Universitat Autònoma de Barcelona

2023/2024

Thermodynamics and Kinetics

Code: 100888
ECTS Credits: 6

Degree	Type	Year	Semester
2500252 Biochemistry	FB	1	2

Contact

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Teaching groups languages

You can check it through this link. To consult the language you will need to enter the CODE of the subject.
Please note that this information is provisional until 30 November 2023.

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

- Act with ethical responsibility and respect for fundamental rights and duties, diversity and democratic values.
- 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.
- Take account of social, economic and environmental impacts when operating within one's own area of knowledge.
- Take sex- or gender-based inequalities into consideration when operating within one's own area of knowledge.
- 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. Act with ethical responsibility and respect for fundamental rights and duties, diversity and democratic values.
2. Apply the principles of thermodynamics and kinetics to biochemical processes.
3. Be able to self-evaluate.
4. Collaborate with other work colleagues.
5. Describe the laws that govern the chemical equilibrium of the various biochemical reactions.
6. Describe the reaction mechanisms operating in the principal biochemical processes.
7. Interpret experimental results and identify consistent and inconsistent elements.
8. Manage information and the organisation and planning of work.
9. Show initiative and an entrepreneurial spirit.
10. Take account of social, economic and environmental impacts when operating within one's own area of knowledge.
11. Take sex- or gender-based inequalities into consideration when operating within one's own area of knowledge.

Content

BLOCK 1. KINETICS

1. Fundamentals of chemical kinetics.

Reaction rate. Speed equation. Reaction orders: differential method. Integration of velocity equations. Half-reaction time. Insulation method. Experimental techniques. Reaction rate and temperature. Microscopic interpretation of the rate of a reaction.

2. Reaction mechanisms.

Reaction mechanism. Reversible reactions. Parallel reactions. Consecutive reactions. Steady state approximation. Pre-equilibrium approximation. Rate-determining step. Reactions in solution. Catalysis. Acid-base catalysis. Enzymatic catalysis. Michaelis-Menten mechanism.

BLOCK 2. FUNDAMENTALS OF THERMODYNAMICS

3. Introduction to thermodynamics.

Introduction to thermodynamics. The ideal gas. Energy, heat and work. Types of systems. Expansion work. Reversible processes. Energy transfer in the form of heat. Principles of Thermodynamics.

4. Thermochemistry.

Enthalpy. Phase change enthalpies. Reaction enthalpies. Calorimetry. Enthalpies of standard formation. Link enthalpy. Enthalpy of solution. Enthalpy of reaction and internal energy. Variation of the enthalpy of reaction with temperature. Thermodynamic properties of fuels.

5. Spontaneity and equilibrium.

Second principle. Entropy variation in some processes. Reversible adiabatic expansion of an ideal gas. Molecular interpretation of entropy. Third principle. Absolute entropies and reaction entropy. Gibbs energy. Fundamental equations of a closed system. Gibbs energy and maximum work. Composition as a variable. Material equilibrium.

BLOCK 3. MATERIAL EQUILIBRIUM

6. Phase equilibrium. Phase equilibrium in one-component systems. P-T phase diagram. Heating and cooling curves. Triple point and critical point. Clapeyron equation. Clausius-Clapeyron equation. Solid-solid phase equilibrium. The phase rule.

7. Solutions.

Partial molar properties. Chemical potential. Raoult's law. Thermodynamics of mixtures. Ideal solution. Deviations from ideal behavior. Ideal dilute solution. Henry's law. Collective properties. Gibbs energy of mixing in a real solution.

8. Chemical equilibrium.

Introduction. Gibbs reaction energy. Degree of reaction advance and Gibbs reaction energy. Reaction quotient and equilibrium constant. Gibbs energy of standard reaction. Reactions in solution. Heterogeneous equilibria. Variation of the equilibrium constant with temperature. Balance shift. Acid-base reactions.

Methodology

The subject will consist of three types of teaching activities:

1. Theoretical classes

The teacher will develop the contents of the program in-person or virtually, according to the instructions of the academic authorities. The contents of the theoretical classes will be available in advance on the Virtual Campus.

2. Problem classes

Several problems will be proposed for each topic, which will be solved by the students under the supervision of the teacher. Problem classes will be devoted to the discussion of the results of the problems in relation with the contents of the subject.

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	2, 5, 7
Theory lectures	30	1.2	2, 6, 5, 7
Type: Supervised			
Team work	10	0.4	2, 4, 8, 7
Type: Autonomous			
Study and problem solving	87	3.48	2, 6, 5, 8, 7

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 mark obtained in the recovery will replace the mark obtained in the first attempt. It is also possible to come up with the recoveries to improve note. In this case, the last mark obtained in each partial exam 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 mark of each partial exam must be equal to or greater than 4

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

The subject will be considered non-evaluable 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.

Students who have opted for single assessment will have to take a final test that will consist of an examination of the entire syllabus of the subject to be carried out on the day on which the students of the continuous evaluation take the second partial exam. The student's grade will be the mark of this test.

If the final grade does not reach 5, the student has another opportunity to pass the subject through the recovery exam that will be held on the date set by the coordination of the degree.

Assessment Activities

Title	Weighting	Hours	ECTS	Learning Outcomes
Group evaluation	20%	3	0.12	1, 11, 10, 2, 4, 6, 5, 8, 7, 3, 9
Parcial exam 1	30%	2	0.08	2, 6, 5
Partial exam 2	50%	3	0.12	2, 6, 5, 7

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.