Universitat Autònoma de Barcelona

2020/2021

Thermodynamics and Kinetics

Code: 105039
ECTS Credits: 6

Degree	Type	Year	Semester
2502444 Chemistry	OB	2	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

Teachers

Àngels González Lafont
Josep Maria Lluch López

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, w

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 ones 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 ones 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. Phases equilibrium in systems of one component
2. Dissolutions
3. Phases equilibrium in systems of more than one component
4. Introduction to statistical thermodynamics
5. Thermodynamic properties of the ideal gas

6. Molecular interpretation of chemical equilibrium
7. Introduction to chemical kinetics
8. Mechanisms of reaction
9. Transition State Theory

Methodology

Guided activities:

Theoretical classes, problem classes, laboratory practices
Autonomous activities:
Study, problem solving, readings and obtaining information, preparation

Activities

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

Assessment

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. Only those students who do not get the minimum mark at the partial assessments are eligible for the recovery. To participate in the final exam, 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 last session 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.
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.

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

Bibliography

- Thermodynamics and Statistical Mechanics, John M. Seddon and Julian D. Gale, Royal Society of Chemistry,2002.

- Fisicoquímica, Raymond Chang, McGraw Hill, 2008 (Tercera Ed.).

- Quimica Fisica, Peter Atkins y Julio de Paula, Editorial Medica Panamericana, 2008 (Octava Ed.).

- Química Molecular Estadística, Iñaki Tuñón y Estanislao Silla, Editorial Sintesis, 2008.- FisicoQuímica, Ira N. Levine, Editorial McGaw Hill, 2004