## •DESCRIPCIÓN DE LA ASIGNATURA

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| **Grado:** | Biotecnology |
| **Doble Grado:** | |
| **Asignatura:** | **Chemical Thermodynamic and Kinetics** |
| **Módulo:** | **Quimica para las ciencias biomoleculares** |
| **Departamento:** | Sistemas Físicos, Químicos y Naturales |
| **Año académico:** | **2016-2017** |
| **Semestre:** | 1º |
| **Créditos totales:** | **6** |
| **Curso:** | 2º |
| **Carácter:** | Obligatorio |
| **Lengua de impartición:** | Español |

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| **Modelo de docencia:** | B1 |
| **•Enseñanzas Básicas (EB):** | 27 horas |
| **•Enseñanzas de Prácticas y Desarrollo (EPD):** | 18 horas |
| **•Actividades Dirigidas (AD):** | |

## •EQUIPO DOCENTE

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| **2.1. Responsable de la asignatura** Juan Antonio Anta Montalvo |

| **2.2. Profesores** | |
|---|---|
| **Nombre:** | **Juan Antonio Anta Montalvo** |
| **Centro:** | **Facultad de CC Experimentales** |
| **Departamento:** | **Sistemas Fisicos, químicos y Naturales** |
| **Área:** | **Química Fisica** |
| **Categoría:** | **Profesor Titular de Universidad** |
| **Horario de tutorías:** | **Martes y Jueves de 13:00 a 16:00** |
| **Número de despacho:** | **Ed 22, tercera planta despacho 13** |
| **E-mail:** | **anta@upo.es** |
| **Teléfono:** | **954349314** |

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|---|---|
| **Nombre:** | **Reyes de la Vega Sánchez** |
| **Centro:** | **Facultad de Ciencias Experimentales** |
| **Departamento:** | **Sistemas Físicos Químicos y Naturales** |
| **Área:** | **Química Física** |
| **Categoría:** | **Prof. Asociado** |
| **Horario de tutorías:** | **Concertar cita por email** |
| **Número de despacho:** | **E22. 3.12** |
| **E-mail:** | **mrvegsan@upo.es** |
| **Teléfono:** | |

# 1. Teaching Team

The main teacher in charge is Juan Antonio Anta Montalvo from the Physical Chemistry Section of the Department of Natural Science, School of Experimental Sciences.

The teaching team is composed of the following teachers:

| Teacher | EB credits | EPD credits |
|---|---|---|
| *Juan Antonio Anta Montalvo* | 3.3 | |
| *Reyes de la Vega* | | 1.2 |

Personal tutorials will be held in the teachers' offices, all of them located at Building 22, 3rd floor. The students should contact the teachers via e-mail to make an appointment for the tutorials.

# 2. Course goals

Biotechnology deals with the use of living organisms or chemicals of biological origin to obtain products which involve an economical, health or social added value. For this reason, learning Biotechnology at an undergraduate degree level brings about acquiring basic knowledge in Chemistry and Biology, so that students can understand technological processes which are used in living organisms.

In the Academic *Memo* for undergraduate studies in Biotechnology of the School of Experimental Science of the Universidad Pablo de Olavide, the following general skills are explicitly indicated (among others):

*To understand the Scientific Method.*

*To get insight and to apply tools, techniques and protocols for experimental work in the laboratory, and to gain the capability to observe and interpret the results obtained.*

*To develop basic experimental skills for every course, by means of the description, quantification, analysis and critical evaluation of experimental results obtained in an autonomous way.*

*To be able to work adequately in biological, chemical or biochemical laboratory, including and adequate knowledge of the required safety and hygienic procedures, as well as waste disposal and animal test handling.*

*To show a correct and integrated vision of the R&D procedures and to be able to connect and interrelate all fields of Biotechnology, from basic physicochemical and biological principles to new scientific findings, in order to develop novel applications and new biotechnological products of commercial interest.*

On the other hand, the *Memo* includes the following <u>specific</u> skills:

*1.To know the Laws of Thermodynamics and their practical application to study a chemical reaction from the thermochemical and thermodynamic point of view. To understand the concept of Chemical Equilibrium and Equlibrium Constant as well as to be able to identify the factors on which they depend.*

*2.To know the basic features which are characteristic of typical physicochemical transport processes like diffusion, osmosis and, electroforesis, among others.*

*3.To master the concepts of reaction rate and rate constant, as well as to know how to identify the factors that influence these magnitudes. To be able to describe proton-transfer and electron-transfer chemical reactions, applying thermodynamic concepts.*

