(*)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

Grado en Química

Subjects

Year 3rd

Code	Name	Quadmester	Total Cr.
V11G201V01301	Chemical engineering	1st	6
V11G201V01302	Analytical Chemistry III: Electroanalytical Methods and Separations	1st	6
V11G201V01303	Physical Chemistry III: Quantum Chemistry	1st	6
V11G201V01304	Inorganic Chemistry III: Coordination Chemistry	1st	6

V11G201V01305	Organic Chemistry III: Concerted, Radical and Photochemical Reactions	1st	6
V11G201V01306	Analytical Chemistry IV: Chromatographic and Affine Methods	2nd	6
V11G201V01307	Physical Chemistry IV: Molecular Structure and Spectroscopy	2nd	6
V11G201V01308	Physical Chemistry V: Chemical Kinetics	2nd	6
V11G201V01309	Inorganic Chemistry IV: Transition Metals and Solid State	2nd	6
V11G201V01310	Organic Chemistry IV: Design of Organic Synthesis	2nd	6

IDENTIFYING DATA

Chemical engineering

Subject	Chemical engineering			
Code	V11G201V01301			
Study programme	Grado en Química			
Descriptors	ECTS Credits	Choose	Year	Quadmester
	6	Mandatory	3rd	1st
Teaching language	#EnglishFriendly Spanish			
Department				
Coordinator	González de Prado, Begoña			
Lecturers	González de Prado, Begoña			
E-mail	bgp@uvigo.es			
Web				
General description	This subject is an introduction to Chemical Engineering, where the knowledge gained in the previous Chemistry degree courses is related to Chemical industry processes. The mail goal is to enable the students to learn the basic knowledge about material and energy balances so that they can applied it to the design of separation processes such as distillation or liquid-liquid extraction. English Friendly subject: International students may request from the teachers: a) materials and bibliographic references in English, b) tutoring sessions in English, c) exams and assessments in English. This subject gives the basis to understand other subjects such as Environmental Quemistry, Food Chemistry and Industrial Chemistry.			

Training and Learning Results

Code	
A1	Students can apply their knowledge and understanding in a manner that indicates a professional approach to their work or vocation, and have competences typically demonstrated through devising and sustaining arguments and solving problems within their field of study
B4	Ability for analysis and synthesis
C3	Recognize and analyze chemical, qualitative and quantitative problems, proposing strategies to solve them through the evaluation, interpretation and synthesis of data and chemical information
C23	Know the principles and procedures of chemical engineering
D1	Ability to solve problems

Expected results from this subject

Expected results from this subject	Training and Learning Results			
Know and identify the diverse operations of separation and their fields of application.	A1	B4	C3 C23	D1
Draw and interpret liquid vapour equilibria, liquid- liquid equilibria and liquid-gas equilibria diagrams	A1	B4	C3 C23	D1
Design the different operations of separation based in liquid vapour, liquid-liquid and liquid-gas equilibria	A1		C23	D1
Design chemical reactors ideals.	A1		C3 C23	D1

Contents

Topic	
Subject 1. Introduction to Chemical Engineering	Origin, concept and evolution of the Chemical Engineering. Discontinuous and continuous operation. Stationary and non stationary state. Cocurrent and countercurrent operations. Classification of the unit operations. Systems of units.
Subject 2. Mass and energy balances	General equation of balance. Mass balances in systems without chemical reaction in steady and non-steady state. Recycle, purge and bypass. Mass balances in systems with chemical reaction in steady and non-steady state. Energy balances. Energy balances in systems with chemical reaction in steady state.
Subject 3. Distillation	Vapour-liquid equilibria. Phase diagrams for binary mixes. Simple and flash distillation. Multistage distillation

Subject 4. Liquid-liquid extraction	Liquid-liquid equilibrium for binary and ternary systems: binodal curve and distribution coefficients. Liquid-liquid extraction in cocurrent and countercurrent contact.
Subject 5. Chemical reactors	Speed of reaction. Ideal reactors: batch stirred tank reactor, continuos stirred tank reactor and plug flow reactor
Subject 6. Heat transfer	Mechanisms of heat transfer. heat transfer through flat walls, cylindrical and spherical. Heat exchangers.

Planning

	Class hours	Hours outside the classroom	Total hours
Lecturing	12	25	37
Problem solving	20	25	45
Collaborative Learning	2	0	2
Autonomous problem solving	0	11	11
Case studies	0	20	20
Objective questions exam	2	19	21
Problem and/or exercise solving	2	12	14

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

Methodologies

	Description
Lecturing	During these classes (one hour per week) the teacher will explain the most relevant aspects of the subject. The students will have the available documentation on Moovi.
Problem solving	There will be a set of exercises of each subject available for the students. Some of these exercises will be solve in class and other ones will be solved by each student and presented to the teacher in order to be corrected.
Collaborative Learning	In some classes of resolution of problems will propose some problem so that they resolve it in groups reduced.
Autonomous problem solving	The students will have to solve some exercises and questions and they will have to present them to through the platform Moovi
Case studies	It will propose a global problem that cover the greater part of the contents of the subject that will have to resolve of individual form and deliver through the platform Moovi for its evaluation

Personalized assistance

Methodologies	Description
Problem solving	In the assigned hours of tutoring the professor will solve any doubts regarding the subject
Collaborative Learning	During the sessions of collaborative learning the professor will resolve the doubts that can arise
Autonomous problem solving	In the assigned hours of tutoring the professor will solve any doubts regarding the subject
Case studies	In the assigned hours of tutoring the professor will solve any doubts regarding the subject

