

## **COURSE DATA**

Data Subject				
Code	34063			
Name	Physical Chemistry			
Cycle	Grade			
ECTS Credits	6.0			
Academic year	2018 - 2019			

Study (s)			
Degree	Center	Acad. year	Period
1201 - Degree in Pharmacy	Faculty of Pharmacy and Food Sciences	1	Second term
1211 - D.D. in Pharmacy-Human Nutrition and Dietetics	Faculty of Pharmacy and Food Sciences	261	Second term
Subject-matter			
Degree	Subject-matter	Character	
1201 - Degree in Pharmacy	3 - Physical chemistry	Obligatory	
1211 - D.D. in Pharmacy-Human Nutrition and Dietetics	<ul><li>1 - Asignaturas obligatorias del PDG Farmacia-Nutrición Humana y Dietética</li></ul>	Obligatory	

#### Coordination

Name Department

GARCIA DOMENECH, RAMON 315 - Physical Chemistry

## SUMMARY

The physical chemistry is a mandatory subject located in the first course, second semester of the Pharmacy degree with 6 ECTS credits

If the pharmaceutical is considered as a medicament expert professional, the aim of this lecture is that the student goes deep and be familiar with the physical chemistry processes that happen during the different states of the life of a drug, since its discovery, synthesis and/or extraction, isolation, chemical stability and kinetics, till their formulation, dosage and distribution into the organism.



Starting from the Thermodynamic Principles studied in the Physics subject during the first semester, the Physical Chemistry will consider the study of the energy interchange, spontaneity and equilibrium criteria of the chemical processes, the phase transitions for pure substances and binary systems, distribution and extraction effects, colligative properties of dilute solutions, rate and mechanisms of the chemical reactions, surface effects, matter transfer through the diffusion and the optical, kinetic, osmotic and electrical properties of macromolecular systems.

It contains a Theoretical and Practical part that will be given in the classroom with complete group and another Laboratory part that it will carry out at the lab with groups 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, studied in the 1st semester, is basic and essential for the development and the adequate learning of this discipline.

### **OUTCOMES**

#### 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.

### LEARNING OUTCOMES

To know the features of solution reactions, the different forms of matter and its application to the pharmaceutical sciences.

To know and apply the physical chemistry laws and principles for determining the properties of the pharmaceutical systems.



To know the principles of chemical kinetics and their application to the stability study of drugs and to the pharmacokinetics.

To know the colligative properties and its application into the formulation and preparation of injectable

To know the surface effects and their influence into the physical chemistry properties of some particular system

To know the basis of diffusion processes in solution, drug delivery from polymeric matrices and capsules, etc...

To understand at basic level the behaviour of the macromolecules regarding to their physical chemistry properties

To offer the necessary knowledge for facing up with success other subjects of the degree, in the same course or in highest.

To know how applying the acquired knowledge for the resolution of the physical chemistry problems and prepare and defend arguments

To develop laboratory experiences enclosing the preparation of experimental assemblies, the obtaining of measurements, its mathematical treatment, their interpretation in physical chemistry terms and its presentation as a scientific report. It is expected that the student would be able to interpret the results and to discuss if them are reasonable.

To be able that the student can study and plan their activities for learning, either individually or in group, searching and summarising the information from the different bibliography sources.

To develop skills of learning needed for undertaking further studies with a high autonomy level.

### **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 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. Second-order phase 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 of the diffusion.- Ficks laws.- Stokes-Einstein equation.- Diffusion coefficient determination.- Diffusion and viscosity in liquids.- Sedimentation and centrifugation: applications

#### 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	Acad -	

## 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. 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, that it will be made together with the theoretical exam.



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**

Student learning assessment will take into account all training aspects addressed in this matter and will take place in a continuous way by the professor.

A 15% of the global rating will come from continuous assessment (questionnaires, problems workshops, tutorials, supplies, assistance,...)

At the end of the semester a written theory test will be done consisting of conceptual or reasoning questions and numeric problems that will enable the student to demonstrate the degree of assimilation of the fundamental concepts. Sometimes topics to be developed allowing demonstrating the capacity of synthesis and exposure may be included. The grade of the examination will be 60% of the global rating.

Laboratory practices, of compulsory attendance, will be 25% of the final grade (60% of the note, will evaluate the work and the participation of the student in the laboratory as well as the delivery of results, the remaining 40% will evaluate the examination on matters relating to the development of lab practices carried out). Repeater students, who have passed lab practices from previous courses, will be kept the grade three academic years.

FINAL GRADE = Theory grade x 0.60 + Lab practices grade x 0.25 + Ass.grade x 0.15

Students, who do not appear for the final theory exam, will be qualified in the record corresponding to the  $1^{ST}$  call, as "NO APPEAR". The rating in the  $2^{ND}$  call will be "FAIL", still not appearing for the final exam of theory, if they had participated in any academic activities, assessable for this matter, scheduled in this teacher guide.

### **REFERENCES**

#### **Basic**

- J.L. Moreno Frigols, R. García Doménech y G.M. Antón Fos. Introducción a la Fisicoquímica, 2ª Edición, PUV, Universitat Valencia (2011)
  - -P. Atkins, J. de Paula. Química Física Ed. Médica panamericana, 8ª Edición, (2008)
  - -Sanz Pedrero. Fisicoquímica para Farmacia y Biología. Ed. Salvat. (1992)





#### **Additional**

- T. Engel, P. Reid. Química Física, Editorial Pearson, Addison Wesley, (2006)
  - -F. Daniels, R.A. Alberty. Fisicoquímica Editorial C.E.C.S.A. (1990)
  - -Química Física para estudiantes de Farmacia y Biología. S.C. Wallbork, D.J.W. Grant Universidad (1987)