*4.To know the basic principles of Surface Chemistry and Adsorption phenomena, applying thermodynamic and kinetic concepts.*

***The main goal of the CHEMICAL THERMODYNAMICS AND KINETICS course is to help develop all***

***these skills and give the students a more solid theoretical background to understand concepts from more advanced courses in their Biotechnology studies.***

*Thus,* this course aims at developing a number of general and specific skills which are explicitly indicated in the Biotechnology Memo of the School and that are important for their education. The concrete goal of this course is that students master the following points:

1. To know the origin, contents and implications of the Laws of Thermodynamics
2. The know the concept of Chemical Potential
3. To be able to describe Phase Equilibrium and interpret Phase Diagrams
4. To understand the Thermodynamics of Chemical Reactions and to be able to calculate equilibrium constants starting from thermodynamic concepts
5. To know the basic features of the Thermodynamics of solutions of Biomolecules
6. To know the basic features of Transport Phenomena: diffusion, viscosity and heat and charge transport
7. To understand and use correctly formal Chemical Kinetics: Rate equation and integrated Rate equations
8. To understand a chemical mechanism and to know how to derive the Rate equation from it: Steady state approximation and rate-limiting step approximation.
9. To understand the principles of Catalysis and its classification: homogeneous, heterogeneous and enzymatic.
10. To know the main interfacial and adsorption processes.
11. To know the determining factors for stability and aggregation of colloids and macromolecules.

# 3. Working Plan: student groups and time distribution

Thermodynamics and Chemical Kinetics is taught in the first semester of the second year. It contains a total academic burden of 6 ECTS (European Credits Transfer System). According to the university regulations, 1 ECTS is equivalent to 7.5 hours of in-class/ teaching (time coincidence of teacher and student). Furthermore, this course falls within the B1 category, which implies that 60% of its academic contents correspond to "Basic Education" (EB, 27 hours), whereas 40% is "Practical and Development Education (EPD, 18 hours).

In-class work will be carried in groups of 20 students, for both the EB and the EPD.

The time distribution for the students per ECTS (25 hours) is as follows :

- 7.5 hours of in-class work: 4.5 hours EB and 3 hours EPD
- 15 hours of individual work
- 2.5 hours of evaluation and examination.

**Therefore: 6 ECTS are equivalent to 27 hours of class attendance for EB, 18 hours for laboratory exercises and seminars, 90 hours of individual work and 15 hours for evaluation.**

# 5. Contents

In order to accomplish the aforementioned goals, the contents of this course are distributed in 10 Units, as described in the table below. Each Unit has a number of EB and EPD hours which depend on their relative importance for the learning of Chemical Kinetics and Thermodynamics for Biotechnology students. There will four 3-hour laboratory exercises and three slots of 2-hour seminars.

### Part A: Introduction and Chemical Thermodynamics

| | **Contents** | Hours | Hours |
|---|---|---|---|

| | | EB | EPD |
|---|---|---|---|
| **Unit 1:** Introduction | *Course organization and general concepts* | 1 | |
| **Unit 2:** Basic definitions and the First Law | *of "system" and "variable" in Thermodynamics. Thermodynamic Equilibrium. Response functions. Equations of State: The ideal gas equation and the virial equation. Heat and Work. Mechanical Work, electric Work, surface Work and chemical Work. Equivalence betwen Heat and Work. Internal energy and the First Law. Enthalpy. Thermochemistry and Hess Law.* | 4 | **Seminar 1:** *Solving Exercises of mid-term exam 1 (Units 2 and 3)* (2 hours) |
| **Unit 3:** The Second and the Third Laws | *Spontaneity and directionality of the physicochemical processes. Entropy and the Second Law. Fundamental Equation of Thermodynamics. The concept of Thermodynamic Potential and Free Energy. Calculations involving variables and thermodynamic derivatives. The Third Law and Absolute Entropies. The Microscopic Basis of Thermodynamics: an introduction to Statistical Thermodynamics.* | 3 | |
| **Unit 4:** Phase Equilibria | *Mass as a thermodynamic variable. Chemical Potential. Gibbs-Duhem equation. The relationship between activity and chemical potential. Reference states. Phase transitions and Phase Diagrams in pure substances. Clapeyron and Clausius-Clapeyron Equations. Phase diagrams for binary mixtures. Raoult 's Law and Henry's Law. Colligative properties.* | 4 | **Laboratory Exercise 1:** *Determination of the partition coefficient of Acetic Acid in the water/organic system* (3 hours) |
| **Unit 5:** Chemical Equilibrium | *Determination of the reaction free energy. Thermodynamic Description of Chemical Equilibrium. Definition of Equilibrium Constant. Factors affecting the Chemical Equilibrium: composition and temperature. Van't Hoff's Law.* | 3 | **Seminar 2:** *Solving Exercises of mid-term exam 2 (Units 4 and 5)* (2 hours) |
| | **TOTAL** | 15 | 7 |