Assessment

	Description	Qualification	Training and Learning Results			
Collaborative Learning	Resolution of exercises in small groups	5		B4	C3 C23	D1
Autonomous problem solving	The students will have to deliver, in the terms indicated, the problems and activities proposed of each subject.	10		B4	C3	D1
Case studies	It will propose a global problem that cover the greater part of the contents of the subject	15	A1		C3 C23	D1
Objective questions exam	It will make a long proof of all the matter of the subject.	40	A1	B4	C3 C23	D1
Problem and/or exercise solving	They will make two short proofs, one of the subjects 1 and 2 and another of the subjects 3 and 4.	30	A1	B4	C3 C23	D1

Other comments on the Evaluation

There will be two short written tests throughout the quarter that do not eliminate matter. At the date set by the centre, the entire subject matter will be evaluated and a minimum of 3 out of 10 points must be reached to take account of the other evaluation elements. If the minimum grade is not reached, the final test note is the grade of the subject.

The different activities carried out in the classroom and autonomously by the students together account for 30% of the final grade. To overcome the subject it is essential to have a minimum score of 3.5 out of 10 points in these sections (collaborative learning, problem solving autonomously, case studies).

The participation of the student in some of the evaluation tests, the delivery of 20% or more of the work ordered by the teacher, implies the condition of "presented" and the assignment of a grade.

Second chance. There will be a long test of all the material that will make up 70% of the grade. The grades corresponding to the activities carried out in the classroom and autonomously obtained, by the students, throughout the course

Sources of information

Basic Bibliography

G. Calleja, F. García, A. de Lucas, D. Prats, J.M. Rodriguez, **Introducción a la Ingeniería Química**, Síntesis, 1999

D.M. Himmelblau,, **Principios Básicos y Cálculos en Ingeniería Química**, Prentice-Hall, 2002

C.J. GEANKOPLIS, **Procesos de transporte y principios de procesos de separación**, CECSA, 2006

W.L. McCabe, J.C. Smith, P. Harriot, **Operaciones Unitarias en Ingeniería Química**, McGraw-Hill, 2002

Complementary Bibliography

C.J. King, **Procesos de Separación**, Reverté, 1986

H.S. Fogler, **Elementos de Ingeniería de la Reacción Química**, Prentice-Hall, 2001

R.M. Felder, R.W. Rousseau, **Principios elementales de los procesos químicos**, Limusa,

Recommendations

IDENTIFYING DATA

Analytical Chemistry III: Electroanalytical Methods and Separations

Subject	Analytical Chemistry III: Electroanalytical Methods and Separations			
Code	V11G201V01302			
Study programme	Grado en Química			
Descriptors	ECTS Credits	Choose	Year	Quadmester
	6	Mandatory	3rd	1st
Teaching language	#EnglishFriendly Spanish Galician English			
Department				
Coordinator	González Romero, Elisa			
Lecturers	Costas Rodríguez, Marta González Romero, Elisa			
E-mail	eromero@uvigo.es			
Web				
General description	Give knowledge of the analysis of compound (organic and inorganic, ions, atoms and molecules) of environmental interest, clinical, biomedical, in the food and pharmaceutical industries, in laboratories quality control, etc, by means of the main Electrometric Techniques of analysis and Classical Separation methods. Inside the process/analytical procedure, will take into account the conditions for the direct measurement and those other situations in which it would be necessary the previous separation of the analyte and/or interferences of the matrix (treatment of sample). It will give a wide and current vision of the versatility of these techniques like tool to resolve problems in the areas of application mentioned, already was carried out the analysis in the chemical laboratories (involves transport and storage of the sample) or directly in the place of sample collection (analysis in situ or decentralised), because of its advantages of miniaturisation and, therefore, of portability, its easy handle and its rapidity of answer (methods of screening). With all this, pretends that the student can acquire the sufficient skill, in the first place, in the handle of the sources of bibliographic documentation and, second, in the set up and maintenance of teams, so that it can apply the analytical methodology in the resolution of real problems. Matter of the program English Friendly: the international students will be able to follow the classes without difficulty then , so much the visual material (presentations in PowerPoint) like the bibliography recommended, presents in English, in addition to having to his disposal another material of support for the follow-up of the matter in English and to be able to request to the professors any another material or additional bibliographic references in this language. They will attend the interventions in class, the tutorial and the realisation of the proofs and evaluations also in English. Matter Offered for the Elderly Program; to the students of this program that select this matter, will facilitate them material of support in Spanish (books of text, monographs, articles, etc) so that they can follow fluently the contents, in addition to having of the bibliography recommended.			

Training and Learning Results

Code	
A1	Students can apply their knowledge and understanding in a manner that indicates a professional approach to their work or vocation, and have competences typically demonstrated through devising and sustaining arguments and solving problems within their field of study
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
B5	Ability to adapt to new situations and to make decisions
C6	Know the basics and tools for resolution of analytical problems and characterization of chemical substances
C13	Know the principles and applications of electrochemistry
C26	Perform correctly usual procedures in the laboratory, including the use of standard chemical instrumentation for synthetic and analytical work
D1	Ability to solve problems

Expected results from this subject

Expected results from this subject	Training and Learning Results		
Identify and distinguish properly the different steps of the analytical process	A3		D1
Know and apply the main systems of sampling, storage and treatment of samples for electroanalytical purposes	A1	C13	D1

