COURSE DATA

Data Subject	
Code	36451
Name	Química Física II
Cycle	Grade
ECTS Credits	6.0
Academic year	2018 - 2019

Study (s)			
Degree	**Center**	**Acad. year**	**Period**
1110 - Degree in Chemistry	Faculty of Chemistry	3	First term

Subject-matter		
Degree	**Subject-matter**	**Character**
1110 - Degree in Chemistry	7 - Physical Chemistry	Obligatory

Coordination	
Name	**Department**
VIRUELA MARTIN, PEDRO MANUEL	315 - Physical Chemistry

SUMMARY

With the subject ***Physical Chemistry II***, it is intended essentially that students acquire basic knowledge of two fundamental parts of Physical Chemistry, such as Quantum Chemistry and Spectroscopy. Quantum Chemistry is the application of quantum physics to the study of atomic and molecular structure. Spectroscopy can be defined as the study of the interaction of electromagnetic radiation with matter and uses primarily quantum chemistry knowledge. Both subjects are increasingly interdisciplinary, as they are commonly used in other branches of chemistry.

Therefore, this subject will set the foundations for the student to successfully address subsequently the study of different parts of Chemistry and Physical Chemistry itself, usually using the concepts of Quantum Chemistry and Spectroscopy.

PREVIOUS KNOWLEDGE

Relationship to other subjects of the same degree

There are no specified enrollment restrictions with other subjects of the curriculum.

Other requirements

This course has no enrolment requirements with other Degrees courses. In any case, in order to successfully address the subject, it is essential that the student has a prior knowledge, according to the level required in the first year of the Degree in Chemistry. This knowledge comprises:

Basic knowledge of Mechanics and Electromagnetism (Physics I and II).
Basic concepts of Atomic and Molecular Structure (Chemistry I).
Basic concepts of Mathematics, such as: logarithms and exponential management, complex numbers, calculate simple derivatives and integrals, ordinary differential equations and statistical and combinatory fundamentals (Mathematics I and II).

OUTCOMES

1110 - Degree in Chemistry

- Develop capacity for analysis, synthesis and critical thinking.
- Show inductive and deductive reasoning ability.
- Demonstrate leadership and management skills, entrepreneurship, initiative, creativity, organization, planning, control, leadership, decision making and negotiation.
- Solve problems effectively.
- Demonstrate ability to work in teams both in interdisciplinary teams and in an international context.
- Demonstrate ability to communicate information, ideas, problems and solutions to both specialist and non-specialist audiences and using information technology, as appropriate.
- Demonstrate a commitment to ethics, equality values and social responsibility as a citizen and as a professional.
- Learn autonomously.
- Demonstrate the ability to adapt to new situations.
- Demonstrate knowledge of the main aspects of chemical terminology, nomenclature, conventions and units.
- Interpret the variation of the characteristic properties of chemical elements according to the periodic table.
- Demonstrate knowledge of the principles of quantum mechanics and their application to the description of the structure and properties of atoms and molecules.

- Solve qualitative and quantitative problems following previously developed models.
- Recognise and analyse new problems and plan strategies to solve them.
- Relate theory and experimentation.
- Recognise and evaluate chemical processes in daily life.
- Understand the qualitative and quantitative aspects of chemical problems.
- Students must be able to apply their knowledge to their work or vocation in a professional manner and have acquired the competences required for the preparation and defence of arguments and for problem solving in their field of study.
- Students must have the ability to gather and interpret relevant data (usually in their field of study) to make judgements that take relevant social, scientific or ethical issues into consideration.
- Students must be able to communicate information, ideas, problems and solutions to both expert and lay audiences.
- Students must have developed the learning skills needed to undertake further study with a high degree of autonomy.
- Express oneself correctly, both orally and in writing, in any of the official languages of the Valencian Community.
- Have basic skills in the use of information and communication technology and properly manage the information obtained.

LEARNING OUTCOMES

In this course, the following learning outcomes will be addressed, as contained in the document of the Bachelor Degree, within the field of Physical Chemistry

1. Demonstrate the ability to understand and predict the behaviour and reactivity of atoms and molecules from the analysis of its structure, which can be determined from spectroscopic data.
2. Effective understanding and use of bibliographic and technical information relating to the physical and chemical phenomena.
3. Perform effectively his/her assignments as a member of a team and with a gender perspective.
4. Solve problems with rigor.
5. Demonstrate adaptation to new situations.
6. Demonstrate the ability to analyze and synthesize.
7. Demonstrate inductive and deductive ability.
8. Demonstrate the ability to organize and plan.
9. Write and present in native languages properly and able to express and understand a foreign EU language.
10. Manage information with rigor.
11. Demonstrate ethical compromise and with gender perspective.
12. Learn autonomously.

