(*)Facultade de Química

Presentation

The studies of Chemistry have a large tradition at the University of Vigo, where it has been taught during more than 30 years. The stablisment of the Universitary System of Galicia in the 90s and the current process of implantation of the European Space of Higher Education (EEES) modified the offer of degrees, but no the pioneering spirit of the chemists in research of in the quest for a better service to the society.

Degrees given in the Faculty

Degree in Chemistry

- Masters And Doctorates:
  - Industry and Chemical Research and Industrial Chemistry
  - Theoretical chemistry and Computational Modelling
- Master:
  - Science and Technology of Conservation of Fishing Products

Web page

Information about the Faculty of Chemistry:

http://quimica.uvigo.es

(*)Grao en Química

Subjects

Year 2nd

Code	Name	Quadmester	Total Cr.
V11G200V01301	Physics III	1st	6
V11G200V01302	Analytical chemistry I	1st	9
V11G200V01303	Physical chemistry I	1st	6
V11G200V01304	Organic chemistry I	1st	9
V11G200V01401	IT tools and communication in chemistry	2nd	6
V11G200V01402	Numerical methods in chemistry	2nd	6
V11G200V01403	Physical chemistry II	2nd	9

V11G200V01404	Inorganic chemistry I	2nd	9

IDENTIFYING DATA				
Physics III				
Subject	Physics III			
Code	V11G200V01301			
Study programme	(*)Grao en Química			
Descriptors	ECTS Credits	Choose	Year	Quadmester
	6	Mandatory	2nd	1st
Teaching language	Spanish			
Department				
Coordinator	Flores Rodríguez, Jesús Ramón			
Lecturers	Flores Rodríguez, Jesús Ramón Martínez Piñeiro, Manuel			
E-mail	flores@uvigo.es			
Web				
General description	The matter pretends to be an introduction to Quantum Mechanics and Statistical mechanics, oriented to theirs applications in Chemistry.			

Competencies	
Code	
C3	Demonstrate knowledge and understanding of essential facts, concepts, principles and theories in: principles of quantum mechanics and its application in the description of the structure and properties of atoms and molecules
C14	Demonstrate knowledge and understanding of essential facts, concepts, principles and theories: relationship between macroscopic properties and properties of individual atoms and molecules, including macromolecules
C19	Apply knowledge and understanding to solve basic problems of quantitative and qualitative nature
C20	Evaluate, interpret and synthesize data and chemical information
C22	Process and perform computational calculations with chemical information and chemical data
C23	Present oral and written scientific material and scientific arguments to a specialized audience
D1	Communicate orally and in writing in at least one of the official languages of the University
D3	Learn independently
D4	Search and manage information from different sources
D5	Use information and communication technologies and manage basic computer tools
D6	Use mathematics, including error analysis, estimates of orders of magnitude, correct use of units and data representations
D7	Apply theoretical knowledge in practice
D8	Teamwork
D9	Work independently
D12	Plan and manage time properly
D13	Make decisions
D14	Analyze and synthesize information and draw conclusions
D15	Evaluate critically and constructively the environment and oneself

Learning outcomes		
Expected results from this subject		Training and Learning Results
Describe *unificadamente the electromagnetic field by means of the laws of Maxwell. Apply the basic conditions of border in the empty or in presence of material means.	C3	D1 D12 D14
Derive the equation of propagation of an electromagnetic wave, characterised through his main characteristic. Relate this concept with the electromagnetic spectrum.	C3	D12 D14
Explain the empirical phenomena related with the interaction radiation matter no explained by the Classical Theory, and the solutions proposed for his resolution (duality wave corpuscle, *cuantización of the radiation).	C3	D12 D14 D15
Bill the postulates of the Quantum Mechanics and his consequences in the reformulation of the microscopic theory of the Classical Physics.	C3	D1 D12 D14 D15
Explain the foundations of the theory of mathematical operators, including the concepts of function and own value, spectrum, *linealidad and *hermiticidad, space of functions, etc.	C3	D1 D9 D12 D14

Write the fundamental operators of the Quantum Mechanics (position, linear and angular moment, Hamiltonian of simple systems).	C3 C19	D1 D9 D12 D14
Apply the previous concepts to the mechanical study-quantum of simple systems, like a particle subjected to a potential of *pozo square infinite, or to a harmonic potential, resolving the equation of Schrödinger independent of the time.	C3 C19	D1 D3 D6 D8 D12 D13 D14
Calculate the functions and own values of the for the moment angular operator.	C3 C19	D6 D12 D14
Resolve the equations of wave of the atom of hydrogen, calculating his orbital.	C3 C19	D6 D8 D12 D14
Resolve the equation of Schrödinger for atoms *polielectrónicos by means of approximate methods.	C3 C19 C20	D1 D5 D6 D9 D12 D13 D14
Explain of simple form the transitions between states and the spectrums of broadcast or resultant absorption.	C3 C19 C20 C22 C23	D1 D6 D8 D9 D12 D14 D15
Bill the laws of the Statistical mechanics that govern the behaviour of systems of particles, *particularizado to the statistics of Maxwell *Boltzmann. Derive the function of partition of a system and know in detail his physical meaning.	C14 C20 C22 C23	D1 D4 D5 D6 D7 D8 D12 D13
Apply the statistics of Maxwell *Boltzmann to the case of the ideal gases monkey and polyatomic to estimate thermodynamic properties from microscopic properties like mass, molecular geometry and frequencies of vibration.	C14 C19	D1 D4 D5 D6 D7 D8 D12 D13

Contents

Topic	
Electromagnetic field: equations of Maxwell.	Displacement current. Maxwell equations. Energy. Waves equations.
Quantización Of radiation. Wave-corpuscle duality	Ultraviolet catastrophe photoelectric Effect X-rays. Bragg condition. Braking radiation. Compton effect Wave-corpuscle duality
Principles of Quantum Mechanics	Limitations of Classical Physics and origin of Quantum Mechanics De Broglie Hypothesis Uncertainty Relationship Quantum Mechanics Postulates Virial Theorem
Quantum-mechanical Study of model systems	Introduction. Particle in a box of potential. Harmonic oscillator. Angular moment and rigid rotor.

Approximate methods	Introduction. Method of variations. Method of perturbations.
Hydrogen-like Atoms	Introduction. Resolution of the radial part of the equation of Schrödinger. Hydrogen-like Orbitals. Angular and magnetic moments electronic. Electronic spin. Spin-orbit coupling. Hyperfine structure. Spectra of Hydrogen-like atoms
Polielectronic atoms	Approximation of independent electrons. Antisymmetry Principle. Slater orbitals and basic functions. SCF-HF Method Terms and electronic levels. Spectra of polielectronic atoms
Statistical mechanics	Nomenclature and postulates. Canonical ensemble. Canonical partition function. Systems of non-interacting particles. Molecular partition function. Canonical partition function for a pure ideal gas. Boltzmann distribution law for non-interacting molecules. Statistical thermodynamics for ideal gases. Introduction to the study of real systems.

Planning

	Class hours	Hours outside the classroom	Total hours
Master Session	26	49.4	75.4
Troubleshooting and / or exercises	26	39	65
Introductory activities	1	0.6	1.6
Short answer tests	4	0	4
Long answer tests and development	4	0	4

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

Methodologies

	Description
Master Session	*Expoisición Of the fundamental appearances of each subject and approach of those that go to tackle in the seminars
Troubleshooting and / or exercises	Resolution of numerical problems, theoretical questions and development of the theoretical appearances posed in the Masterclasses with the participation of the student.
Introductory activities	Class of presentation of the *asignatura with exhibition: of parts of the *temario, contents, distribution in short proofs and final examination, general norms of evaluation, etc.

Personalized attention

Methodologies	Description
Master Session	Answers to the questions related with the matter that pose the students in the classes of resolution of problems and in *tutorías. The students will know from principle of course the schedules of *tutorías of the professors of the matter. In the *tutorías the students will be able to review his examinations
Troubleshooting and / or exercises	Answers to the questions related with the matter that pose the students in the classes of resolution of problems and in *tutorías. The students will know from principle of course the schedules of *tutorías of the professors of the matter. In the *tutorías the students will be able to review his examinations

Assessment

	Description	Qualification	Training and Learning Results
Troubleshooting and / or exercises	Basically it will centre in the resolution of exercises in the classroom. Nevertheless, it will be able to *tambien ask to the student that deliver exercises proposed and that the resolve of autonomous way. In this case the professor will be able to ask to the student that explain him *indivdualmente as it has resolved the exercise.	15	

Short answer tests	They will celebrate 2 proofs of short answer. They will refer , respectively, to the matter of the subjects 1 to 3 and 4 to 8. The *superación of each one of them will allow that the students can not going back to examine of this matter in the final examination of the *cuatrimestre, but no like this in the examination of second opportunity (June-July).	42.5
Long answer tests and development	When finishing the course will celebrate a complete proof in which the students that wish it will be able to repeat those appearances that did not surpass in the short proofs realised.	42.5

Other comments on the Evaluation

During the course will realise two short proofs referred to the subjects
1-3, the first, and to the subjects 4-8, the second. Both will contain
problems and questions and his *superación will free to the students of this
part of the *asignatura. Of voluntary way, the students will be able to participate in the resolution of exercises in the seminars or deliver exercises proposed.Also will be able to present to a final examination, that will include all the matter, that will allow them increase the punctuation reached in
the partial.All student will have to reach at least a qualification of 3.5 on 10
in the global of his proofs written to be able to accumulate the corresponding
punctuation to resolution of exercises.
In the second announcement will keep the punctuation reached
by means of the resolution of exercises. This examination will value of
similar way to the final examination.
The student that do not present to any proof during the course will be described in first announcement as no presented.

Sources of information

R. Eisberg, y R. Resnick, **Fisica Cuantica**, 1983,
M. Alonso y E.J. Finn, **Física**, 2000,
I. N. Levine, **Fisicoquímica**, 2004,
P.W. Atkins y J. de Paula, **Atkin's Physical Chemistry**, 2014,
J. Bertrán y otros, **Química Cuántica**, 2000,
I.N. Levine, **Química Cuántica**, 2001,

Recommendations

Subjects that continue the syllabus

Physical chemistry II/V11G200V01403

Subjects that it is recommended to have taken before

Physics: Physics I/V11G200V01102
Physics: Physics II/V11G200V01201
Mathematics: Mathematics I/V11G200V01104
Mathematics: Mathematics II/V11G200V01203

IDENTIFYING DATA

Analytical chemistry I

Subject	Analytical chemistry I			
Code	V11G200V01302			
Study programme	(*)Grao en Química			
Descriptors	ECTS Credits	Choose	Year	Quadmester
	9	Mandatory	2nd	1st
Teaching language	Spanish Galician			
Department				
Coordinator	Pérez Cid, Benita			
Lecturers	Bendicho Hernández, José Carlos González Romero, Elisa Leao Martins, Jose Manuel Pérez Cid, Benita			
E-mail	benita@uvigo.es			
Web				
General description	The main objective of the course Analytical Chemistry (I) is to provide students with an overview on qualitative and quantitative chemical analysis, in both applied and theoretical issues. The different subjects addressed in the course will establish the basis for learning other more advanced topics, particularly those associated with the design and application of more complex analytical methods. Classrooms will be supplemented by hands-on experiments and seminars.			

