Subject Guide

1. Information about the subject

SUBJECT	Physical Chemistry III		**CODE**	GQUIMI01-3-003
EDUCATIONAL OFFER	Bachelor´s Degree in Chemistry	**CENTER**	Facultad de Química	
TYPE	Compulsory	**N° TOTAL CREDITS**	6.0	
PERIOD	Second Semester	**LANGUAGE**	Spanish	
COORDINATORS/ES		**EMAIL**		
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LECTURERS		**EMAIL**		
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2. Context

The current course belongs to the so-called "Fundamental" module and to the "Physical Chemistry" discipline in the ‘BSc in Chemistry’ plan of the University of Oviedo (BOE: July 15th, 2010, pp. 62634-62638), and it is a required (compulsory) subject which is located in the second term of the third year in the mentioned degree.

This subject is closely related to the other theoretical courses of the “Fundamental” module in this degree, particularly to those belonging to the same "Physical Chemistry" discipline, but also to those of "Analytical Chemistry", "Organic Chemistry", "Inorganic Chemistry", "Materials Science", and "Biochemistry" disciplines. Nevertheless, the two courses which have the closest relation with the current subject are “*Physical Chemistry I*”, in the second year of the degree, and “*Physical Chemistry II*”, in the first term of the third year. The non-equilibrium phenomena studied in the current course, from both a macroscopic and a microscopic point of view, have a clear precedent in the equilibrium phenomena studied in the two mentioned courses, from a macroscopic point of view in the second year and from a microscopic point of view in the first term of the third year.

Additionally, this subject develops the essential theoretical formalism needed for the proper gain of other courses’ contents, particularly those included in “*Physical Chemistry Lab II*”, a course in the fourth year of the degree, where several experiments on ‘Chemical Kinetics’ and ‘Surface and Transport Phenomena’ are carried out, not to mention that it is precisely in the current course where bridges between macroscopic and microscopic views of the states of matter are built through the study of ‘Statistical Thermodynamics’ and ‘Physical Kinetics’, among other topics treated along the course.

3. Requirements

In order to enrol in this course, students must have passed the examinations of the following subjects from the first year of the degree: *“Basic Laboratory Operations and Information Technology Tools”*, *“General Chemistry”*, *“General Physics I”*, *“General Physics II”*, and *“Mathematics”*, as well as the subject *“Physical Chemistry I”*, from the second year of the degree.

On the other hand, although it is not compulsory, it is highly advisable that students have also passed the examinations of *“Physical Chemistry II” (PCII)*, a subject located in the first term of the same third year of the degree as the current course, since theoretical models and theories for the microscopic behaviour of matter in equilibrium studied in that subject are profusely used in the current course. For instance, the theoretical description of rotational, vibrational, and electronic molecular energy levels using quantum mechanical tools, which is made in *PCII*, is a critical factor to a proper understanding of the partition function concept, which is at the core of ‘Statistical Thermodynamics’ and ‘Molecular Dynamics’ theoretical models.

4. Competencies and learning results

a) General objectives (Competences).

CG-1: To develop the ability for analysis and synthesis of scientific knowledge.

CG-2: To solve scientific problems efficiently.

CG-3: To obtain knowledge in Informatics applied to Chemistry.

CG-4: To show competency in time organization and planning.

CG-5: To develop the ability of taking complex decisions.

CG-6: Proper managing of scientific information.

CG-8: To correctly communicate scientific information, both orally and in writing.

CG-9: Self-learning.

CG-12: To gain awareness about environmental issues.

CG-17: To develop a critical awareness.

CG-18: Working in a team.

CG-20: To gain basic competency in the use of ICTs.

b) Specific objectives (Skills).

CE-2: To correlate macroscopic properties of matter with its microscopic composition (atoms, ions, and molecules).

CE-8: To understand the kinetics of a chemical transformation, including catalysis phenomena and reaction mechanisms.

CE-20: To solve quantitative and qualitative scientific problems according to previously developed models and theories.

CE-22: To acquire skills in order to correctly evaluate, interpret, and summarize chemical information.

CE-24: To process and compute data related to chemical information and knowledge.

CE-30: To correctly interpret experimental data on theoretical grounds.

CE-32: To properly use inductive and deductive methods in the field of chemistry.

CE-35: To perform calculations with the right magnitudes and units.

c) Learning outcomes (Qualifications).

- To gain knowledge and understanding of concepts, empirical laws, experimental facts, theoretical models, and physical theories related to ‘Physical Kinetics’, ‘Statistical Thermodynamics’, ‘Chemical Kinetics’, and ‘Surface and Transport Phenomena’ from the point of view of the ‘Chemical Physics’ discipline.

- To be able to solve both algebraic and numerical problems and exercises of ‘Physical Kinetics’, ‘Statistical Thermodynamics’, ‘Chemical Kinetics’, and ‘Surface and Transport Phenomena’, as well as to correctly interpret the obtained results.

- To use and understand relevant bibliographic sources.

- To correctly communicate scientific information, both orally and in writing.

