

UNIVERSIDAD DE CASTILLA - LA MANCHA **GUÍA DOCENTE**

Course: PHYSICAL-CHEMISTRY IV: KINETICS IN CHEMISTRY Type: CORE COURSE

Degree: 409 - CHEMISTRY

Center: 1 - FACULTY OF SCIENCE AND CHEMICAL TECHNOLOGY

Year: 3 Main language: Spanisl

Use of additional languages:

ECTS credits: 6 demic year: 2023-24 Group(s): 20 23 Duration: C2 language: English English Friendly: Y

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|---|-----------------------|--------------|-------|---------------------------|---|--|--|--|--|--|
| Lecturer: MARÍA ANTIÑOLO NAVAS - Group(s): 20 23 | | | | | | | | | | |
| Building/Office | | Phone number | Email | il | Office hours | | | | | |
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| Lecturer: ELENA JIMENEZ MARTINEZ - Group(s): 20 23 | | | | | | | | | | |
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| Lecturer: FRANCISCO JAVIER POBLETE MARTIN - Group(s): 20 23 | | | | | | | | | | |
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| EDIFICIO MARIE CURIE 2ª PLANTA, DESPACHO | S 2.03 QUÍMICA FÍSICA | 926052177 | | fcojavier.poblete@uclm.es | | Wendesday-Thursday: 9.00-10.00h and 11.00-13.00 h. Monday: 17:00-18:00 h | | | | |
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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. Lii

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 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 CB01 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 Know the kinetics of chemical change, including catalysis and reaction mechanisms E09 F14 Know and know how to apply the metrology of chemical processes, including quality management 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) 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 G01 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 Know how to apply the theoretical-practical knowledge acquired in the different professional contexts of Chemistry G03 G04 Know how to communicate, orally and in writing, the knowledge, procedures and results of chemistry, both specialized and non-specialized T07 Ability to work as a team and, where appropriate, exercise leadership functions, fostering the entrepreneurial character TOS Motivation for quality, job security and awareness of environmental issues, with knowledge of internationally recognized systems for the correct management of these aspects Ability to obtain bibliographic information, including Internet resources T11

Course learning outcomes

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

Ability to solve chemical problems applying the proper methodologies of physical chemistry

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

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 et solvation. General mechanism of catalysis. Acid-base catalysis. Enzymatic catalysis 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

Unit 8: EXPERIMENT 1. KINETICS OF THE REACTION OF HI WITH H202 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 \$2082 + 2 I- BY THE METHODS OF THE INITIAL RATES. The partial reaction orders and the rate constant of the reaction

rature by the method of initial rates. The formation of I2 in this reaction is follow ed in the presence of sodium thiosulfate. The partial reaction orde 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 to mperatures, the Arrhenius parameters are then determined. The thermody namic formulation of the TST is used to determine the activation enthalpy and

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 measurin 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 (HCI). 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 | 0.88 | 2 | 2 1 | ١ . | Theory classes dedicated to explaining the contents of the syllabus. The Powerpoint presentations used will be available in Campus Virtual. |
| Workshops or seminars [ON-SITE] | Problem solving and exercises | CB01 E17 G02 G04 T03 T11 | 0.48 | 1 | 2 | r N | Doubts from seminars previously raised and worked on autonomously by the students will be resolved and clarified. This activity is not evaluable in the non-continuous mode. |
| Problem solving and/or case studies [ON-SITE] | Problem solving and exercises | E09 G01 G02 G04 T03 | 0.24 | | 1 0 | ١ . | Discussion of concepts and resolution of doubts while solving the exercises and problems of the seminar classes |
| Class Attendance (practical) [ON-SITE] | Practical or hands-on activities | CB01 CB02 E14 E15 E16 E17 G02 G04 T03 T07 T09 T11 | 0.64 | 1 | 6 | | The student learn in the laboratory the concepts of the syllabus and the work methodology of Physical Chemistry. They will learn to handle basic chemical instrumentation necessary to carry out the experiments. The understanding of the practice will be evaluated daily by means of a FORMS questionnaire as a PRE-LABORATORY. |
| Practicum and practical activities report writing or preparation [OFF-SITE] | Self-study | G02 G04 T03 T11 | 0.48 | 1 | 2 , | | A conventional memory of the laboratory practices will not be elaborated by the student, instead practical skills and abilities in the laboratory will be evaluated. Students must upload the data files obtained and their treatment to Campus Virtual. |

| Assessment tests | 50 | | Inis test is the sum of the two mid-terms exams. Total class time hours: 60 |
|---|------|-----|--|
| | 50 | | Inis test is the sum of the two mio-terms exams. |
| Final test [ON-SITE] Assessment tests E09 E17 G01 G04 T03 0 | | | this test is the sum of the two mid-terms exams. |
| | 0 Y | r Y | The final test will be carried out only for Non-Continuous Assessment students. Therefore, the hours corresponding to this test is the sum of the two mid-terms exams. |
| Mid-term test [ON-SITE] Assessment tests E09 E17 G01 G04 T03 0.08 | 2 Y | | Second mid-term exam corresponding to topics 5, 6 and 7. This activity is not evaluable in non-continuous mode. |
| Mid-term test [ON-SITE] Assessment tests E09 E17 G01 G04 T03 0.08 | 2 Y | | First mid-term exam corresponding to the first 4 topics. This activity is not evaluable in non-continuous mode. |
| Striking and reports proprojects (REF-STFE) Self-study E63 E97 587 Tib 2.18 | 34 N | 1 - | Study of the laboratoy manual. Autonomous study of the theoretical contents of the program. |

