

NON-CONTINUING EVALUATION SYSTEM
For students who do not follow the continuous evaluation, the evaluation criteria are 20% Lab practicals cases + 80% Exam.

Non-continuous evaluation:

Evaluation criteria not defined

Specifications for the resit/retake exam:

Students will answer to some theoretical-practical questions corresponding to the whole program of the subject, which will represent 80% of their grade. The remaining 20% will correspond to the evaluation of the experimental work. If passed, the student will keep the grade obtained in the ordinary call for the lab work. In the case of not having passed the lab activities, the student must repeat the written test.

Specifications for the second resit / retake exam:

Students will do an exam with some theoretical-practical questions corresponding to the whole program of the subject (theory+seminars+lab).

9. Assignments, course calendar and important dates

Not related to the syllabus/contents

Hours **hours**

Unit 1 (de 11): KINETIC THEORY OF GASES. Molecular model of an ideal gas. Pressure of an ideal gas. Temperature. Maxwell speed distribution. Distribution of energies. Molecular collisions with a wall. Effusion speed. Intermolecular collisions. Mean free path.

Activities	Hours
Class Attendance (theory) [PRESENCIAL][Lectures]	3
Workshops or seminars [PRESENCIAL][Problem solving and exercises]	1.5
Group tutoring sessions [PRESENCIAL][Group tutoring sessions]	.5
Writing of reports or projects [AUTÓNOMA][Self-study]	3
Study and Exam Preparation [AUTÓNOMA][Self-study]	6.5
Progress test [PRESENCIAL][Assessment tests]	.5
Progress test [PRESENCIAL][Assessment tests]	.5

Unit 2 (de 11): TRANSPORT PHENOMENA. Transport properties of an ideal gas. Phenomenological equations for viscosity, diffusion and thermal conductivity. Transport coefficients according to the kinetic theory of gases. Transport in condensed phases in the absence of applied electric fields. Fick's laws for diffusion. Statistical vision of the diffusion.

Activities	Hours
Class Attendance (theory) [PRESENCIAL][Lectures]	3
Workshops or seminars [PRESENCIAL][Problem solving and exercises]	1.5
Group tutoring sessions [PRESENCIAL][Group tutoring sessions]	.5
Writing of reports or projects [AUTÓNOMA][Self-study]	3
Study and Exam Preparation [AUTÓNOMA][Self-study]	6.5
Progress test [PRESENCIAL][Assessment tests]	.5
Progress test [PRESENCIAL][Assessment tests]	.5

Unit 3 (de 11): INTRODUCTION TO FORMAL KINETICS. Elementary and complex reactions: Molecularity. Reaction rate. Rate equation. Empirical kinetic equations: order of reaction and rate constant. Obtaining kinetic data: Experimental methods in chemical kinetics. Kinetic data analysis: Differential method and integration method. Half-life period. Influence of temperature on the reaction rate.

Activities	Hours
Class Attendance (theory) [PRESENCIAL][Lectures]	3
Workshops or seminars [PRESENCIAL][Problem solving and exercises]	1.5
Group tutoring sessions [PRESENCIAL][Group tutoring sessions]	.5
Writing of reports or projects [AUTÓNOMA][Self-study]	3
Study and Exam Preparation [AUTÓNOMA][Self-study]	6.5
Progress test [PRESENCIAL][Assessment tests]	.5
Progress test [PRESENCIAL][Assessment tests]	.5

Unit 4 (de 11): KINETICS OF COMPLEX REACTIONS. Kinetic equations of complex reactions. Reversible, parallel and consecutive reactions. Approximate methods to solve the rate equation. Steady state approximation. Approximation of the rate limiting step. Influence of temperature on the rate of a complex reaction. Chain reactions. Polymerization reactions.

Activities	Hours
Class Attendance (theory) [PRESENCIAL][Lectures]	4
Workshops or seminars [PRESENCIAL][Problem solving and exercises]	1.5
Group tutoring sessions [PRESENCIAL][Group tutoring sessions]	.5
Writing of reports or projects [AUTÓNOMA][Self-study]	3
Study and Exam Preparation [AUTÓNOMA][Self-study]	9
Progress test [PRESENCIAL][Assessment tests]	.5
Progress test [PRESENCIAL][Assessment tests]	.5

Unit 5 (de 11): THEORIES OF REACTION RATES. Collision theory. Collision cross section and reaction cross section. Potential energy surfaces and reaction path. Molecular dynamics of the reaction. Transition state theory (TST). Trimolecular and unimolecular reactions.

Activities	Hours
Class Attendance (theory) [PRESENCIAL][Lectures]	4
Workshops or seminars [PRESENCIAL][Problem solving and exercises]	2.25
Group tutoring sessions [PRESENCIAL][Group tutoring sessions]	.75
Writing of reports or projects [AUTÓNOMA][Self-study]	4.5
Study and Exam Preparation [AUTÓNOMA][Self-study]	9

Unit 6 (de 11): KINETICS AND CATALYSIS IN LIQUID PHASE. Effect of the solvent. Collisions in liquid phase. Reactions controlled by diffusion. Application of TST to reactions in solution: Brønsted-Bjerrum equation. Primary salt effect. Influence of solvation. General mechanism of catalysis. Acid-base catalysis. Enzymatic catalysis. Autocatalysis and oscillating reactions.

Activities	Hours
Class Attendance (theory) [PRESENCIAL][Lectures]	4
Workshops or seminars [PRESENCIAL][Problem solving and exercises]	2.25
Group tutoring sessions [PRESENCIAL][Group tutoring sessions]	.75
Writing of reports or projects [AUTÓNOMA][Self-study]	4.5
Study and Exam Preparation [AUTÓNOMA][Self-study]	8

Unit 7 (de 11): PHOTOCHEMISTRY. Principles of photochemistry. Primary photophysical and photochemical processes. Diagrams of Jablonski. Secondary photochemical processes. Quantum yields. Kinetics of photophysical and photochemical processes. Quenching: Stern-Volmer equation. Intermolecular energy transfer processes.

