Subject Guide

1. Information about the subject

SUBJECT	Physical Chemistry I		CODE	GQUIMI01-2-003
EDUCATIONAL OFFER	Bachelor´s Degree in Chemistry	**CENTER**	Facultad de Química	
TYPE	Compulsory	**N° TOTAL CREDITS**	6.0	
PERIOD	First Semester	**LANGUAGE**	Spanish	
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2. Context

This is the first course in Physical Chemistry. It is one of the fundamental (core material) courses taken by undergraduate chemistry students. The characteristic approach of Physical Chemistry is the study of chemical systems in terms of physical laws and concepts. This course, *Physical Chemistry I* (PC-I), is focused on the fundamentals and applications of classical (Chemical) Thermodynamics to the study of chemical systems in *equilibrium*. Besides providing a macroscopic description of any equilibrium system using state variables and functions, the thermodynamic laws will allow us to predict the feasibility of a given transformation between two or more equilibrium states that may be accessible to the system of interest.

Dr. Dimas Suárez is the assigned professor for oral lectures (CE), practice sessions (PA) and tutorial group (TG) sessions (English-group only).

3. Requirements

Students must have passed the following first-year courses: General Chemistry, Laboratory Basic Operations and Computer Tools. General Physics I and II. Mathematics.

In addition, PC-I is a prerequisite course for the third-year Physical Chemistry III course.

4. Competencies and learning results

From the various abilities listed in the Project Book of the Chemistry Degree at the University of Oviedo, we highlight the following ones:

Broad competences and skills

Students should be able to:

- CG1. Carry out information analysis and synthesis.
- CG6. Properly manage information.
- CG7. Use a foreign language, preferably English.
- CG9. Engage in autonomous learning activities.
- CG17. Develop critical thinking.

Specific competences and skills:

Students should have a knowledge of:

- CE4. The characteristic properties of the various states of matter and how theory can describe them.
- CE7. The thermodynamic principles and how they are applied in Chemistry.

Students should be able to

- CE20: Solve quantitative problems and concept questions using the previously-introduced theoretical models.
- CE22. Assess and summarize chemical information.
- CE30. Interpret experimental data and observations in terms of the underlying concepts and theories.
- CE32. Use either inductive or deductive reasoning in Chemistry.

Overall learning outcome: Students should demonstrate knowledge and understanding of the facts, concepts, principles and theories related to Thermodynamics and its application to problem solving in chemical sciences.

5. Contents

The Project Book of the Chemistry Degree at the University of Oviedo enumerates the following topics for PC-I:

- Introduction to Chemical Thermodynamics.
- Material Equilibrium.
- Thermodynamics of Solutions.
- Thermodynamics of Electrochemical Systems.

These broad topics will be adapted to the following program.

1. Introduction to Thermodynamics: Goals and application framework. Basic concepts and definitions. Gases as simple thermodynamic systems: State equations. Thermometry.
2. Laws of Thermodynamics: First law. Internal energy. Heat capacity. Enthalpy. Second law: Entropy.
3. Material equilibrium: Gibbs and Helmholtz energies. Chemical potential. Chemical equilibrium: reactions among ideal gases. Phase equilibria: one component systems.
4. Application of the thermodynamic laws to the study of chemical reactions: Thermochemistry, Third Law of Thermodynamics.
5. Ideal solutions: partial molar quantities and mixing quantities. Ideal solutions: Raoult's law. Ideal diluted solutions: Henry's law.
6. Non-ideal solutions: fugacity, fugacity coefficient. Activity, activity coefficients. Standard states. Electrolyte solutions. Electrochemical systems.

6. Methodology and working plan

Lectures (CE, 42 hours): The lectures will analyze and develop, in a didactic manner, the contents of the program. Students will be encouraged to get involved by raising issues and questions during the lectures.

The core explanations provided by the instructor will point the students towards the essential mathematical proofs and transformations that they have to work out on their own (with the help of the recommended bibliography) and again in the practical sessions. Similarly, the instructor will set questions and numerical problems to all students that will be further analyzed during the practical sessions/group tutorials to be held in the classroom and/or in the *Virtual Campus*.

Practical sessions (PA 7 hours/group): Students will analyze the thermodynamic data and mathematical questions that are previously introduced in the lectures. In order to apply the acquired knowledge to practical problems of interest, students will work out many numerical problems among those included in the supporting materials. During the practical sessions, students are expected to play an active role and use numerical software tools like Octave/MATLAB with the support of the instructor.

Group tutorials (TG 4 hours/group): The first part of these sessions will be open to discussions raised by the students on the basis of the materials and topics treated during the lectures. On the other hand, students working in teams will solve additional problems and/or deliver short presentations about other topics. The selected topics and the statements of the additional problems will develop other aspects of the program showing how Thermodynamics can be put to work. The required materials will be available in the Virtual Campus at least two weeks before the TG session.

Other activities (OA 4 hours/group): Students will attend to two computer seminars oriented to reinforcing their skills in using numerical software for data analysis and problem solving. These seminars, which will be organized at the beginning of the semester, will provide hands-on learning. Students will work out selected problems requiring data plotting, searching numerical solutions of non-linear equations, etc. The acquired knowledge will be useful in PC-I and in other courses.

7. Evaluation of the student's learning results

During the regular semester, the global grade will be based on:

(a) Two written examinations (a first partial exam and a second partial or final exam) that will count 80% of the final grade (40% each partial exam). The exams will consist of both questions (Theory) and numerical problems, being required a minimum score of 4 out of 10 points in each part.

(b) Grading class participation during the TGs and homework. These activities, which will count 20% of the final grade (a minimum of 4 out of 10 points being required to pass the course), will be graded basing on the written materials uploaded to the *Virtual Campus* by the students and on the short presentations/solution to assigned exercises carried out by students during the TG sessions. Under extraordinary circumstances, students may ask the instructor to consider other alternative tasks specially adapted to his/her personal situation for grading his/her personal work.

The global average score resulting from (a) and (b) must be at least 5 out of 10 points to pass the PC-1 subject.

The grade of students who attend *extraordinary calls* will be that corresponding to a written exam, a minimum of 5 out of 10 points will be required to pass the course (4 out of 10 points in each of the two parts of the written exam: Theory and Problems).

8. Resources, bibliography and complementary documentation

One of the following textbooks can be used:

- Physical Chemistry, Thomas Engel y Philip Red, Pearson New International Edition (3rd edition), 2013.
- Physical Chemistry, Ira N. Levine, 6th edition, McGraw-Hill International Editions. 2009.

Additionally, other specific bibliographic references that could help students to better understand the topics of study will be provided during the course.