UNIVERSIDADE DA CORUÑA

Teaching Guide				
Identifying Data				2016/17
Subject (*)	Química Física 3		Code	610G01018
Study programme	Grao en Química			
Descriptors				
Cycle	Period	Year	Type	Credits
Graduate	1st four-month period	Third	Obligatoria	6
Language	SpanishEnglish			
Teaching method	Face-to-face			
Prerequisites				
Department	Química Física e Enxeñaría Química 1			
Coordinador	Herrero Rodriguez, Roberto	E-mail	r.herrero@udc.es	
Lecturers	Barriada Pereira, José Luis	E-mail	jose.barriada@udc.es	
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Web	campusvirtual.udc.es/moodle			
General description	Physical Chemistry consists in the study of fundamental physical principles that govern the properties and behavior of chemical systems. A chemical system can be studied from a microscopic or a macroscopic point of view. In this course of Physical Chemistry the methodology to study the macroscopic equilibrium is introduced (Chemical Thermodynamics) The subjects taught in this course are the essential theoretical foundations for the subsequent subjects in Physical Chemistry. They are also a framework for all other branches of chemistry that necessarily apply many of the concepts studied in this course in the development of their specific programs.			

Study programme competences	
Code	Study programme competences
A1	Ability to use chemistry terminology, nomenclature, conventions and units
A3	Knowledge of characteristics of the different states of matter and theories used to describe them
A5	Understanding of principles of thermodynamics and its applications in chemistry
A14	Ability to demonstrate knowledge and understanding of concepts, principles and theories in chemistry
A15	Ability to recognise and analyse new problems and develop solution strategies
A16	Ability to source, assess and apply technical bibliographical information and data relating to chemistry
A21	Understanding of qualitative and quantitative aspects of chemical problems
B2	Effective problem solving
B3	Application of logical, critical, creative thinking
C3	Ability to use basic information and communications technology (ICT) tools for professional purposes and learning throughout life

Learning outcomes			
Learning outcomes	Study programme competences		
To know the principles of thermodynamics and their applications in chemistry	A1 A3 A5 A14 A15 A16 A21	B2 B3	C3
To solve complex problems through the use of spreadsheets.	A1 A14 A15 A16 A21	B2 B3	C3

To adquire skills in literature search of real and research applications about the subject contents of the course	A14 A15 A16 A21	B3	C3

Contents	
Topic	Sub-topic
1. Introduction to Chemical Thermodynamics.	Previous concepts and mathematical properties
2. The principles of Thermodynamics.	First law: internal energy, enthalpy, heat capacities. Second law: entropy, calculating the entropy change in simple systems.
3. Thermodynamic potentials and evolution of systems	Equilibrium conditions in closed systems: the Gibbs and Helmholtz functions. Thermodynamic relationships for a closed system. Applications: thermodynamic equations of state, the difference between the heat capacities, the Joule-Thomson coefficient.
4. Thermodynamics standard reaction functions	Standard enthalpy: Kirchhoff's and Hess's law. Standard Entropy: the third law of thermodynamics, conventional entropy determination. Standard Gibbs energy. Using thermodynamic tables.
5. Thermodynamics of systems of variable composition	The chemical potential. Partial molar properties. Material equilibrium conditions: phase equilibrium and chemical equilibrium.
6. Gas state thermodynamics	The ideal gas: chemical potential and properties, ideal gas mixture. Real gases: equation of state and fugacity, fugacity calculation.
7.Phase equilibria in systems of one component	The phase rule. Phase diagram for one-component systems. Clapeyron and Clausius-Clapeyron equations. Classification of phase transitions.
8. Solutions	Ideal solution: Raoult's Law. Ideally dilute solution: Henry's Law. Mixing functions. Nonideal solutions of nonelectrolytes: activity and activity coefficients, the Gibbs-Duhem equation, excess functions. Solutions of electrolytes: the activity coefficient of ionic species.
9. Phase equilibria in multicomponent systems	Liquid-vapor equilibrium: ideal solution at constant T and P constant, fractional distillation, azeotropic mixtures. Liquid-liquid equilibrium: miscibility. Solid-liquid equilibrium: temperature-composition diagrams, simple eutectic, compound formation with congruent and incongruent melting, thermal analysis. Solution-crystalline solid equilibrium. Colligative properties: freezing point depression, boiling point elevation, osmotic pressure, vapor-pressure lowering. Nernst's distribution law.
10. Chemical equilibrium	Chemical equilibrium in gas mixtures: the equilibrium constant, changes in chemical equilibrium-Le Chatelier's principle. Chemical equilibrium in solution. Chemical equilibrium with pure solids and liquids.
11. Surface thermodynamics	The interface: surface tension. Curved interfaces: capillary rise. Adsorption on solid: physisorption and chemisorption, adsorption isotherms.
12. Electrochemical equilibrium	Electrochemical systems. Thermodynamics of electrochemical systems: the electrochemical potential. Galvanic and electrolytic cells. Nernst equation and standard electrode potentials. Types of reversible electrodes. Liquid junction potentials. Determination of thermodynamic parameters.