Competencies

Code	
A5	Students have developed those learning skills that are necessary for them to continue to undertake further study with a high degree of autonomy
C1	Demonstrate knowledge and understanding of essential facts, concepts, principles and theories: Major aspects of chemical terminology, nomenclature, units and unit conversions.
C2	Demonstrate knowledge and understanding of essential facts, concepts, principles and theories: types of chemical reactions and its main characteristics
C4	Demonstrate knowledge and understanding of essential facts, concepts, principles and theories: Basics and tools for solving analytical problems and characterization of chemical substances
C17	Demonstrate knowledge and understanding of essential facts, concepts, principles and theories in: metrology of chemical processes including quality management
C18	Demonstrate knowledge and understanding of essential facts, concepts, principles and theories: principles of electrochemistry
C19	Apply knowledge and understanding to solve basic problems of quantitative and qualitative nature
C20	Evaluate, interpret and synthesize data and chemical information
C21	Recognize and implement good scientific practices for measurement and experimentation
C22	Process and perform computational calculations with chemical information and chemical data
C25	Handle chemicals safely, considering their physical and chemical properties, including the evaluation of any specific risks associated with its use
C26	Perform common laboratory procedures and use instrumentation in synthetic and analytical work
C27	Monitor, by observation and measurement of physical and chemical properties, events or changes, and document and record them in a consistent and reliable way
C28	Interpret data derived from laboratory observations and measurements in terms of their significance and relate them to the appropriate theory
C29	Demonstrate skills for numerical calculations and interpretation of experimental data, with special emphasis on precision and accuracy
D1	Communicate orally and in writing in at least one of the official languages of the University
D3	Learn independently
D4	Search and manage information from different sources
D5	Use information and communication technologies and manage basic computer tools
D6	Use mathematics, including error analysis, estimates of orders of magnitude, correct use of units and data representations
D7	Apply theoretical knowledge in practice
D8	Teamwork
D9	Work independently
D12	Plan and manage time properly
D13	Make decisions
D14	Analyze and synthesize information and draw conclusions
D15	Evaluate critically and constructively the environment and oneself

Learning outcomes			
Expected results from this subject		Training and Learning Results	
Recognise the importance of the Analytical Chemistry in function of its aims.		C4 C19	D4 D14
Identify the fundamental stages of the analytical process like methodology for the resolution of analytical problems and select the appropriate analytical method.	A5	C4 C19	D4 D14
Describe the basic analytical properties (accuracy, precision, sensitivity and selectivity) and the types of errors that can affect to the experimental results.		C19 C20	D1 D4 D6 D14
Describe the fundamentals of sampling and sample preparation for the determination of different analytes.		C4 C19	D1 D4 D14
Calibration, use and cleaning of the material used in the analytical laboratory.	A5	C21 C26	D7 D9 D12
Prepare solutions of exact concentration (primary pattern) and approximate (secondary and reactive pattern auxiliaries) in function of its purpose and handle properly the concentration units.	A5	C1 C17 C21 C25	D6 D7 D9 D12 D13
Explain and interpret the basic knowledges of the separation and identification of chemical species in solution using a systematic separation approach.	A5	C2 C4 C19 C21 C26	D3 D7 D9 D12 D13 D14
Describe the principles of the quantitative chemical analysis (volumetric and gravimetric) and its experimental limitations.		C2 C4 C19	D1 D14
Identify and evaluate the possible interaction between concurrent reactions: acid-base, complexes, precipitation and redox.	A5	C2 C18 C19 C20	D7 D9 D12 D14
Elaborate and interpret titration curves of acid-base, complexes, precipitation and redox and know select the most suitable indicators.	A5	C2 C18 C19 C20	D5 D7 D9 D12 D14
Describe the foundations of the gravimetric analysis and the factors that influence the purity of precipitates.		C2 C20	D1 D4 D14
Carry out, in the laboratory, the precipitation and the separation by filtration in gravimetric analysis.		C2 C17 C19 C21 C25 C26 C28	D7 D8 D12
Use properly the gravimetric and volumetric techniques, including the suitable handling of the necessary equipment.	A5	C17 C19 C21 C26 C27	D7 D9 D12 D14
Handle the systematic calculation in the volumetric (direct, indirect and back titrations) and gravimetric analysis and learn how to interpret the results obtained.	A5	C20 C22 C28 C29	D6 D7 D14 D15 D16

Contents
Topic

Subject 1: Analytical Chemistry and analytical process.	The Analytical Chemistry as a metrological science. Classification of the analytical methods. The analytical process: steps. Types of analytical problems and working scales. Conceptual and technical hierarchy.
Subject 2: Evaluation of the analytical results.	Analytical properties. Errors in Analytical Chemistry: classification. Basic statistics applied to the expression of the results. Comparison and rejection of the results. Concept of traceability.
Subject 3: Introduction to the qualitative and quantitative Chemical Analysis .	Previous operations to the analysis. Sampling and sample treatment. Decomposition and dissolution. Introduction to the analytical separations. Qualitative analysis: characteristics of the binary answers. Classical quantitative analysis and instrumental. Methodologies of quantification. Calculable and relative methods.
Subject 4: Quantitative analysis: volumetric and gravimetric.	Volumetric reactions. Pattern solutions. Direct, indirect and back titrations. Formation, properties and purity of the precipitates. Calculations in volumetric and gravimetric analysis .
Subject 5: Acid-base titrations	Behaviour of monoprotic, polyprotic and amphoteric species. Titration curves. Detection of the end point: acid-base indicators. Titrant reagents. Analytical applications.
Subject 6: Complexometric titrations	Stability of the complexes. Masking reactions. Titration curves . Detection of the end point: metallochromic indicators. Analytical applications.
Subject 7: Precipitation titrations.	Factors affecting the solubility of precipitates. Titration curves. Detection of the end point: Mohr, Volhard and Fajans methods. Analytical applications.
Subject 8: Redox titrations	Factors influencing the redox potential. Titration curves. Detection of the end point: redox and specific indicators. Analytical applications.
Qualitative analysis (Laboratory)	Separation and identification of chemical species. (3 sessions) Resolution of an analytical problem by using a systematic separation procedure. (2 sessions)
Gravimetric analysis (Laboratory)	Gravimetric determination of nickel with dimethylglyoxime. (1 session)
Acid-base titrations (Laboratory)	Determination of the acidity of a vinegar sample. (1 session) Determination of acetylsalicycil acid in analgesics. (1 session)
Complexation titrations (Laboratory)	Standarization of an AEDT solution with Zn (II). (1 session) Determination of the hardness of a water sample. (1 session)
Precipitation titrations (Laboratory)	Determination of chloride in seawater using the Mohr method. (1 session)
Redox titrations (Laboratory)	Determination of wealth in oxygen in a hydrogen peroxide sample. (1 session) Determination of active chlorine in a bleach sample . (1 session)

Planning

	Class hours	Hours outside the classroom	Total hours
Master Session	26	33	59
Troubleshooting and / or exercises	26	36	62
Laboratory practises	45.5	12.5	58
Reports / memories of practice	0	6	6
Short answer tests	4	11	15
Long answer tests and development	3.5	12	15.5
Practical tests, real task execution and / or simulated.	3.5	6	9.5

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

Methodologies

	Description
Master Session	They are theoretical classes (two hours each week) in which the professor will offer a global vision of each one of the subjects of the program, specially in the most relevant issues and in those with more difficulty for the student. Classroom sessions will develop in an interactive way with the students, commenting with them the on-line material (available in the platform Tem@) and the most adapted bibliography for the preparation, in depth, of each subject.

Troubleshooting and / or exercises	Two hours per week will be devoted to problems and/or exercices solving (seminars) aimed at reinforcing the knowledges acquired during the classroom sessions. In some sessions the professor will explain to the students the problems-type that allow them to solve the worksheet exercises. Instead, in other sessions, the own students will solve and will explain in the blackboard the exercises proposed (on-line material). Will be able to request to the students that deliver, of individual form, some of these solved exercises , that will be corrected by the professor.
Laboratory practises	Students will do experiments in the laboratory, in an individual way, in 3.5 hours per session. The student will have the scripts of the practices in the platform Tem@, so that they can have a previous knowledge of the experiments to perform. During the development of the practices the student will elaborate a notebook in which they will annotate all the relative to the experiment carried out (reactions, procedures, observations, results, etc.).Those students who have approved the laboratory practices in the academic year 2015-16, do not need to repeat them. In this case, marks reached in the laboratory sessions will be maintained.

Personalized attention

Methodologies	Description
Laboratory practises	Time devoted by the teacher to solve all doubts and queries raised by students during the course. The teacher will inform students in advance on the suitable timetable for tutorials.
Troubleshooting and / or exercises	Time devoted by the teacher to solve all doubts and queries raised by students during the course. The teacher will inform students in advance on the suitable timetable for tutorials.
Tests	**Description**
Reports / memories of practice	Time devoted by the teacher to solve all doubts and queries raised by students during the course. The teacher will inform students in advance on the suitable timetable for tutorials.

Assessment

	Description	Qualification		Training and Learning Results	
Troubleshooting and / or exercises	The teacher will evaluate the exercices/problems included in the worksheets and solved by students.	8		C1 C2 C4 C18 C19 C22	D4 D5 D6 D7 D9 D14
Laboratory practises	The teacher will carry out a follow-up the performance of students in the laboratory sessions (skills acquired). It is important to indicate that it is COMPULSORY the assistance to all the laboratory sessions. If the number of absences is equal or upper than 25 % of the laboratory sessions, students will not be allowed to pass the course.	15	A5	C1 C2 C4 C17 C18 C19 C20 C21 C22 C25 C26 C27 C28 C29	D6 D7 D8 D9 D12 D13 D14 D15 D16
Reports / memories of practice	During the laboratory sessions, students will elaborate a noteboodk in which reflects the experimental work performed (reactions, procedures, observations, results, etc.). This notebook will be evaluated by the professor.	5		C20	D1 D3 D6 D9 D12 D14 D15 D16

Short answer tests	Students will carry out a first short proof about formulation of chemical compounds and calculation of concentrations that will represent a 7 % of the final mark. Students will carry out a second short exam corresponding to the four first subjects of the program (20% of the final mark). If students pass this exam, they only need to pass the examination corresponding to the rest of subjects in the final exam.	27	A5	C1 C2 C4 C19 C20 C22	D1 D3 D4 D5 D6 D7 D9 D12 D13 D14 D16
Long answer tests and development	Students will carry out a final written exam corresponding to the four last subjects of the program. Students who have not passed the exam corresponding to the first four subjects, will need to pass the examination of the whole course.	30	A5	C1 C2 C4 C18 C19 C20 C22	D1 D3 D4 D5 D6 D7 D9 D12 D13 D14 D16
Practical tests, real task execution and / or simulated.	At the end of the laboratory sessions, students will carry out a exam so that practical skills acquired can be evaluated. It is mandatory to overcome this examination to pass the practical part of the course.	15	A5	C28 C29	D1 D3 D6 D7 D9 D12 D13 D15 D16

Other comments on the Evaluation

First Announcement: To pass the course, it is compulsory to pass individually each one of the parts: theory and laboratory practices. For this, it is necessary to pass the written and laboratory examinations. The corresponding mark of the laboratory practices will be only taken into account once students have passed the theoretical examination. The participation of the student in any of the acts of evaluation of the course will involve the condition of presented and, therefore, the allocation of a mark. For this effect, they are considered acts of evaluation the assistance to practical laboratory sessions (two or more) and the realisation of written exams.