These learning outcomes are to allow that, at the end of the course, the student should be able to:

- Define the terms: operator, commutator, eigenvalue equation, eigenvalue and eigenfunction
- Establish the relationship between operators and observables
- Describe the meaning of the wave function and extract the information of this function by applying the various postulates of quantum chemistry
- Define the average or expected value of an observable
- Formulate the uncertainty principle and its relation to the simultaneous measurement of multiple properties
- Set up and solve the Schrödinger equation for a particle confined in a one-dimensional box
- Set up the Schrödinger equation for a particle confined in a two-or three-dimensional box using the technique of separation of variables
- Define the concept of degeneration and the difference between state and energy level
- Formulate the Schrödinger equation for an harmonic oscillator and analyze their solutions
- Formulate the problem of orbital angular momentum and analyze the possible values of the simultaneous measurement of the angular momentum module and its projection on an axis. Apply the model to the rotation of a diatomic rotor
- Set up the resolution of the Schrödinger equation for the hydrogen atom, showing that it can be separated into radial and angular equations
- Define the energies and wave functions of hydrogen-like orbitals and use their different representations
- Define the general concept of spin and spin properties of an electron
- Set up the Hamiltonian of a many-electron atom
- Use approximate methods for solving the Schrödinger equation-electron systems: variational method
- Set up the Schrödinger equation for helium atom and its resolution at different levels of approximation. Describe the orbital model
- Set the anti-symmetry principle for identical particles systems and apply it to the helium and lithium atoms. Formulate the Slater determinant
- State the self-consistent field method (SCF-HF) for electron atoms
- Differentiate between atomic orbital and function of state of the atom, orbital energy and total energy of the atom. Discuss electronic configurations
- Formulate the Hamiltonian operator for a polyatomic molecule
- Describe the Born-Oppenheimer approximation and the concept of potential energy surface
- Analyze the exact solutions of the hydrogen molecule ion and those obtained with the MO-LCAO approximation method
- Describe the application of the MO-LCAO method to the hydrogen molecule
- Discuss the electronic structure of diatomic molecules using qualitative models MOs and SCF-HF. Represent MOs using a graphical interface (ChemOffice)
- Apply the Hückel method to aromatic conjugated systems
- Describe correctly the spectroscopic phenomenon and the types of spectroscopy
- Describe the semi-classical approximation for radiation-matter interaction
- Define the transition dipole moment and differentiate between generic and specific selection rules
- Describe the various factors on which depends the intensity and width of a spectroscopic signal
- Formulate the Boltzmann distribution law and relate the intensity of a spectroscopic signal to the population of the energy levels and transition probability
- Define the experimental measurement of the intensity of a spectroscopic signal
- Formulate the separation of different types of nuclear motion
- Set up the rotational energy levels of diatomic and linear rotors, and interpret the pure rotational

spectrum shape using the selection rules
- Set up the vibrational energy levels for a diatomic molecule using harmonic and anharmonic approximations
- Outline the transitions composing a pure vibration spectrum and interpret the effects of anharmonicity on such transitions
- Explain the characteristics of rotation-vibration spectra of diatomic molecules and extract structural information from the P, Q and R branches
- State the properties of the vibrational motion of polyatomic molecules and the concept of normal modes of vibration
- Analyze in a simple way the vibrational spectrum of a polyatomic molecule
- Represent the normal vibrational modes using a graphical interface (ChemOffice)
- Describe the characteristics of the rotational and vibrational Raman spectroscopy
- Analyze the electronic spectrum of a diatomic molecule and explain its vibrational structure using the Franck-Condon principle
- Define the concept of chromophore group and differentiate the types of transitions that occur in the electronic spectra of polyatomic molecules
- Describe the phenomena of fluorescence and phosphorescence and their properties

DESCRIPTION OF CONTENTS

1. Basic concepts. Principles of Quantum Mechanics

Development of quantum theory. Wave-particle duality. Schrödinger equation. Mathematical formalism. Postulates of Quantum Mechanics. Stationary states. Uncertainty Principle.

