Subject Guide

1. Information about the subject

SUBJECT	Physical Chemistry II		**CODE**	GQUIMI01-3-002
EDUCATIONAL OFFER	Bachelor´s Degree in Chemistry	**CENTER**	Facultad de Química	
TYPE	Compulsory	**N° TOTAL CREDITS**	6.0	
PERIOD	First Semester	**LANGUAGE**	Spanish	
COORDINATORS/ES		**EMAIL**		
LECTURERS		**EMAIL**		
García Granda Santiago		sgg@uniovi.es	(English Group)	
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2. Context

Physical Chemistry II (QFII) is a course from the third year of the Degree in Chemistry. It is the second theoretical course of the field Physical Chemistry and it includes contents related to Quantum Mechanics, Quantum Chemistry, Molecular Spectroscopy and Diffractometry. The first notions on Quantum Chemistry from the Degree in Chemistry are introduced in the course General Chemistry, from the first year, and they are necessary in order to take QFII. Some of the contents from the fields of Mathematics (lineal algebra and differential and integral calculation) and Physics (mechanics, waves and electromagnetism) are essential tools to approach the field of Physical Chemistry, in particular in order to address the quantum models and their application to spectroscopy and diffraction (specific contents of QFII).

As regards the rest of the courses from the field of Physical Chemistry, there exists a direct relationship with Thermodynamic Statistics from Physical Chemistry III (third year, second term), in which the microscopic levels of energy intervene to assess the partition functions.

The connection with Analytical Chemistry is produced through spectroscopic analytical techniques, studied in Analytical Chemistry II, which require knowledge on Physics and Chemistry related to spectroscopy delivered in QFII. The chemical and physical treatment of spectroscopy is also necessary in the identification of substances: the vibration seal characteristic of certain functional groups in the infrared spectrum, the detailed information from the connection between spins in the nuclear magnetic resonance, or the comparison between spectrums of any sort with known patterns constitute important tools within the scope of Organic and Inorganic Chemistry. Moreover, the methodology introduced by Quantum Chemistry plays an important role in these two fields from Chemistry; for instance, in the application of the molecular orbital theory to organic structure and reactivity (Organic Chemistry I and II) and the formation, structure and stability of inorganic and organometallic complexes. Finally, the importance of diffraction techniques in the characterization and structure of crystalline materials builds relations between the contents introduced in QFII through Biochemistry and Chemistry of the Materials, from the last year of the Degree. However, according to the Verification Report, in order to take any other course from the Degree in Chemistry, students do not have to pass QFII.

3. Requirements

Requirements to take QFII are those necessary in order to take any other course from the field of Physical Chemistry: students must have passed all the courses from the field of Chemistry (General Chemistry and Laboratory Basic Operations and Computing Tools), and Physics (General Physics I and General Physics II) and a course from the field of Mathematics (Mathematics).

4. Competencies and learning results

General competences

- To show the ability of analysis and synthesis (CG-1).
- To have computing knowledge related to the field of chemistry (CG-3).
- To solve problems in an effective way (CG2).

- To learn in an autonomous way (CG-9).
- To develop critical thinking (CG-17).

Specific Competences (knowledge)

- To relate macroscopic properties with those of the atoms and individual molecules (CE-2).
- To apply the principles of quantum mechanics to the description of the structure and properties of atoms and molecules (CE-12).
- To gain the basics to apply and assess the interaction matter-radiation, the principles of spectroscopy and the main techniques of structural research (CE-13).

Specific Competences (abilities)

- To solve quantitative and qualitative problems according to previously developed models (CE-20).
- To gain the skills to assess, interpret and synthesize chemical information (CE-22).
- To process and compute data, in relation to chemical data and information (CE-24).
- To interpret data from laboratory observations and laboratory measures in terms of meaning and the theory it supports (CE-30).
- To use in a correct way the inductive and deductive methods in Chemistry (CE-32).
- To make calculations and error analysis using magnitudes and units correctly (ce-35).
- To prepare, present and defend scientific reports, both in written and oral form, before an audience (CE-36).

Learning Results

- To check and use scientific information effectively.
- To identify and analyse new problems in the field of Chemistry and to propose strategies to solve them.
- To prepare and present correctly a report both in oral and written form.
- To use computing programs in the field of Chemistry.
- To prove understanding and knowledge of facts, concepts, principles and theories related to quantum chemistry and spectroscopy as well as their application in the solution of problems.
- To relate the fundamentals of analytical, spectroscopic and structural research practices to its applications.

5. Contents

Unit 1. The principles of quantum mechanics. Precedents to quantum mechanics. The wave function. Operators. Eigenvalues and measurement. Schrödinger's equation.

Unit 2. One and two-particle problems with analytical solution. The free particle. The particle in a box. The harmonic oscillator. Angular moment in a particle. The rigid rotor. The hydrogenoid atom.

Unit 3. The Atomic Theory: the two-electron atom. Variation theorem. Lineal variation method. Perturbative methods. The He atom. Spin and Pauli's principle.

Unit 4. The atomic theory: atoms with more than two electrons. Coupling of angular moments. L and S angular moment of an atom. Slater determinants. Russell-Saunders' terms. Hund's rules. Hartree-Fock's method. Spin-orbit coupling. Atomic fine electronic structure.

