2021/2022

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

Name: Vicenç Branchadell Gallo

Email: Vicenc.Branchadell@uab.cat

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.

Annotation: Within the schedule set by the centre or degree programme, 15 minutes of one class will be reserved for students to evaluate their lecturers and their courses or modules through questionnaires.

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

Written exams

Throughout the course there will be two partial exams. The weights of these exams in the final mark will be 30% and 50%, respectivelly, so that the whole of the two partial exams will represent 80% of the final mark.

The minimum mark of a partial exam that allows to calculate the average of the course is 4. If these minimum ones can not be reached, at the end of the course one or both partial exams can be retrieved. The note obtained in the recovery will replace the note obtained in the first attempt. It is also possible to come up with the recoveries to improve note. In this case, the last note obtained in each partial is the one that prevails. In order to be entitled to a recovery, it is compulsory to have submitted to both partial exams.

Trace work

Throughout the course, a certain number of student tracking tests (problems solved individually or in groups, short classroom tests, etc.) will be collected. The average grade of these tests will represent 20% of the final mark

The requirements to pass the subject are:

1. The note of each partial exam must be equal to or greater than 4

2. The average mark of the subject must be equal or superior 5

The subject will be considered non-evaluable if if the weigth of the evaluation activities done represents less than 50% of the final mark for the subject. To qualify for the "Matrícula d'Honor" qualification, the marks obtained in the partial exams will be taken into account preferably.

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.

Software

None.