Describe and explain the fundamentals and the analytical applications of separation techniques (no chromatographic ones) in the treatment of sample and the electroanalysis in the determination	A3		C13	D1
Purchase critical trial to evaluate and select the ideal technique, so much electroanalytical as of separation, to resolve a real analytical problem, taking into account to the analyte, to the type of sample and the analytical quality that demands to the results.	A1	B5	C13 C26	D1
Differentiate, choose and correctly handle the instrumentation involved in electroanalysis and the material used in non-chromatographic separations	A1	B5	C13 C26	D1
Acquire skills to plan and develop an analysis method, as well as to calibrate, measure and interpret the results obtained when solving, experimentally, the analytical problem that is proposed and successfully evaluate / defend any situation, simulated or real, that arises at the laboratory.	A3	B5	C26	D1
Acquire skills to discuss and defend the choice of an analysis method in different situations and its validation.	A3	B5	C13 C26	D1
Correctly carry out calculations in the preparation of solutions, in the calibration and in the evaluation of the results and recognize errors.	A1 A3	B5	C6 C26	D1
Collect information to prepare, argue and present reports.	A1	B5		D1
Handle chemicals correctly, assess risks and manage the waste produced in the lab.	A3	B5		D1

Contents

Topic	
UNIT 1.- Electroanalysis in the measurement step. Fundamentals of electrometric methods.	Redox and electrochemical chemical reactions. Interface electrode / dissolution. Transportation phenomena. Electrolysis and model of stationary diffusion. Classification of electrometric techniques. Instrumentation: basic components in potentiometric systems, conductimetric and potentiostatic / galvanostatic.
UNIT 2.- Electrodes and cells.	Working, reference and auxiliary electrodes. Working Electrodes: ISE, ISFET, solids (metallic and carbon), liquids (Hg), screen-printed electrodes (SPE) and modified. Supporting electrolytes and solvents. Cell configuration in electroanalysis and equivalent circuit. Calibration, the role of blank in electroanalysis and calculation of analytical parameters. Direct measurement and measurement after sample treatment: separation and derivatization in electroanalysis. Validation.
UNIT 3.- Conductimetry and potentiometry.	Conductometric analysis. Potentiometric analysis. Conductometric and potentiometric titrations. Analytical applications
UNIT 4.- Electroanalysis in dynamic systems I.	Coulombimetry, chronocoulombimetry and coulometric titrations. Analytical applications. Chronoamperometry and amperometry.Linear sweep voltammetry (LSV) and cyclic (CV). Processes of electrode for organic and inorganic compounds and criteria. Analytical applications.
UNIT 5.- Electroanalysis in dynamic systems II.	Pulse techniques: normal pulse voltammetry (NPV), differential pulse(DPV), square wave (SWV). Alternate current techniques (AC). Stripping techniques. Hybrid techniques and couplings. Analytical applications. Reflections and comparative study with others analytical techniques.
UNIT 6.- Fundamentals and aims of the separations in analytical chemistry.	Treatment of sample by digestion. Preparation of the sample: purification and pre-concentration. Studies of recovery.
UNIT 7.- Non-chromatographic Separations.	Precipitation, Leaching, Volatilisation and Distillation (lyophilisation, Kjeldhal, Willard-Winter), Electrodeposition and stripping.
UNIT 8.- Extraction	Liquid-liquid extraction, S-L extraction (Soxhlet, Assisted Extraction by Ultrasonic, microwave and accelerated-ASE), microextraction and solid phase extraction (SPE).
LABORATORY EXPERIMENTS	Experiments related to the contents in electroanalysis and non-chromatographic separations, applying the analytical process and including the evaluation and data processing, as well as the delivery of reports.

Planning

	Class hours	Hours outside the classroom	Total hours
Lecturing	24	18	42
Seminars	12	4	16
Laboratory practical	26	14	40
Workshops	0	6	6
Objective questions exam	1	8	9
Essay questions exam	2	12	14
Report of practices, practicum and external practices	0	12	12

Laboratory practice	1	10	11

*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 master classes (55 min) aim to give a global and real vision of electroanalysis, both from organic and inorganic compounds, by direct measurement or prior separation of the analyte. Each one of the topics will be documented with scientific articles, the contents of which will serve to establish and expand the knowledge acquired in the theoretical classes, and with representative examples of the fundamental concepts that are collected in each topic. The teaching-learning methodology will be centered on the student, so the classes will be aimed at motivating / encouraging a high participation on the part of these in the classroom. Therefore, the classes will be developed in a very interactive with the students, using the didactic material for their development online, as well as the most appropriate bibliography. The use of ICTs (MooVi and My Moodle) will be the resource that allows the student to communicate with the teacher (in addition to e-mail and the tutorials) and their peers, at the same time being the source of information of immediate access for them. In the tele-teaching platform, they will be able to find the basic information and documentation on the subject being taught, the schedule of activities, the exercises proposals, practice guide, workshop planning and qualifications.
Seminars	After the lectures, the seminars will be dedicated to solving problems / exercises, in which it is intended to strengthen the level of understanding of the students in the topic under study. These problems / exercises, in principle, are worked on in class in small groups, then there is a general debate on them and later the student will have to solve them individually. The seminars aim to reinforce knowledge acquired in the theoretical classes. There will also be a discussion of practical cases and work scientists related to the contents of the subject.
Laboratory practical	The practical laboratory classes play a fundamental role in teaching the subject. On the one hand, they are essential for understanding the theories and concepts taught in the lessons; and on the other, they allow the student to be trained in the handling of analytical methodology, as well as norms and rules of scientific work, both at the level of group and individual work, including report writing. Ultimately, these are procedural objectives. The use of ICTs (MooVi and My Moodle) will be the resource that allows the student to communicate with the teacher and their colleagues, at the same time being the source of information of immediate access for them. In the tele-teaching platform, you will be able to find basic information and documentation on the subject that is taught, the agenda of activities, the proposed exercises, the practice guide, the workshop planning and qualifications.
Workshops	They would be part of the seminars and laboratory practices in which students must solve by themselves, under the teacher's supervision but with greater autonomy, assumptions real practicals of electrochemical processes, detection and determination of compounds of interest (pollutants, drugs, biomolecules, etc.) and design analytical strategies. Both in the seminars and workshops will monitor the personal work that is being carried out by the student at all times. Discussions will be held that will serve to solve problems real, as well as to expose complementary concepts, addressed or not in other subjects, but necessary in the approach to this problem. This task will be subject to the evolution of the student in the learning process.