## Part B: Kinetics and Complex Systems

| | **Contents** | Horas EB | Horas EPD |
|---|---|---|---|
| **Unit 6:** Transport processes | *Introduction of the time variable in physicochemical processes. Concept of thermodynamic gradient and flux. Continuity equation. Diffusion, viscosity, thermal conductivity and electrical conductivity. Fick's Laws. Equations of Stokes-Einstein and Einstein-Smoluchowski.* | 3 | **Lab exercise 2:** *Measurement of the Isoelectric point of Casein.* **(3 hours)** |
| **Unit 7:** Physical chemistry of electrolytic | *Ions in solution. Debye-Hückel law. Relationship between free energy and electric potential. Ion transport and electrochemical potential. Membrane potential. Electron-transfer chemical reactions: Nernst equation. Colloidals systems. Stability and aggregation* | 3 | **Lab Exercise 3:** *Kinetic study of the hydrolysis of the methyl acetate in acid* |

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| solutions and electron-transfer reactions. | *of macromolecules and colloids.* | | *medium* (3 hours)<br><br>**Seminar 3:** *Solving Exercises of mid-term exam 3* (2 hours) |
| **Unit 8:** Formal Chemical Kinetics | *Concept of reaction rate. Rate equation and reaction orders. Integrated rate equation. First order and Second order chemical reactions. Concept of lifetime.* | 3 | |
| **Unit 9:** Molecular Chemical Kinetics | *Concept of molecularity and reaction mechanism. Concept of steady state and rate-limiting step. Temperature effect and Arrhenius Equation. Catalysis. Types of Catalysis: homogenous, heterogenous and enzymatic. Michaelis-Menten mechanism.* | 3 | **Lab Exercise 4:** *Numerical study of enzymatic kinetics* (3 hours) |
| | **TOTAL** | 12 | 11 |

**EB Schedule and location:** Wednesday and Thursday at 4 pm. Classroom to be confirmed.

**EPD schedule**: lab and seminar sessions are held on Fridays and start at 3 pm

| | Week | Dates | Location |
|---|---|---|---|
| Lab Exercise 1 | | | |
| Seminar 1 | | | |
| Lab Exercise 2 | | | |
| Seminar 2 | | | |
| Lab Exercise 3 | | | |
| Lab Exercise 4 | | | |
| Seminar 3 | | | |

# 6. Course evaluation

Evaluation is organized as follows:

•Final EB exam: 3 hours (January 2016)

•Final EPD-laboratory: exam 1 hour (January 2016)

•Final EB exam (retake): 3 hours (June-July 2016 )

•Final EPD-laboratory exam (retake): 1 hour (June-July 2016)

•Three mid-term (partial) exams: 3 hours (1 hour each)

•Poster session plus MoleQla paper: 3 horas.

The students should bear in mind the following aspects:

1. The **Final EB exam** will be composed of 3 or 4 numerical problems from Parts A and B

2. The **Final EPD-laboratory exam** will be composed of one question for each of the practical exercise done in the laboratory. The students may bring their laboratory notes to the exam to help them answer the questions. It is then important to carry out the laboratory exercises properly and correctly annotate the main results and conclusions

3. **Mid-term exams and seminars** are organized as follows: a 1 hour exam containing 2 problems on the topics taught so far in the course will be presented. Students will be allowed to choose any one of the two problems for their answer. Next week, a two hours seminar will be held, where the two problems will be solved and discussed. Some of the students can be required to solve the problems on the blackboard for public discussion.

4. At the end of the semester, a 2-hours **poster session** will be held, where groups of 3-4 students will give a presentation, in the form of a poster, on one of the following topics: Enzymatic Kinetics, Biomolecules, Interfases, Colloidal Systems, or related. The groups should also submit a paper with the MoleQla journal format (www.upo.es/moleqla/) on the topic of the poster. The poster mark will be calculated from the quality of the presentation (50%) and the quality of the paper (50%). If the papers have sufficient quality, they will be published in MoleQla in the Spring issue.

