(*)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 3	1st	6
V11G200V01302	Analytical chemistry 1	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 3				
Subject	Physics 3			
Code	V11G200V01301			
Study programme	(*)Grao en Química			
Descriptors	ECTS Credits	Choose	Year	Quadmester
	6	Mandatory	2nd	1st
Teaching language	Spanish			
Department	Applied Physics Physical Chemistry			
Coordinator	Flores Rodríguez, Jesús Ramón			
Lecturers	Flores Rodríguez, Jesús Ramón Martínez Piñeiro, Manuel			
E-mail	flores@uvigo.es			
Web				
General description	The matter intends 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
To describe in an unified way the electromagnetic field by means of Maxwell's laws. Apply the basic boundary conditions in the vacuum or in materials.	C3	D1 D12 D14
To derive the equation of propagation of an electromagnetic wave, and describe its main characteristics. Relate this concept with the electromagnetic spectrum.	C3	D12 D14
To explain the empirical phenomena related with the interaction of radiation with matter which cannot be explained by the Classical Theory, and the solutions proposed (wave-corpuscle duality, quantization of the radiation).	C3	D12 D14 D15
To know the postulates of Quantum Mechanics and their consequences in the reformulation of the microscopic theory of the Classical Physics.	C3	D1 D12 D14 D15
To explain the essentials of the theory of mathematical operators, including the concepts of eigenfunction and eigenvalue, spectrum, linearity and hermiticity, complete sets of eigenfunctions, etc.	C3	D1 D9 D12 D14

To write the fundamental operators of Quantum Mechanics (position, linear and angular moment, Hamiltonian of simple systems).	C3 C19	D1 D9 D12 D14
To apply the previous concepts to the quantum- mechanical study of simple systems, like a particle in a square well potential, or to a harmonic oscilator potential, by resolving the time-independent Schrödinger equation.	C3 C19	D1 D3 D6 D8 D12 D13 D14
To calculate the eigenfunctions and eigenvalues of the angular momentum operator.	C3 C19	D6 D12 D14
To resolve the wave equation of the hydrogen atom, and calculate its eigenfunctions (orbitals).	C3 C19	D6 D8 D12 D14
To resolve the Schrödinger equation for many-electron atoms by means of approximate methods.	C3 C19 C20	D1 D5 D6 D9 D12 D13 D14
To explain in a simple way the transitions between states and the absorption and emission spectra.	C3 C19 C20 C22 C23	D1 D6 D8 D9 D12 D14 D15
To know the laws of Statistical Mechanics, which govern the behaviour of many-particle systems, in particular the Maxwell-Boltzmann statistics. Derive the partition function of a system and know in detail its physical meaning.	C14 C20 C22 C23	D1 D4 D5 D6 D7 D8 D12 D13
To apply the Maxwell-Boltzmann statistics to the case of the ideal gases of atoms and polyatomic particles to estimate thermodynamic properties, using microscopic properties like the mass, the molecular geometry and the vibrational frequencies.	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
Lecturing	25	50	75
Problem solving	26	39	65
Introductory activities	1	1	2
Short answer tests	4	0	4
Essay questions exam	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
Lecturing	Discussion of the fundamental points of each subject and presentation of those which are going to be tackled in the seminars
Problem solving	Resolution of numerical problems, theoretical questions and development of the theoretical points proposed in the masterclasses with the participation of the student.
Introductory activities	Presentation of the subject with a brief desription of: sections, contents, distribution of the sections in the short tests and in the final exam general norms of evaluation,etc.

Personalized attention

Methodologies	Description
Lecturing	Discussion of the main points of the subject. Answers to the questions related with the points raised by the students not only in the master session but also in the seminars. The students will know before the beginning of the course the schedules of the the tutorial sessions offered by the professors of the subject. In those tutorials the student will be able to review his/her examinations
Problem solving	Answers to the questions related with the points the students may have raised in the classes devoted to problem resolution and in the tutorial sessions. The students will know before the beginning of the course, the schedules of the the tutorial sessions offered by the professors of the subject. In those tutorials the student will be able to review his/her examinations