Personalized assistance	
Methodologies	**Description**
Lecturing	The tutoring program is configured as a study support element, where the student will have personalized academic assistance that results in a better use of the training and knowledge provided by the subject. In addition to face-to-face tutorials and / or via email, student work, individually or in groups, will also be tutored at through the MooVi Platform or through the remote campus.
Seminars	The tutoring program is configured as a study support element, where the student will have personalized academic assistance that results in a better use of the training and knowledge provided by the subject. In addition to face-to-face tutorials and / or via email, student work, individually or in groups, will also be tutored at through the MooVi Platform or through the remote campus.
Laboratory practical	The tutoring program is configured as a study support element, where the student will have personalized academic assistance that results in a better use of the training and knowledge provided by the subject. In addition to face-to-face tutorials and / or via email, student work, individually or in groups, will also be tutored at through the MooVi Platform or through the remote campus.
Workshops	The tutoring program is configured as a study support element, where the student will have personalized academic assistance that results in a better use of the training and knowledge provided by the subject. In addition to face-to-face tutorials and / or via email, student work, individually or in groups, will also be tutored at through the MooVi Platform or through the remote campus.

Tests	Description
Report of practices, practicum and external practices	The tutoring program is configured as a study support element, where the student will have personalized academic assistance that results in a better use of the training and knowledge provided by the subject. In addition to face-to-face tutorials and / or via email, student work, individually or in groups, will also be tutored at through the MooVi Platform or through the remote campus.

Assessment

	Description	Qualification	Training and Learning Results
Seminars	PRACTICAL CASES: application of techniques in the RESOLUTION OF environmental, clinical, food industry PROBLEMS, etc. There will be a personalized follow-up of the student and evaluable by the teacher, considering the degree of participation by the students in the practical cases that arise in the seminar classes for the resolution of analytical problems in different fields of application. The ability to resolve questions and issues that arise related to the topic will be taken into account, both in the way of presenting them (ability to synthesize, explain and transmit the information) and in defending them vehemently.	10	A1 B5 C6 D1 A3 C13 C26
Laboratory practical	EXPERIMENTAL IN THE LABORATORY The teachers involved will carry out personalized monitoring of the experimental work carried out by the student in the laboratory sessions, their progress, autonomy, attitude, aptitude and skills developed, as well as their ability to work in a group. It is important to indicate that it is MANDATORY AND ESSENTIAL to attend ALL laboratory sessions and pass the activity to qualify for approval in the matter. Logically, the laboratory practices will be suspended for students who do not complete or fail this activity. A minimum grade of 4/10 must be achieved to qualify for the pass of the subject.	15	A1 B5 C6 D1 A3 C13 C26
Workshops	Resolution of PRACTICAL ASSUMPTIONS (design of experiments, laboratory introduction) A personalized monitoring of the student will be carried out and the way of defending/presenting the information will be evaluated, endorsed by the reliable bibliographic search (ability to search, value, classify and select information), as well as the ability to structure, synthesize, criticize and interrelate the contents for the resolution of the practical case or case raised.	5	A1 B5 C6 D1 A3 C13 C26
Objective questions exam	There will be a short test of objective questions on the topics covered in seminars/workshops that may include theoretical-practical questions/problems or multiple choice. This test serves, at the same time, for the student to assess and evaluate their study methodology. In order to compensate with the rest of the evaluation, a total final grade of 4/10 must be achieved (and a minimum grade of 4/10 in each part of the test). The day and time, as well as the classroom, will be public and the information will be included in the academic program of the center, previously approved by the Faculty Board.	10	A1 B5 C6 D1 A3 C13 C26
Essay questions exam	It corresponds to the official test (ordinary and/or extraordinary calls) and MANDATORY for all enrolled students. It is made up of three parts: theoretical (5%), theoretical-practical (15%) and problems (15%) that integrates the development of an analytical procedure and/or resolution of a practical case. In order to compensate with the rest of the evaluation, a total final grade of 4/10 must be achieved (and a minimum grade of 4/10 in each part of the test). The day and time, as well as the classroom, will be public and the information will be included in the academic program of the center, previously approved by the Faculty Board. OBSERVATION: If there are several teachers involved in the subject (in theory/seminars), the grade that the student must obtain in the part taught and evaluable by each teacher will have to be greater than or equal to 3.5/10, being the necessary requirement for the overall weighting of the exam to take place. Not reaching this qualification, the final result is fail.	40	A1 B5 C6 D1 A3 C13 C26

