



| 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<br>Herrero Rodriguez, Roberto   | E-mail | jose.barriada@udc.es<br>r.herrero@udc.es |         |
| 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)<br>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 / results |   |
|---------------------------------------|---|
| Code                                  | Study programme competences / results   |
| 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 / results      |          |    |
|  | results                                    |          |    |
| To know the principles of thermodynamics and their applications in chemistry | A1<br>A3<br>A5<br>A14<br>A15<br>A16<br>A21 | B2<br>B3 | C3 |



|   |                                |          |    |
|---|--------------------------------|----------|----|
| To solve complex problems through the use of spreadsheets.  | A1<br>A14<br>A15<br>A16<br>A21 | B2<br>B3 | C3 |
| To acquire skills in literature search of real and research applications about the subject contents of the course | A14<br>A15<br>A16<br>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 / Results        | Teaching hours (in-person & virtual) | 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<br>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<br>B3     | 2                                    | 0                             | 2           |
| Speaking test                   | A3 A5 A14 B3                  | 0                                    | 10                            | 10          |
| Mixed objective/subjective test | A1 A3 A5 A14 A15<br>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.<br>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 attend to two individual tutorial sessions 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<br>Critical bibliographical<br>Problem solving<br>Speaking test | These works are proposed in the class and students must solve them supported by individual tutorials with the teacher.<br>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 / Results | 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

|                      |  |
|----------------------|--|
| <b>Basic</b>         | §LEVINE, I.N. (2004). Fisocoquímica.5ª Ed Vol 1 y 2. McGraw-Hill. §ATKINS, P.W. Química Física. (Cualquier edición)  |
| <b>Complementary</b> | § 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.