Assessment

	Description	Qualification	Training and Learning Results

Problem solving	It will consist on the resolution of exercises and tests in the classroom. Nevertheless, the teacher will be able too to ask the student to deliver the solution to previously proposed exercises, that he/she has resolved in an autonomous way. In this case the teacher may ask the student tho explain to him indivdually how he/she has resolved the exercise.	25	C19 C20 C22 C23	D1 D3 D4 D5 D6 D7 D8 D9 D12 D13 D14 D15
Short answer tests	During the course two short written tests will take place. They will correspond, respectively, to the contents of the sections 1 to 3 and 4 to 8 respectively. If any of those written tests is not passed the student must take on the corresponding part of the final exam (December/January). The student must take on the whole subject in the second-opportunity exam (June/July).	37.5	C3 C14 C19 C20	D6 D7 D9 D12 D13 D14
Essay questions exam	At the end of the course a full written test will take place in which the students can take on those aspects that they did not pass in the short written tets or improve in those they did pass.	37.5	C3 C14 C19 C20	D6 D7 D9 D12 D13 D14

Other comments on the Evaluation

During the course two short written tests will take place corresponding to sections 1-3, the first one, and to sections 4-8, the second. Both will contain problems and questions and, if they are passed, the student, is not obliged to take on the corresponding part of the subject in the (first-call) final exam (December/January), although he/she can do so in order to improve his/her mark. On a voluntary basis the student may participate in the seminars by solving exercises on the board. Also voluntarily the student may solve at home some proposed exercises and deliver them to the teacher. The final exam will include the whole subject but is divided into two parts corresponding to the two tests so the student can take on any or both of them, even if they have passed the short written test of that part.

The student though, must reachin the written tests a global minimum mark of 3.5/10 in order to accumulate the points obtained by resolving exercises independently or in the classroom.

In the second-opportunity evaluation (July) the student should do a full written test; the points obtained by exercise resolution (troubleshooting section) will be mantained.

On a voluntary basis, the students will be able to participate in the resolution of exercises in the seminars or deliver the answer to the written exercises proposed in the classroom.

It will be understood that any student who has not taken any written test (short or the final exam) has not really followed the subject and will not be given a mark (his/her qualification will be "no presentado").

Sources of information

Basic Bibliography

Complementary Bibliography

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 2/V11G200V01201

IDENTIFYING DATA

Analytical chemistry 1

Subject	Analytical chemistry 1			
Code	V11G200V01302			
Study programme	(*)Grao en Química			
Descriptors	ECTS Credits	Choose	Year	Quadmester
	9	Mandatory	2nd	1st
Teaching language	Spanish Galician			
Department	Analytical and Food Chemistry			
Coordinator	Pérez Cid, Benita			
Lecturers	Bendicho Hernández, José Carlos 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
D16	Develop an ethical commitment

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.
Subject 2: Sampling and sample treatment.	Sampling. Previous opertions to the analysis. Decomposition and dissolution. Introduction to the analytical separations.

Subject 3: 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.
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)	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
Lecturing	26	35	61
Problem solving	26	39	65
Laboratory practices	42.5	12	54.5
Practices report	0	6	6
Short answer tests	2	9	11
Essay questions exam	3.5	16	19.5
Laboratory practice	2	6	8

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

Methodologies

	Description
Lecturing	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.
Problem solving	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 practices	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 2017-18, do not need to repeat them. In this case, marks reached in the laboratory sessions will be maintained.

Personalized attention

Methodologies	Description
Laboratory practices	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.
Problem solving	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
Practices report	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	
Problem solving	The teacher will evaluate the exercices/problems included in the worksheets and solved by students.	15		C1 C2 C4 C18 C19 C22	D4 D5 D6 D7 D9 D14
Laboratory practices	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.The lack of assistance, even being justified, will penalize the mark (in case of justified absences are recommended to made the practice in another group). If the number of absences is 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
Practices report	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 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.	20	A5	C1 C2 C4 C19 C20 C22	D1 D3 D4 D5 D6 D7 D9 D12 D13 D14 D16
Essay questions exam	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

Laboratory practice	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. Written exams will consist of theoretical questions and numerical exercises. To pass these exams it will be necessary to have a balance in the marks of both parts. 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

Basic Bibliography

D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, **Fundamentos de Química Analítica**, 9ª Ed., Cengage Learning, 2015

Gary D. Christian, **Química Analítica**, 6ª Ed., McGraw-Hill, 2009

D.C. Harris, **Análisis Químico Cuantitativo**, 3ª Ed., Reverté, 2007

F. Burriel, S. Arribas, F. Lucena y J. Hernández, **Química Analítica Cualitativa**, 18ª Ed., Thomson, 2002

M. Valcárcel, **Principios de Química Analítica**, Springer-Verlag Ibérica, 1999

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P. Yañez-Sedeño Orive, J.M. Pingarrón Carrazón, F.J. Manuel de Villena Rueda, **Problemas Resueltos de Química Analítica**, Síntesis, 2003