2. Model Systems

Translational motion: particle in a one-dimensional box. Particle in a two-dimensional box. Separation of variables technique. Finite tunneling barriers. Vibrational motion: Harmonic Oscillator.

3. Hydrogen Atom

Introduction. Orbital angular momentum. Rigid rotor. Hydrogen Atom: approach to the formal solution of the Schrödinger equation. Energy and functions of the bound states. Spin angular momentum.

4. Many-electron atoms

Many-electron atoms: general approach. Approximate methods. Helium Atom. Orbital approach. Anti-symmetry principle. Self-consistent field (SCF) orbitals. Electronic states.

5. Molecular structure

Many-electron molecules: general approach. Born-Oppenheimer approximation. The hydrogen ion-molecule (MO-LCAO method). The hydrogen molecule. Diatomic molecules. Polyatomic molecules. pi-electronic systems. Hückel method.

6. Foundations of Spectroscopy

Electromagnetic radiation. Spectroscopy: types of spectra. Radiation-matter interaction: semi-classical approximation. Boltzmann distribution law. The spectroscopic signal: position, intensity and width. Spectroscopic signal intensity. Lambert-Beer Law. Laser emission.

7. Rotation and Vibration Spectroscopies

Collective nuclear motion spectroscopies. Rotational energy levels of diatomic and linear molecules. Pure rotational spectra. Microwave spectroscopy. Vibrational energy levels. Vibration spectra of diatomic molecules. Rotation-vibration spectra. Vibration spectra of polyatomic molecules: vibration normal modes. IR spectroscopy. Raman spectroscopy.

8. Electronic Spectroscopy

Quantum interpretation of the electronic spectra: diatomic molecules. Vibrational structure: Franck-Condon principle. Selection rules. Electronic spectroscopy of polyatomic molecules. Fluorescence and phosphorescence.

WORKLOAD

ACTIVITY	Hours	% To be attended
Theory classes	51,00	100
Tutorials	9,00	100
Study and independent work	90,00	0
TOTAL	**150,00**	

TEACHING METHODOLOGY

The development of the course is structured around the following axis:

- lectures
- tutorials

With respect to the former, they will give an overview of the main topics and they will make emphasis on those key concepts necessary for their understanding. The most recommended resources for further preparation in depth of the subject will be indicated.

Tutorials will be devoted to the approach and resolution of problems and questions, which will allow for identifying the essential elements and concepts of each subject. For these sessions, a list of questions and problems will be provided that will serve for reinforcing the knowledge of the student and to exercise themselves in each subject discussed. The student must deliver the solved problems and questions as indicated by the teacher.

EVALUATION

The following assessment systems will be used:

- Tests consisting of written, oral, and/or practical exams
- Evaluation of group mentoring sessions, seminars, assignments and/or oral presentations
- Continuous assessment of each student based on classroom activities, participation and degree of involvement in the teaching-learning process.

The assessment of the student learning will take into account all aspects stated in the methodology section of this syllabus. Students who do not attend class regularly must choose the modality B.

Mode A:

FIRST CALL

The final grade will consist of:

- The written examination (80%), that consists of a series of theoretical questions and numerical problems, which will deal with the basic concepts taught in class. The exam will be the same for all groups.
- Continuous assessment (20%) comprising short exams conducted throughout the academic year in the form of multiple choice tests or short answers, the assessment of group tutoring sessions, by performing and/or delivery of exercises and questions and continuous assessment of each student based on classroom activities, participation and degree of involvement in the teaching-learning process.

The grade of the written exam must be equal to or greater than 4.0 over 10 in order to do average with the grade from continuous assessment. The minimum overall grade to pass the subject is 5.0 over 10.

SECOND CALL

In the second call students will conduct a written exam consisting of a series of theoretical questions and numerical problems, which will deal with the basic concepts taught in class. The exam will be the same for all groups. The final evaluation will include the rest of the student activities of that academic year taking the same weighting as in the first round. The minimum overall grade to pass the subject is 5.0 over 10.

Mode B

FIRST AND SECOND CALL

Students may choose to be evaluated only with a written exam that in both first and second call will consist of a series of theoretical questions and numerical problems, which will deal with the basics taught in class. The exam will be the same for all groups. The minimum overall grade to pass the subject is 5.0 over 10.

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