



IDENTIFYING DATA

Physical chemistry I: Chemical thermodynamics

Subject	Physical chemistry I: Chemical thermodynamics			
Code	V11G201V01203			
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	Fernández Nóvoa, Alejandro Hervés Beloso, Juan Pablo Ramos Berdullas, Nicolás			
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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	
A2	Students can apply their knowledge and understanding in a manner that indicates a professional approach to their work or vocation, and have competences typically demonstrated through devising and sustaining arguments and solving problems within their field of study
B1	Autonomous learning ability
B3	Ability to manage information
C11	Know the principles of Thermodynamics and its applications in Chemistry
C13	Know the principles and applications of electrochemistry
C28	Interpret data derived from laboratory observations and measurements in terms of their meaning and relate them to the appropriate theory
C29	Demonstrate ability for numerical calculations and interpretation of experimental data, with correct use of units and estimation of uncertainty
D1	Ability to solve problems
D3	Ability to communicate in both oral and written form in Spanish and / or Galician and / or English

Learning outcomes

Expected results from this subject	Training and Learning Results			
Obtain the entropy of a substance from calorimetric measures	A2	B1 B3	C11 C28 C29	D1 D3
Establish if a process that suffers a pure substance is spontaneous or no from the calculation of the variations of the thermodynamic properties	A2	B1 B3	C11 C29	D1 D3

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	A2	B1 B3	C11 C28	D1 D3
Calculate the thermodynamic characteristics of a change of phase, and know the interval of applicability of the equations employed	A2	B1 B3	C11 C29	D1 D3
Calculate the thermodynamic properties of an ideal solution from his composition	A2	B1 B3	C11 C29	D1 D3
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	A2	B1 B3	C11 C28 C29	D1 D3
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	A2	B1 B3	C11 C13 C28 C29	D1 D3
Calculate the thermodynamic constant of reactions in solution, from the concentrations of the species or from the thermodynamic functions	A2	B1 B3	C11 C28 C29	D1 D3
Apply the theoretical knowledge acquired to obtain experimentally equilibrium constants, activity coefficients and other thermodynamic paramaters.	A2	B1 B3	C11 C28 C29	D1 D3

Contents

Topic	
The laws of the thermodynamic in Chemistry.	First Law of thermodynamics. Internal energy. Enthalpy. Heat capacities . Thermochemistry. Second law of thermodynamics. Entropy. Molecular interpretation of the entropy. Third law of thermodynamics. Calculation of the variations of entropy.
Thermodynamic functions	Gibbs Equations. Maxwell relationships. Calculation of variations of the state functions . Open systems. Partial Molar quantities. Chemical potential. Chemical potential of an ideal gas. Chemical potential of the real gases.
Phase equilibrium in systems of one component.	Concepts of component, phase and degree of freedom. Equilibrium conditions between phases. Phases Rule. First order transitions. Clapeyron and Clausius Equations.
Ideal Solutions.	Molar partial Volume. Gibbs-Duhem Equation. Ideal solutions: Raoult law. Vapour pressure diagrams. Ideal diluted solutions: Henry Law. Colligative Properties
Non-ideal Solutions.	Deviations of the Raoult law. Activity and activity coefficient . Electrolytic solutions. Debye-Hückel theory.
Chemical equilibrium	Equilibrium conditions . Extent of reaction. Perfect gas equilibria. Equilibrium in solution reactions. Response of equilibria to temperature. Le Chatelier´s principle. Acid-base equilibria. Solubility Product. Salt effects. Electrochemical cells. Nerst Equation.
(*)Prácticas de Laboratorio	(*)- Determinación experimental de constantes de equilibrio empregando técnicas espectrofotométricas ou potenciométricas. - Determinación experimental de entalpías de combustión, disolución, neutralización, fusión ou vaporización. - Determinación experimental de propiedades coligativas. - Determinación experimental de coeficientes de actividade

Planning

	Class hours	Hours outside the classroom	Total hours
Lecturing	26	33	59
Seminars	26	33	59
Laboratory practical	14	0	14
Problem and/or exercise solving	2.5	0	2.5
Self-assessment	0	4	4
Essay questions exam	3	0	3
Report of practices, practicum and external practices	0	6	6
Laboratory practice	0.5	2	2.5

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

Methodologies

Description

Lecturing	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.
Laboratory practical	Completion of laboratory practices under the supervision of a teacher in an autonomous way in sessions of 3,5 hours. With advance enough, students will have in the TEM@ platform guide notes for the practices together with all the additional necessary material. Guide notes will present the essential elements to realise the experimental practices, as well as the fundamental theoretical points and further data treatment. After practice completion, in the terms set by the teacher, it will be necessary to deliver the corresponding report, elaborated following the guidelines given by the teacher.