J. Guiteras, R. Rubio, G. Fonrodona, **Curso Experimental en Química Analítica**, Síntesis, 2003

Complementary Bibliography

D.A. Skoog, D.M. West , F.J. Holler, S.R. Crouch, **Química Analítica**, 7ª Ed., McGraw-Hill, 2001

D. Harvey, **Química Analítica Moderna**, McGraw-Hill, 2002

M. Válcarcel, A.I. López Lorente, M.A., López Jiménez, **Fundamentos de Química Analítica: una aproximación docente-discente**, Universidad de Córdoba, 2016

J. A. López Cancio, **Problemas Resueltos de Química Analítica**, Thompson, 2005

Recommendations

Subjects that continue the syllabus

Analytical chemistry II/V11G200V01503
Analytical chemistry 3/V11G200V01601

Subjects that are recommended to be taken simultaneously

Physics 3/V11G200V01301
Physical chemistry I/V11G200V01303
Organic chemistry I/V11G200V01304

Subjects that it is recommended to have taken before

Chemistry, physics and biology: Integrated laboratory 1/V11G200V01103
Chemistry, physics and geology: Integrated laboratory 2/V11G200V01202
Chemistry: Chemistry 1/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	Physical Chemistry			
Coordinator	Hervés Beloso, Juan Pablo			
Lecturers	Hervés Beloso, Juan Pablo Mandado Alonso, Marcos			
E-mail	jherves@uvigo.es			
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	
The laws of the thermodynamic in Chemistry.	First Law of thermodynamics. Internal energy. ** Enthalpy. Heat capacities . Thermochemistry. Second law of thermodynamics. ** Entropy. Molecular interpretation of the ** entropy. Third law of thermodynamics. Calculation of the variations of ** entropy.
Thermodynamic functions	Gibbs Equations. Maxwell relationships. Calculation of variations of the state functions . Open systems. Partial Molar quantities. Chemical potential. Chemical potential of an ideal gas. Chemical potential of the real gases.
Phase equilibrrium in systems of one component.	Concepts of component, phase and degree of *freedom. Equilibrium conditions between phases. Phses Rule. First order changes phases. Clapeyron and Clausius Equations.
Ideal Solutions.	Molar partial Volume. Gibbs-Duhem Equation. Ideal solutions: Raoult law. Vapour pressure diagrams. Ideal diluted solutions: Henry Law. Colligative Properties
Non-ideal Solutions.	Deviations of the Raoult law. Activity and activity coefficient . Electrolitic solutions. Debye-Hückel theory.

Chemical equilibrium	Equilibrium Conditions . Extent of reaction. perfect gas equilibria. Equilibrium is solution reactions. Response of equilibria to temperature. Le Chatelier´s principle. Acid-base equilibria. Solubility Product. salt effects. Electrochemical Cells. Nerst Equation.

Planning

	Class hours	Hours outside the classroom	Total hours
Lecturing	26	31	57
Seminars	26	38	64
Problem solving	0	14	14
Self-assessment	0	10	10
Essay questions exam	5	0	5

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

Methodologies

	Description
Lecturing	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	Students will solve autonomously questionnaires-type test through the TEMA platform and will be individually tutorized by the professor.
Problem solving	Students will solve autonomously proposed problems and will be individually tutorized by the professor.

Assessment

	Description	Qualification	Training and Learning Results	
Problem solving	Problems proposed stop each subject of the subject.	Hasta un 12,5	C6 C18 C19 C20 C23	D1 D3 D4 D6 D7 D8 D9 D12 D13 D14 D15
Self-assessment	Proofs type test in the platform SUBJECT.	Hasta un 12,5	C6 C18 C19 C20	D3 D4 D5 D7 D9 D12 D13 D14 D15
Essay questions exam	Examination written especially *los contents of the subject.	Mínimo un 75	C6 C18 C19 C20	D1 D3 D4 D6 D7 D9 D12 D13 D14

Other comments on the Evaluation

Sources of information
Basic Bibliography
Complementary Bibliography
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 2/V11G200V01203
Chemistry: Chemistry 1/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	Organic Chemistry			
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	http://secretaria.uvigo.gal/docnet-nuevo/guia_docent/index.php?centre=311&ensenyament=V11G200V01&assignatura=V11G200V01304&any_academic=2017_18			
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.
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. Three sessions.

Planning			
	Class hours	Hours outside the classroom	Total hours
Lecturing	25	25	50
Problem solving	26	50	76
Laboratory practices	42	10	52
Essay	0	10	10
Short answer tests	8	29	37
*The information in the planning table is for guidance only and does not take into account the heterogeneity of the students.			