Report of practices, practicum and external practices	Upon the teacher's indication, the work team will prepare the practical reports (limited number of pages), which will reflect the work done in the laboratory by the team. Two models will be followed: scientific and technical. The fact of adjusting to the norms, the title proposal, layout, discussion of results, ability to synthesize the conclusions, etc. will be valued. The scientific articles/technical reports handled in the practices will serve as a model. Taking as a model does not mean PLAGIARIASING, which will be penalized with a ZERO in the qualification of the reports. These reports, whether scientific or technical, must be delivered within the established period and will be corrected by the professor. A minimum grade of 4/10 must be achieved to qualify for the pass of the subject.	10	A1 B5 C6 D1 A3 C13 C26
Laboratory practice	A laboratory test will be practiced, at an individual level, which will allow the evaluation of the competencies and skills acquired by the student during the laboratory sessions. Said test will be carried out at the end of the laboratory sessions and is mandatory, and a minimum grade of 4/10 must be achieved to opt for the subject's approval.	10	A1 B5 C6 D1 A3 C13 C26

Other comments on the Evaluation

1.-The ***EVALUACIÃ*N continuous** *harÃ taking into account the *calificaciÃ*n of the distinct activities/test that they describe in this section (see Ã*tems of *evaluaciÃ*n up). It is **indispensable to reach a *calificaciÃ*n of 5/10 in each one of split them/activities/test that *evalÃ*an to SURPASS the matter**. *AdemÃ*s, beÃ necessary to reach a *calificaciÃ*n ***mÃ*nima of 4/10 in each one of these activities/test proposed to OPT To THE APPROVED of the matter**. In **case of not achieving the note *mÃ*nima** demanded in any of the activities/test, supposes the ***calificaciÃ*n of SUSPENSE** in the matter; the ***calificaciÃ*n that appearÃ in the record beÃ the note *ponderada *mÃ*s high reached**, reflecting aceÃ the *calificaciÃ*n *mÃ*s faithful and real of the activities/test made by the student (Regulation on *evaluaciÃ*n, the *calificaciÃ*n and the quality of the teaching and of the process of learning of the student, approved in the *claustro of 18 April 2023,*TÃ*tulo V. Of the *calificaciÃ*n of the student, *Art. 31.2.).

The ASSISTANCE To THE *PRÃ*CTICAS And To THE SEMINARS/WORKSHOPS, aceÃ like **the development and the *realizaciÃ*n of the activities/test associated** (see Ã*tems of *evaluaciÃ*n), **is COMPULSORY for ALL THE STUDENTS ENROLLED**, receive to the *evaluaciÃ*n continuous or global. **The *prÃ*cticas, the reports and the seminars/workshops are not recoverable** in the second neither successive announcements. The **ABSENCE in the *prÃ*cticas and/or seminars/workshops, aceÃ like the does not deliver of the reports in group, are not recoverable** in the second neither successive announcements, preventing *tambiÃ*n surpass the *evaluaciÃ*n global (in the case of the students that had opted by this way of *evaluaciÃ*n).

THE DELIVERY OF THE REPORTS OF *PRÃ*CTICAS, inside the term established by the *profesorado, is **COMPULSORY**. All the reports happenÃ*n by programs *anti-plagiarism and only allowÃ a *mÃ*ximo of 10% of similarity. The ***detecciÃ*n of plagiarism** with an upper similarity to 10% *tendrÃ like consequence the **SUSPENSE in the activity, with a *calificaciÃ*n of ZERO** and without *opciÃ*n to recover (Regulation on *evaluaciÃ*n, the *calificaciÃ*n and the quality of the teaching and of the process of learning of the student, approved in the *claustro of 18 April 2023,*TÃ*tulo VII. Of the use of half *ilÃ*citos, *Art. 40.).

The *calificaciÃ*n obtained in the distinct activities/test of *evaluaciÃ*n compulsory, whenever it reach the *mÃ*nimo of 4/10, *mantendrÃ for the announcement of July, by what in this announcement the student presentÃ only to the parts that have not surpassed in the first announcement.

2.- ***EVALUACIÃ*N GLOBAL:** to the *calificaciÃ*n definite of this proof moveÃ*n the qualifications obtained in the activities of *carÃ*cter compulsory and developed in the *prÃ*cticas of laboratory and in the seminars/workshops. **The student that wish to receive to the *evaluaciÃ*n global, have toÃ deliver to the coordinator of the matter**, **IN THE TERM OF TWO WEEKSfrom the start of the teaching**, a writing **signed in which it certify that opts by said *evaluaciÃ*n global**, what him preventÃ go back to the *evaluaciÃ*n continuous.

3.-Regarding the *realizaciÃ*n of the proofs or any official examination of the subject, is **COMPULSORY to carry achieve to be able to access to the classroom: *DNI/*NIF or *carnet to drive, SIMPLE CALCULATOR (no programmable or *electrÃ*nica) and 2 BOWLÃ*GRAFOS BLUE**. No allowÃ the use of an extraneous calculator. Therefore, no allowÃ the access to the classroom with the following UNAUTHORISED material: correctors (*tipex),*lapiceros, *TELÃ*FONO MÃ*VILE, INTELLIGENT CLOCK Or ANY ANOTHER DEVICE *ELECTRÃ*NICO, coats, hunters, *parcas, sweatshirts marsupials, scarves and similar, etc.

The no allowed material and detected in the interior of the classroom during the *realizaciÃ*n of the proofs beÃ

confiscated by the *profesorado and no *tendrÃ right to *devoluciÃ*n. *AdemÃ*s, the *incumplimiento of these norms, established by the *profesorado and known by the students with quite *antelaciÃ*n to the proofs and/or exÃ*menes when being published in the *GUÃ*To EDUCATIONAL OF THE MATTER, considerÃ fraudulent behaviour and *tendrÃ consequences of Ã*ndole discipline (Regulation on *evaluaciÃ*n, the *calificaciÃ*n and the quality of the teaching and of the process of learning of the student, approved in the *claustro of 18 April 2023, *TÃ*tulo VII. Of the use of half *ilÃ*citos, *Art. 41.)