Personalized assistance

Methodologies	Description
Lecturing	In tutorial sessions, the teacher may solve in an individual and more personal way those doubts of the students that can arise along the course in any one of its parts (theory lessons, seminars, laboratory practice and the several types of autonomous activities to realise).
Seminars	In tutorial sessions, the teacher may solve in an individual and more personal way those doubts of the students that can arise along the course in any one of its parts (theory lessons, seminars, laboratory practice and the several types of autonomous activities to realise).
Laboratory practical	In tutorial sessions, the teacher may solve in an individual and more personal way those doubts of the students that can arise along the course in any one of its parts (theory lessons, seminars, laboratory practice and the several types of autonomous activities to realise).
Tests	Description
Problem and/or exercise solving	In tutorial sessions, the teacher may solve in an individual and more personal way those doubts of the students that can arise along the course in any one of its parts (theory lessons, seminars, laboratory practice and the several types of autonomous activities to realise).
Essay questions exam	In tutorial sessions, the teacher may solve in an individual and more personal way those doubts of the students that can arise along the course in any one of its parts (theory lessons, seminars, laboratory practice and the several types of autonomous activities to realise).
Report of practices, practicum and external practices	In tutorial sessions, the teacher may solve in an individual and more personal way those doubts of the students that can arise along the course in any one of its parts (theory lessons, seminars, laboratory practice and the several types of autonomous activities to realise).
Laboratory practice	In tutorial sessions, the teacher may solve in an individual and more personal way those doubts of the students that can arise along the course in any one of its parts (theory lessons, seminars, laboratory practice and the several types of autonomous activities to realise).
Self-assessment	In tutorial sessions, the teacher may solve in an individual and more personal way those doubts of the students that can arise along the course in any one of its parts (theory lessons, seminars, laboratory practice and the several types of autonomous activities to realise).

Assessment

	Description	Qualification	Training and Learning Results			
Problem and/or exercise solving	Proposed problems for each chapter of the subject. The students will solve part of them in short tests carried out in the seminars.	12.5	A2	B1 B3	C11 C13 C29	D1 D3
Self-assessment	Test tries in Tem@ platform	7.5	A2	B1 B3	C11 C13 C29	D1 D3
Essay questions exam	Global written exam	65	A2	B1 B3	C11 C13 C29	D1 D3
Report of practices, practicum and external practices	The report of a practice proposed by the teaching staff will be made, which must be presented taking care of the formal aspects related to the organization, the correct use of the units, the correct preparation of the graphics and the presentation of the results. The critical analysis of these and drawing conclusions will also be valued. In addition, all the practices carried out will be evaluated by means of oral questions that the students will be able to answer to the sight of their laboratory notebook.	5	A2	B1 B3	C11 C28 C29	D1 D3

Laboratory practice	The effort, attitudes, skills and competencies developed by the students during the performance of the different practices are scored here.	10	A2	B1	C11	D1
				B3	C28	C29

Other comments on the Evaluation

- The student's voluntary work (self-evaluating tests + proposed problems) may constitute up to 20% of the final grade.
- A written test of the first half of the subject will be made. This test can eliminate material if the mark is ≥ 5 .
- There will be a global written test at the end of the semester about all the content of the subject. This global test will involve at least 65% of the final grade. If the students have passed the written test of the first half of the subject (≥ 5) they may choose either the global written test exam or the second half of the subject. In the first case, the mark of the global test will be the average of the exams of the first and second half of the subject.

IMPORTANT:

- To pass the subject, it is mandatory to achieve a minimum score of 4 points out of 10 in the global test.
- To pass the subject, it is mandatory not to fail laboratory practical lessons.
- The participation of the student in any written test or in the laboratory lessons is the minimum condition for the subject to be qualified.

July exam: The marks obtained by the student during the course in the voluntary work and laboratory practical lessons will be maintained.

Sources of information

Basic Bibliography

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

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

Complementary Bibliography

Engel, **Química Física**, Pearson,

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

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

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

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

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

Recommendations

Subjects that continue the syllabus

Physical Chemistry II: Surfaces and Colloids/V11G201V01208

Contingency plan