Planning				
Methodologies / tests	Competencies	Ordinary class hours	Student?s personal work hours	Total hours
Guest lecture / keynote speech	A1 A3 A5 B3	28	56	84
Problem solving	A1 A5 A14 A15 A21 B2 B3	11	33	44
ICT practicals	A14 B2 B3 C3	0.5	1.5	2

Critical bibliographical	A16 C3	0.5	1.5	2
Mixed objective/subjective test	A1 A3 A5 A14 A21 B2 B3	2	0	2
Speaking test	A3 A5 A14 B3	0	10	10
Mixed objective/subjective test	A1 A3 A5 A14 A15 A21 B2 B3	4	0	4
Personalized attention		2	0	2
(*)The information in the planning table is for guidance only and does not take into account the heterogeneity of the students.				

Methodologies	
Methodologies	**Description**
Guest lecture / keynote speech	Lectures, where the theoretical concepts will be introduced
Problem solving	Seminars in small groups where it will be shown the application of the theoretical contents from the lectures into problem solving
ICT practicals	Practical exercises where students will solve complex problems using computer programs
Critical bibliographical	Students will be taught to do bibliographic search. They will be asked to perform searches about topics related with the subject. Reading of papers related with topics from the subject will be also proposed
Mixed objective/subjective test	Students will be asked to solve a problem which combines the theoretical concepts and their application. Resolution will be achieved jointly with lecturer's guidance
Speaking test	Students will attent to two individual tutorial sesions where they will present test questions developed by themselves about the theoretical concepts of the course. Those questions will be discussed with the lecturer. This activity constitutes the assessment of the theoretical concepts of the subject.
Mixed objective/subjective test	A final test will be done at the end of the semester. Students will be asked solving problems on their own

Personalized attention	
Methodologies	**Description**
ICT practicals Critical bibliographical Problem solving Speaking test	These works are proposed in the class and students must solve them supported by individual tutorials with the teacher. Part-time students and those with special academic leave permission will have access to the materials of the subject in the moodle application. They could ask for presential or email tutorials when necessary while they prepare for the final test.

Assessment			
Methodologies	**Competencies**	**Description**	**Qualification**
ICT practicals	A14 B2 B3 C3	Complex problem solving through calculation programs are proposed. Solved problems are delivered individually.	5
Critical bibliographical	A16 C3	Bibliographic searches of research articles related with practical applications of the subject proposed. Search results are delivered individually.	5
Mixed objective/subjective test	A1 A3 A5 A14 A15 A21 B2 B3	Final examination of the contents of the subject based on the autonomous, individual resolution of problems.	70

Mixed objective/subjective test	A1 A3 A5 A14 A21 B2 B3	It will be assessed the individual contribution to the resolution of all activities. The goal is for all students to be able to successfully complete the exercise.	10
Speaking test	A3 A5 A14 B3	Students are asked to make question test. These questions will be discussed with the lecturer and used to evaluate the theoretical knowledge acquired by the students.	10

Assessment comments
The student who engages in at least two of the activities or in the final exam will be considered to have attended on the subject at the time of the final mark. The above marks rating corresponds to January (first opportunity). Exceptionally, the rating of both opportunities will be made with the final test, scoring 10 out of 10, for those student at part time or with special academic leave permission. The rating of the second opportunity will be made only with a final test, scoring 10 out of 10. Honors grade: priority is given in the first opportunity. Honors grade may only be granted in the second opportunity if their number have not be exhausted in the first opportunity final qualifications. Should it be more candidates to honors grade than honors available, allocation will be done through a extraordinary exam. Scheduled activities dates: 1st activity: to be established 2nd activity: to be established Final testing will take place at the following dates and times(pending approval by the Faculty Board): -First Opportunity: Check the official dates approved by the Faculty Board -Second Opportunity: Check the official dates approved by the Faculty Board

Sources of information	
Basic	§LEVINE, I.N. (2004). Fisocoquímica.5ª Ed Vol 1 y 2. McGraw-Hill. §ATKINS, P.W. Química Física. (Cualquier edición)
Complementary	§ DENBIGH, K. (1985). Equilibrio Químico. AC. Madrid. § McQUARRIE, D.A., SIMON, J.D. (1997).Physical Chemistry. Univ. Science Books.. § DÍAZ PEÑA, M., ROIG MUNTANER, A. (1988).Química Física. Alhambra. § KLOTZ, I.M., ROSENBERG, R.M. (1981) Termodinámica Química. AC. § AVERY, H.E., SHAW, D.J. (1978). Cálculos básicos en Química Física.Reverté. § AVERY, H.E., SHAW, D.J. (1974). Cálculos superiores en Química Física.Reverté. § LABOWITZ, L.C., ARENTS, J.S. (1986). Fisicoquímica: Problemas y soluciones. AC. § GANDÍA, V. (1977). Problemas de Termología. Artes Gráficas Soler S.A. § METZ, C.R. (1991).Teoría y problemas de Química Física. McGraw-Hill (Schaum)

Recommendations
Subjects that it is recommended to have taken before
Matemáticas 1/610G01001 Matemáticas 2/610G01002 Física 1/610G01003 Física 2/610G01004 Química 2/610G01008
Subjects that are recommended to be taken simultaneously
Experimentación en Química Física/610G01019
Subjects that continue the syllabus
Química Física Avanzada/610G01020 Experimentación en Química Física/610G01019
Other comments

(*)The teaching guide is the document in which the URV publishes the information about all its courses. It is a public document and cannot be modified. Only in exceptional cases can it be revised by the competent agent or duly revised so that it is in line with current legislation.