COURSE DATA

Data Subject	
Code	36451
Name	Physical Chemistry II
Cycle	Grade
ECTS Credits	6.0
Academic year	2023 - 2024

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
ORTI GUILLEN, ENRIQUE	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, exponentials, complex numbers, simple derivatives and integrals, ordinary differential equations and fundamentals of statistics.

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.
- Have basic skills in the use of information and communication technology and properly manage the information obtained.

LEARNING OUTCOMES

The previous section includes the competences contained in the document VERIFICA. This subject addresses part of the learning results of the matter Physical Chemistry that allow to acquire specific knowledge of chemistry, cognitive skills and general skills recommended by the EUROPEAN CHEMISTRY THEMATIC NETWORK (ECTN) for the Chemistry Eurobachelor® Label. The following table lists the learning outcomes acquired in the subject Phyical Chemistry II related to the competences of the degree in Chemistry.

SPECIFIC KNOWLEDGE OF CHEMISTRY	
The learning process should allow the degree graduates to demonstrate:	
Major aspects of chemical terminology, nomenclature, conventions and units.	Demonstrate knowledge of the main aspects of chemical terminology, nomenclature, conventions and units..(CE1)
The characteristics of the different states of matter and the theories used to describe them.	Demonstrate knowledge of the characteristics and behaviour of the different states of matter and the theories used to describe them..(CE3).

The principles of quantum mechanics and their application to the description of the structure and properties of atoms and molecules	Demonstrate knowledge of the principles of quantum mechanics and their application to the description of the structure and properties of atoms and molecules..(CE5).

COMPETENCES AND COGNITIVE SKILLS	
The learning process should allow the degree graduates to demonstrate:	
Ability to apply this knowledge and understanding to the solution of common qualitative and quantitative problems.	Solve qualitative and quantitative problems following previously developed models..(CE14). Recognise and analyse new problems and plan strategies to solve them..(CE15). Understand the qualitative and quantitative aspects of chemical problems..(CE24).
Ability to calculate and process data, related to information and chemistry data.	Solve qualitative and quantitative problems following previously developed models..(CE14). Recognise and analyse new problems and plan strategies to solve them..(CE15).

GENERAL COMPETENCES	
The learning process should allow the degree graduates to demonstrate:	
Ability to apply practical knowledge to solve problems	Solve problems effectively..(CG4).

related to qualitative and quantitative information.	Solve qualitative and quantitative problems following previously developed models..(CE14). Relate theory and experimentation..(CE22). Recognise and evaluate chemical processes in daily life..(CE23). Understand the qualitative and quantitative aspects of chemical problems..(CE24).
Calculation and arithmetic capabilities, including aspects such as analysis error, estimates of orders of magnitude, and correct use of the units.	Develop capacity for analysis, synthesis and critical thinking.. (CG1). Show inductive and deductive reasoning ability..(CG2). Solve problems effectively..CG4).
Planning and time management skills..	Develop capacity for analysis, synthesis and critical thinking. (CG1). Demonstrate leadership and management skills, entrepreneurship, initiative, creativity, organization, planning, control, leadership, decision making and negotiation..(CG3).
Competences in oral and written communication, in one of the main European languages, in addition to the language of the country of origin	Demonstrate ability to work in teams both in interdisciplinary teams and in an international context..(CG5). Demonstrate a commitment to ethics, equality values and social responsibility as a citizen and as a professional. (CG7). Express oneself correctly, both orally and in writing, in any of the official languages of the Valencian Community. (CT1). Students must be able to communicate information, ideas, problems and solutions to both expert and lay audiences..(CB4). Have basic skills in the use of information and communication technology and properly

	manage the information obtained.(CT2).
Study skills necessary for professional development. These will include the ability to work autonomously.	Demonstrate leadership and management skills, entrepreneurship, initiative, creativity, organization, planning, control, leadership, decision making and negotiation..(CG3). Demonstrate ability to work in teams both in interdisciplinary teams and in an international context..(CG5). Learn autonomously.(CG8). Demonstrate the ability to adapt to new situations..(CG9). Students must have developed the learning skills needed to undertake further study with a high degree of autonomy.(CB5).