The use of means or material *ilÃ*citos involveÃ the *finalizaciÃ*n of the proof and the immediate abandonment of the classroom, appearing a SUSPENSE in Records (certifying the fault in the file) and losing the rights to make ANY ACTIVITY, PROOF or EXAMINATION OF THE SUBJECT during the rest of the course. *TambiÃ*n NotifyÃ the fault committed to the managers of the Centre and of the *Dpto. So that they notify, to his time, to the upper authorities so that they take the timely measures (Regulation on *evaluaciÃ*n, the *calificaciÃ*n and the quality of the teaching and of the process of learning of the student, approved in the *claustro of 18 April 2023, *TÃ*tulo VII. Of the use of half *ilÃ*citos, *Art. 42.).

4.-All the activities that develop in the classroom or in the laboratories, the material of support (presentations), etc. *estÃ*n subject to the rights of the copyright and of image. The educational of the matter do not allow to be recorded, neither by *vÃ*deos neither by audios or any another format like the *pantallazos, during the development of the face-to-face classes or in the *telemÃ*ticas. What communicates for the timely effects by the possible consequences of Ã*ndole disciplinary that can produce .

NOTE: it recommends the reading of the document Regulation on *evaluaciÃ*n, the *calificaciÃ*n and the quality of the teaching and of the process of learning of the student, approved in the *claustro of 18 April 2023, that beÃ available in *MooVi to the start of the course.

***EVALUACIÃ*N OF THE STUDENTS OF THE PROGRAM OF GREATER**

1.- Assistance to the activities programmed 40%

2.- Follow-up of the activities made 30%

3.- The *anÃ*lisis home (sensors and devices *portÃ*tiles) 30%

Sources of information

Basic Bibliography

Hernández, L y González, C, **Introducción al análisis instrumental**, Ariel, 2002

Skoog, DA; Holler, FJ y Crouch, SR, **Principios de análisis instrumental**, 7, Cengage Learning Editores, 2018

Wang, J, **Analytical Electrochemistry**, 3, Wiley, 2006

Cela, R; Lorenzo, RA y Casais, MC, **Técnicas de separación en química analítica**, Síntesis, 2002

Complementary Bibliography

Monk, PMS, **Fundamentals of Electroanalytical Chemistry**, Wiley, 2001

Riley, T y Watson, A, **Polarography and other Voltammetric Methods**, Wiley, 1987

Kissinger, PT y Heineman, WR, **Laboratory Techniques in Electroanalytical Chemistry**, Marcel Dekker, INC, 1984

Valcárcel, M y Silva, M, **Teoría y práctica de la extracción líquido-líquido**, Alhambra, 1984

Miller, JM, **Separation Methods in Chemical Analysis**, Wiley, 1974

Recommendations

Subjects that continue the syllabus

Analytical Chemistry IV: Chromatographic and Affine Methods/V11G201V01306

Subjects that are recommended to be taken simultaneously

Chemical engineering/V11G201V01301
Inorganic Chemistry III: Coordination Chemistry/V11G201V01304
Organic Chemistry III: Concerted, Radical and Photochemical Reactions/V11G201V01305

Subjects that it is recommended to have taken before

Physics: Physics 2/V11G201V01107
Chemistry: Chemistry Lab I/V11G201V01105
Chemistry: Chemistry Lab II/V11G201V01110
Chemistry: Chemistry 1/V11G201V01104
Chemistry: Chemistry 2/V11G201V01109
Biochemistry/V11G201V01201
Analytical Chemistry I: Principles of Analytical Chemistry/V11G201V01202
Analytical Chemistry II: Optical Methods of Analysis/V11G201V01207
Physical chemistry I: Chemical thermodynamics/V11G201V01203

IDENTIFYING DATA

Physical Chemistry III: Quantum Chemistry

Subject	Physical Chemistry III: Quantum Chemistry			
Code	V11G201V01303			
Study programme	Grado en Química			
Descriptors	ECTS Credits	Choose	Year	Quadmester
	6	Mandatory	3rd	1st
Teaching language	#EnglishFriendly Galician			
Department				
Coordinator	Mosquera Castro, Ricardo Antonio			
Lecturers	Hermida Ramón, José Manuel Mosquera Castro, Ricardo Antonio Peña Gallego, María de los Ángeles Pérez Barcia, Álvaro			
E-mail	mosquera@uvigo.es			
Web				
General description	The foundations of the quantum chemistry are presented and applied to simple models to describe: nuclear movements in molecules and the electronic structure of the atoms. English Friendly subject: International students may request from the teachers: a) materials and bibliographic references in English, b) tutoring sessions in English, c) exams and assessments in English.			

