Universitat Autònoma de Barcelona

2019/2020

Physical Chemistry

Code: 102504
ECTS Credits: 6

Degree	Type	Year	Semester
2502444 Chemistry	OB	3	1

Contact

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Use of Languages

Principal working language: catalan (cat)
Some groups entirely in English: No
Some groups entirely in Catalan: No
Some groups entirely in Spanish: No

Teachers

Iluminada Gallardo García
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Prerequisites

It is advisable to have studied "Fundamentals of Chemistry", "Quantum Chemistry", and "Chemical Thermodynamics".

Objectives and Contextualisation

The objective of this subject is for the student to consolidate their training in Physical Chemistry. Therefore, the main concepts of Chemical Kinetics, one of the fundamental areas of Physical Chemistry that the student has yet to know, will be presented. On the other hand, the study will address other areas of Physical Chemistry of particular nature and, therefore, more difficult to classify. Thus, Transport Phenomena will be studied, both in the gas phase and in the liquid phase, Surface Chemistry and Heterogeneous Kinetics, Electrochemistry, both equilibrium and dynamics, and Macromolecules and Colloids. All this will be done so that the student can grasp the different strategies with which Physical Chemistry attacks the problem of the study of chemical systems: from microscopic or macroscopic visions, or in situations of balance or change. In those occasions in which the simplicity of the systems under study allows it, an attempt will be made to relate these different strategies.

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.
- Show sensitivity for environmental issues.
- 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 surface adsorption processes and adapt them to different isothermals.
4. Be ethically committed.
5. Classify and analyse the properties of colloids and macromolecules.
6. Communicate orally and in writing in ones own language.
7. Define colloids and macromolecules.
8. Define surface chemistry.
9. Describe the components of electrochemistry.
10. Explain chemical kinetics.
11. Have numerical calculation skills.
12. Identify the English names of fundamental physical and chemical variables.
13. Identify the phenomena of transport.
14. Interpret data referring to surface tension (surfactants), wetting (angles of contact) and detergence.
15. Interpret intensity/potential graphs (I/E) and their relation with the operation of batteries.
16. Interpret the evolution of the concentration of species over time and their relation with the reaction mechanism.
17. Learn autonomously.
18. Manage the organisation and planning of tasks.
19. Manage, analyse and synthesise information.
20. Obtain information, including by digital means.
21. Operate with a certain degree of autonomy and integrate quickly in the work setting.
22. Propose creative ideas and solutions.
23. Reason in a critical manner
24. Recognise and analyse problems related with surface chemistry (adherence and detergence).
25. Recognise, analyse and resolve electrochemical problems (batteries).
26. Resolve problems and make decisions.
27. Resolve qualitative problems related to transport phenomena, colloids and macromolecules.
28. Resolve quantitative problems in surface chemistry, chemical kinetics and electrochemistry.
29. Show initiative and an enterprising spirit.
30. Show motivation for quality.
31. Show sensitivity for environmental issues.
32. Summarise a scientific text related with the subject in the English language
33. Use IT to treat and present information.
34. Use the English names for the different states of matter and their changes.

Content

Unit 1. HOMOGENEOUS KINETICS

Reaction rate.

Rate equation. Reaction order.

Elementary reactions and complex reactions.

Experimental methods

Determination of the reaction order.

Integration of the rate equation. Reactions of order 0, 1, 2 and n.

Half-life.

Differential method of Van't Hoff.

Temperature dependence of rate constants. Arrhenius equation.

Activation energy, an experimental magnitude.

Complex reactions. Reaction mechanisms.

Reversible reactions

Consecutive reactions. Parallel reactions

Approximations of steady state and equilibrium.

Reactions in linear and branched chain. Explosion limits.

Basic foundations of Statistical Thermodynamics. Partition function.

Transition state theory.

Thermodynamic formulation of the theory of the transition state.

Interpretation of the different magnitudes. Relationship between them.

Tunneling effect.

Reactions in solution.

Reactions controlled by diffusion and activation.

Catalysis. Types of catalysis.

Homogeneous catalysis.

Enzyme catalysis. Michaelis-Menten equation.

Mechanism of Michaelis-Menten.

Mechanism of Briggs-Haldane.

Unit 2. TRANSPORT PHENOMENA

Definition. Types.

Kinetic theory of gases.

Speed distribution.

Molecular collisions and mean free path.

Effusion rate. Law of Graham.

Transport in an ideal gas. Fick's first law of diffusion.

Thermal conductivity.

Phenomena of transport in liquids.

Conductance and conductivity.

Strong and weak electrolytes.

Law of Kohlrausch.

Dilution law of Ostwald.

Mobility of ions.

Transport numbers

Diffusion.

Nernst-Einstein equation.

