Bachelor´s Degree in Chemistry

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	**Nº TOTAL CREDITS**	6.0	
PERIOD	Second Semester	**LANGUAGE**	Spanish English	
COORDINATORS/ES		**EMAIL**		
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LECTURERS		**EMAIL**		
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2. Context

Let me introduce the notation (I, II, III, IV / a, b) to refer to I (first course of this Degree), II (second) and so one, and a (first semester), b (second semester). Therefore, the present course corresponds to III/b and the relationships with other chemistry courses will be discussed here.

The current course belongs to the so-called “Fundamental” module and to the “Physical Chemistry” discipline in the “Bachelor’s Degree in Chemistry” of the University of Oviedo (BOE: July 15th, 2010, pp. 62634- 62638), and it is a required (compulsory) subject.

The subject is closely related to the other theoretical courses of the “Fundamental” module, particularly to those belonging to the same “Physical Chemistry” tree, 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 II/a, and *Physical Chemistry II*, in III/a. I will refer to them as PhysChem-I and PhysChem-II from now on. 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 PhysChem-I and from a microscopic point of view in PhysChem-II. Our course has connecting both perspectives as its main objective.

Additionally, our subject develops the essential theoretical formalism needed for the proper understanding of other courses' contents, particularly those included in *Experimentation in Physical Chemistry II*, in IV/a, 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 enroll on this course, students must have passed the examinations of the following subjects from the first year of the degree: *Basic Operations in the Laboratory and Informatic Tools*, *General Chemistry*, *General Physics I*, *General Physics II*, and *Mathematics* (all in I/a or I/b), as well as the subject *Physical Chemistry I*, in II/a.

In practice I will provide as lesson zero a short description of the mathematical statistics concepts essential to our current subject and a description of the energy levels corresponding to the quantum models representing the different degrees of molecular motion.

Students would benefit from a good knowledge of the previous Physical Chemistry courses: both PhysChem-I and PhysChem-II.

4. Competencies and learning results

The next paragraphs describe a list of wishful elements students are intended to acquire.

a) General competences expected:

- CG-01: Developing abilities for analysis and synthesis of scientific knowledge.
- CG-02: Solving scientific problems efficiently.
- CG-03: Being able to use computer science tools as applied to Chemistry.
- CG-04: Acquiring competency in time organization and planning.
- CG-05: Developing abilities for taking complex decisions.
- CG-06: Proper managing of scientific information.
- CG-08: Communicating correctly scientific information, both in writing and orally.
- CG-09: Self-learning.
- CG-17: Developing critical awareness.
- CG-18: Being able to work in a team and also leading it.
- CG-20: Showing gain basic competency in the use of ICTs.

b) Specific competences expected:

- CE-02: Correlating micro and macroscopic properties. This is a core aspect of the statistical thermodynamics subject.
- CE-08: Understanding the kinetics of chemical transformations, both on a macroscopic description (formal kinetics) and on a microscopic perspective (molecular kinetics).
- CE-20: Solving quantitative and qualitative scientific problems.

- CE-22: Acquiring the skills to evaluate, interpret, and summarize chemical information.
- CE-24: Processing data related to chemical information and concepts.
- CE-30: Learning to interpret experimental data on theoretical grounds.
- CE-32: Using inductive and deductive methods in the field of chemistry.
- CE-35: Dominate using the right magnitudes and units.

All this these competences appear in relation to the main subjects of the course: statistical thermodynamics, chemical kinetics, and surface and transport phenomena.

5. Contents

Chapter 1: Kinetic theory and statistical thermodynamics.

Probability theory and probability distributions. Velocity distributions. Basic kinetic theory of transport phenomena: diffusion, thermal conduction, electric conduction, viscosity. Distributions in the phase space. Basic concepts in Statistical Mechanics: definitions of stationary state and equilibrium state. The microcanonical ensemble in a gas and in a crystal. The canonical ensemble in a gas and in a crystal. Other ensembles: calculation of thermodynamic magnitudes. Statistical Thermodynamics of a monoatomic and polyatomic gas. Mixtures of gases and chemical equilibrium: calculation of equilibrium constants.

(Estimated: 23 in-classroom hours = 20 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. Homogeneous catalysis: acid and base catalysis, autocatalysis, enzimatic catalysis. Theoretical models in Chemical Kinetics: collision theory and activated complex theory. Potential

Energy Surfaces (PES): reactants, products, and transition states in a PES.

(Estimated: 12 in-classroom hours = 10 CEX + 2 PA)

Chapter 3: Surface phenomena.

Surface phenomena with uncharged interphase. Thermodynamic study of the uncharged interphase: Gibbs adsorption isotherm. Empirical adsorption isotherms: gas/solid, liquid/solid, and solute/solid interphases. Heterogeneous catalysis. Surface phenomena with charged interphase: the electrical double layer. Theoretical models of the electrical double layer. Electrokinetic phenomena. Electrochemical kinetics.

(Estimated: 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. The general equation of transport phenomena.

(Estimated: 6 in-classroom hours = 5 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, in order for them to raise specific questions previously to proceed during the sessions to their analysis and discussion. The professor will solve in detail in these sessions some of the proposed exercises.

Group Mentoring (TG, 4 in-classroom hours): These sessions will be held in small groups of students. Students should have an active role in these sessions. Students will explain orally their results on their solutions to selected exercises, 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.

7. Evaluation of the student's learning results

In the regular examination a final written test must be taken by every student and their qualification, in the range 0-10, provides 80% of the final note. A minimal score of 4 is required on the test.

The remaining 20% of the final note must come from the activities, challenges and projects done by the students during the course.

In the case of students that, by whatever reason, were not able to participate on the class activities the final test provides a 100% of the note. This applies both to the regular test call and the second or extraordinary call, if required. In other words, class activities, if any, will be taken into account in both cases.

8. Resources, bibliography and complementary documentation

a) Recorded magistral lectures by the instructor will be available. A textbook is also planned. Both are the basic bibliography for the course.

b) Essential references:

- D. A. McQuarrie, *Statistical Mechanics*, University Science Books, 2000.
- B. Widom, *Statistical Mechanics: A concise introduction for chemists*, Cambridge University Press, 2002.
- I. N. Levine, *Physical Chemistry*, McGraw-Hill, 2008.
- P. W. Atkins and J. de Paula, *Physical Chemistry*, (2 vols.), Freeman, 2014.