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 | | | |
| Mid-term tests | 30.00% | 0.00% | First mid-term exam corresponding to topics 1 to 4. | | | |
| Mid-term tests | 40.00% | | Second mid-term exam corresponding to topics 5, 6 and 7 (30%). There will also be some questions related to the laboratory sessions (10%). | | | |
| Assessment of problem solving and/or case studies | 20.00% | | 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 | 10.00% | 10.00% | Attendance to all practical laboratory sessions is mandatory. The work prior to the laboratory (pre- laboratory) will be assessed through a FORMS questionnaire (5%). Capabilities, skills and practical abilities will be assessed through rubrics and the data collected and processed (5%) will be uploaded to Campus Virtual. | | | |
| Final test | 0.00% | | This final test consists of a theoretical part + problem solving (80%) and some questions about the laboratory practices (10%). | | | |
| 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

- CONTINUOUS EVALUATION 575 LEM
 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 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.

In the case of not passing the first mid-term exam, students have the possibility of retaking itm in the ordinary call, together with the second mid-term exam, maintaining the previous evaluation criteria.

It is recalled that, according to the UCLM Student Evaluation Regulations, if the student does less than 60% of the face-to-face training activities, they will be marked NOT PRESENTED.

Non-continuous evaluation:

For students who do not follow the continuous evaluation, the evaluation criteria are 20% Lab practical cases + 80% Final test.

Specifications for the resit/retake exam:

There will be a test with theoretical and practical questions corresponding to the entire syllabus of the subject, which will account for 80% of the grade. The remaining 20% ¿¿will correspond to the evaluation of laboratory practices.

- 1) If the student has passed this part of the subject in the ordinary call, the grade will be kept.
 2) If in the ordinary call you have obtained LESS THAN 4.0 in the written test on laboratory questions, you must repeat this test, but you will keep the qualification of the pre-lab questionnaire and of the skills in the laboratory obtained in the call ordinary.