Second Announcement: In the extraordinary announcement the students will have to repeat those exams (theory and/or laboratory) that have not passed in the ordinary announcement. It will be preserved the mark reached by the student, during the course, in the other activities that appear in the evaluation section.

Sources of information

J. Guiteras, R. Rubio, G. Fonrodona, **Curso Experimental en Química Analítica**, Síntesis,

D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, **Fundamentos de Química Analítica**, 9ª Ed., Thompson, Madrid,

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Gary D. Christian, **Química Analítica**, 6ª Ed., McGraw-Hill,

D.A. Skoog, D.M. West , F.J. Holler, S.R. Crouch, **Química Analítica**, 7ª Ed., McGraw-Hill, Madrid,

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D. Harvey, **Química Analítica Moderna**, McGraw-Hill, Madrid,

M. Valcárcel, **Principios de Química Analítica**, Springer,

J. A. López Cancio, **Problemas Resueltos de Química Analítica**, Thompson,

P. Yañez-Sedeño Orive, J.M. Pingarrón Carrazón, F.J. Manuel de Villena Rueda, **Problemas Resueltos de Química Analítica**, Síntesis,

J. N. Miller y J.C. Miller, **Estadística y Quimiometría para Química Analítica**, 4ª Ed., Prentice Hall,

Recommendations

Subjects that continue the syllabus

Analytical chemistry II/V11G200V01503

Analytical chemistry 3/V11G200V01601

Subjects that are recommended to be taken simultaneously

Physics III/V11G200V01301
Physical chemistry I/V11G200V01303
Organic chemistry I/V11G200V01304

Subjects that it is recommended to have taken before

Chemistry, physics and biology: Integrated laboratory I/V11G200V01103
Chemistry, physics and geology: Integrated laboratory II/V11G200V01202
Chemistry: Chemistry I/V11G200V01105
Chemistry: Chemistry 2/V11G200V01204

IDENTIFYING DATA				
Physical chemistry I				
Subject	Physical chemistry I			
Code	V11G200V01303			
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	Hervés Beloso, Juan Pablo Mandado Alonso, Marcos			
E-mail	jherves@uvigo.es			
Web	http://webs.uvigo.es/qf1_web/			
General description	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. 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.			

Competencies	
Code	
C6	Demonstrate knowledge and understanding of essential facts, concepts, principles and theories in: principles of thermodynamics and their applications in chemistry
C18	Demonstrate knowledge and understanding of essential facts, concepts, principles and theories: principles of electrochemistry
C19	Apply knowledge and understanding to solve basic problems of quantitative and qualitative nature
C20	Evaluate, interpret and synthesize data and chemical information
C23	Present oral and written scientific material and scientific arguments to a specialized audience
D1	Communicate orally and in writing in at least one of the official languages of the University
D3	Learn independently
D4	Search and manage information from different sources
D5	Use information and communication technologies and manage basic computer tools
D6	Use mathematics, including error analysis, estimates of orders of magnitude, correct use of units and data representations
D7	Apply theoretical knowledge in practice
D8	Teamwork
D9	Work independently
D12	Plan and manage time properly
D13	Make decisions
D14	Analyze and synthesize information and draw conclusions
D15	Evaluate critically and constructively the environment and oneself

Learning outcomes		
Expected results from this subject	Training and Learning Results	
Employ the concept of function of state to calculate the variations of the distinct functions of thermodynamic state of a pure substance.	C6 C19 C20 C23	D1 D3 D4 D5 D6 D7 D8 D9 D12 D13 D14 D15

Obtain the entropy of a substance from calorimetric measures	C6 C19 C20 C23	D1 D3 D4 D5 D6 D7 D8 D9 D12 D13 D14 D15
Establish if a process that suffers a pure substance is spontaneous or no from the calculation of the variations of the thermodynamic properties	C6 C19 C20 C23	D1 D3 D4 D5 D6 D7 D8 D9 D12 D13 D14 D15
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	C6 C19 C20 C23	D1 D3 D4 D5 D6 D7 D8 D9 D12 D13 D14 D15
Calculate the fugacity function for a real gas from his equation of state or from experimental measures	C6 C19 C20 C23	D1 D3 D4 D5 D6 D7 D8 D9 D12 D13 D14 D15
Calculate the thermodynamic constant of reactions in solution, from the concentrations of the species or from the thermodynamic functions	C6 C19 C20 C23	D1 D3 D4 D5 D6 D7 D8 D9 D12 D13 D14 D15

Calculate the thermodynamic characteristics of a change of phase, and know the interval of applicability of the equations employed	C6 C19 C20 C23	D1 D3 D4 D5 D6 D7 D8 D9 D12 D13 D14 D15
Calculate the thermodynamic properties of an ideal solution from his composition	C6 C19 C20 C23	D1 D3 D4 D5 D6 D7 D8 D9 D12 D13 D14 D15
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	C6 C19 C20 C23	D1 D3 D4 D5 D6 D7 D8 D9 D12 D13 D14 D15
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	C6 C18 C19 C20 C23	D1 D3 D4 D5 D6 D7 D8 D9 D12 D13 D14 D15
Employ pertinent experimental measures of the galvanic cells to determine functions of state of reaction	C6 C18 C19 C20 C23	D1 D3 D4 D5 D6 D7 D8 D9 D12 D13 D14 D15

Determine the activity and/or the mean ionic activity coefficient of an electrolite by means of experimental measures of EMF of galvanic cells	C6 C18 C19 C20 C23	D1 D3 D4 D5 D6 D7 D8 D9 D12 D13 D14 D15
Analyse the importance of the interphase and of the distinct phenomena associated to the interphase in the thermodynamic processes of the material systems	C6 C19 C20 C23	D1 D3 D4 D5 D6 D7 D8 D9 D12 D13 D14 D15
Establish the importance of the superficial tension and the distinct processes associated in function of the nature of the system	C6 C19 C20 C23	D1 D3 D4 D5 D6 D7 D8 D9 D12 D13 D14 D15
Differentiate between processes of physical and chemical adsorption and describe the models employed for his description	C6 C19 C20 C23	D1 D3 D4 D5 D6 D7 D8 D9 D12 D13 D14 D15

Contents	
Topic	
Principles of the thermodynamics in Chemistry.	First principle of the Thermodynamics. Internal energy. Enthalpy. Heat capacity. Thermochemistry. Second principle of the thermodynamics. Entropy. Molecular interpretation of the entropy. Third principle of the Thermodynamics. Calculation of the variations of entropy.
Thermodynamic functions	Equations of Gibbs. Relations of Maxwell. Calculation of variations of the functions of state. Open systems. Partial molar magnitudes. Chemical potential. Chemical potential of an ideal gas. Chemical potential in a mix of ideal gases. Chemical potential of the real gases. Fugacity.
Chemical equilibrium between gases.	Conditions of thermodynamic equilibrium. Degree of advance. Constant of thermodynamic balance in reactions in gas phase. Influence of the temperature in the constant of balance. Factors that affect to the position of the equilibrium: principle of Le Châtelier.

Balance of phases in systems of a component.	Concepts of component, phase and degree of freedom. Conditions of balance between phases. Rule of the phases. Changes of phase of prime importance. Equations of *Clapeyron and *Clausius-*Clapeyron. Changes of phase of upper order.
Ideal solutions.	Partial molar volumes. Equation of *Gibbs-*Duhem. Ideal dissolution: Law of *Raoult. Diagrams *P-*x and *T-*x. Ideal dilute solution: Law of Henry. Colligative Properties.
Non ideal solutions.	Deviations of the law of *Raoult. Activity and coefficient of activity. Coefficients of activity in the scales of molality and molarity. Electrolyte solutions. Theory of *Debye-*Hückel.
Chemical equilibrium in solution.	Constant of thermodynamic equilibrium in reactions in solution. Acid-base equilibria. Product of solubility. Saline effects. Electrochemical systems. Galvanic and electrolytic cells. Measure of the electromotive strength of a galvanic cell. Equation of *Nernst. Potential of electrode.
Thermodynamics of surfaces.	Surfaces and interfaces. Superficial tension. Phenomena derived of the superficial tension. Adsorption. Physorption and Chemisorption Isotherms.

Planning

	Class hours	Hours outside the classroom	Total hours
Master Session	26	31	57
Seminars	26	38	64
Troubleshooting and / or exercises	0	14	14
Self-assessment tests	0	10	10
Short answer tests	2	0	2
Long answer tests and development	3	0	3

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

Methodologies

	Description
Master Session	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.

Personalized attention

Tests	Description
Self-assessment tests	Students will solve autonomously questionnaires-type test through the TEMA platform and will be individually tutorized by the professor.
Troubleshooting and / or exercises	Students will solve autonomously proposed problems and will be individually tutorized by the professor.

Assessment

	Description	Qualification	Training and Learning Results	
Troubleshooting and / or exercises	Problems proposed for each subject of the matter.	Hasta un 7,5	C6	D1
			C18	D3
			C19	D4
			C20	D6
			C23	D7
				D8
				D9
				D12
				D13
				D14
				D15

Self-assessment tests	Quiz-tests in the TEMA platform	Hasta un 7,5	C6 C18 C19 C20	D3 D4 D5 D7 D9 D12 D13 D14 D15
Short answer tests	Short-writing exams on some parts of matter.	Hasta un 20	C6 C18 C19 C20	D1 D3 D4 D6 D7 D9 D12 D13 D14 D15
Long answer tests and development	Written examination of the contents of the matter.	Mínimo un 65	C6 C18 C19 C20	D1 D3 D4 D6 D7 D9 D12 D13 D14

Other comments on the Evaluation

- The voluntary work of the student (tests + problems proposed) will be able to constitute until 15% of the final qualification whenever the student realise, at least, the half of the activities proposed along the course.

- It will be done a short written proof (of two hours of length) of the first-half of the matter. This proof can eliminate contents. The realisation of this proof is the minimum condition so that the matter was described in record. This short proof will be able to suppose until 20% of the final qualification.