The final mark of the course will be the largest of either of these two mathematical formulae:

**MARK 1 = 0.5 x Final EB + 0.25 x mid-term exams + 0.15 x Final EPD-laboratory + 0.1 x Poster-Paper**

**MARK 2 = 0.75 x Final EB + 0.15 x Final EPD-laboratory + 0.1 x Poster-Paper**

To pass the course, a minimum of 5 points out of 10 will be required, provided a minimum of 4 points in each of the Final Exams of EB and EPD-laboratory is achieved. This means that realization of the EB and EPD Final Exams is mandatory to pass the course, whereas the rest of the elements in the evaluation are facultative.

Once the retake exams for both EB and EPD-lab (July call) are held, the marks obtained from the mid-term exams and the Poster-Paper during the normal teaching period will be kept and considered to calculate the final mark of the course. However, upon student request, and after renouncing to the marks previously obtained (by written and signed permission), a special exam covering a 100% of the total mark of the course will be presented to the students. This exam will include the examination of all skills taught during the course. In case the student does not pass the course, partial marks (EPD, Seminars, etc.) will not be kept for subsequent years.

Attendance to the lab sessions is mandatory, although the students can miss one and only one session if their absence is properly justified (medical certificate). According to the article 8.2.d of the Evaluation Regulations of the University, the attendance to the lab sessions is not required when the course is evaluated by a single exam covering the 100% of the total mark.

## 7. References

This course is not based on any single textbook, so managing several books is recommended. Note that some of the books in the list have a higher level and scope than that required to pass the course, but they can be very useful to gain further knowledge in some topics. Specific books for some parts of the course will be recommended in due course.

**Theory** (Those in the UPO library are marked with *)


•*Físicoquímica**, P.W. Atkins y J. De Paula, 4th Edition, Oxford University Press (2003)

•*Physical chemistry for the Life Sciences**, P.W. Atkins y J. De Paula, Oxford : Oxford University Press, cop. 2006

•*The elements of Physical Chemistry**, P. Atkins, Oxford : Oxford University Press, 2001

•*Quimica Física I y II**. J. Bertrán Rusca y Javier Núñez Delgado (coords). Ariel 2002

•*Physical chemistry for the Biological Sciences**, Gordon G. Hammes Publicación Hoboken, NJ : John Wiley, cop. 2007

•Thermodynamics and kinetics for the biological sciences

•*Termodinámica (I y II)**, Y.A. Çengel y M.A. Boles, Ed. McGraw Hill, 2001

•*Termodinámica**, Kenneth Wark, McGraw-Hill, D. L. 2003

•*Termodinámica Química y de los procesos irreversibles**, Criado Sancho, Manuel
Madrid [etc.] : Pearson Educación : Addison Wesley, 2004

•*Termodinámica Química**, J. Rodríguez-Renuncio, Editorial Síntesis (2000)

•*Fundamentos de Cinética Química**, S. R. Logan, Addison Wesley Publishing Company (2000).

•*Cinética Química para Sistemas Homogéneos (libro electrónico)**, Jorge Ancheyta Juárez, Miguel ángel Valenzuela Zapata. Publicación México : Instituto Politécnico Nacional, 2002.

•*Molecular Driving Forces*.* Ken a Dill y Sarina Bromberg. Garland Science

•*Curso de Termodinámica** A. Peris, Alhambra Universidad (2006)

•*Calor y termodinámica,* M.W. Zemansky y R.H. Dittman, Ed. McGraw-Hill, 1990.


**Problems**


•*Problemas resueltos de termodinámica**, María del Barrio Casado, Eduardo Bravo Guil, Francisco J. Lana, Pons, David O Pérez, Perez, et al. (Paraninfo), ISBN: 8497323491. ISBN-13: 9788497323499, 2005

•*Termodinámica: 100 problemas y ejercicios resueltos**, Hubert Lumbroso, Barcelona Reverté, D.L. 2005

•*100 problemas de termodinámica**, Julio Pellicer y José Antonio Manzanares. Alianza Editorial, 1996

•*Teoría y problemas de termodinámica*, M. M. Abbot, H. C. van Ness. McGraw-Hill, 1990.

•*Problemas de termodinámica**, J.M. Lacalle, R. Nieto, M.C.Gonzalez. E.T..S. de Ingenieros Industriales, Universidad Politécnica de Madrid, 1993

•*Termodinamica: 100 ejercicios y problemas resueltos,* Hubert Lumbroso. Ed. Reverté, 1979

•*Problemas de termodinámica y mecánica estadística*, J. Aguilar Peris, J. de la Rubia Pacheco, C. Fernandez Pineda. Ed. Saber, 1971

•*Problemas programados de termodinámica**, E.Braun, E.T. Wait. Ed. Reverté, 1973