Thermodynamics and Kinetics

Code: 105039
ECTS Credits: 6

2024/2025

Degree	Type	Year
2502444 Chemistry	OB	2

Contact

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Teachers

Maria dels Angels Gonzalez Lafont

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Teaching groups languages

You can view this information at the end of this document.

Prerequisites

Fundamentals of Chemistry I and II, Physics I and II, Mathematics I and II, Quantum Chemistry

Objectives and Contextualisation

The objective of this subject is that the student advances in their training in Physical Chemistry. In this subject, we intend to deepen the application of the laws of Thermodynamics to specific chemical systems, using the concept of chemical potential in homogeneous and heterogeneous systems of one or more components. On the other hand, we also want to introduce the complementarity of the macroscopic and microscopic visions of matter to calculate and interpret their thermodynamic properties using the bases of Statistical Thermodynamics. Finally, we will do an introduction to Chemical Kinetics, emphasizing the study of reaction mechanisms using the microscopic interpretation of reaction rates given by the Transition State Theory.

Competences

- "Interpret data obtained by means of experimental measures, including the use of IT tools; identify their meaning and relate the data with appropriate chemistry, physics or biology theories."
- Adapt to new situations.
- Apply knowledge of chemistry to problem solving of a quantitative or qualitative nature in familiar and professional fields.

- Be ethically committed.
- Communicate orally and in writing in one's own language.
- Have numerical calculation skills.
- Learn autonomously.
- Manage the organisation and planning of tasks.
- Manage, analyse and synthesise information.
- Obtain information, including by digital means.
- Operate with a certain degree of autonomy and integrate quickly in the work setting.
- Propose creative ideas and solutions.
- Reason in a critical manner
- Recognise and analyse chemical problems and propose suitable answers or studies to resolve them.
- Resolve problems and make decisions.
- Show an understanding of the basic concepts, principles, theories and facts of the different areas of chemistry.
- Show initiative and an enterprising spirit.
- Show motivation for quality.
- Use IT to treat and present information.
- Use the English language properly in the field of chemistry.

Learning Outcomes

1. Adapt to new situations.
2. Analyse and resolve problems in the field of homogenous chemical kinetics.
3. Analyse and resolve problems of a thermodynamic nature.
4. Apply the aforesaid models for predictive purposes, knowing how to appreciate limitations.
5. Apply the theoretical aspects of phase equilibrium to understand distillation processes.
6. Be ethically committed.
7. Communicate orally and in writing in one's own language.
8. Enumerate and describe the basics of statistical thermodynamics.
9. Explain chemical kinetics.
10. Explain the principles of classical thermodynamics and their applications to chemistry.
11. Have numerical calculation skills.
12. Identify the English names of fundamental physical and chemical variables.
13. Interpret molecular behaviours and the equilibrium phenomena of ideal gases.
14. Interpret the evolution of the concentration of species over time and their relation with the reaction mechanism.
15. Learn autonomously.
16. Manage the organisation and planning of tasks.
17. Manage, analyse and synthesise information.
18. Obtain information, including by digital means.
19. Operate with a certain degree of autonomy and integrate quickly in the work setting.
20. Propose creative ideas and solutions.
21. Reason in a critical manner
22. Recognise the phenomena of energy exchange and the laws that govern them in natural or industrial processes.
23. Relate a theoretical model with the phenomena of chemical equilibriums.
24. Relate macroscopic properties and the properties of individual atoms and molecules.
25. Resolve problems and make decisions.
26. Resolve quantitative problems in surface chemistry, chemical kinetics and electrochemistry.
27. Show initiative and an enterprising spirit.
28. Show motivation for quality.
29. Understand how the presence of solute affects the properties of dissolutions.
30. Use IT to treat and present information.
31. Use entropic bases to define the spontaneity of a process.
32. Use the English names for the different states of matter and their changes.
33. Use the concepts and formulations of chemical and electrochemical potentials in real processes.

Content

1.Introduction to statistical thermodynamics

2. Thermodynamic properties of the ideal gas

3. Molecular interpretation of chemical equilibrium

4. Introduction to chemical kinetics

5. Mechanisms of reaction

6. Transition State Theory

7. Material equilibrium, Gibbs energy and chemical potential

8. Phases equilibrium in systems of one component

9. Dissolutions

Activities and Methodology

Title	Hours	ECTS	Learning Outcomes
Type: Directed			
Laboratory practices	16	0.64	1, 5, 15, 27, 28, 29, 17, 6, 18, 19, 20, 21, 25, 30
Problems classes	13	0.52	3, 2, 4, 16, 17, 18, 21, 26, 25, 11, 33, 30
Theoretical classes	33	1.32	3, 2, 5, 7, 31, 29, 8, 9, 16, 12, 13, 14, 24, 23, 25, 32
Type: Autonomous			
Personal work	65	2.6	1, 4, 15, 31, 27, 8, 10, 9, 16, 17, 13, 6, 18, 20, 21, 22, 24, 23, 26, 25, 33, 30

Guided activities:

Theoretical classes, problem classes, laboratory practices

Autonomous activities:

Study, problem solving, readings and obtaining information, preparation of laboratory practices, bibliographic search.

By order of the Vice-Rector for Quality and Academic Accreditation, the teaching guides will indicate that the teacher must allocate approximately 15 minutes of some class to allow their students to answer the evaluation surveys of the teaching and evaluation of the subject or module.

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.