-It will be realised a global written proof at the end of term (around three hours of length) on the whole of the contents of the matter. This global proof will suppose at least 65% of the final qualification. In case that the student surpass the short proof (> 5) students will be able to opt in the global written proof between examining only of the second half of the matter or of the whole of the subject. In the first case, the note of the global proof will do average with the short proof.

IMPORTANT: To surpass the matter in record is indispensable requirement reach in the global proof a minimum note of 4 points on 10.

- In the following callings of the matter the previous percentages will be respected and the qualifications obtained in the voluntary work and in the short proof realised during the course will be kept, except in the case of change of professor, who will be the one who establish new norms.

Sources of information

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

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

Engel, **Química Física**, Pearson,

Chang, **Fisicoquimica**, McGraw-Hill,

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

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

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

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

Recommendations

Subjects that continue the syllabus

Physical chemistry II/V11G200V01403

Subjects that it is recommended to have taken before

Mathematics: Mathematics II/V11G200V01203
Chemistry: Chemistry I/V11G200V01105
Chemistry: Chemistry 2/V11G200V01204

IDENTIFYING DATA

Organic chemistry I

Subject	Organic chemistry I			
Code	V11G200V01304			
Study programme	(*)Grao en Química			
Descriptors	ECTS Credits	Choose	Year	Quadmester
	9	Mandatory	2nd	1st
Teaching language	Spanish Galician			
Department				
Coordinator	Iglesias Antelo, María Beatriz			
Lecturers	Cid Fernández, María Magdalena Iglesias Antelo, María Beatriz Muñoz López, Luis Terán Moldes, María del Carmen			
E-mail	bantelo@uvigo.es			
Web				
General description	In this subject, students reach an understanding of the fundamental principles of Organic Chemistry, regarding organic compounds structure and reactivity. Following two lessons on general concepts, the reactivity of functional groups with multiple carbon-oxygen and carbon-carbon bonds, including aromatic compounds, is studied.			

Competencies

Code	
C2	Demonstrate knowledge and understanding of essential facts, concepts, principles and theories: types of chemical reactions and its main characteristics
C10	Demonstrate knowledge and understanding of essential facts, concepts, principles and theories: properties of aliphatic, aromatic, heterocyclic and organometallic compounds
C11	Demonstrate knowledge and understanding of essential facts, concepts, principles and theories: nature and behavior of functional groups in organic molecules
C12	Demonstrate knowledge and understanding of essential facts, concepts, principles and theories: structural features of chemical elements and their compounds, including stereochemistry
C13	Demonstrate knowledge and understanding of essential facts, concepts, principles and theories: main synthetic routes in organic chemistry, including interconversions of functional groups and the formation of carbon-carbon and carbon-heteroatom bonds
C19	Apply knowledge and understanding to solve basic problems of quantitative and qualitative nature
C20	Evaluate, interpret and synthesize data and chemical information
C21	Recognize and implement good scientific practices for measurement and experimentation
C23	Present oral and written scientific material and scientific arguments to a specialized audience
C25	Handle chemicals safely, considering their physical and chemical properties, including the evaluation of any specific risks associated with its use
C26	Perform common laboratory procedures and use instrumentation in synthetic and analytical work
C27	Monitor, by observation and measurement of physical and chemical properties, events or changes, and document and record them in a consistent and reliable way
C28	Interpret data derived from laboratory observations and measurements in terms of their significance and relate them to the appropriate theory
D1	Communicate orally and in writing in at least one of the official languages of the University
D3	Learn independently
D4	Search and manage information from different sources
D5	Use information and communication technologies and manage basic computer tools
D7	Apply theoretical knowledge in practice
D8	Teamwork
D9	Work independently
D12	Plan and manage time properly
D13	Make decisions
D14	Analyze and synthesize information and draw conclusions
D15	Evaluate critically and constructively the environment and oneself

Learning outcomes

Expected results from this subject	Training and Learning Results

Distinguish the most usual reactions in Organic Chemistry. Relate the energetic profile to a particular reaction. Differentiate the types of reagents. Differentiate the types of reaction intermediates.	C2 C19	D1 D3 D4 D7 D9 D12 D14
Establish the influence of the structure and the chemical features of the functional groups present in a molecule on its reactivity.	C2 C11	D1 D3 D4 D7 D9 D12 D14
Explain the reactivity of carbonyl compounds by means of a nucleophilic addition mechanism and the reactivity of carboxylic acids and their derivatives by means of an addition-elimination mechanism.	C2 C10 C11 C13	D1 D3 D4 D7 D9 D12 D14
Explain the reactivity of organic compounds with multiple carbon-carbon bonds by means of an electrophilic addition mechanism.	C2 C10 C11 C13	D1 D3 D4 D7 D9 D12 D14
Explain the reactivity of aromatic compounds through an electrophilic substitution mechanism.	C2 C10 C11 C13	D1 D3 D4 D7 D9 D12 D14
For each transformation, describe in detail the reaction mechanism, indicating reaction steps, transition states, intermediates etc.	C2 C11	D1 D3 D4 D7 D9 D12 D14
Predict the result of the reaction of a specific substrate with a given reagent in specific conditions, regarding regioselectivity and stereoselectivity of the process.	C11 C12 C13 C19	D1 D3 D4 D7 D9 D12 D14
Apply the rules for safety and health in laboratory work and carry out the treatment and correct elimination of the waste generated.	C25	D1 D3 D4 D7 D9 D12 D13 D14 D15
Carry out correctly the usual experimental procedures in simple organic preparations.	C21 C26	D1 D3 D4 D7 D9 D12 D13 D14

Carry out the work up of the reaction product, as well as its isolation and purification by means of usual techniques (extraction, distillation, recrystallization and chromatography).	C21 C26 C27	D1 D3 D4 D7 D9 D12 D13 D14
Write and describe appropriately the completed experiments in the laboratory notebook, so that they can be reproduced.	C23 C27 C28	D1 D3 D4 D7 D9 D12 D13 D14 D15
Look for and select information regarding the subjects studied.	C20	D4 D5 D8 D14 D15

Contents

Topic	
Lesson 1. Configurational stereoisomerism	Functional groups. Three-dimensional representation of organic structures. Absolute configuration of stereogenic centres, cyclic compounds and alkenes.
Lesson 2. Reactivity of organic compounds	Acid-base reactivity of organic compounds. Reaction mechanisms: stepwise reactions. Energetic profile of a reaction. Heterolytic bond cleavage. Ionic reactions. Reaction intermediates: carbanions. Redox reactivity of organic compounds. Formal states of oxidation.
Lesson 3. Addition reactions to carbon-carbon multiple bonds	Structure and general reactivity of functional groups with carbon-carbon multiple bonds: alkenes and alkynes. Hydrogenation: heats of hydrogenation and stability of alkenes and dienes; homolytic bond cleavage; concerted reactions. Electrophilic addition reactions to alkenes. Addition of HX; reaction intermediates: carbocations; regioselectivity; electrophiles and nucleophiles. Hydration reactions; orientation and stereochemistry. Addition of halogens (X2). Dihydroxylation reactions. Addition reactions to alkynes.
Lesson 4. Aromatic substitution reactions	Structure and general reactivity of aromatic compounds. General mechanism for the electrophilic aromatic substitution reaction. Reactions with non-carbon electrophiles. Reactions with carbon electrophiles. Electrophilic aromatic substitution reactions in substituted systems: orientation and reactivity. Modulation of the reactivity of aromatic rings. Nucleophilic aromatic substitution reactions.
Lesson 5. Reactions of nucleophilic addition to the carbonyl group	Structure and general reactivity of the carbonyl group (aldehydes and ketones). General mechanism for the nucleophilic addition reaction. Non reversible nucleophilic additions: addition of organometallic compounds (alkynyl anions, organolithium and organomagnesium reagents); addition of stabilized carbanions; addition of hydride. Reversible nucleophilic additions: addition of oxygen and sulphur compounds (water, alcohols and thiols); addition of nitrogen compounds (amines and other nitrogen compounds); addition of hydrogen cyanide.
Lesson 6. Reactions of nucleophilic substitution at the carbonyl group	Structure and general reactivity of carboxylic acids and their derivatives. Relative reactivity of acid derivatives: basicity and electrophilic character. Non reversible addition-elimination reactions: leaving group. Reversible addition-elimination reactions: basic catalysis and acid catalysis. Reactions with water and alcohols; reactions with ammonia and amines. Structure and reactivity of nitriles. Reactions of nitriles.
Practice 1	Separation of organic compounds mixtures by using two techniques: acid-base extraction (liquid-liquid extraction) and column chromatography. Four sessions.
Practice 2	Electrophilic addition to a double bond. One session.

Practice 3	Electrophilic aromatic substitution. One session.
Practice 4	Reduction of a ketone. One session.
Practice 5	Preparation of a hydrazone. One session.
Practice 6	Hydrolysis of an ester. One session.
Practice 7	Synthesis project. Four sessions.

Planning

	Class hours	Hours outside the classroom	Total hours
Master Session	26	26	52
Troubleshooting and / or exercises	26	49	75
Laboratory practises	45.5	9.5	55
Jobs and projects	0	9	9
Short answer tests	10	24	34

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

Methodologies

	Description
Master Session	Exposition by the teaching staff of the syllabus' general aspects, with special emphasis in its fundamental features. The teaching staff will facilitate, through Tema, all the material needed for the student's personal work. Prior to class, the student must use this material and consult the recommended bibliography to complete the information, in order to improve his/her academic progress in the subject.
Troubleshooting and / or exercises	Two hours each week will be devoted to discussing the most prominent aspects of the topic, to solve questions arisen in the development of the lesson and to the resolution of the proposed exercises.
Laboratory practises	Laboratory experiments will be carried out, individually, in 3.5 h sessions. The students will find, in advance, in Tema, the material needed for the preparation of the experiments. At the start of each session the professor will do an exposition of the contents to be developed. During the experiments the student will elaborate a laboratory notebook recording all the observations pertinent to the experiment. At the end of the session the student will answer some questions regarding the work done.

Personalized attention

Methodologies	**Description**
Troubleshooting and / or exercises	The teaching staff will attend the students' queries regarding the different topics within the subject. Attention to students schedules will be available through the Faculty of Chemistry webpage (http://quimica.uvigo.es/profesorado.php).
Tests	**Description**
Jobs and projects	The teaching staff will tutor the students while preparing and carrying out a short laboratory project.

