VNIVERSITAT DE VALÈNCIA

Course Guide
34063 Physical Chemistry

COURSE DATA

Data Subject	
Code	34063
Name	Physical Chemistry
Cycle	Grade
ECTS Credits	6.0
Academic year	2023 - 2024

Study (s)

Degree	Center	Acad. year	Period
1201 - Degree in Pharmacy	Faculty of Pharmacy and Food Sciences	1	Second term
1211 - Double Degree in Pharmacy and Human Nutrition and Dietetics	Faculty of Pharmacy and Food Sciences	1	Second term

Subject-matter

Degree	Subject-matter	Character
1201 - Degree in Pharmacy	3 - Physical chemistry	Obligatory
1211 - Double Degree in Pharmacy and Human Nutrition and Dietetics	1 - Asignaturas obligatorias del PDG Farmacia-Nutrición Humana y Dietética	Obligatory

Coordination

Name	Department
TORDERA SALVADOR, DANIEL	315 - Physical Chemistry

SUMMARY

Physicochemistry is a compulsory subject located in the first year, second semester, of the Degree in Pharmacy and it is endowed with 6 ECTS credits.

The pharmacist is the professional expert in the medical drug and with this course the student is expected to deepen and become familiar with the physicochemical processes that accompany the different stages of the life of a medical drug, from its discovery, synthesis and/or extraction, isolation, chemical stability and kinetics, to its formulation, dosage and distribution in the organism.

Taking as a starting point the Principles of Thermodynamics studied in the Physics course during the first term, Physicochemistry will deal with the study of energy exchange, criteria of spontaneity and

equilibrium of chemical processes, phase equilibria in systems of one or more components, partitioning and extraction phenomena, the colligative properties of dilute solutions, the speed and mechanisms of chemical reactions, surface phenomena, the transport of matter through diffusion and the optical, kinetic, osmotic and electrical properties of macromolecular systems.

It has a part of Theory and Problems that is taught in the classroom with the whole group and another part of Laboratory Practices that will be carried out in the laboratory in subgroups of 16 students.

PREVIOUS KNOWLEDGE

Relationship to other subjects of the same degree

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

Other requirements

It is very convenient that the students had study Mathematics II and Physics in 2nd Bachillerato. The course of Physics (34108), studied in the 1st semester, is basic and essential for the development and the adequate learning of this discipline.

COMPETENCES (RD 1393/2007) // LEARNING OUTCOMES (RD 822/2021)

1201 - Degree in Pharmacy

- Students must have developed the learning skills needed to undertake further study with a high degree of autonomy.
- Module: Chemistry - Capability to know the physico-chemical characteristics of the substances used for the manufacture of drugs.
- Module: Chemistry - To know and understand the characteristics of the reactions in solution, the different states of matter and the principles of thermodynamic and their application to the pharmaceutical sciences.
- Know and apply physicochemical laws and principles to determine the properties of pharmaceutical systems.
- Know the physico-chemical properties of active ingredients and excipients and the possible interactions between them.
- Be able to apply the knowledge acquired to solve physico-chemical problems and to develop and defend arguments.
- Conduct laboratory experiments and know how to evaluate scientific data related to medicinal and healthcare products.
- Know the principles of chemical kinetics and their application to the study of drug stability and pharmacokinetics.

- Know the properties of true solutions.
- Know the basics of adsorption processes.
- Know the basics of diffusion processes in dissolution processes, drug release from polymeric matrices, release from capsules, etc.
- Understand the basics of the behaviour of macromolecules based on their physico-chemical properties.

LEARNING OUTCOMES (RD 1393/2007) // NO CONTENT (RD 822/2021)

The previous section includes the competencies contained in the VERIFICA document.

As a basic core subject taught in the first cycle of the Degree, the subject must:
• Serve as a link between the subjects that the student has already studied and the demands that will be made throughout the Degree.
• Provide the necessary knowledge for an adequate understanding of the physicochemical characteristics of the substances that the pharmacist needs in his professional practice.
• To provide the necessary basis for an adequate understanding of the concepts and methods exposed in other subjects of the Degree such as Pharmaceutical Chemistry, Pharmacology, Pharmacognosy, Pharmaceutical Technology, Biological Analysis and Laboratory Diagnosis, Biochemistry, Microbiology or Parasitology among others.
• To provide the physicochemical knowledge necessary for the rational study of the drug in its preparative, analytical, stability, mechanism of action, etc. aspects.

The learning outcomes should allow that, at the end of the course "Physicochemistry", the student should have acquired a solid foundation on the essential facts, concepts and principles of physicochemistry so that they are able to use them properly. These concepts include thermochemistry, phase equilibria of one and two components, colligative properties, chemical kinetics of simple and complex reactions, including catalysis and photochemistry, adsorption surface phenomena, transport of matter due to diffusion and properties of colloids and macromolecules. The description of the contents is detailed in the corresponding section of this Guide.

