2020/2021

Thermodynamics and Kinetics

Code: 100888
ECTS Credits: 6

Degree	Type	Year	Semester
2500252 Biochemistry	FB	1	2

The proposed teaching and assessment methodology that appear in the guide may be subject to changes as a result of the restrictions to face-to-face class attendance imposed by the health authorities.

Contact

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Use of Languages

Principal working language: catalan (cat)

Some groups entirely in English: No

Some groups entirely in Catalan: Yes

Some groups entirely in Spanish: No

Prerequisites

Although there are no official prerequisites, it is advisable for the student to review the calculation of derivatives and integrals and
the concepts included in Baccalaureate Chemistry.

Objectives and Contextualisation

The general objective of the subject is to introduce the student, for the first time, to the theoretical study of the chemical and biochemical phenomena, that is to say, to the contributions of Physical Chemistry to a life science like Biochemistry.

In the long run, the student has to become aware of the importance of Physical Chemistry as the theoretical basis of Biochemistry, and become familiar with its theoretical and experimental methodology.

The most general objective of the program is to help the student to understand the chemical and biochemical phenomena
of the macroscopic world. The basic concepts of Thermodynamics and Chemical Kinetics will be studied.

At the same time, we also want the student to be aware of the dual-theoretical-experimental character of the Physical Chemistry. Another general objective is to give the student an interdisciplinary view of Biochemistry, in
particular, its close relationship with Chemistry, Physics, and Mathematics.

Specific objectives:

1) Understand the laws of Classical Thermodynamics and be able to apply them to the study of chemical and biological systems.

2) Know the basic foundations of the Chemical Kinetics and be able to apply them in the study of chemical and biochemical reactions.

3) Distinguish between phenomena governed by Thermodynamics and phenomena governed by Kinetics.

Competences

- Be able to self-evaluate.
- Collaborate with other work colleagues.
- Identify molecular structure and explain the reactivity of the different biomolecules: carbohydrates, lipids, proteins and nucleic acids.
- Interpret experimental results and identify consistent and inconsistent elements.
- Manage information and the organisation and planning of work.
- Show initiative and an entrepreneurial spirit.
- Use the basics of mathematics, physics and chemistry that are required to understand, develop and evaluate the chemical procedures of living matter.

Learning Outcomes

1. Apply the principles of thermodynamics and kinetics to biochemical processes.
2. Be able to self-evaluate.
3. Collaborate with other work colleagues.
4. Describe the laws that govern the chemical equilibrium of the various biochemical reactions.
5. Describe the reaction mechanisms operating in the principal biochemical processes.
6. Interpret experimental results and identify consistent and inconsistent elements.
7. Manage information and the organisation and planning of work.
8. Show initiative and an entrepreneurial spirit.

Content

Block 1: Chemical Kinetics

Unit 1: Foundations of Chemical Kinetics. Reaction rate. Rate equation. Order of reaction.
Elemental and complex reactions. Experimental methods. Determination of the reaction order and the rate constant. Integration of the rate equation. Half-life. Differential method of Van't Hoff. Effect
of the temperature on the rate constant. Arrhenius Equation. Activation energy.

Unit 2: Mechanisms of reaction. Mechanisms of first order: reversible, consecutive and
competitive reactions. Approximations of the steady state and equilibrium. General mechanism of chemical catalysis.
Enzyme catalysis. Equation of Michaelis-Menten.

Block 2: Fundamentals of Thermodynamics

Unit 1: Energy. Thermodynamic systems. Laws of Thermodynamics.

Unit 2: Energy transfer: heat and work. Internal energy and enthalpy. Heat capacity at
constant volume and constant pressure. Reversible and irreversible processes. Examples: ideal gas, chemical and biochemical reactions (Thermochemistry).

Unit 3: Distribution of energy and spontaneity of processes. Entropy. Microscopic interpretation. Criteria of spontaneous change and equilibrium in a system of fixed composition. Gibbs Energy. Application to reactions.

Block 3: Phase equilibrium and chemical equilibrium

Unit 1: Phase transitions. Phase equilibrium condition. Equations of Clapeyron and Clausius-Clapeyron. Phase diagrams. Gibbs phase rule.

Unit 2: Dissolutions. Partial molar quantities. Specific case: chemical potential. Thermodynamics of mixtures. Binary mixtures of volatile liquids. Law of Raoult. Henry's Law. Colligative properties.

Unit 3: Chemical equilibrium. Termodynamics equilibrium constant. The response of equilibria to the conditions. Examples of chemical equilibria.

*Unless the requirements enforced by the health authorities demand a prioritization or reduction of these contents.

Methodology

Students will learn by working. They will have to learn to find knowledge and build them, to work on team, face and solve problems and find strategies for action.

Theory lectures: they will be carried out by performing developments on the board. It will be treated to encourage the participation of students during classes. Some practical cases will be solved to exemplify the theory.

Problem sessions: they are essential for the correct understanding of the subject and for the application of the concepts studied to the resolution of real problems. The student will have a collection of problems that will be resolved throughout the course. When the teacher determines it, the delivery of problems will be mandatory.

*The proposed teaching methodology may experience some modifications depending on the restrictions to face-to-face activities enforced by health authorities.

Activities

Title	Hours	ECTS	Learning Outcomes
Type: Directed			
Problem sessions	15	0.6	1, 4, 6
Theory lectures	30	1.2	1, 5, 4, 6
Type: Supervised			
Team work	10	0.4	1, 3, 7, 6
Type: Autonomous			
Study and problem solving	87	3.48	1, 5, 4, 7, 6

Assessment

In this subject a continuous evaluation will be carried out. The final grade will be obtained using the following concepts:

- Work to deliver, 20% (not recoverable).

- Partial exams, 80% (2 in total, 30% the first one and 50% the second one).

To pass the subject per course as a result of the continuous evaluation, the weighted average of the two partial exams and the works to be delivered will be made.

The mark obtained must be at least 5.0. In addition, the two partial exam grades must be at least 4.0 each, and it is mandatory to have a qualification in each work to be delivered.

Final exam: Those students who have not passed the subject per course as a result of the continous evaluation must go to a final exam, which will cover all the subject. The grade of the final exam will replace the joint note of the two partial exams (80%) and the mark of the works (20%) will be kept.

To participate in the final exam, the students must have been previously evaluated in a set of activities the weight of which equals to a minimum of two thirds of the total grade of the subject. The students will obtain the qualification of "Not Evaluable" if the number of their evaluation activities is less than 67% of the programmed ones for the subject.

*Student's assessment may experience some modifications depending on the restrictions to face-to-face activities enforced by health authorities.

Assessment Activities

Title	Weighting	Hours	ECTS	Learning Outcomes
Group evaluation	20%	3	0.12	1, 3, 5, 4, 7, 6, 2, 8
Parcial exam 1	30%	2	0.08	1, 5, 4
Partial exam 2	50%	3	0.12	1, 5, 4, 6

Bibliography

1) I. N. Levine, Physical Chemistry, 6th Edition, McGraw Hill, 2009. (Translated edition: Principios de fisicoquímica, 6ª edició, McGraw Hill, 2014).

2) P.W. Atkins, J. de Paula, Physical Chemistry for the Life Sciences, Oxford University Press, 2006.

3) R. Chang, Fisicoquímica para las ciencias químicas y biológicas, McGraw-Hill, 2008, 3a ed.

4) S.R. Logan, Fundamentos de Cinética Química, Addison Wesley iberoamericana, 2000.

5) R. Chang, Physical Chemistry for the Biosciences, University Science books, 2005.