Training and Learning Results

Code	
A1	Students can apply their knowledge and understanding in a manner that indicates a professional approach to their work or vocation, and have competences typically demonstrated through devising and sustaining arguments and solving problems within their field of study
A5	Students have developed those learning skills that are necessary for them to continue to undertake further study with a high degree of autonomy
B1	Ability for auronomous learning
B2	Organization and planning capacity
B4	Ability for analysis and synthesis
C1	Ability to know and understand essential facts, concepts, principles and theories related to Chemistry
C4	Use computer tools properly to obtain information, process data, perform computational calculations and calculate matter properties
C14	To know the principles of quantum mechanics and its application in the description of the structure and properties of atoms and molecules
D1	Ability to solve problems

Expected results from this subject

Expected results from this subject	Training and Learning Results			
Write and apply the fundamental operators of the quantum mechanics using the basic concepts of the theory of operators to calculate functions and own values, half values and more likely in the systems model (particle in the box, harmonic oscillator, rigid rotor, electrostatic model of the atom *monoelectrónico).		B2 B4	C1 C14	D1
Describe the functions and own values of the systems model.		B1 B2 B4	C1 C14	
Use the methods of variations and perturbations to treat systems more complex (atoms *polielectrónicos, oscillator *anarmónico, etc.)	A1 A5	B1 B2 B4	C1 C4 C14	D1
Pose approximate solutions for the equation of Schrödinger of atoms *polielectrónicos and describe his electronic structure using models of attachment of angular moments.		B1 B2 B4	C1 C14	D1
Describe the spectrums of atoms *monoelectrónicos and *polielectrónicos.	A1 A5	B1 B2 B4	C1 C4 C14	D1
Apply the theory of groups of symmetry in the context of the chemistry	A1 A5	B2	C1	D1

Contents

Topic	
1. Foundations of the quantum mechanics.	1.1. Origin of the quantum mechanics (experimental facts). Formalisms of the quantum mechanics. Non relativistic quantum mechanics. Atomic units. 1.2. Wavefunction. Constrains of the wavefunction. Wavefunctions for a single particle and a set of particles. Slater Determinants. Interpretation of the wavefunction. Normalization. Molecular and atomic wavefunctions. Separation of movements. 1.3. Operators. Hermiticity. Values for a magnitude. Eigenvalues. Orthogonality. Conmutation. Angular momentum operators. Ladder operators. Symmetry operators. Point groups. Symmetry classification of the wavefunctions (symmetry species). Character tables. 1.4. Half value. Most probable values. Uncertainty. Hypervirial and virial theorems. 1.5. Time-dependent Schrödinger equation. Stationary States (Non-time dependent Schrödinger equation).
2. Molecular translation	2.1. Free particle in 1-dimension and 3-dimension spaces. 2.2. Particle in a monodimentional box of infinite potential walls. 2.3. Particle in a 3-dimentional box. Level degeneration. 2.4. Infinite thick barriers. Reflection and transmission coefficients. 2.5. Finite thick barriers. Tunnelling.
3. Approximate treatments to resolve the equation of Schrödinger.	3.1. Variational Method. Eckart's Theorem. 3.2. Variational functions (linear combinations). Secular determinant. 3.3. Theory of time-independent perturbations in non degenerated levels. 3.4. Theory of independent perturbations of the time in degenerate levels. 3.5. Treatment *semiclásico of the interaction radiation-matter: theory of dependent perturbations of the time. Consequences in the interaction *inelástica radiation-matter. Integral moment *dipolar of transition. Coefficients of absorption and broadcast stimulated. Coefficient of spontaneous broadcast. Half life of the states aroused. 3.6. Distribution of a sample of particles between his levels of energy (statistics of Maxwell-*Boltzmann). Intensity of absorption and broadcast of radiation.
4. Molecular rotation.	4.1. Diatomic molecules: rigid Rotor. 4.2. Polyatomic molecules: spherical, symmetric and asymmetric tops. Rigid polyatomic rotors. 4.3. Centrifugal distortion in diatomic molecules.
5. Molecular vibration.	5.1. Harmonic oscillator (diatomic molecules). 5.2. Systems with connected harmonic oscillators (polyatomic molecules). 5.3. Effect of the molecular symmetry. 5.4. Limitations of the harmonic model. Anharmonic oscillator (diatomic molecules).
6. Electronic structure: one electron atoms.	6.1. Electrostatic model. Time-independent Schrödinger equation. 6.2. Results of the electrostatic model. Orbitals. 6.3. Electronic spin. Spin-orbit coupling. Fine structure. 6.4. Hyperfine structure. 6.5. Interpretation of electronic spectra of 1-electron atoms. Zeeman effect.
7. Electronic structure: many electron atoms.	7.1. Electrostatic model. Impossibility to solve Schrödinger equation exactly. 7.2. Description of the Hartree-Fock method. Limitations. 7.3. Angular momentum coupling. 7.4. Interpretation of electronic spectra of polyelectronic atoms.

Planning

	Class hours	Hours outside the classroom	Total hours
Lecturing	24	48	72
Problem solving	12	30	42
Laboratory practical	14	14	28
Essay questions exam	2	3	5
Essay questions exam	0	3	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	The professor will expose the concepts, methods and main knowledges of each subject. It will orient the autonomous work of the student marking objectives and proposing questions and/or exercises. In the classroom the student has to pay attention to the exposiition, take his/her notes and formulate the questions that he/she considers. In the autonomous work the student has to complete the elements of the subject that remained as autonomous work, resolve the questions that have been proposed, assimilate this information and, if necessary, elaborate new questions to formulate to the professor in next sessions or in tutorials.
Problem solving	The professor will resolve the exercises that he considers fundamental in each subject. Problems for autonomous resolution will be proposed to students. The participation of the students will be motivated, thus, in part of the sessions the students are those who resolve the problems. Students have to assist to these classes with participatory spirit, procuring to understand the resolution of the exercises and connect it with the knowledges purchased in theory. Modelling of problems and its mechanical resolution should be avoided. In the autonomous work the student has to solve the problems proposed and even look for other related.
Laboratory practical	The professors will propose exercises, longer than those usual in problem solving lectures. In its majority the problems will be solved with computers. The students will obtain results to the exercises proposed. In the autonomous work thye will have to analyse the results obtained. It is always important that they relate the work made with that studied in lecturing.