 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 ene | rgies. Molecular collisions with a wall. Effusion speed. Intermolecular collisions. |
| Mean free path. | |
| Activities | Hours |
| Class Attendance (theory) [PRESENCIAL][Lectures] | 3.1 |
| Workshops or seminars [PRESENCIAL][Problem solving and exercises] | 1.7 |
| Problem solving and/or case studies [PRESENCIAL][Problem solving and exercises] | .8 3 |
| Writing of reports or projects [AUTONOMA][Self-study] | |
| Study and Exam Preparation [AUTONOMA][Self-study] Mid-term test [PRESENCIAL][Assessment tests] | 7.5 .5 |
| wid-tern lest [PRESENCIA_[IAssessment tests] Wid-tern lest [PRESENCIA_[IAssessment tests] | .5 .5 |
| Juit 2 (de 11): TRANSPORT PHENOMENA. Transport properties of an ideal gas. Phenomenological equations for viscosity, diffusion and thermal conductivity. Tran | |
| unit 2 (de 11): INANSPORT FEROMENA. Hansport properties of an integrass. Professional equations for viscosity, diffusion and thermal conductivity. Han phases in the absence of applied electric fields. Fick's laws for diffusion. Statistical vision of the diffusion. | sport coefficients according to the kinetic theory of gases. Transport in condens |
| Activities | Hours |
| Class Attendance (theory) [PRESENCIAL [Lectures] | 3.1 |
| Workshops or seminars [PRESENCIAL][Problem solving and exercises] | 1.5 |
| Problem solving and/or case studies [PRESENCIAL][Problem solving and exercises] | .8 |
| Writing of reports or projects [AUTÓNOMA][Self-study] | 3 |
| Study and Exam Preparation [AUTÓNOMA][Self-study] | 7.5 |
| Mid-term test [PRESENCIAL][Assessment tests] | .5 |
| Mid-term 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 method |
| chemical kinetics. Kinetic data analysis: Differential method and integration method. Half-life period. Influence of temperature on the reaction rate. Activities | Hours |
| Activities Class Attendance (theory) [PRESENCIAL][Lectures] | 3 |
| orass Attendance (intensy) in resource_irectures; Workshops or seminars [PRESENCIAL]Problem solving and exercises] | 1.5 |
| Problem solving and/or case studies [PRESENCIAL][Problem solving and exercises] | .9 |
| Writing of reports or projects [AUTÓNOMA][Self-study] | 4 |
| Study and Exam Preparation [AUTÓNOMA][Self-study] | 7.7 |
| Mid-term test [PRESENCIAL []Assessment tests] | .5 |
| Mid-term 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 rat |
| limiting step. Influence of temperature on the rate of a complex reaction. Chain reactions. Polymerization reactions. | , |
| Activities | Hours |
| Class Attendance (theory) [PRESENCIAL][Lectures] | 3.1 |
| Workshops or seminars [PRESENCIAL][Problem solving and exercises] | 1.7 |
| Problem solving and/or case studies [PRESENCIAL][Problem solving and exercises] | .9 |
| Writing of reports or projects [AUTÓNOMA][Self-study] | 4 |
| Study and Exam Preparation [AUTÓNOMA][Self-study] | 7.6 |
| Mid-term test [PRESENCIAL][Assessment tests] | .5 |
| Mid-term 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. I unimolecular reactions. | Molecular dynamics of the reaction. Transition state theory (TST). Trimolecular at |
| Activities | Hours |
| Class Attendance (theory) [PRESENCIAL][Lectures] | 3.1 |
| Workshops or seminars [PRESENCIAL][Problem solving and exercises] | 2 |
| Problem solving and/or case studies [PRESENCIAL][Problem solving and exercises] | .9 |
| Writing of reports or projects [AUTÓNOMA][Self-study] | 3 |
| Study and Exam Preparation [AUTÓNOMA][Self-study] | 7.7 |
| 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 |
| solvation. General mechanism of catalysis. Acid-base catalysis. Enzymatic catalysis. Autocatalysis and oscillating reactions. Activities | Hours |
| Activities Class Attendance (theory) [PRESENCIAL][Lectures] | 3.5 |
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| workships or seminats [FRESENCHE_[Froblem solving and exercises] Problem solving and/or case studies [PRESENCHE_[Froblem solving and exercises] | 9 |
| Writing of reports or projects [AUTONOMA][Self-study] | 4 |
| witing of reports projects for Oncompligational by Study and Exam Preparation (AUTÓNOMISelf-study) | 7 |
| Unit 7 (de 11): PHOTOCHEMISTRY. Principles of photochemistry. Primary photophysical and photochemical processes. Diagrams of Jablonski. Secondary photoch | • |
| processes. Quenching: Stern-Volmer equation. Intermolecular energy transfer processes. | |
| Activities | Hours |

| Class Attendance (theory) [PRESENCIAL][Lectures] | 3.1 |
|---|---|
| Workshops or seminars [PRESENCIAL][Problem solving and exercises] | 1.6 |
| Problem solving and/or case studies [PRESENCIAL][Problem solving and exercises] | .8 |
| Writing of reports or projects [AUTÓNOMA][Self-study] | 3 |
| Study and Exam Preparation [AUTÓNOMA][Self-study] | 7 |
| Unit 8 (de 11): EXPERIMENT 1. KINETICS OF THE REACTION OF HI WITH H202 IN ACID MEDIUM FOLLOWED BY VOLUMETRY. The partial ord | der of reaction with respect to each reagent is determined. The time evolution of the reaction is followed |
| volumetry, assessing the iodine formed with sodium thiosulfate in the presence of starch. By varying the initial concentration of I-, the pseudo | |
| 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 \$2082 reaction between persulfate ions and iodide ions in aqueous solution will be determined at room temperature by the method of initial rates. Th 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 |
| used to monitor the temporal evolution of the reaction. The reaction kinetics is performed at three temperatures, the Arrhenius parameters a and entropy. Activities | Hours |
| Class Attendance (practical) [PRESENCIAL][Practical or hands-on activities] | 10013 |
| | |
| | 3 |
| Practicum and practical activities report writing or preparation [AUTÓNOMA][Self-study] | 3 5 |
| Practicum and practical activities report writing or preparation [AUTÓNOMA][Self-study] Study and Exam Preparation [AUTÓNOMA][Self-study] | .5 |
| Practicum and practical activities report writing or preparation [AUTÓNOMA][Self-study] Study and Exam Preparation [AUTÓNOMA][Self-study] Unit 11 (de 11): EXPERIMENT 4. ACID CATALYSIS: KINETICS OF THE REACTION OF MUTAROTATION OF ALPHA-D-GLUCOSE BY POLARIMI | .5 ETRY. The mutarotation reaction of alpha-D-glucose to produce beta-D-glucose can be followed by |
| Practicum and practical activities report writing or preparation [AUTÓNOMA][Self-study] | .5 ETRY. The mutarotation reaction of alpha-D-glucose to produce beta-D-glucose can be followed by d beta-D-glucose is levorotatory, a decrease in the total rotation angle will be observed. This mutarotatic |
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