Assessment

	Description	Qualification	Training and Learning Results	
Troubleshooting and / or exercises	Class participation and resolution by the student of all the problems and/or exercises proposed in time/conditions established by the teaching staff will be evaluated.	25	C2 C10 C11 C12 C13 C19 C20	D1 D4 D7 D8 D9 D14
Laboratory practises	Assistance to practical classes is mandatory. Monitoring of laboratory work will be evaluated as APT/NO APT. The following aspects will be considered in this section: pre-lab questionnaires, development of the experimental work, laboratory notebook, final questions. In order to pass the subject it is indispensable to be evaluated as APT.	0	C21 C25 C26 C27 C28	D12 D13 D14 D15

Jobs and projects	The student will elaborate a report prior to the execution of a short project in the laboratory during the last week of practical classes.	15	C20 C23 C25	D1 D4 D5 D9 D14
Short answer tests	First test: 15%. It will cover contents corresponding to the first three lessons. Second test: 15%. It will cover contents corresponding to the last three lessons. Written test for the experimental part: 15%. To be taken by the students that have achieved the mention APT in the monitoring of the laboratory work. In this test, student acquisition of competencies and skills related to the experimental aspects of the subject will be evaluated. Global test: 15%. In this test, student acquisition of competencies and skills related to the theoretical aspects of the subject will be evaluated.	60	C2 C10 C11 C12 C13 C19	D3 D7 D12 D14

Other comments on the Evaluation

In order to pass the subject in January, it will be required :

- Achieve mention **APT** in the evaluation of the laboratory work.
- Achieve a **minimum mark of 3 points out of 10** in each of the two short theoretical tests (first test and second test) and in the written test for the experimental part.
- Achieve a **minimum mark of 4 points out of 10** in the global test.

  If any of the previous conditions is not fulfilled, the final mark for the subject will be the mark obtained for the Short answer tests section multiplied by 0.6 (60%).

- Achieve a minimum mark of 5.0 in the weighted addition of the marks for all the sections (troubleshooting and/or exercises, short answer tests, jobs and projects).

The participation of the student in any of the acts of evaluation for the subject will involve the condition of "presentado/a" and, therefore, the assignment of a mark. The acts of evaluation that will be considered are: assistance to laboratory practices (25% or more) or the delivery of reports/exercises (25% or more) or taking any examination.

Students of 2nd and subsequent enrollment . Those students who have passed the laboratory practices during the courses 2014-15 or 2015-16 will be awarded the APT mention for the monitoring of laboratory work in the academic course 2016-17, not being necessary the completion of the experimental work again. However, they must elaborate the report of the project (15%) and take the written test for the experimental part (15%) to achieve the mark for the experimental part of the subject in the academic course 2016-17.

EVALUATION IN JULY

45% of the Short answer tests section can be repeated in July, in the following way:

- **Tests (30%)**. It will be carried out a global test in which the competences acquired in the theoretical aspects of the subject will be evaluated. The student must achieve **a minimum mark of 4 points out of 10** so that the result of this test will be taken into account in the global mark of the subject. This result will substitute the two lower marks obtained for the three theoretical tests carried out during the semester (first test, second test and global test), keeping the higher mark of the three, as long as it exceeds the required minimum.
- **Written test for the experimental part (15%)**. **A minimum mark of 3 points out of 10** must be achieved. The new mark will substitute the one achieved in the written test for the experimental part taken at the end of the semester.

The final mark will be the weighted addition of the marks for all the sections (troubleshooting and/or exercises, short answer tests, jobs and projects), as long as all the required minima are reached. If this is not the case, the final mark for the subject will be the mark obtained for the Short answer tests section multiplied by 0.6 (60%). In case that this mark was lower than the one obtained in the end of semester evaluation, the official mark will be this last one.

Sources of information
KLEIN, D., **Química Orgánica**, 1ª edición en español,
VOLLHARDT, K.P.C.; SCHORE, N.E, **Química Orgánica**, 5ª edición en español,
WADE, L.G., **Química Orgánica**, 7ª edición en español,

Supplementary bibliography

- CAREY, F. *Química Orgánica*, 6th edition in Spanish, McGraw-Hill Interamericana, 2006.
- CLAYDEN, J.; GREEVES, N.; WARREN, S. *Química Orgánica*, 2nd edition, Oxford University Press, 2012.
- YURKANIS BRUICE, P. *Fundamentos de Química Orgánica*, 3rd edition in Spanish, Pearson, 2015.
- DOBADO, J. A.; GARCÍA-CALVO, F.: GARCÍA, J. I. *Química Orgánica: ejercicios comentados*, Garceta, 2012.
- PALLEROS, D. R. *Experimental Organic Chemistry*, John Wiley and Sons, 2000.
- QUIÑOÁ, E.; RIGUERA, R. *Cuestiones y ejercicios de Química Orgánica*, 2nd edition, McGraw-Hill Interamericana, 2004.
- QUIÑOÁ, E.; RIGUERA, R. *Nomenclatura y representación de los compuestos orgánicos*, 2nd edition, McGraw-Hill Interamericana, 2005.

Recommendations
Subjects that continue the syllabus
Organic chemistry II/V11G200V01504
Organic chemistry III/V11G200V01704
Subjects that are recommended to be taken simultaneously
Physics III/V11G200V01301
Analytical chemistry I/V11G200V01302
Physical chemistry I/V11G200V01303
Subjects that it is recommended to have taken before
Biology: Biology/V11G200V01101
Chemistry, physics and biology: Integrated laboratory I/V11G200V01103
Chemistry, physics and geology: Integrated laboratory II/V11G200V01202
Chemistry: Chemistry I/V11G200V01105
Chemistry: Chemistry 2/V11G200V01204

IDENTIFYING DATA				
IT tools and communication in chemistry				
Subject	IT tools and communication in chemistry			
Code	V11G200V01401			
Study programme	(*)Grao en Química			
Descriptors	ECTS Credits	Choose	Year	Quadmester
	6	Mandatory	2nd	2nd
Teaching language	English			
Department				
Coordinator	Correa Duarte, Miguel Ángel			
Lecturers	Correa Duarte, Miguel Ángel Pérez Juste, Jorge Silva López, Carlos			
E-mail	macorrea@uvigo.es			
Web				
General description	The course aims to familiarize students with the use of chemical information sources (scientifical and technical in general) with emphasis on its use through the Internet, as well as with the use of all types of software tools for statistical calculations and chemical modeling . Attention is also paid to the acquisition of important communication skills (writing scientific and technical documents, academic, web design, etc).			

Competencies	
Code	
C20	Evaluate, interpret and synthesize data and chemical information
C22	Process and perform computational calculations with chemical information and chemical data
C23	Present oral and written scientific material and scientific arguments to a specialized audience
D1	Communicate orally and in writing in at least one of the official languages of the University
D2	Communicate at a basic level in English in the field of chemistry
D3	Learn independently
D4	Search and manage information from different sources
D5	Use information and communication technologies and manage basic computer tools
D8	Teamwork
D9	Work independently
D10	Work at a national and international context
D14	Analyze and synthesize information and draw conclusions
D15	Evaluate critically and constructively the environment and oneself
D16	Develop an ethical commitment
D18	Generate new ideas and show initiative

Learning outcomes		
Expected results from this subject		Training and Learning Results
(*)Distinguish and handle the distinct sources of scientific and technical information (books, magazines, summaries, databases, pages web, patents, etc.).	C23	D1 D2 D4 D5 D9 D14 D16
(*) Differentiate and classify the scientific magazines and the contributions to the same, respect to their thematic, aim and scope.		D2 D4 D5 D8 D9 D14

(*) Find and absorb information in a fast and effective way.	C23	D1 D2 D3 D5 D8 D9 D10 D15 D18
(*) Resume and classifiy the information for its effective broadcasting.	C23	D1 D2 D5 D8 D10 D16
(*) Argue the own opinions showing critical sense.	C23	D1 D2 D5 D8 D10 D16
(*) Performd simple written documents for the diffusion of knowledges and the scientific and technical results (p.ej. Articles, reports, works).	C23	D1 D2 D5 D8 D10 D16
(*) Handle with critical spirit the network (""""internet"""") as an information source.	C22	D3 D5 D9 D14 D16
(*) Perform academic oral presentations on subjects related with the Chemistry, using audiovisual media.	C23	D1 D2 D14 D18
(*) Organise the bibliography, with or without help of bibliographic tools.	C20	D3 D4 D5 D9 D14 D15
(*) Use computer programs for the preparation of figures and charts.	C22	D4 D5 D9
(*) Comprehend the basic principles and utility of simulation programs of chemical processes.	C22	D5 D9 D14
(*) Comprehend and explain texts in English related with Chemistry.	C23	D1 D2 D3 D8
(*) Draft simple documents and perform short oral presentations in English, on subjects related with Chemistry.	C23	D1 D2 D3 D8 D14
(*) Identify the most important programs of molecular modelling and understand the usefulnes of the results obtained.	C20	D3 D4 D14

Contents	
Topic	
The scietific literature: general aspects.	Structure and classification of the literature. General rules of a literature search. Function, organization and use of a scientific library.

Information Sources	Books. Journals. Technical reports. Conference Proceedings. Patents. Thesis. Government Publications. Standards. Videos. Dictionaries. Directories Encyclopedias Databases
Using Internet	Basic Internet services. Remote connection and file transfer utilities. Search engines. Electronic lists and subscription services. Other services. Structure, function and design of web pages.
Indexing and abstracting services	Identification of a scientific paper. The ISI Web of Knowledge (WOK). The Chemical Abstract Service (CAS) and the Scifinder. Other abstracting services. Handbooks.
Bibliographic Managers	Classification of bibliographic references: general principles. Use of popular software packages: Refworks and Endnote as examples.
Preparation of a scientific, technical or academic document	Parts of a scientific document. References, tables and figures : general principles. Use of computer templates. General aspects of the scientific style and the use of English. How to write: CVs, progress reports, grant requests and other academic documents.

Planning

	Class hours	Hours outside the classroom	Total hours
Master Session	14	28	42
Practice in computer rooms	26	52	78
Troubleshooting and / or exercises	2	22	24
Long answer tests and development	1.5	4.5	6

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

Methodologies

	Description
Master Session	The theoretical aspects of the subject are presented
Practice in computer rooms	Computer lab exercises: literature searches, use of bibliographic managers, use of statistical packages, report writing.
Troubleshooting and / or exercises	Report or article writing in English language. Simple exercises with modelling software

Personalized attention

Methodologies	Description
Practice in computer rooms	
Troubleshooting and / or exercises	

Assessment				
	Description	Qualification	Training and Learning Results	
Practice in computer rooms	Typically, literature searches	20	C22 C23	D1 D2 D3 D4 D5 D9 D15 D16
Troubleshooting and / or exercises	Tipically, database searches and use of utilities of modelling software.	40	C22 C23	D1 D2 D3 D4 D5 D8 D10 D14 D15 D18
Long answer tests and development	Written exam consisting of short questions.	40		D1 D2 D14 D15

Other comments on the Evaluation

Attendance at practical lectures (seminars) is compulsory. The student will be given a rating (0-10) as long as he/she has attended 3 or more seminar sessions, has delivered at least two reports on the exercises or practices proposed by the teacher or has done a written exam.

If the student fails in the first call he/she will be asked to improve some of the exercises or perform new ones provided by the teacher. In addition he/she will have to undergo a more thorough exam, which will weight 50% of the final grade.