5. Contents

Chapter 1: *Kinetic Theory and Statistical Thermodynamics*.

Probability theory and probability distributions. Speed distributions. Basic kinetic theory of transport phenomena. Distributions in the phase space. Basic concepts in Statistical Mechanics. The microcanonical ensemble. The canonical ensemble. Statistical Thermodynamics of a gas.

(22 in-classroom hours = 19 CEX + 3 PA)

Chapter 2: *Chemical Kinetics*.

Basic concepts: reaction rate, rate constant, and kinetic equation. Partial order and overall order of reaction. Integration of kinetic equations. Reaction mechanisms. Temperature variation of reaction rates. Chemical reactions in solution. Theoretical models in Chemical Kinetics.

(11 in-classroom hours = 9 CEX + 2 PA)

Chapter 3: *Surface phenomena*.

Surface phenomena with uncharged interphase. Thermodynamic study of the uncharged interphase. Adsorption isotherms. Heterogeneous catalysis. Surface phenomena with charged interphase. Theoretical models of the electrical double layer.

(8 in-classroom hours = 7 CEX + 1 PA)

Chapter 4: ***Transport phenomena*****.**

Transport phenomena in non-electrolytic solutions. Energy transport in liquids and liquid solutions: Fourier's law and non-linear phenomena. Linear-momentum transport in liquids and liquid solutions: Newton's law. Matter transport in liquids and liquid solutions: Fick's laws. Transport phenomena in electrolytic solutions.

(8 in-classroom hours = 7 CEX + 1 PA)

6. Methodology and working plan

Expositive Lectures (*CEX, 42 in-classroom hours*): In these lectures the professor will present and discuss the subject matter of study, with special emphasis in the most innovative aspects and those of special complexity, integrating both theoretical aspects and examples that facilitate reasoning and analysis of the matter under discussion. For this reason, regular attendance of students at such lectures is highly recommended. It is also necessary for the student to complete the study of the matter with the reading of the recommended bibliography, in order to compare and expand the knowledge transmitted in the classroom.

Seminars (*PA, 7 in-classroom hours*): The specific application of the knowledge that students have acquired in the expositive lectures will take place in these sessions. Students will be provided in advance with the theoretical questions and numerical problems to be solved, and must have worked on them previously to proceed during the sessions to their analysis and discussion, individually and collectively. Students will have an active role in these seminars by explaining the solutions they have found for the proposed exercises.

Group mentoring (*TG*, 4 in-classroom hours): These sessions will be held in small groups of students. Each group will be assigned a task at the start of the course to be worked by them along the course. Each student team will explain orally their results on their own task in the last TG session, with foregoing discussion with the professor and the rest of the class. Wide and deep use of the bibliography is a must for the students to gain proper benefit of these sessions.

TEACHING TYPE		**Hours**	**%**	**Totals**
Contact learning (in-classroom teaching)	Expositive Lectures (*CEX*)	42	70,00	60
	Seminars (*PA*)	7	11,66	
	Group Mentoring (*TG*)	4	6,67	
	Other Activities	4	6,67	
	Exams	3	5,00	
Self-learning (out-of-classroom learning)	Group work	10	11,11	90
	Personal work	80	88,89	
	Total	150		

7. Evaluation of the student's learning results

Aspect	Criteria	Instrument	Grade weight
Subject contents (Chapters 1-4)	Solving numerical and algebraic exercises, as well as answering theoretical questions, related to the subject.	Written exam	80%
Daily work	- Active engagement in PA sessions. - Active engagement in TG sessions. - Oral and written expression.	Seminars and Group mentoring	20%

First call (regular call):

To pass the subject in the regular call (first call) it is imperative to obtain at least a minimum score of 4.5 points out of 10 (4.5/10) in each aspect of the evaluation shown in the previous table, as well as a minimum of 5 points out of 10 (5/10) in the global grade.

Second call (extraordinary call):

In the second call the student has to pass a written exam, with a weight of 100% in the grade.

8. Resources, bibliography and complementary documentation

a) Basic bibliography.

1) P. W. Atkins and J. de Paula, *Physical Chemistry*, (2 vols.), Freeman, 2014.

2) I. N. Levine, *Physical Chemistry*, McGraw-Hill, 2008.

b) Additional bibliography.

1) D. A. McQuarrie, *Statistical Mechanics*, University Science Books, 2000.

2) B. Widom, *Statistical Mechanics: A concise introduction for chemists*, Cambridge University Press, 2002.

3) J. I. Steinfeld, J. S. Francisco, and W. L. Hase, *Chemical Kinetics and Dynamics*, Prentice Hall, 1999.

4) G. A. Somorjai and Y. Li, *Introduction to Surface Chemistry and Catalysis*, John Wiley & Sons, 2010.

5) C. H. Hamann, A. Hamnett, and W. Vielstich, *Electrochemistry*, Wiley-VCH, 2007.

Complementary documentation will be available on-line through the Virtual Campus platform at:

www.uniovi.es/recursos/campusvirtual.