Likewise, the laboratory practices of the course have been designed in order to develop the student's autonomous work in the laboratory, including the realization of experimental setups, the taking of measurements, their mathematical treatment, their interpretation in physicochemical terms and their presentation in the form of a scientific report. The student is expected to know how to interpret the results and discuss their reasonableness.

In addition, the student is expected to develop the following skills:
• To be able to pose and solve numerical problems, correctly handling the units and interpreting the results obtained with an analytical and critical spirit.
• To be able to study and plan their learning activities, either individually or in groups, searching, selecting and synthesizing information from different bibliographic sources.
• Justify with rational arguments scientific facts or opinions in an adequate and rigorous manner.
• Solve new problematic situations related to the aspects seen during the course.
• Relate the chemical contents approached in the course with everyday life phenomena, being able to explain them.

DESCRIPTION OF CONTENTS

0. INTRODUCTION

Physical Chemistry concept. Analysis of the Teaching Guide of the Subject

1. THERMOCHEMISTRY

Heat of reaction. Thermochemistry laws. Reference states. Formation, reaction and combustion entalphies. Calorimeter bomb. Variation of the heat of reaction with temperature: Kirchoff equation. Entropy changes in chemical reactions. Heat of solutions.

2. SPONTANEITY AND EQUILIBRIUM CONDITIONS

Spontaneity of the processes. Concept of thermodynamics potential. Hemholtz and Gibbs energies: their variation in different processes. Chemical potential. Differential forms of the thermodynamics potentials. Spontaneity and equilibrium criteria for thermodynamic processes.

3. PHASE TRANSITIONS: PURE SUBSTANCE

The phase rule. Chemical potential-temperature diagram. Clapeyron equation: Phase diagram. Clasiuss-Clapeyron equation: applications. Vapour pressure: influence of external pressure. Polymorphic transitions. Troutons rule.

4. PHASE TRANSITIONS: BINARY SYSTEMS. L-V EQUILIBRIUMS

Immiscible liquids systems. Fractional by vapour current: application to molecular mass calculation. Miscible liquids systems. Raoult and Henry laws. Gases solubility in liquids. Fractional distillation and azeotrope mixtures.

5. PHASE TRANSITIONS: BINARY SYSTEMS. S-L AND L-L EQUILIBRIUMS

Solids-liquids solubility. Cooling curves. Phase diagrams

6. COLLIGATIVE PROPERTIES

Depression of vapour pressure. Elevation of boiling point. Depression of freezing point. Osmotic pressure. Anomalous colligative properties. Application for the preparation of injectables.

7. DISTRIBUTION AND EXTRACTION EFFECTS

Distribution of a solute between immiscible solvents. Simple and multiple distribution. Association and dissociation influence. Pharmaceutical applications. Ferguson principle and Overton Meyer rule

8. THE RATES OF CHEMICAL REACTIONS

The rates of reactions. Rate equations. Reaction order and molecularity.- Integrated rate laws. Reactions of order 0, 1, 2 and 3. Half-lives and time constants. Reaction order determination

9. REACCIONES COMPLEJAS

Simultaneous, equilibrium and consecutive reactions. Consecutive reactions with one equilibrium step. The steady-state approximation.

10. MOLECULAR KINETICS

Temperature dependence of reaction rates. Arrhenius equation. Collision theory. Transition state theory

11. CATALYSIS AND PHOTOCHEMISTRY

General mechanism. Classification. Homogeneous catalysis: specific and general acid-base catalysis. Heterogeneous catalysis. Enzyme catalysis: general mechanism. Michaelis-Menten mechanism. Enzyme inhibition. Photochemistry: laws. Quantum yield. Photochemistry sequences.

12. SURFACE EFFECTS. ADSORPTION

Generalities. Adsorption types. Experimental study. Physisorption: BET isotherm. Chemisorption: Langmuir and Freundlich isotherm. L-L adsorption: Gibbs adsorption equation.

13. MATTER TRANSFER: DIFFUSION

Thermodynamic approach to diffusion: Fick's laws. Determination of the diffusion coefficient: Stokes-Einstein equation, moving boundary method and porous disk method. Applications: Diffusion and molecular and kinetic parameters, dialysis and ultracentrifugation, isoosmotic and isotonic solutions.

14. COLLOIDS AND MACROMOLECULES

Classification and general properties. Preparation and purification. Stability. Molecular weight distribution. Optical, kinetics, osmotic and electric properties.

15. LABORATORY

Solubility diagram.
Heat of solution.
Colligative properties.
Kinetic study.
Surface effects.

WORKLOAD

ACTIVITY	Hours	% To be attended
Theory classes	37,00	100
Laboratory practices	20,00	100
Tutorials	3,00	100
Development of group work	5,00	0
Development of individual work	5,00	0
Study and independent work	21,00	0
Readings supplementary material	6,00	0
Preparation of evaluation activities	18,00	0
Preparing lectures	16,00	0
Preparation of practical classes and problem	19,00	0
TOTAL	**150,00**	

TEACHING METHODOLOGY

Learning processes. The development of the subject will be organized , mainly, throughout three activity types: theoretical and practical classes, laboratory practical classes and presence tutorials.