Methodologies	
	Description
Lecturing	Exposition by the teaching staff of the syllabus' general aspects, with special emphasis in its fundamental features. The teaching staff will facilitate, through the virtual classroom, 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.
Problem solving	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 practices	Laboratory experiments will be carried out, individually, in 3.5 h sessions. The students will find, in advance, in the virtual classroom, 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**
Problem solving	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) and other ways provided by the university. Additionally, the teaching staff will use online channels to communicate with the students (electronic mail and tools within the virtual classroom).
Tests	**Description**
Essay	The teaching staff will tutor the students while preparing and carrying out a short laboratory project.

Assessment				
	Description	Qualification	Training and Learning Results	
Problem solving	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 practices	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

Essay	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, short answer tests, works).

The final grade for the students who pass the subject could be standardized so that the highest mark can reach a value of up to 10 points.

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 passed the laboratory practices during the 2014-15 or 2015-16 courses or were evaluated as APT during the 2016-17 or 2017-18 courses will be awarded the APT mention for the monitoring of laboratory work in the academic course 2018-19, 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 2018-19.

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, short answer tests, works), 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

Basic Bibliography

KLEIN, D., **Química Orgánica**, 1ª edición en español, Médica Panamericana, 2013
VOLLHARDT, K.P.C.; SCHORE, N.E, **Química Orgánica**, 5ª edición en español, Edicións Omega, 2007
WADE, L.G., **Química Orgánica**, 9ª edición en español, Pearson-Educación, 2017

Complementary Bibliography

CAREY, F., **Química Orgánica**, 9ª edición en español, McGraw-Hill Interamericana, 2014
CLAYDEN, J.; GREEVES, N.; WARREN, S., **Organic Chemistry**, 2ª edición, Oxford University Press, 2012
YURKANIS BRUICE, P., **Fundamentos de Química Orgánica**, 3ª edición, 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**, 2ª edición, McGraw-Hill Interamericana, 2004
QUIÑOÁ, E.; RIGUERA, R., **Nomenclatura y representación de los compuestos orgánicos**, 2ª edición, 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 3/V11G200V01301
Analytical chemistry 1/V11G200V01302
Physical chemistry I/V11G200V01303

Subjects that it is recommended to have taken before

Chemistry, physics and biology: Integrated laboratory 1/V11G200V01103
Chemistry, physics and geology: Integrated laboratory 2/V11G200V01202
Chemistry: Chemistry 1/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	Physical Chemistry Organic Chemistry			
Coordinator	Silva López, Carlos			
Lecturers	Hermida Ramón, José Manuel Pérez Juste, Jorge Silva López, Carlos			
E-mail	csilval@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
Lecturing	14	28	42
Computer practices	26	52	78
Problem solving	2	22	24
Essay questions exam	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
Lecturing	The theoretical aspects of the subject are presented
Computer practices	Computer lab exercises: literature searches, use of bibliographic managers, use of statistical packages, report writing.
Problem solving	Report or article writing in English language. Simple exercises with modelling software

Personalized attention

Methodologies	Description
Computer practices	Hands-on exercises in a computer laboratory
Problem solving	Monitored problem solving tasks

Assessment

	Description	Qualification	Training and Learning Results	
Computer practices	Typically, literature searches	20	C22 C23	D1 D2 D3 D4 D5 D9 D15 D16
Problem solving	Tipically, database searches and use of utilities of modelling software.	40	C22 C23	D1 D2 D3 D4 D5 D8 D10 D14 D15 D18
Essay questions exam	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

Basic Bibliography

Complementary Bibliography

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 2/V11G200V01201
Chemistry: Chemistry 1/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	Mathematics Analytical and Food Chemistry Physical Chemistry			
Coordinator	Besada Morais, Manuel			
Lecturers	Besada Morais, Manuel Calle González, Inmaculada de la Peña Gallego, María de los Ángeles			
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. Derivation 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. Optimization.	Direct methods of solving optimization problems. One Variable. Several variables. Without restrictions. With restrictions.

Planning			
	Class hours	Hours outside the classroom	Total hours
Lecturing	13	26	39
Computer practices	26	52	78
Objective questions exam	4	12	16
Problem solving	2	8	10
Essay	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
Lecturing	Exhibition of the theoretical bases and orientation by part of the *profesorado on the contents of the matter
Computer practices	Development in the classrooms of computing of the exercises that propose in the theoretical classrooms using the scientific calculator **MATLAB.

