



## IDENTIFYING DATA

### Physical chemistry I

Subject	Physical chemistry I			
Code	V11G200V01303			
Study programme	(*)Grao en Química			
Descriptors	ECTS Credits	Choose	Year	Quadmester
	6	Mandatory	2nd	1st
Teaching language	Spanish Galician			
Department				
Coordinator	Hervés Beloso, Juan Pablo			
Lecturers	Hervés Beloso, Juan Pablo Mandado Alonso, Marcos			
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General description	<p>Physical Chemical I is one of the first contacts of a student of Chemistry with the Physical Chemistry. This discipline studies the properties and the behaviour of the chemical systems employing the methods of the Physics. This matter presents the rigorous macroscopic treatment of chemical systems in equilibrium, systems already entered in Chemistry I. Taking advantage of the basic knowledge of the principles of the Thermodynamics, they will be applied to systems of chemical interest to obtain a quantitative description of them. For this purpose, it is fundamental to be familiarised with differential calculus in more than a variable and integral calculus in one variable, skill already seen in Mathematics II.</p> <p>The knowledge on the macroscopic description of the chemical systems that will be reached in this subject are complementary with the contents of the subject Physical Chemistry III the following year. The experimental applications of these knowledges will be studied in the subject of the second tern Physical Chemistry II.</p>			

## Competencies

Code	
C6	Demonstrate knowledge and understanding of essential facts, concepts, principles and theories in: principles of thermodynamics and their applications in chemistry
C18	Demonstrate knowledge and understanding of essential facts, concepts, principles and theories: principles of electrochemistry
C19	Apply knowledge and understanding to solve basic problems of quantitative and qualitative nature
C20	Evaluate, interpret and synthesize data and chemical information
C23	Present oral and written scientific material and scientific arguments to a specialized audience
D1	Communicate orally and in writing in at least one of the official languages of the University
D3	Learn independently
D4	Search and manage information from different sources
D5	Use information and communication technologies and manage basic computer tools
D6	Use mathematics, including error analysis, estimates of orders of magnitude, correct use of units and data representations
D7	Apply theoretical knowledge in practice
D8	Teamwork
D9	Work independently
D12	Plan and manage time properly
D13	Make decisions
D14	Analyze and synthesize information and draw conclusions
D15	Evaluate critically and constructively the environment and oneself

## Learning outcomes

Expected results from this subject	Training and Learning Results
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Employ the concept of function of state to calculate the variations of the distinct functions of thermodynamic state of a pure substance.	C6 C19 C20 C23	D1 D3 D4 D5 D6 D7 D8 D9 D12 D13 D14 D15
Obtain the entropy of a substance from calorimetric measures	C6 C19 C20 C23	D1 D3 D4 D5 D6 D7 D8 D9 D12 D13 D14 D15
Establish if a process that suffers a pure substance is spontaneous or no from the calculation of the variations of the thermodynamic properties	C6 C19 C20 C23	D1 D3 D4 D5 D6 D7 D8 D9 D12 D13 D14 D15
Handle thermodynamic tables to obtain values of the distinct functions of thermodynamic state of reaction and calculate the thermodynamic functions of reaction to distinct temperatures	C6 C19 C20 C23	D1 D3 D4 D5 D6 D7 D8 D9 D12 D13 D14 D15
Calculate the fugacity function for a real gas from his equation of state or from experimental measures	C6 C19 C20 C23	D1 D3 D4 D5 D6 D7 D8 D9 D12 D13 D14 D15

