UNIVERSIDADE DA CORUÑA

Teaching Guide				
Identifying Data				2014/15
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			
Prerequisites				
Department	Química Física e Enxeñaría Química 1			
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General description	A Química Física é o estudo dos principios físicos fundamentais que gobernan as propiedades e o comportamento dos sistemas químicos. Un sistema químico pode estudarse dende un punto de vista microscópico ou macroscópico. Neste curso de Química Física introdúcese a metodoloxía do estudo macroscópico de equilibrio (Termodinámica Química) Os contidos que se imparten nesta asignatura constituen os fundamentos teóricos imprescindibles para as seguintes asignaturas de Química Física e un marco de referencia para todas as demáis ramas da Química que, necesariamente, aplican boa parte dos conceptos estudiados nesta asignatura no desenvolvemento dos seus programas específicos.			

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			
Subject competencies (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	**Ordinary class hours**	**Student?s personal work hours**	**Total hours**
Guest lecture / keynote speech	21	42	63
Problem solving	13	39	52
ICT practicals	3	9	12
Critical bibliographical	1	4	5

Mixed objective/subjective test	2	0	2
Case study	2	8	10
Mixed objective/subjective test	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
Case study	A real case study, directly related with the application of Thermodynamics, will be posed to the students. Students will be asked explaining this case study using the basis of Thermodynamics and they will be asked proposing possible alternatives. Solution of the case study could be achieved with bibliographic search or even completed with simple experiments in the laboratory. Work will be developed in groups
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**
Case study Problem solving ICT practicals Critical bibliographical	These works are proposed in the class and students must solve them supported by individual tutorials with the teacher.

Assessment		
Methodologies	**Description**	**Qualification**
Mixed objective/subjective test	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. Competencies assessed: A1, A3, A5, A14, A21, B2, B3	10
Case study	Students are asked to make a group work. The contribution of each member to the overall work will be assessed. Competencies assessed: A5, A14, A15, A16, B3, C3	5
ICT practicals	Complex problem solving through calculation programs are proposed. Solved problems are delivered individually. Competencies assessed: A14, B2, B3, C3	7.5
Critical bibliographical	Bibliographic searches of research articles related with practical applications of the subject proposed. Search results are delivered individually. Competencies assessed: A16, C3	7.5

Mixed objective/subjective test	Final examination of the contents of the subject based on the autonomous, individual resolution of problems. Competencies assessed: A1, A3, A5, A14, A15, A21, B2, B3	70

Assessment comments
The student who engages in any of the activities 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). To facilitate completion of the course, there will be an extraordinary, optional test. To carry out this test regular attendance at lectures and seminars in small groups is required and also participation in all the other methodologies proposed. This optional test will score 7 out of 10 to calculate the final mark. Those students achieving a final mark of 5 out of 10 would not require to attend to the final test. In any case, students wishing to improve their final mark may be re-examined of the entire matter in the final test. The date of this extraordinary test shall be established by consensus among students, teachers and coordinator. 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 3rd 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	
Complementary	

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