Sources of information

Douville, J.A., **The literature of chemistry**, 1st,
Kaplan, S.M., **The English-Spanish Spanish-English dictionary of chemistry**, 2ª,
Day, R.A.; Gastel, B., **How to write and publish a scientific paper**, 7ª,

Recommendations

Subjects that are recommended to be taken simultaneously

Numerical methods in chemistry/V11G200V01402
Physical chemistry II/V11G200V01403
Inorganic chemistry I/V11G200V01404

Subjects that it is recommended to have taken before

Physics: Physics I/V11G200V01102
Physics: Physics II/V11G200V01201
Chemistry: Chemistry I/V11G200V01105
Chemistry: Chemistry 2/V11G200V01204

IDENTIFYING DATA				
Numerical methods in chemistry				
Subject	Numerical methods in chemistry			
Code	V11G200V01402			
Study programme	(*)Grao en Química			
Descriptors	ECTS Credits	Choose	Year	Quadmester
	6	Mandatory	2nd	2nd
Teaching language	Galician			
Department				
Coordinator	Besada Morais, Manuel			
Lecturers	Besada Morais, Manuel Hermida Ramón, José Manuel Leao Martins, Jose Manuel			
E-mail	mbesada@uvigo.es			
Web				
General description	"Machine translation into english of the original teaching guide" This matter is the mathemetical practical version of application to observed data and of numerical solution of numerous problems that have difficult, or impossible, analytical solution. It will allow to the student to obtain skills to handle big amounts of numerical information and consolidate the handle of a scientific calculator of big power.			

Competencies	
Code	
A3	Students have the ability to gather and interpret relevant data (usually within their field of study) to inform judgments that include reflection on relevant social, scientific or ethical issues
A5	Students have developed those learning skills that are necessary for them to continue to undertake further study with a high degree of autonomy
C19	Apply knowledge and understanding to solve basic problems of quantitative and qualitative nature
C22	Process and perform computational calculations with chemical information and chemical data
C29	Demonstrate skills for numerical calculations and interpretation of experimental data, with special emphasis on precision and accuracy
D3	Learn independently
D4	Search and manage information from different sources
D5	Use information and communication technologies and manage basic computer tools
D6	Use mathematics, including error analysis, estimates of orders of magnitude, correct use of units and data representations
D7	Apply theoretical knowledge in practice
D9	Work independently
D12	Plan and manage time properly
D13	Make decisions
D14	Analyze and synthesize information and draw conclusions

Learning outcomes			
Expected results from this subject	Training and Learning Results		
Use the numerical and symbolic packages of **MATLAB.		C22 C29	D5
Control distinct bases of numbering and *enterarse of the existence of errors committed in the approximations	A3	C29	D6 D9 D13 D14
Look for approximations of roots of equations of a variable and systems of equations.	A3 A5	C19 C22 C29	D3 D4 D5 D6 D7 D9 D12 D13 D14

Use *polynomials that adjust to several points of the plane.	A3 A5	C19 C22 C29	D3 D4 D5 D6 D7 D9 D12 D13 D14
Derive and integrate numerically, relate these numerical and analytical concepts and understand the because of his need.	A3 A5	C19 C22 C29	D3 D4 D5 D6 D7 D9 D12 D13 D14
Handle adjust of data to distinct types of curves of previous election by means of computer packages.	A3 A5	C19 C22 C29	D3 D4 D5 D6 D7 D9 D12 D13 D14

Contents	
Topic	
Subject 1. *Introduction the analysis **numerica.	Systems of numbering Need of the numerical methods. *Fontes And analysis of the error. Available *software.
Subject 2. Approximation of roots of equations of a variable.	*Condicionamiento Of the calculation of roots. Methods of separation of roots- Method of the *bisection. Method of Newton-**Raphson. *Theorem of the point did.
Subject 3. *Numerical interpolation.	The general problem of *interpolation. *Interpolation of *Lagrange. Error of *interpolation and excellent election of *nodes. *Interpolation **polinomial.
Subject 4. It adjust of curves.	It adjust of data. Straight of regression by square minima. Approximation of functions by square minima. *Interpolation **polinomial to *pieces.
Subject 5. *Derivación And numerical integration.	Diagrams of *derivación numerical *based in *interpolation. Formulas of *derivación *finite. Error of *derivación. Formulas of integration with *polynomial *interpolation. Error of integration. Formulas of *quadratures.
Subject 6. Numerical resolution of systems of equations.	Direct methods of resolution of linear systems: *Gauss. Classical *iterative methods. Methods of descent: Máximo descend and *gradient *conjugado. Resolution of systems no linear.

Planning			
	Class hours	Hours outside the classroom	Total hours
Master Session	13	26	39
Practice in computer rooms	26	52	78
Multiple choice tests	4	12	16
Troubleshooting and / or exercises	2	8	10
Jobs and projects	0	7	7
*The information in the planning table is for guidance only and does not take into account the heterogeneity of the students.			

Methodologies	
	Description
Master Session	Exhibition of the theoretical bases and orientation by part of the *profesorado on the contents of the matter
Practice in computer rooms	Development in the classrooms of computing of the exercises that propose in the theoretical classrooms using the scientific calculator **MATLAB.

Personalized attention	
Methodologies	**Description**

Practice in computer rooms	The students will work of autonomous way with the permanent supervision of the professor

Assessment

	Description	Qualification	Training and Learning Results	
Practice in computer rooms	At the end of the sessions in the classrooms of computing, the student will resolve some exercises of the even type that the ones of the realised in the classroom.	25	C19 C22 C29	D6
Multiple choice tests	During the course will realise **alomenos three partial proofs short type test and practical type that will explain a 25 by one hundred in the final qualification. Besides, in a final proof, will realise another tests type test of **tódala matter that *contabilizará another 10 by one hundred in the final qualification.	35	C19 C22 C29	D6
Troubleshooting and / or exercises	When finalising the course **realizaráse a practical proof resolving some practical exercises in the classroom of computing	30	C19 C22 C29	D6
Jobs and projects	**Participacion With *aprovechamiento in all the activities proposed by the *profesorado, are these to realise inside or out of the classroom.	10	C19 C22 C29	D6

Other comments on the Evaluation

The students that do not surpass the *materiaen the common announcement and pretend to do it in the *convocatoriaextraordinaria, will keep the qualifications obtained during the course in each *unode the previous sections, except the qualifications of the practical proofs of computing, that will be able to be recovered, and *lasdos proofs realised at the end of course that will be evaluated in the *examencorrespondiente. In this case, the student has to put in contact with the professor with sufficient *antelación to agree the work to realise before the final proofs.The participation of the student in any of the acts of evaluation of the matter will involve the condition of &*quot;presented&*quot; and, therefore, the allocation of a qualification. They consider acts of evaluation the assistance to the practices of computing (four or more), the realisation of some proof or the delivery of a minimum of 25% of the problems or exercises commissioned by the professor.

Sources of information

Chapra, S.C.; Canale, R.P., **Métodos numéricos para ingenieros**, 2010,

Besada, M., **MATLAB: todo un mundo**, 2007,

Mathews, J.H.; Fink, K.D., **Métodos numéricos con MATLAB**, 2000,

Nakamura, S., **Análisis numérico y visualización gráfica con MATLAB**, 1997,

Recommendations

Subjects that it is recommended to have taken before

Mathematics: Mathematics I/V11G200V01104

Mathematics: Mathematics II/V11G200V01203

IDENTIFYING DATA				
Physical chemistry II				
Subject	Physical chemistry II			
Code	V11G200V01403			
Study programme	(*)Grao en Química			
Descriptors	ECTS Credits	Choose	Year	Quadmester
	9	Mandatory	2nd	2nd
Teaching language	Spanish Galician			
Department				
Coordinator	Mosquera Castro, Ricardo Antonio			
Lecturers	Graña Rodríguez, Ana María Hermida Ramón, José Manuel Mosquera Castro, Ricardo Antonio Pastoriza Santos, Isabel Peña Gallego, María de los Ángeles Pérez Juste, Ignacio			
E-mail	mosquera@uvigo.es			
Web				
General description	Application of the principles and methods of Quantum Mechanics to the study of molecular structure and spectroscopy.			

Competencies	
Code	
C3	Demonstrate knowledge and understanding of essential facts, concepts, principles and theories in: principles of quantum mechanics and its application in the description of the structure and properties of atoms and molecules
C6	Demonstrate knowledge and understanding of essential facts, concepts, principles and theories in: principles of thermodynamics and their applications in chemistry
C8	Demonstrate knowledge and understanding of essential facts, concepts, principles and theories: main techniques for structural determination, including spectroscopy
C19	Apply knowledge and understanding to solve basic problems of quantitative and qualitative nature
C20	Evaluate, interpret and synthesize data and chemical information
C21	Recognize and implement good scientific practices for measurement and experimentation
C22	Process and perform computational calculations with chemical information and chemical data
C23	Present oral and written scientific material and scientific arguments to a specialized audience
C27	Monitor, by observation and measurement of physical and chemical properties, events or changes, and document and record them in a consistent and reliable way
C28	Interpret data derived from laboratory observations and measurements in terms of their significance and relate them to the appropriate theory
C29	Demonstrate skills for numerical calculations and interpretation of experimental data, with special emphasis on precision and accuracy
D1	Communicate orally and in writing in at least one of the official languages of the University
D3	Learn independently
D4	Search and manage information from different sources
D5	Use information and communication technologies and manage basic computer tools
D6	Use mathematics, including error analysis, estimates of orders of magnitude, correct use of units and data representations
D7	Apply theoretical knowledge in practice
D8	Teamwork
D9	Work independently
D12	Plan and manage time properly
D13	Make decisions
D14	Analyze and synthesize information and draw conclusions
D15	Evaluate critically and constructively the environment and oneself

Learning outcomes	
Expected results from this subject	Training and Learning Results

Formulate molecular Hamiltonians, with use of the Born-Oppenheimer approximation and discussion of their consequences.	C3 C20 C22 C23	D1 D3 D4 D5 D6 D7 D9 D12 D13 D14
Work with potential energy profiles and surfaces and understand related concepts.	C3 C19 C20 C22 C28 C29	D1 D3 D4 D5 D6 D7 D9 D12 D13 D14
Apply MO and EV methods for describing the chemical bond in simple systems and understand the limitations of these methods.	C3 C8 C19 C20 C21 C22 C23 C27 C28 C29	D1 D3 D4 D5 D6 D7 D9 D12 D13 D14 D15
Describe orbital localization techniques and the basis for atomic orbital hybridisation.	C3	D1 D3 D4 D6 D9
Apply, with understanding of their foundations and their limitations, the main calculation methods (HF, DFT, post-HF) for the study of molecular structures.	C3 C19 C20 C22 C23 C28 C29	D1 D3 D4 D5 D6 D7 D9 D12 D13 D14
Describe the forms of radiation-matter interactions and formulate the selection rules of electrical dipole.	C8	D1 D3 D4 D6 D9
Relate the radiation frequency with the molecular motion responsible of a spectroscopic transition.	C8	D1 D3 D4 D6 D7 D9
Justify the broadening of spectral lines and the enviromental effects on different spectra.	C8	D1 D3 D4 D6 D9