Assessment

Continous Assessment Activities

Title	Weighting	Hours	ECTS	Learning Outcomes
Exams	70	10	0.4	3, 2, 5, 4, 7, 31, 29, 8, 10, 9, 13, 14, 21, 22, 24, 23, 26, 33
Individual work	15	5	0.2	1, 3, 2, 5, 4, 15, 31, 27, 28, 29, 8, 10, 9, 17, 12, 13, 14, 18, 20, 21, 22, 24, 23, 26, 25, 11, 33, 30, 32
Laboratory practices	15	8	0.32	3, 2, 15, 16, 17, 6, 18, 19, 20, 21, 25, 11, 30

Continuous Evaluation

Written exams: Two partial exams will be carried out during the course, on the dates set by the coordination. Each of these exams will weight 35% on the final grade. The minimum mark required at each partial assessment to average with the rest of evaluating activities is 4,0. If these minimum requirements are not satisfied at the end of the term, there will be a recovery exam on the whole contents of the course. The note obtained in the recovery exam will replace the grade got in the first attempt. The students must have been previously evaluated in a set of activities the weight of which equals 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.

Laboratory practices: The laboratory practices will be evaluated based on the results obtained in each practice and from a quizz that will have to be answered at the end of the period of practices. The average mark obtained from the practices in the laboratory will be equivalent to 15% of the final mark of the subject.

Individual Work: During the course, several avaluable exercises to be resolved in the classroom or outside the classroom will be proposed. The marks obtained in these exercises will have a weight of 15% on the final mark of the subject.

The requirements to pass the subject are:

1) The mark of each partial exam must be equal to or greater than 4,0. The minimum mark in the recovery exam must be 4,0.

2) The average mark of the subject must be equal to or greater than 5,0.

3) Attendance to the sessions of laboratory practices is obligatory. The mark of the laboratory practices must be equal or greater than 5,0.

Single Evaluation

The students who have taken advantage of the single assessment modality will have to take a final test that will consist of an examination of the entire theoretical syllabus and problems of the subject.

This test will take place on the day that the continuous assessment students take the second partial exam.

The student's grade will be:

Subject grade = (Final test grade * 80 + Practice grade * 20)/100

If the final mark 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. In this test it will be possible to recover 80% of the mark corresponding to the theory part. The practice part is not recoverable. The students will obtain the qualification of "Not Evaluable" if they have taken neither the exam of the final test nor the recovery exam.

Bibliography

Available books in the Biblioteca de Ciència i Tecnología (UAB):

Físicoquímica / Ira N. Levine ; traducción: Ángel González Ureña ; con la colaboración de Antonio Rey Gayo [i 4 més]	Levine, Ira N., 1937-, autor	Document físic
Fisicoquímica para las ciencias químicas y biológicas / Raymond Chang ; traducción técnica Rosa Zugazagoitia Herranz ; revisión técnica Alberto Rojas Hernández ... [et al.]	Chang, Raymond	Document físic
Physical chemistry / Ira N. Levine	Levine, Ira N.	Document físic
Physical chemistry for the life sciences / Peter Atkins, Julio de Paula	Atkins, P. W. (Peter William), 1940-	Document físic
Química física / Peter Atkins, Julio de Paula	Atkins, P. W. (Peter William), 1940-	Document físic
Química física / Peter Atkins y Julio de Paula ; traducido por Ernesto Timmermann... [et. al.]	Atkins, P. W. (Peter William), 1940- autor	Document electrònic
Química molecular estadística : termodinámica estadística para químicos y bioquímicos / Iñaki Tuñón, Estanislao Silla	Tuñón, Iñaki	Document físic
Thermodynamics and statistical mechanics [Recurs electrònic] / John M. Seddon & Julian D. Gale	Seddon, John M.	Document electrònic
Fundamentos de cinética química / S. R. Logan ; traducción Concepción Pando García-Pumarino	Logan, S. R.	Document físic
Physical chemistry for the biosciences / Raymond Chang	Chang, Raymond	Document físic

Principios de fisicoquímica / Ira N. Levine ; revisión técnica: Carlos Amador Bedolla, René Huerta Cevallos ; [traducción: Gabriel Nagore Cázares]	Levine, Ira N.	Document físic
Principios de fisicoquímica / Ira N. Levine (Chemistry Department Brooklyn College City University of New York, Brooklyn, New York) ; revisión técnica, Carlos Amador Bedolla (Universidad Nacional Autón	Levine, Ira N. 1937- autor	Document electrònic

Software

For the computational practices the following programs will be used:

Gaussview 6.0.16

Gaussian 16, B.01

Language list

Name	Group	Language	Semester	Turn
(PAUL) Classroom practices	1	Catalan	second semester	morning-mixed
(PAUL) Classroom practices	2	Catalan	second semester	morning-mixed
(PLAB) Practical laboratories	1	Catalan	second semester	morning-mixed
(PLAB) Practical laboratories	2	Catalan	second semester	morning-mixed
(PLAB) Practical laboratories	3	Catalan	second semester	morning-mixed
(PLAB) Practical laboratories	4	Catalan	second semester	morning-mixed
(PLAB) Practical laboratories	5	Catalan	second semester	afternoon
(PLAB) Practical laboratories	6	Catalan	second semester	afternoon
(PLAB) Practical laboratories	7	Catalan	second semester	afternoon
(PLAB) Practical laboratories	8	Catalan	second semester	afternoon
(TE) Theory	1	Catalan	second semester	morning-mixed
(TE) Theory	2	Catalan	second semester	morning-mixed