# UNIVERSIDADE DA CORUÑA

**Teaching Guide**

| Identifying Data | | | | 2020/21 |
|---|---|---|---|---|
| Subject (*) | Physical Chemistry 3 | | Code | 610G01018 |
| Study programme | Grao en Química | | | |

| Descriptors | | | | |
|---|---|---|---|---|
| Cycle | Period | Year | Type | Credits |
| Graduate | 1st four-month period | Third | Obligatory | 6 |
| Language | SpanishEnglish | | | |
| Teaching method | Hybrid | | | |
| Prerequisites | | | | |
| Department | Química | | | |
| Coordinador | Herrero Rodriguez, Roberto | E-mail | r.herrero@udc.es | |
| Lecturers | Barriada Pereira, José Luis | E-mail | jose.barriada@udc.es | |
| | Herrero Rodriguez, Roberto | | 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) 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. | | | |
| Contingency plan | 1. Modifications to the contents<br><br>2. Methodologies<br>*Teaching methodologies that are maintained<br><br>*Teaching methodologies that are modified<br>Teaching methodologies will be adapted to be followed through online media<br><br>3. Mechanisms for personalized attention to students<br><br>e-mail, Moodle Platform and Microsoft Teams<br><br>4. Modifications in the evaluation<br><br>*Evaluation observations: Evaluation will not be changed, just adapted to be done through online tools<br><br>5. Modifications to the bibliography or webgraphy | | | |

| 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 | | |
| 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 / Results | Teaching hours (in-person & virtual) | Student?s personal work hours | Total hours |
| Problem solving | A1 A5 A14 A15 A21 B2 B3 | 11 | 33 | 44 |
| Guest lecture / keynote speech | A1 A3 A5 B3 | 30 | 60 | 90 |
| 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 | 8 | 0 | 8 |
| Mixed objective/subjective test | A1 A3 A5 A14 A15 A21 B2 B3 | 4 | 0 | 4 |
| Personalized attention | | 0 | 0 | 0 |

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

| Methodologies | |
|---|---|
| Methodologies | Description |
| Problem solving | Seminars in small groups where it will be shown the application of the theoretical contents from the lectures into problem solving |
| Guest lecture / keynote speech | Lectures, where the theoretical concepts will be introduced |
| 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 collection of problems which combines the theoretical concepts and their application. Two of these tests will be done in the semester. |
| 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 |

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 / Results | Description | Qualification |
|---|---|---|---|
| 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.<br>The final qualification obtained it will be the best of the following results:<br><br>20% of the tests done in the semester + 80% of the final test<br><br>OR<br><br>100% of the final test | 80 |
| Mixed objective/subjective test | A1 A3 A5 A14 A21 B2 B3 | The tests will be done along the semester. It will be assessed the individual contribution to the resolution of all activities. These tests do not eliminate contents to be evaluated in the final test. The qualifications obteined can contribute up to a 20% of the final qualification (10% each test) | 20 |

## Assessment comments

The student who engages in any of the two tests will be considered to have attended on the subject at the time of the final mark. The qualifications obtained will correspond 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 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.

## 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

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|---|---|
| Mathematics 1/610G01001 | |
| Mathematics 2/610G01002 | |
| Physics 1/610G01003 | 5/5 |
| Physics 2/610G01004 | |
| General Chemistry 2/610G01008 | |

<div align="center">**Subjects that are recommended to be taken simultaneously**</div>

Experimental Physical Chemistry/610G01019

<div align="center">**Subjects that continue the syllabus**</div>

Experimental Physical Chemistry/610G01019

Advanced Physical Chemistry/610G01020

<div align="center">**Other comments**</div>