Calculate the thermodynamic constant of reactions in solution, from the concentrations of the species or from the thermodynamic functions	C6	D1
	C19	D3
	C20	D4
	C23	D5
		D6
	D7	
	D8	
	D9	
	D12	
	D13	
	D14	
	D15	
Calculate the thermodynamic characteristics of a change of phase, and know the interval of applicability of the equations employed	C6	D1
	C19	D3
	C20	D4
	C23	D5
		D6
	D7	
	D8	
	D9	
	D12	
	D13	
	D14	
	D15	
Calculate the thermodynamic properties of an ideal solution from his composition	C6	D1
	C19	D3
	C20	D4
	C23	D5
		D6
	D7	
	D8	
	D9	
	D12	
	D13	
	D14	
	D15	
Calculate the colligative properties of a solution from the concentration of the solute and the properties of the dissolvent. Establish when these results can be applied to a real case	C6	D1
	C19	D3
	C20	D4
	C23	D5
		D6
	D7	
	D8	
	D9	
	D12	
	D13	
	D14	
	D15	
Calculate the activities and activity coefficients of non-electrolytic solutions and employ the suitable model for the calculation of the mean ionic activity coefficient. Obtain this coefficient from experimental measures	C6	D1
	C18	D3
	C19	D4
	C20	D5
	C23	D6
	D7	
	D8	
	D9	
	D12	
	D13	
	D14	
	D15	

Employ pertinent experimental measures of the galvanic cells to determine functions of state of reaction	C6 C18 C19 C20 C23	D1 D3 D4 D5 D6 D7 D8 D9 D12 D13 D14 D15
Determine the activity and/or the mean ionic activity coefficient of an electrolyte by means of experimental measures of EMF of galvanic cells	C6 C18 C19 C20 C23	D1 D3 D4 D5 D6 D7 D8 D9 D12 D13 D14 D15
Analyse the importance of the interphase and of the distinct phenomena associated to the interphase in the thermodynamic processes of the material systems	C6 C19 C20 C23	D1 D3 D4 D5 D6 D7 D8 D9 D12 D13 D14 D15
Establish the importance of the superficial tension and the distinct processes associated in function of the nature of the system	C6 C19 C20 C23	D1 D3 D4 D5 D6 D7 D8 D9 D12 D13 D14 D15
Differentiate between processes of physical and chemical adsorption and describe the models employed for his description	C6 C19 C20 C23	D1 D3 D4 D5 D6 D7 D8 D9 D12 D13 D14 D15

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## Contents

Topic

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Principles of the thermodynamics in Chemistry.	First principle of the Thermodynamics. Internal energy. Enthalpy. Heat capacity. Thermochemistry. Second principle of the thermodynamics. Entropy. Molecular interpretation of the entropy. Third principle of the Thermodynamics. Calculation of the variations of entropy.
Thermodynamic functions	Equations of Gibbs. Relations of Maxwell. Calculation of variations of the functions of state. Open systems. Partial molar magnitudes. Chemical potential. Chemical potential of an ideal gas. Chemical potential in a mix of ideal gases. Chemical potential of the real gases. Fugacity.
Chemical equilibrium between gases.	Conditions of thermodynamic equilibrium. Degree of advance. Constant of thermodynamic balance in reactions in gas phase. Influence of the temperature in the constant of balance. Factors that affect to the position of the equilibrium: principle of Le Châtelier.
Balance of phases in systems of a component.	Concepts of component, phase and degree of freedom. Conditions of balance between phases. Rule of the phases. Changes of phase of prime importance. Equations of *Clapeyron and *Clausius-*Clapeyron. Changes of phase of upper order.
Ideal solutions.	Partial molar volumes. Equation of *Gibbs-*Duhem. Ideal dissolution: Law of *Raoult. Diagrams *P-*x and *T-*x. Ideal dilute solution: Law of Henry. Colligative Properties.
Non ideal solutions.	Deviations of the law of *Raoult. Activity and coefficient of activity. Coefficients of activity in the scales of molality and molarity. Electrolyte solutions. Theory of *Debye-*Hückel.
Chemical equilibrium in solution.	Constant of thermodynamic equilibrium in reactions in solution. Acid-base equilibria. Product of solubility. Saline effects. Electrochemical systems. Galvanic and electrolytic cells. Measure of the electromotive strength of a galvanic cell. Equation of *Nernst. Potential of electrode.
Thermodynamics of surfaces.	Surfaces and interfaces. Superficial tension. Phenomena derived of the superficial tension. Adsorption. Physisorption and Chemisorption Isotherms.