Activities	Hours
Class Attendance (theory) [PRESENCIAL][Lectures]	3
Workshops or seminars [PRESENCIAL][Problem solving and exercises]	1.5
Group tutoring sessions [PRESENCIAL][Group tutoring sessions]	.5
Writing of reports or projects [AUTÓNOMA][Self-study]	3
Study and Exam Preparation [AUTÓNOMA][Self-study]	6.5

Unit 8 (de 11): EXPERIMENT 1. KINETICS OF THE REACTION OF HI WITH H2O2 IN ACID MEDIUM FOLLOWED BY VOLUMETRY. The partial order of reaction with respect to each reagent is determined. The time evolution of the reaction is followed by volumetry, assessing the iodine formed with sodium thiosulfate in the presence of starch. By varying the initial concentration of I-, the pseudo-first order rate constants are determine from the slope of the appropriate graphical representation. From them and knowing the concentration of I- the bimolecular rate constant is determined.

Activities	Hours
Class Attendance (practical) [PRESENCIAL][Practical or hands-on activities]	4
Practicum and practical activities report writing or preparation [AUTÓNOMA][Self-study]	3
Study and Exam Preparation [AUTÓNOMA][Self-study]	.5

Unit 9 (de 11): EXPERIMENT 2. DETERMINATION OF THE ORDER OF REACTION AND THE RATE CONSTANT OF THE REACTION OF S2O82- + 2 I- BY THE METHODS OF THE INITIAL RATES. The partial reaction orders and the rate constant of the reaction between persulfate ions and iodide ions in aqueous solution will be determined at room temperature by the method of initial rates. The formation of I2 in this reaction is followed in the presence of sodium thiosulfate. The partial reaction order with respect to persulfate is determined by keeping the iodide in excess and vice versa.

Activities	Hours

Class Attendance (practical) [PRESENCIAL][Practical or hands-on activities]	4
Practicum and practical activities report writing or preparation [AUTÓNOMA][Self-study]	3
Study and Exam Preparation [AUTÓNOMA][Self-study]	.5

Unit 10 (de 11): EXPERIMENT 3. KINETICS OF HYDROLYSIS OF TERT-BUTYL YODIDE BY CONDUCTIMETRY. Taking advantage that a significant variation of the conductivity of the solution occurs in the course of the reaction, the conductimetry is used to monitor the temporal evolution of the reaction. The reaction kinetics is performed at three temperatures, the Arrhenius parameters are then determined. The thermodynamic formulation of the TST is used to determine the activation enthalpy and entropy.

Activities	**Hours**
Class Attendance (practical) [PRESENCIAL][Practical or hands-on activities]	4
Practicum and practical activities report writing or preparation [AUTÓNOMA][Self-study]	3
Study and Exam Preparation [AUTÓNOMA][Self-study]	.5

Unit 11 (de 11): EXPERIMENT 4. ACID CATALYSIS: KINETICS OF THE REACTION OF MUTAROTATION OF ALPHA-D-GLUCOSE BY POLARIMETRY. The mutarotation reaction of alpha-D-glucose to produce beta-D-glucose can be followed by measuring the change in the rotation angle of the polarized light as it passes through the solution. Since alpha-D-glucose is dextrorotatory and beta-D-glucose is levorotatory, a decrease in the total rotation angle will be observed. This mutarotation reaction is catalyzed in acidic medium (HCl). Under pseudo-first order conditions and varying the catalyst concentration, the catalysis rate constant and the mutarotation rate constant can be determined from the proper graphical plot.

Activities	**Hours**
Class Attendance (practical) [PRESENCIAL][Practical or hands-on activities]	4
Practicum and practical activities report writing or preparation [AUTÓNOMA][Self-study]	3
Study and Exam Preparation [AUTÓNOMA][Self-study]	.5

Global activity

Activities	**hours**
Class Attendance (theory) [PRESENCIAL][Lectures]	24
Workshops or seminars [PRESENCIAL][Problem solving and exercises]	12
Group tutoring sessions [PRESENCIAL][Group tutoring sessions]	4
Class Attendance (practical) [PRESENCIAL][Practical or hands-on activities]	16
Practicum and practical activities report writing or preparation [AUTÓNOMA][Self-study]	12
Writing of reports or projects [AUTÓNOMA][Self-study]	24
Study and Exam Preparation [AUTÓNOMA][Self-study]	54
Progress test [PRESENCIAL][Assessment tests]	2
Progress test [PRESENCIAL][Assessment tests]	2
Total horas:	150

10. Bibliography and Sources

Author(s)	Title/Link	Publishing house	Citv	ISBN	Year	Description
Bertrán, J., Núñez, J.	QUÍMICA FÍSICA	Ariel Ciencia			2002	
González Ureña, A.	CINÉTICA QUÍMICA	Síntesis			2001	
Jiménez, E.	Apuntes proporcionados por el Profesor				2012	
Levine, I. N.	FISICOQUÍMICA	McGraw-Hill			2014	6ª Ed.
Logan, S. R.	FUNDAMENTOS DE CINÉTICA QUÍMICA	Addison Wesley			2000	
Robert G. Mortimer	PHYSICAL CHEMISTRY	Academic Press		978-0-12-370617-1	2008	
SILBEY, R. J. and ALBERTY, R. A.,	Physical Chemistry	Wiley, New York,		0471658979	2004	4ª Ed
Atkins, P.W.	FISICOQUÍMICA.	Addison-Wesley			2006	8ª Ed. Español