Theoretical and practical classes. The students must acquire the basic knowledge enclosed in the subject contents through their individual study and the assistance to the theoretical classes. In these classes, to which the student must assist among 2-3 week hours, the professor will provide a global vision of the theme, stress in those critical concepts for the understanding of them, answer to eventual doubts and questions and give special importance to the problem solutions.

For the individual study and the preparation of the chapter with some depth, it will provide to the students with a basic and complementary bibliography, web sites and supporting informatics material, and as well instructions and advices for the management of the information sources. In addition, the student will have in the “virtual aula” of the whole complementary information that it would be considered adequate for the best comprehension of each chapter, and as well with he material show in the supporting presentations used in each class.

Laboratory classes. In first place, the student must complete a preliminary work previous to the assistance to the lab consisting in the comprehension of the guide of each lab practice, the review of the

theoretical concepts implying the preparation of a scheme of the work procedure. In the lab, the professor will do a summary exposition of the most important aspects of the experimental work and will help to the student during the session.The selection and consumption optimization of reagents for the generation of least waste have been deeply considered in the preparation of the Lab Sessions, in order to raise awareness of the students in the proper use of them as a part of sustainable development. Once finished the experimental work, the student will examine the observed facts and carry out the needed calculations, using the calculation pages prepared for that in the lab computers. Likewise, it will be mandatory the presentation of the practical notebook, individually prepared, that it will be evaluated by the professor, together with a exam about questions related to the development of the lab practices.

Tutorials. The students will come to them in groups of 16 students (3 sessions of 1 hour). In those tutorials the doubts that could appear during the theoretical classes will be solved and the students will be directed about the methods of work more useful to improve their performance of learning, proposing, in this case, new activities improving the previous knowledge.

EVALUATION

The evaluation of the students' learning will take into account all the formative aspects that are addressed in this subject and will be carried out in a continuous way by the teacher.

The evaluation will be divided into 15% of continuous evaluation, 25% of laboratory practices and 60% of the exam. The grade, therefore, will be calculated as follows:

FINAL GRADE = Theory exam grade x 0.60 + Global laboratory grade x 0.25 + Continuous evaluation grade x 0.15.

To pass the course it is necessary to obtain:
- A minimum grade of 5 points out of 10 in the theory exam.
- A minimum grade of 4 points out of 10 in the laboratory exam.
- A minimum grade of 5 points out of 10 in the global laboratory grade.
- A minimum grade of 5 points out of 10 in the final grade of the course obtained in the calculation of the above equation.

Continuous evaluation: 15% of the grade will come from this section and may consist of questionnaires, problem workshops, tutorials, deliveries, attendance, etc.

Theory exam: It will correspond to 60% of the grade. At the end of the semester there will be a written theory exam consisting of conceptual or reasoning questions and numerical problems that will allow the student to demonstrate the degree of assimilation of the fundamental concepts. Occasionally, topics to be developed may be included to demonstrate the capacity of synthesis and exposition.

Laboratory: It will correspond to 25% of the grade, of which 60% will evaluate the work and participation of the student in the laboratory and the delivery of results and the remaining 40% will evaluate the examination on matters relating to the development of lab practices carried out. It will be allowed to miss a single practice as long as the absence is justified by a force majeure cause and it could not be recovered in another group. In this regard, the realization of any practice in a laboratory group other than the one initially assigned must always be done with prior notice to the professors involved. Students who repeat

the course and who have passed the laboratory practicals of previous courses (grade equal to or higher than 5 points out of 10 in the overall laboratory grade), will keep the grade for three academic years.

Evidence of copying or plagiarism in any of the assessable tasks will result in failure to pass the subject and in appropriate disciplinary action being taken. Please note that, in accordance with article 13. d) of the Statute of the University Student (RD 1791/2010, of 30 December), it is the duty of students to refrain from using or participating in dishonest means in assessment tests, assignments or university official documents. In the event of fraudulent practices, the "Action Protocol for fraudulent practices at the University of Valencia" will be applied (ACGUV 123/2020): https://www.uv.es/sgeneral/Protocols/C83sp.pdf

REFERENCES

Basic

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- P. Atkins y J. de Paula. Química Física. 8ª Edición. Ed. Médica panamericana (2008).
- R.H. Petrucci, F. G. Herring, J. D. Madura y C. Bissonnette. Química General. Principios y Aplicaciones Modernas. 11ª Edición. Pearson (2017).

Additional

- Sanz Pedrero. Fisicoquímica para Farmacia y Biología. Ed. Masson (1996).
- T. Engel y P. Reid. Química Física. Editorial Pearson (2006).
- I. Levine. Principios de Fisicoquímica. 6ª Edición. Editorial McGraw Hill Education (2014)