## Planning

	Class hours	Hours outside the classroom	Total hours
Master Session	26	31	57
Seminars	26	38	64
Troubleshooting and / or exercises	0	14	14
Self-assessment tests	0	10	10
Short answer tests	2	0	2
Long answer tests and development	3	0	3

\*The information in the planning table is for guidance only and does not take into account the heterogeneity of the students.

## Methodologies

	Description
Master Session	They will consist in the brief exposition by the professor of the fundamental aspects of each subject, employing the available material in the TEMA platform. Also numerical problems will be proposed for helping to comprise and settle concepts.
Seminars	Seminar will be devoted to the resolution of problems and will deepen on those aspects that present greater difficulties to the students. These classes will be mainly a task for the students under the supervision of the professor.

## Personalized attention

Tests	Description
Self-assessment tests	Students will solve autonomously questionnaires-type test through the TEMA platform and will be individually tutorized by the professor.
Troubleshooting and / or exercises	Students will solve autonomously proposed problems and will be individually tutorized by the professor.

## Assessment

Description	Qualification Training and Learning Results

Troubleshooting and / or exercises	Problems proposed for each subject of the matter.	Hasta un 7,5	C6 C18 C19 C20 C23	D1 D3 D4 D6 D7 D8 D9 D12 D13 D14 D15
Self-assessment tests	Quiz-tests in the TEMA platform	Hasta un 7,5	C6 C18 C19 C20	D3 D4 D5 D7 D9 D12 D13 D14 D15
Short answer tests	Short-writing exams on some parts of matter.	Hasta un 20	C6 C18 C19 C20	D1 D3 D4 D6 D7 D9 D12 D13 D14 D15
Long answer tests and development	Written examination of the contents of the matter.	Mínimo un 65	C6 C18 C19 C20	D1 D3 D4 D6 D7 D9 D12 D13 D14

### Other comments on the Evaluation

- The voluntary work of the student (tests + problems proposed) will be able to constitute until 15% of the final qualification whenever the student realise, at least, the half of the activities proposed along the course.

- It will be done a short written proof (of two hours of length) of the first-half of the matter. This proof can eliminate contents. The realisation of this proof is the minimum condition so that the matter was described in record. This short proof will be able to suppose until 20% of the final qualification.

-It will be realised a global written proof at the end of term (around three hours of length) on the whole of the contents of the matter. This global proof will suppose at least 65% of the final qualification. In case that the student surpass the short proof (> 5) students will be able to opt in the global written proof between examining only of the second half of the matter or of the whole of the subject. In the first case, the note of the global proof will do average with the short proof.

IMPORTANT: To surpass the matter in record is indispensable requirement reach in the global proof a minimum note of 4 points on 10.

- In the following callings of the matter the previous percentages will be respected and the qualifications obtained in the voluntary work and in the short proof realised during the course will be kept, except in the case of change of professor, who will be the one who establish new norms.

### Sources of information

Levine, **Fisicoquímica**, McGraw-Hill. 5ª Ed,

Atkins, **Química Física**, Panamerica, 8ª Ed,

Engel, **Química Física**, Pearson,

Chang, **Fisicoquímica**, McGraw-Hill,

Rodríguez Renuncio, **Termodinámica Química**, Síntesis, 2ª Ed,

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Levine, **Problemas de Físicoquímica**, McGraw-Hill,

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Rodríguez Renuncio, **Problemas resueltos de Termodinámica Química**, Síntesis,

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Metz, **Físicoquímica. Problemas y Soluciones**, McGraw-Hill,

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### **Recommendations**

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#### **Subjects that continue the syllabus**

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Physical chemistry II/V11G200V01403

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#### **Subjects that it is recommended to have taken before**

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Mathematics: Mathematics II/V11G200V01203

Chemistry: Chemistry I/V11G200V01105

Chemistry: Chemistry 2/V11G200V01204

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