Interpret rotation and vibration-rotation spectra to obtain structural information, making use of simple quantum-mechanical models (rigid and flexible rotor and harmonic and anharmonic oscillators), selections rules and line assignment techniques.	C3 C8 C19 C20 C22 C23 C27 C28 C29	D1 D3 D4 D5 D6 D7 D9 D12 D13 D14
Discuss the Franck-Condon principle and its consequences.	C3 C8	D1 D3 D4 D6 D9
Interpret electronic and photoelectronic spectra and obtain structural information.	C3 C8 C19 C22	D1 D3 D4 D5 D6 D7 D9
Describe the different deactivation processes of excited electronic states and their representation in a Jablonski diagram.	C8 C19	D1 D3 D4 D6 D9
Describe the foundations of magnetic resonance spectroscopies, and interpret the physical origin of chemical shifts and couplings in NMR spectra.	C8 C19 C22	D1 D3 D4 D6 D9
Describe the instrumental peculiarities of the spectroscopic techniques in different spectral regions, as well as the foundations and applications of laser and Fourier-transform based techniques.	C8	D1 D3 D4 D6 D9
Apply the theoretical knowledge of Physical Chemistry I to determine experimentally chemical equilibrium constants, activity coefficients and thermochemical magnitudes.	C6 C19 C20 C21 C23 C27 C28 C29	D1 D3 D4 D5 D6 D7 D8 D9 D12 D13 D14 D15
New		

Contents	
Topic	
Introduction to group symmetry theory in chemistry	- Symmetry elements and operations. - Symmetry point groups. - Matrix representations. - Irrdeducible Representations. Character tables. - Chemical applications.
Qualitative spects of molecular electronic structure.	- Born-Oppenheimer approximation. - The H2+ molecule. - The MO method for homonucler and heteronuclear diatomic molecules. - The MO method in polyatomic molecules. - The VB method.
Quantitative treatments for the study of the molecular electronic structure.	- Hartree-Fock method. - post-Hartree-Fock methods. - Semiempirical methods. - Calculation of molecular properties

Introduction to Molecular Spectroscopy.	- Radiation-matter interaction: General approach. - Transition dipole moment integral. Selection rules. - Intensity and position of the spectral transitions. - Instrumentation.
Rotational spectroscopy.	- Pure rotation spectra of diatomic molecules. Rigid and elastic rotor models. - Pure rotation spectra of polyatomic molecules. - Pure rotation Raman spectra. - Instrumentation and applications.
Spectroscopy of Vibration-rotation.	- Vibration-rotation spectra of diatomic molecules. Harmonic and anharmonic oscillator models with rotation depending on vibration. - Vibration-rotation spectra of polyatomic molecules. - Vibration-rotation Raman spectroscopy. - Instrumentation and applications.
Electronic spectroscopy.	- Molecular Electronic states. - Vibration-rotation structure: Franck-Condon principle - Chromophore and auxochrome Groups. - Electronic deactivation Processes. - Instrumentation and applications. - Lasers. - Photoelectron Spectroscopy and related techniques.
Spectroscopies of Resonance.	- Introduction to the magnetic resonance. - Chemical shift. - Spin-spin interaction. Coupling Constant. - Electronic spin resonance Spectroscopy.
Practices of Chemical Thermodynamics (six sessions)	- Experimental determination of chemical equilibrium constants employing spectroscopic or potentiometric techniques. - Experimental determination of combustion, dissolution, neutralisation, fusion or vaporisation enthalpies. - Colligative Properties. - Experimental determination of activity coefficients employing potentiometric techniques.
Practices of Quantum Chemistry and Spectroscopy (seven sessions).	- Computational study of the electronic structure of different molecules - Computational Study of conformational isomery. - Computational study of simple chemical processes. - Prediction, theoretical interpretation and resolution of the vibration-rotation spectrum of HCl in gas phase. - Electronic spectroscopy: Spectrum of the I2 molecule in gas phase.

Planning

	Class hours	Hours outside the classroom	Total hours
Master Session	26	39	65
Seminars	26	39	65
Laboratory practises	45.5	4.5	50
Autonomous troubleshooting and / or exercises	0	10	10
Long answer tests and development	4	8	12
Reports / memories of practice	0	9	9
Short answer tests	2	5	7
Multiple choice tests	0	4	4
Practical tests, real task execution and / or simulated.	1	2	3

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

Methodologies

	Description
Master Session	They will consist in the presentation of the fundamental aspects of each subject by the teacher, using the material available in the TEM@ platform (diagrams, bulletins of problems, ...). In addition, numerical problems will be proposed for a better understanding of theoretical concepts.
Seminars	The classes of seminar will be mainly work of the student, under the supervision of the professor, and will be used for: - Problems solving, individually or by groups. - Once the student has worked the basic concepts, reinforce those contents of each subject that can present a greater complexity.

Laboratory practises	Completion of laboratory or computational chemistry practices under the supervision of a teacher in an autonomous way. Lab practices will be done by pairs 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 neccessary material. Guide notes will present the essential elements to realise the experimental or computational 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.
Autonomous troubleshooting and / or exercises	For each one of the subjects, some problems or other works to be solved by the student and delivered to the teacher in due time will be proposed.

Personalized attention

Methodologies	Description
Master Session	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 practises	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).
Autonomous troubleshooting and / or exercises	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**
Long answer tests and development	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).
Reports / memories of 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).
Short answer tests	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).
Multiple choice tests	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).
Practical tests, real task execution and / or simulated.	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
Laboratory practises	This mark comprises the effort and the attitude, the skills and the competitions developed by the student during the realisation of the laboratory practices.	ata 10,0	C3 D1 C6 D4 C8 D5 C19 D6 C20 D7 C21 D8 C22 D12 C27 D13 C28 D14 D15

Autonomous troubleshooting and / or exercises	For each one of the subjects or groups of subjects, problems or additional work to be done by the students will be proposed.	ata 3,75	C3 C8 C19 C20 C22 C23	D1 D3 D4 D5 D6 D9 D12 D13 D14 D15
Long answer tests and development	Realisation of one global writing test at the end of the term, in a date set by the Faculty of Chemistry.	como mínimo 52,5	C3 C8 C19 C20 C22	D1 D3 D6 D9 D12 D14 D15
Reports / memories of practice	Students must present a report for a laboratory practice proposed by the teachers. Students have to take care on format aspects related to the organisation, the correct use of the units, and the correct preparation of graphics and exhibition of the results. It will be also evaluated the critical analysis of results and getting right conclusions. Besides, all the practices will be evaluated by means of oral questions that the students can answer with the help of their laboratory notebook.	ata 5,0	C3 C6 C8 C19 C20 C22 C23 C27 C28 C29	D1 D3 D4 D5 D6 D8 D9 D12 D14
Short answer tests	Realisation of two short writing test (not liberatory) along the term, in dates set by the Faculty of Chemistry.	hasta 15	C3 C8 C19 C20 C22	D1 D3 D6 D9 D12 D14 D15
Multiple choice tests	For each each subject or group of subjects the student will have the opportunity of answer quiz tests through the TEM@ platform.	ata 3,75	C3 C8 C19	D3 D4 D6 D7 D9 D12 D14 D15
Practical tests, real task execution and / or simulated.	This written proof will be done in the date fixed by the Faculty of Chemistry and about the contents and skills that the student has to have purchased during the development of the laboratory practices. The questions will be situated, in some cases, in the context of some of the experiences realised by the student and, in others, will be more general. These questions will be used to evaluate the capacity to solve the problems presented.	ata 10,0	C3 C6 C8 C19 C21 C22 C28 C29	D1 D3 D4 D6 D7 D9 D12 D13 D14 D15

Other comments on the Evaluation

The evaluation of the course will take into account the part mentioned above, with distinction between the theoretical and the practical parts of the subject.

Theoretical part: The evaluation will suppose, in his group (short proofs (20%), long proof (70%), problems solving (5%), quiz-tests (5%)), 75% of the final qualification of the subject.

It is required to pass the subject to obtain in the long proof a minimum qualification of 4,0 on 10,0 points. In the case of not reaching this punctuation the qualification that will reflect in the record will be only the qualification of this examination, no taking into account any of the other sections.

Besides, it will be necessary to obtain an average of 3,0 in the theoretical questions of the examinations (short and long proofs). If it did not reach this punctuation the note reflected in the record will not be able to surpass 4,0.

Practical part: The evaluation will contribute, in his group (practices of laboratory (40%), reports and oral questions(20%) and proof written of practices (40%)), 25% to the final qualification of the matter.

It is indispensable requirement to surpass the matter to obtain in the practical part a minimum qualification of 5,0 on 10 points. In the case of not reaching said punctuation the qualification that will reflect in the record will not be able to surpass 4,0.

The assistance to the practical sessions is compulsory (absences to sessions should be properly justified) and, therefore, is not possible to approve the matter in the case of not to have them realised.

Condition of presented/no presented: The realisation of the two short proofs, or of the proof written of practices, or of the long proof or the assistance to but of five sessions of laboratory, will involve the condition of presented/to and, therefore, the allocation of a qualification.

Second Opportunity: For the evaluation in the second opportunity, will keep the qualifications and the percentages of the short proofs, of the problems/works proposed, of the practices of laboratory and the corresponding reports and of the quiz-tests. In the case to have an equal or upper qualification to 5,0 points in the global proof (long) or the same or upper to 4,0 in the proof written of practices, will keep said qualification (and the percentage) and only will be necessary to realise to another.

Sources of information

ATKINS, P. W.; DE PAULA, J., **Química Física**, 8ª edición,

BERTRÁN, J.; BRACHANDELL, V.; MORENO, M.; SODUPE, M., **"Química Cuántica"**, 2ª edición,

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LEVINE I.N., "Química Cuántica" (5ª ed.), Prentice Hall (2001).

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LEVINE I.N., "Fisicoquímica" (5ª ed.), McGraw Hilll (2004).

REQUENA A., ZÚÑIGA J., "Espectroscopía", Pearson Prentice Hall (2004).

Libros de problemas:

CARBALLEIRA OCAÑA L., PÉREZ JUSTE I., "Problemas de Espectroscopía Molecular", Netbiblo (2008).

LEVINE I.N., "Problemas de Fisicoquímica" (5ª ed.), McGraw Hilll (2005).

Libros de prácticas:

GARLAND C.W., NIBLER J.W., SHOEMAKER D.P., "Experiments in Physical Chemistry" (7ª ed.), McGraw-Hill (2003).

FORESMAN J.B., FRISH A., "Exploring Chemistry with Electronic Structure Methods: a guide to using Gaussian" (2ª ed.), Gaussian Inc (1996).