Stokes-Einstein equation.

Fick's second law of diffusion.

Diffusion with convection.

Einstein-Schmoluchowski equation.

Unit 3. THE INTERFACE (SURFACE CHEMISTRY)

Interfaces

Surface tension.

Curved interfaces

Law of Laplace.

Capillarity rise

Surface thermodynamics: Gibbs adsorption isotherm. Adsorption and surfactants.

Unit 3b. HETEROGENEOUS KINETICS

Physisorption and chemisorption.

Surface coverage.

Adsorption isotherms: Langmuir, Freundlich, BET and Temkin.

Heterogeneous catalysis.

Mechanism of Langmuir-Hinshelwood.

Mechanism of Eley-Rideal.

Unit 4. ELECTROCHEMISTRY

Electrochemical Equilibrium.

Introduction.

Nernst equation

Thermodynamic parameters.

Galvanic cells

Transport Cells

Applications.

Electrochemical kinetics.

Introduction

Charge transfer kinetics in the electrodes.

Effect of the Transport of Matter

Electrochemical methods.

Unit 5. COLOIDS AND MACRO-MOLECULES

Colloids

Classification, preparation and applications.

Structure, surface and stability of colloids. Zeta potential. Flocculation.

Association of colloids. Micelles, bilayers and vesicles / liposomes. Membranes.

Macromolecules

Natural and synthetic macromolecules.

Molecular weight distributions. Mass spectrometry. Dispersion of light. Sedimentation. Electrophoresis. Viscosity.

Structures of macromolecules

Methodology

Activities Directed
Theory Lectures
Problem solving sessions

Autonomous activities
Study, Problem Solving, Reading and Information Obtaining

Activities

Title	Hours	ECTS	Learning Outcomes
Type: Directed			
Problems	12	0.48	
Theory Lectures	38	1.52	3, 5, 6, 7, 8, 9, 10, 19, 13, 16, 15, 4, 31, 20, 22, 23, 24
Type: Autonomous			
Study, Problem solving, Readings and Information Obtaining	90	3.6	18, 19, 20, 21, 23, 26

Assessment

Evaluation

This subject will use continuous evaluation to verify that the student has achieved the competences determined in the curriculum.

For evaluation purposes, the subject is divided into two parts: exams and follow-up work

Exams: (80%)

Throughout the course two partial exams will be carried out (P1, P2). Each of the exams will be scored with a grade between 0 and 10.

Follow-up work (Evidences): (20%)

Throughout the course there will be two series of evidences (S1, S2) (collect problems made at home, work, test or problems in the classroom, etc.) that will be considered evidence of the student's personal work. Each of the series of tests corresponding to the evidences of the follow-up work will give rise to a score between 0 and 10, and they are not recoverable.
Grades:

Students who pass the subject per course:

In order to pass the subject per course, the following three conditions must be met:

1) The final grade of COURSE (CFG) must be at least 5.0.

CFG = 0.80 [0.50 (P1 + P2)] + 0.20 [0.50 (S1 + S2)]

2) The two exam grades P1 and P2 must be at least 4.0.

3) It is mandatory to have a qualification in the two series of follow-up work.

Students who do not pass the subject per course
and students who want to improve their course grade:

Students who do not pass the subject per course, according to the previous paragraph, or who want to improve theirqualification, must go to a final exam that will include all the subject.

The grade of the final exam will replace the grade that could be had of the sets of both partial ones and, therefore, it will have a weight of 80% (the note of the follow-up works will not be able to recover).

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 grade of Not evaluable will be applied if the number of evaluation activities is less than 50% of the programmed ones for the subject.

Assessment Activities

Title	Weighting	Hours	ECTS	Learning Outcomes
Evidences	20%	2	0.08	2, 3, 17, 5, 6, 7, 8, 29, 30, 9, 10, 18, 19, 13, 12, 16, 14, 15, 4, 31, 20, 21, 22, 23, 24, 25, 27, 28, 26, 32, 11, 33, 34
Final exam	80%	2	0.08	1, 2, 3, 5, 7, 8, 30, 9, 10, 19, 13, 16, 14, 15, 22, 23, 24, 25, 27, 28, 26, 11
Partial Exam 1	40%	3	0.12	1, 2, 6, 30, 10, 19, 13, 16, 22, 23, 27, 28, 26, 11
Partial exam 2	40%	3	0.12	1, 3, 5, 6, 7, 8, 30, 9, 19, 14, 15, 22, 23, 24, 25, 27, 28, 26, 11

Bibliography

Physical Chemistry, P.W. Atkins, 8th edition, Oxford University Press, 2006

Fisicoquímica, (Vol. 1 i 2), Ira N. Levine, 5ª edició, McGraw Hill, 2004