Personalized attention	
Methodologies	**Description**
Computer practices	The students will work of autonomous way with the permanent supervision of the professor

Assessment				
	Description	Qualification	Training and Learning Results	
Computer practices	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
Objective questions exam	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
Problem solving	When finalising the course **realizaráse a practical proof resolving some practical exercises in the classroom of computing	30	C19 C22 C29	D6
Essay	**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

Basic Bibliography

Chapra, S.C.; Canale, R.P., **Métodos numéricos para ingenieros. Sexta edición.**, 2015, McGraw-Hill, 2015

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

Bober, W.; Tsai, C.; Masory, O., **Numerical and Analytical Methods with Matlab**, 2009, CRC Press,

Complementary Bibliography

Recommendations

Subjects that it is recommended to have taken before

Mathematics: Mathematics 1/V11G200V01104
Mathematics: Mathematics 2/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	Physical Chemistry			
Coordinator	Mosquera Castro, Ricardo Antonio Fernández Nóvoa, Alejandro			
Lecturers	Fernández Nóvoa, Alejandro Mosquera Castro, Ricardo Antonio Peña Gallego, María de los Ángeles Pérez Juste, Jorge			
E-mail	mosquera@uvigo.es afnovoa@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
Lecturing	26	39	65
Seminars	26	39	65
Laboratory practices	45.5	4.5	50
Autonomous problem solving	0	10	10
Essay questions exam	4	8	12
Practices report	0	9	9
Short answer tests	2	5	7
Objective questions exam	0	4	4
Laboratory practice	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
Lecturing	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 practices	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 problem solving	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
Lecturing	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 practices	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 problem solving	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**
Essay questions exam	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).
Practices report	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).
Objective questions exam	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 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).

Assessment

	Description	Qualification	Training and Learning Results	
Laboratory practices	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 C6 C8 C19 C20 C21 C22 C27 C28	D1 D4 D5 D6 D7 D8 D12 D13 D14 D15

Autonomous problem solving	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
Essay questions exam	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
Practices report	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
Objective questions exam	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
Laboratory practice	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 (proofs (90%), problems solving (5%), quiz-tests (5%)), 75% of the final qualification of the subject. 2 proofs will be done during the course.

If the student passes the first proof (it will take place around the midle of the 4-months periode, he/she could only answer the questions related to the second part of the subject. Proofs qualification will be the average of the two proofs. When the first proof is repeated the best qualification is the only one to be used for the average,

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 not larger than 4,0.

Besides, it will be necessary to obtain an average of 2,5 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 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 proofs, or of the proof written of practices, or the assistance to 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 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

Basic Bibliography

Complementary Bibliography

BERTRÁN RUSCA, J.; NÚÑEZ DELGADO, J., **"""Química Física""" (vol. I)**, 1ª edicion,

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

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

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 1/V11G200V01104
Mathematics: Mathematics 2/V11G200V01203
Physics 3/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	Inorganic Chemistry			
Coordinator	García Bugarín, Mercedes			
Lecturers	Carballo Rial, Rosa Castro Fojo, Jesús Antonio Couce Fortúnez, María Delfina García Bugarín, Mercedes García Fontán, María Soledad García Martínez, Emilia			
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 5-6	Obtaining and reactivity of compounds of the group 16.
Practice 7-8	Obtaining and reactivity of compounds of the group 15.

Practice 9	Obtaining and reactivity of compounds of the group 14.
Practice 10-11	Obtaining and reactivity of compounds of the group 13.
Practice 12	Practice to determine

Planning

	Class hours	Hours outside the classroom	Total hours
Lecturing	26	15	41
Problem solving	26	23	49
Laboratory practices	42	6	48
Essay questions exam	4	70	74
Laboratory practice	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
Lecturing	Exhibition by part of the professor on the subject to develop, doing special emphasis 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.
Problem solving	They will devote two weekly hours to argue and resolve questions on the matter that previously the student will have to work.
Laboratory practices	The experiments will realise along 12 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
Problem solving	

Assessment

	Description	Qualification	Training and Learning Results	
Problem solving	It will value the resolution by part of the student of a series of problems and/or exercises proposed in the time/condition established 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 practices	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
Essay questions exam	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 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 Julio. 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

Basic Bibliography

RAYNER-CANHAM, G., **Química Inorgánica Descriptiva**, 2.ª Ed,
SHRIVER & ATKINS, **Química Inorgánica**, 4º ed.,

Complementary Bibliography

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**, 6ª 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 1/V11G200V01103
Chemistry, physics and geology: Integrated laboratory 2/V11G200V01202
Chemistry: Chemistry 1/V11G200V01105
Chemistry: Chemistry 2/V11G200V01204