Recommendations

Subjects that are recommended to be taken simultaneously

IT tools and communication in chemistry/V11G200V01401
Numerical methods in chemistry/V11G200V01402
Inorganic chemistry I/V11G200V01404

Subjects that it is recommended to have taken before

Mathematics: Mathematics I/V11G200V01104
Mathematics: Mathematics II/V11G200V01203
Physics III/V11G200V01301
Physical chemistry I/V11G200V01303

IDENTIFYING DATA				
Inorganic chemistry I				
Subject	Inorganic chemistry I			
Code	V11G200V01404			
Study programme	(*)Grao en Química			
Descriptors	ECTS Credits	Choose	Year	Quadmester
	9	Mandatory	2nd	2nd
Teaching language	Spanish			
Department				
Coordinator	García Bugarín, Mercedes			
Lecturers	Bolaño García, Sandra Carballo Rial, Rosa Couce Fortúnez, María Delfina García Bugarín, Mercedes			
E-mail	mgarcia@uvigo.es			
Web				
General description	"Machine translation into english of the original teaching guide" In this asignatura studies the chemistry of the elements of the main groups and his compounds. It pretends give an overview of the different types of chemical behaviour and of the existent compounds.			

Competencies	
Code	
C1	Demonstrate knowledge and understanding of essential facts, concepts, principles and theories: Major aspects of chemical terminology, nomenclature, units and unit conversions.
C2	Demonstrate knowledge and understanding of essential facts, concepts, principles and theories: types of chemical reactions and its main characteristics
C9	Demonstrate knowledge and understanding of essential facts, concepts, principles and theories: characteristic properties of the elements and their compounds, including group relationships and variations in the periodic table
C12	Demonstrate knowledge and understanding of essential facts, concepts, principles and theories: structural features of chemical elements and their compounds, including stereochemistry
C14	Demonstrate knowledge and understanding of essential facts, concepts, principles and theories: relationship between macroscopic properties and properties of individual atoms and molecules, including macromolecules
C20	Evaluate, interpret and synthesize data and chemical information
C23	Present oral and written scientific material and scientific arguments to a specialized audience
C25	Handle chemicals safely, considering their physical and chemical properties, including the evaluation of any specific risks associated with its use
C26	Perform common laboratory procedures and use instrumentation in synthetic and analytical work
C27	Monitor, by observation and measurement of physical and chemical properties, events or changes, and document and record them in a consistent and reliable way
C28	Interpret data derived from laboratory observations and measurements in terms of their significance and relate them to the appropriate theory
D1	Communicate orally and in writing in at least one of the official languages of the University
D3	Learn independently
D4	Search and manage information from different sources
D5	Use information and communication technologies and manage basic computer tools
D6	Use mathematics, including error analysis, estimates of orders of magnitude, correct use of units and data representations
D7	Apply theoretical knowledge in practice
D8	Teamwork
D9	Work independently
D12	Plan and manage time properly
D13	Make decisions
D14	Analyze and synthesize information and draw conclusions
D15	Evaluate critically and constructively the environment and oneself

Learning outcomes		
Expected results from this subject	Training and Learning Results	
Distinguish the different chemical behaviour of the elements of the main groups inside each group.	C1 C2 C9	D1 D3 D4 D9

Choose the general method more adapted for the obtaining of the elements of the main groups from his present compounds in the nature.	C1 C2 C9	D1 D3 D4 D9
Identify in each group of elements of the main groups those types of singular compounds and of particular importance by his structure or his reactivity.	C1 C2 C9 C12 C14	D1 D3 D4 D9
Deduce the physical properties of a compound from the type of link between his components and his structure.	C9 C12 C14 C20 C23	D1 D3 D4 D9
Relate the physical and chemical properties of the elements of the main groups and of his compounds with his applications.	C2 C9 C12 C14 C23	D1 D3 D4 D9
Carry out in the laboratory the preparation and the study of some physical and chemical properties of elements of the main groups and of his compounds.	C25 C26 C27 C28	D4 D5 D6 D7 D8 D9 D12 D13 D14 D15

Contents

Topic	
1. Hydrogen	Obtaining. Physical and chemical properties. Hydrides: classification and general study of the same. The water.
2. Noble gases	General characteristics. Properties and uses. Fluorides of xenon. Combinations of xenon with oxygen.
3. *Halógenos	General characteristics. Obtaining, properties and reactivity. Halides. Oxides, *oxoácidos and *oxosales. Compound *interhalógenos and ions *polihalogenuro. *Pseudohalógenos. *Fluorocarbonos.
4. Elements of the group 16	General characteristics. Specific study of the oxygen. Obtaining, properties and reactivity. Peroxide of hydrogen. Sulphur. Obtaining, properties and reactivity. Combinations hydrogenated and *halogenadas of the sulphur. Oxides, *oxoácidos and *oxosales of sulphur.
5. Elements of the group 15	General characteristics. Obtaining, properties and reactivity. Combinations hydrogenated and *halogenadas. Oxides, *oxoácidos and *oxosales of nitrogen and phosphorus. Arsenic and bismuth.
6. Elements of the group 14	General characteristics. Carbon. Obtaining, properties and reactivity. Oxides and carbonates. Carbides. Combinations *halogenadas and nitrogenous. Silicon, germanium, tin and lead. Obtaining, properties and reactivity. Hydrides and halides. Oxides. Silicates. Silicones.
7. Elements of the group 13	General characteristics. Boron. Obtaining, properties and reactivity. Hydrides and halides. Composed with nitrogen. Oxides, *oxoácidos and *oxosales. Aluminium. Obtaining, properties and reactivity. Chemistry in aqueous dissolution of the *ion aluminium. Hydrides, halides and oxides. Compounds more important of gallium, Indian and *talio.
8. Elements of the group 1	Physical and chemical properties. Reactivity. Obtaining. Compounds more important.
9. Elements of the group 2	Physical and chemical properties. Reactivity. Obtaining. Compounds more important.
Practice 1-2	Study of the chemical properties of the oxides.
Practice 3-4	Obtaining and chemical behaviour of the *halógenos.
Practice 4-5	Obtaining and reactivity of compounds of the group 16.
Practice 6-7-8	Obtaining and reactivity of compounds of the group 15.
Practice 9-10	Obtaining and reactivity of compounds of the group 14.
Practice 11-12	Obtaining and reactivity of compounds of the group 13.

Planning

	Class hours	Hours outside the classroom	Total hours
Master Session	26	15	41
Troubleshooting and / or exercises	26	20	46
Laboratory practises	45.5	5.5	51
Long answer tests and development	4	70	74
Practical tests, real task execution and / or simulated.	3	10	13
*The information in the planning table is for guidance only and does not take into account the heterogeneity of the students.			

Methodologies

	Description
Master Session	Exhibition by part of the professor on the subject to develop, doing special *enfásis in the most important appearances or of difficult understanding for the student. The professor/to will use the platform *Tem@ to give information on the matter or on his development.
Troubleshooting and / or exercises	They will devote two weekly hours to argue and resolve questions on the matter that previously the student will have to work.
Laboratory practises	The experiments will realise along 13 sessions of 3,5 hours each one. The student will have of the scripts of practices as well as of the material of support in the platform *tem@ with the end that it can have previous knowledge of the experiments to realise. The student will have to elaborate the fascicle of laboratory during the realisation of the practices.

Personalized attention

Methodologies	Description
Troubleshooting and / or exercises	

Assessment

	Description	Qualification	Training and Learning Results	
Troubleshooting and / or exercises	It will value the resolution by part of the student of a series of problems and/or exercises proposed in the time/condition established/ace by the professor. The punctuation will be considered if in each one of the eliminatory proofs reaches an equal or upper qualification to 5 points on 10.	15	C1 C2 C9 C12 C14 C23	D1 D3 D4 D6 D7 D9 D13
Laboratory practises	It is compulsory the assistance to the sessions of laboratory. The professor will realise a follow-up of the experimental work realised by the student in the sessions of laboratory, as well as of the fascicle elaborated (10%). It will realise a proof that will allow to evaluate the competitions and skills purchased by the student (15%). The punctuation will be considered if in each one of the eliminatory proofs reaches an equal or upper qualification to 5 points on 10.	25	C25 C26 C27 C28	D4 D5 D6 D7 D8 D9 D12 D13 D14 D15
Long answer tests and development	2 Proofs on concrete appearances of the contents explained in class and seminars. Each proof will be able to be eliminatory when the student reach a minimum qualification of 5 points on 10. To be able to approve the matter, the student will have to reach in each one of the eliminatory proofs a minimum qualification of 5 points on 10.	60	C1 C2 C9 C12 C14 C20	D1 D6 D7

Other comments on the Evaluation

The assistance to the theoretical classes, practices of laboratory and seminars is compulsory.

The participation of the student in any of the acts of evaluation of the matter will involve the condition of presented/to and, therefore, the allocation of a qualification. They consider acts of evaluation the assistance to the practical classes of laboratory (three or more) and the realisation of proofs.

The students will be able to realise a Final Proof, that will be able to have a value of until a 60 %, in the date of closing of evaluation of the announcement of May-June when they require:
- Surpass any of the eliminatory proofs.

- Go up the note of the eliminatory proofs that allow him reach the minima required to approve the matter.
- Go up the note in the eliminatory proofs to improve the final note of the matter.

Announcement of July.

The students that do not surpass the matter at the end of the cuatrimestre will have to do a proof written in the period of closing of evaluation of the announcement of July. Said proof will substitute the results of the eliminatory proofs realised along the cuatrimestre and will have a value of until a 60 %. The qualification of resolution of problems and practical of laboratory obtained to along the cuatrimestre keeps .

Sources of information

ATKINS, P.; OVERTON, T.; ROURKE, J.; WELLER, M. Y ARMSTRONG, F., **Inorganic Chemistry**, Fifth Edition,
HOUSE, J. E., **Inorganic Chemistry**, 2ª Ed,
HOUSECROFT, C.E. Y SHARPE, A. G., **Inorganic Chemistry**, 3ª Ed,
HOUSECROFT, C. E. ; A. G. SHARPE., **Química Inorgánica**, 2.ª Ed (español),
RAYNER□CANHAM, G., OVERTON, T., **Descriptive Inorganic Chemistry**, 5ª Ed,
RAYNER-CANHAM, G., **Química Inorgánica Descriptiva**, 2.ª Ed,
SHRIVER & ATKINS, **Química Inorgánica**, 4º ed.,

Recommendations

Subjects that are recommended to be taken simultaneously

IT tools and communication in chemistry/V11G200V01401
Numerical methods in chemistry/V11G200V01402
Physical chemistry II/V11G200V01403

Subjects that it is recommended to have taken before

Chemistry, physics and biology: Integrated laboratory I/V11G200V01103
Chemistry, physics and geology: Integrated laboratory II/V11G200V01202
Chemistry: Chemistry I/V11G200V01105
Chemistry: Chemistry 2/V11G200V01204