

THERMODYNAMICS AND CHEMICAL KINETICS

Coordination: DAVID, CALIN ADRIAN

Academic year 2021-22

Subject's general information

Subject name	THERMODYNAM	IICS AND CHEMICAL P	KINETICS			
Code	102216					
Semester	2nd Q(SEMESTE	R) CONTINUED EVAL	UATION			
Typology	Degree		Course	Charac	cter	Modality
	Bachelor's De Science and	_	1	СОММ	ION	Attendance- based
Course number of credits (ECTS)	6					
Type of activity, credits, and groups	Activity type	PRALAB	PRAU	LA		TEORIA
	Number of credits	0.8	1			4.2
	Number of groups	4	1			1
Coordination	DAVID , CALIN A	DRIAN				
Department	CHEMISTRY					
Teaching load distribution between lectures and independent student work	60 contact hours 90 hours of stude	nt work				
Important information on data processing	Consult this link f	or more information.				
Language	Spanish					

Teaching staff	E-mail addresses	Credits taught by teacher	Office and hour of attention
DAVID , CALIN ADRIAN	calinadrian.david@udl.cat	7,2	
DE PAULA PEDROZA, RICARDO HENRIQUE	ricardo.depaula@udl.cat	1,2	

Learning objectives

The student, upon passing the subject, must be able to:

- 1. Know how to use the concept of chemical potential
- 2. Know how to apply the conditions of chemical and phase equilibrium and the main characteristics of each of them
- 3. Know the main features of colloidal systems
- 4. Know the bases that govern the behavior of non-equilibrium systems: Transport phenomena and chemical reactivity
- 5. Know the concepts and methodologies used in determining the speed of a chemical reaction as well as the basis of the main theories that allow justifying the speed of the processes
- 6. Relate the acquired chemical physical concepts with those of mathematics, physics and biology.
- 7. Quantitatively solve the problems that arise in practice in the laboratory with the determinations that involve the concepts mentioned in the subject using specialized computer programs where appropriate

Competences

At least the following basic competences will be guaranteed:

CB4: That students can transmit information, ideas, problems and solutions to both specialized and non-specialized audiences.

CB5: That students have developed those learning skills necessary to undertake further studies with a high degree of autonomy.

General competencies

In addition, the graduate must be able to:

CG2: Interpret studies, reports, data and analyze them numerically.

GC3: Select and use available written and computerized sources of information related to the professional activity.

GC5: Understand and express themselves in the appropriate terminology.

GC6: Discuss and argue in different forums.

GC10: Have a critical and innovative spirit.

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CT3: Use existing computer and communication tools as a support for the development of their professional activity (strategic competence UdL).

Specific competences

CE2: Identify and apply the chemical fundamentals necessary for the development of other disciplines and activities of the profession.

CE5. Apply the basic processes of a laboratory and use equipment, handle reagents, comply with safety conditions and prepare reports.

CE6. To pose and solve problems by correctly applying the acquired concepts to concrete situations.

Translated with www.DeepL.com/Translator (free version)

Subject contents

THEORETICAL CONTENTS:

Unit 1.- Principles of Thermodynamics (2 T + 3 P)

Introduction. First Principle. Enthalpy. The second principle of thermodynamics. Microscopic meaning of entropy.

Unit 2.- Thermodynamic equilibrium (2 T +4 P)

Gibbs and Helmholtz function. Chemical potentials. Phase equilibrium and chemical equilibrium conditions. Thermodynamic relationships. Calculation of variations in state functions for different processes.

Unit 3.- Chemical potential and activity. (4 T +5 P + 4 L)

Partial molar magnitudes. Mixing quantities. Chemical potentials for gases. Ideal solutions. Ideal diluted solutions. Non-ideal solutions. Activity and activity coefficient. Scales. Colligative properties. Electrolyte solutions. Debye-Hückel theory.

Unit 4.- Chemical equilibrium in non-ideal systems. (2 T +4 P)

The equilibrium constant. Dependencies. Balance displacements.

Unit 5.- Phase equilibrium. (2 T +4 P)

Phase balances in 1-component systems. Clapeyron equation. Two-component phase diagrams: Liquid-vapor, liquid-liquid, and solid-liquid balance. Structure of the phase diagrams. Three component systems.

Unit 6.- Chemistry of surfaces. (2 T + 3 P)

Interface. Surface thermodynamics. Superficial films. Adsorption. Colloids.

Unit 7.-Electrochemistry and Battery. (2 T + 3 P)

Redox reactions. Faraday laws. Electrode potentials. Battery thermodynamics: Nernst equation. Concentration stacks. Applications.

Unit 8.- Kinetics of reactions. (4 T + 10 P + 4 L)

Determination of the kinetic equations. Reaction mechanisms. Approximation of the limiting stage and the steady-state. Influence of temperature on kinetic constants. Experimental techniques for the measurement of reaction rates. Solution reactions. Catalysis. Enzymatic catalysis. Inhibition. Heterogeneous catalysis. Photochemistry. Dynamic theories of chemical reactivity.

Methodology

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Master classes.

Problems and questions discussion with small groups.

Laboratory sessions with the aim of knowing the laboratory safety procedures and the techniques useful for the subject.

Development plan

Learning activities

Activity type	Description	Contact activity	student	Activitat no presei Alumne	ncial	Evaluation	Total tim	ne
		Target	Hours	Student work	Hours	Hours	Hours	ECTS
Master class	Master class (Classroom. Large group)	Explanation of the main concepts	20	Study: Gain, understant and synthesize knowledge	28	2	50	2
Problems and cases	Participative session (Classroom. Large group)	Resolution of problems and cases	22	Learn to solve problems and cases	32	2	56	2.2
Seminar	Participative session (Small group)	Conducting discussion activities	10	Solve problems and cases. To argue	20	1	31	1
Laboratory	Laboratory session (Small group)	Practice development: understanding phenomena, measuring	8	Write a report	4	1	13	0.8
Total			60		84	6	150	6

Evaluation

Activity type	Evaluation activity		Percentatge grading
Activity type	Procedure	Number	(%)
Master class	Written tests of the theoretical program of the subject	2	35
Practice cases	Case studies deliveries or written tests	4	5
Laboratory	Delivery of reports. Written or oral tests2		5

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Total 100

FINAL NOTE: average of the partial mark, provided that each partial mark is greater than 3.5.

Bibliography

- LEVINE, I.N. 2003 Físico-química. McGraw-Hill. Quinta edición ATKINS, P.W. 1999 (6ª Ed.) Química Física Ediciones Omega.
- CLARET, J., MAS, F., SAGUÉS, F.- Termodinámica Química y Electroquímica. Libros del Index. Barcelona 1996.

Bibliografía Complementaria

- AGUILAR, A, GÓMEZ, E y LUCAS, J. M. -1997- Cinética Química -Libros del Index. Universidad
- HIEMENZ, P. C-1997 (3ª Ed) Principles of Colloid and Surface Chemistry- Marcel Dekker, Inc.