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.

Modality A:

FIRST CALL

The final grade will consist of:

The exam (75%), that consists of a series of theoretical questions and numerical problems, which deal with the basic concepts taught in class. The exam will be the same for all groups.

Continuous assessment (25%) 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 the participation and degree of involvement in the teaching-learning process. **Only in exceptional cases and within the time limit set by the teachers, the continuous evaluation may be waived.**

The grade of the written exam must be equal to or greater than 4.5 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 an 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 grades, including continuous evaluation, will be calculated using the same weighting as in the first call. The minimum overall grade to pass the subject is 5.0 over 10.

Modality B

This modality will only be accepted in those very exceptional cases in which the teacher has accepted the waver of continuous assessment.

FIRST AND SECOND CALL

Students may choose to be evaluated only with an exam that in both first and second call will consist of a series of theoretical questions and numerical problems, which 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.

Final warning

Copying or plagiarism of any assignment that is part of the evaluation will make it impossible to pass the course, and the student will be subject to the appropriate disciplinary procedures.

Please note that, according to Article 13 d) of the University Student Statute (RD 1791/2010, December 30), "*it is the duty of a student to refrain from using or cooperating in fraudulent procedures in evaluation tests, in the work performed or in official University documents*".

REFERENCES

Basic

- ATKINS, P.W., de PAULA,J., Química Física, 8ª ed., Ed. Médica Panamericana, 2008. ISBN 9789500612487
- LEVINE, I.N., Fisicoquímica, 5ª ed., McGraw-Hill, 2004. ISBN 9788448137861 (v.1) ISBN 978844137878 (v.2)
- ENGEL, T. y REID, P. Química Física, Pearson Education, 2006
  ISBN 10-84-7829-077-X
- ATKINS, P. W, de PAULA, J., Química Física, Physical Chemistry, 9ª ed., Oxford University Press, 2010. ISBN 97801995437878
- LEVINE, I. N., Physical Chemistry, 6ª ed., McGraw-Hill, 2008. ISBN 9780072538625 (v.1) ISBN 9780071276368 (v.2)

Additional

- BERTRAN, J. y col., Química Cuántica: Fundamentos y aplicaciones computacionales, 2ª ed., Síntesis, 2002.
- HANNA, W., Mecánica Cuántica para Químicos, Fondo Educativo Interamericano, 1985.
- PLANELLES, J., CLEMENTE, I. y GABRIEL, J., Noves Notes de Química Cuàntica, Publicacions de la Universitat Jaume I, 2ªed, 2010. www.uji.es/bin/publ/edicions/quimicaq.pdf.

- McQUARRIE, D. A., Quantum Chemistry, 2ª ed, University Science Books; 2007.
- BROWN, J. M., Molecular Spectroscopy, Oxford University Press, 1998.
- BANWELL, C. N. y McCASH, E. M., Fundamentals of Molecular Spectroscopy, 4ª ed., McGraw-Hill, 1994.
- PLANELLES, J. CLEMENTE, I. y GABRIEL, J., Espectroscòpia, Publicacions de la Universitat Jaume I, 2002.
- DIAZ PEÑA, M. y ROIG MUNTANER, A., Química Física, Vol. 1, Alhambra, 1972.
- CRUZ-GARRITZ, D., CHAMIZO, J. A. y GARRITZ, A., Estructura atómica: un enfoque químico, Addison-Wesley Iberoamericana, 1987.
- LEVINE, I.N., Química Cuantica, 5ª ed., Prentice Hall, 2001.
- REQUENA, A. y ZUÑIGA, J., Espectroscopia, Pearson Prentice Hall, 2003.
- HOLLAS, J. M., Modern Spectroscopy, 2ª ed., John Wiley & Sons, 1992.
- BARROW, G. M., Introduction to Molecular Spectroscopy, McGraw-Hill, 1962.