Unit 5. Electronic molecular structure. Born-Oppenheimer's approximation and electronic equation. The H2 ion molecule: the H2 molecule: the Mulliken-Hund and Heitler-London's methods. The LCAO method in lineal molecules. The method of molecular orbitals in non-lineal molecules. Hybridization. Magnetic and electric properties of the molecules.

Unit 6. Rotation and Vibration spectroscopies. Absorption and emission of electromagnetic radiation. Einstein's probability of transition. Selection rules. Nuclear movement of molecules. Roto-vibrational selection regulations. Rotational spectra of diatomic molecules. Rotation-vibration spectra. Raman spectroscopy. Nuclear movement in polyatomic molecules. Rotational spectrum in symmetric and asymmetric top. Microwave spectroscopy. Molecular vibration and symmetry: vibration normal modes. Selection rules. Anharmonicity.

Unit 7. Electronic Spectroscopy. Electronic spectra and Lambert-Beer's Law. Franck-Condon's Principle. Absorption, fluorescence and phosphorescence. Dissociation and predissociation. Lasers: background, types, applications in Chemistry. Photoelectronic Spectroscopy.

Unit 8. Magnetic resonances. Nuclear magnetic resonance: nuclear magnetic moment and selection rules. Chemical shift. Shielding constant. Spin-spin connection. Electronic spin resonance.

Unit 9. Diffraction and its applications. Introduction. General theory of diffraction: introduction to elastic dispersion of the particles (photons, neutrons, electrons) by matter. The structure factor. Laue and Bragg's equations. Diffraction by single crystals. Powder Diffraction method. X-ray spectroscopy. Introduction to the X-rays absorption techniques.

6. Methodology and working plan

Three different types of lectures will be delivered: expositional lecture (CE), problem-solving or practical sessions (PA) and seminars or group tutorials (TG).

Expositional lectures (42 hours) will be devoted to the delivery of the theoretical content of the course. In these sessions the lecturer will present and discuss the subject matter, highlighting the most important and difficult aspects and integrating theoretical questions and examples to facilitate the course comprehension. Thus, it is highly advisable that the students attend regularly to the sessions, although this attendance will have to be implemented with the study of the materials recommended in the lessons.

The practical sessions (7 hours) will involve the application of the knowledge gained in the expositional lectures, and this will be implemented through the integration of theoretical content and exemplifications mentioned above. Before the lecture, students will have access to the problems and questions to be addressed in the lesson, since they are expected to try to solve them on their own in advance.

Seminars or group tutorials (4 hours) will be performed in small groups and its content must have been previously organized so that they are really effective and facilitate the students' learning. The materials used will include exercises and both individual and group tasks which will make reference to the contents delivered in the expositional lectures and also in the practical sessions, especially those themes which might present more difficulties or need to be implemented.

Students will have access to all the course materials which will be uploaded onto the Virtual Campus of the University of Oviedo.

A schedule of the activities is presented below, with the specification of hours corresponding to in-class and off-class activities for each of the units.

	L1	**L2**	**L3**	**L4**	**L5**	**L6**	**L7**	**L8**	**L9**	**Total**	**%**
CE	5	4	4	4	5	6	5	4	5	42	28,00
PA	1,0	1,0	1,0	1,0	0,5	1,0	0,5	0,5	0,5	7	4,66
TG										4	2,66
OA										4	2,66
SE										4	2,00
										60	**40,00**
TNPI	14	10	10	10	10	10	8	8	10	**90**	**60,00**
										150	**100,00**

7. Evaluation of the student's learning results

Students' final grade will be calculated taking into account the following aspects. (i) **continuous assessment** of the students' performance by means of two written tests; the first will cover the contents from the introduction of the subject to the last Friday of October 2016, and the second from the introduction after the first test to the first Friday of December 2016. Both tests will take place immediately after the mentioned dates and during the lectures, and they will represent 30% of the final mark; (ii) **final written exam** (exam of all the contents of the subject covered by the end of the term, taking place in the official date specified by the Faculty), representing 60% of the final mark; and

(iii) **individual tasks** presented during the group tutorials and representing 10% of the final mark.

In order to pass the course in the January exam students must fulfil condition (1) and (2) as specified below:

- **Condition (1)** implies obtaining of a global mark (total sum of the marks of the continuous assessment tests, the final written exam and the individual tasks) which is equal or above 5,0 out of 10,0, with the condition that each of the continuous assessment written tests must have a mark equal or above 3,0 out of 10,0, and that the final written exam must have a mark equal or above 3,5 above 10,0. If a mark under 3,0 out of 10,0 is obtained in any of the continuous assessment tests, students must then fulfil condition (2) to pass the course.
- **Condition (2)** implies obtaining a mark in the final exam equal or above 5,0 out of 10,0.

When both conditions are fulfilled, **the final grade will correspond to the maximum between (1) and (2).**

8. Resources, bibliography and complementary documentation

Course book:

- N. Levine, *Physical Chemistry*, Sixth Edition, McGraw-Hill (Boston, 2009).

Advanced bibliography:

- N. Levine, *Química Cuántica*, 5a edición, Pearson Educación, S. A. (Madrid, 2001).
- N. Levine, *Espectroscopia Molecular*, Editorial AC (Madrid, 1980).
- Giacovazzo, *Fundamentals of Crystallography*, 3rd edition, Oxford University Press / International Union of Crystallography (Oxford, 2011).

Further texts to be consulted:

- D. A. McQuarrie y J. D. Simon, *Physical Chemistry: A Molecular Approach*, University Science Books (Sausalito, 1997).