Personalized assistance

Methodologies	Description
Lecturing	The student can request tutorials to consult the doubts that go generating in his autonomous work.
Problem solving	The student is allowed to request tutorials to consult the doubts that go generating in his autonomous work.
Laboratory practical	The student could request tutorials to consult the doubts that go generating in his autonomous work.
Tests	**Description**
Essay questions exam	The student can request tutorials to consult the doubts that go generating in his autonomous work and to review the results of his examinations.
Essay questions exam	

Assessment

	Description	Qualification	Training and Learning Results			
Problem solving	During problem solving lectures, warning at least one day before, the students can be requeste to solve, alone, one of the problems that had been proposed for the subject under study at that time. Likewise, the voluntary resolution of a problem by the student in front of his mates ("on the blackboard") will be values (only in positive way) .	10	A1 A5	B2	C1 C4 C14	D1
Laboratory practical	The systematic observation of the work made the student, the answers to the questions asked by the professors, as well as, in its case, the contents of the memory of some experiments, will be valued. Satisfactory lab presence and work is an indispensable requirement to pass the course. In case of not passing this part of the subject the global qualification could not exceed 4,0 on 10 points.	10	A1 A5	B1 B2 B4	C1 C4 C14	D1
Essay questions exam	During the course the following examinations will be done: a) A partial proof that will include, probably, subjects 1, 2 and 3.	40	A1 A5	B1 B2 B4	C1 C14	D1
Essay questions exam	b) A final examination, with two opportunities, in the dates fixed by Faculty: January the first and June/July the second. In the first opportunity, this examen will include subjects 4, 5, 6 and 7, excluding those students who have chosen a global exam. In the second opportunity, the exam will include all the course.	40	A1 A5	B1 B2 B4	C1 C4 C14	D1

Other comments on the Evaluation

Rule 1: To pass the matter is indispensable requirement to have attended satisfactorily lab. This requires : a) assisted to all the sessions of practices or present a certificate accrediting a justified reason ; and b) reach a 4.0 punctuation. When both requirements are not full filled the global qualification will not exceed 4.0 points.

Rule 2: Each examination (partial or final) will include theoretical questions and numerical problems. To surpass the examination, in addition to a global qualification of 5.0 points, it is necessary to obtain a minimum punctuation of 4.0 points on 10 in the theoretical questions and of 3.0 points on 10 in the numerical problems. In contrary case the global qualification of the examination could not exceed 4.0 points on 10.

Rule 3. The students that, fulfilling the "rule 2", reach an equal or upper punctuation to 4,2 on 10 points in the partial proof could go to the final examination (in any one of his opportunities) answering only the exercises and questions related with those subjects not reviewed in the partial examination. This option must be indicated to the professor when beginning the final examination. When using this option the global qualification of the examinations will be obtained valuing to 50% the partial and to 50% the final.

Rule 4. When previoius rules are fullfilled, the global qualification of the matter will be the highest of: a) that obtained in the examination (or group of examinations using the rule 3); and b) the resultant of applying the following weighting: resolution of exercises 10%, practices of laboratory 10%, examination/s 80%.

Rule 5. In future trials to pass this course the students that have surpassed lab could request a certificate with the mark obtained in this course. It will serve them to request to future professors the validation of the lab. Access to this validation will depend, obviously, of the rules followed by future professors and does not remain guaranted.

Rule 6. We will not certify that a partial has been passed. It is not contemplated to keep approved parts of the subject between different academic years.

Rule 7. Along the cualification process, teachers could ask any student, in a personal interview, to answer any questions that could make correction more exact. This way could be employed in cases where exams are not easy to read, professor have doubts about original authorship of the examination or any other that could be solved with this method.

Rule 8. The detection of any kind of non-ethical behaviour during the exam (any kind of copy) will give rise to student expeled from exam and 0,0 result, appplied to this opportunity and the following ones within the academic year.

Sources of information

Basic Bibliography

Bertrán, J.; Branchadell, V.; Moreno, M; Sodupe, M., **Química cuántica**, 1, Síntesis, 2000

Complementary Bibliography

Levine, I. N., **Química cuántica**, 5, Prentice-Hall, 2001
Atkins, P.; Friedman, R., **Molecular quantum mechanics**, 5, Oxford University Press, 2011
Pilar, F. L., **Elementary quantum chemistry**, 2, McGraw-Hill, 1990
McQuarrie, D. A., **Quantum chemistry**, 1, Viva Books, 2003

Recommendations

Subjects that continue the syllabus

Physical Chemistry IV: Molecular Structure and Spectroscopy/V11G201V01307

Subjects that it is recommended to have taken before

Physics: Physics I/V11G201V01102
Physics: Physics 2/V11G201V01107
Mathematics: Mathematics 1/V11G201V01103
Mathematics: Mathematics 2/V11G201V01108
Chemistry: Chemistry 1/V11G201V01104

IDENTIFYING DATA

Inorganic Chemistry III: Coordination Chemistry

Subject	Inorganic Chemistry III: Coordination Chemistry			
Code	V11G201V01304			
Study programme	Grado en Química			
Descriptors	ECTS Credits	Choose	Year	Quadmester
	6	Mandatory	3rd	1st
Teaching language	#EnglishFriendly Galician			
Department				
Coordinator	Vázquez López, Ezequiel Manuel			
Lecturers	Couce Fortúnez, María Delfina García Fontán, María Soledad Vázquez López, Ezequiel Manuel			
E-mail	ezequiel@uvigo.es			
Web				
General description	This subject addresses the most relevant aspects of Coordination Chemistry: This type of compound will be studied from the structural, synthetic point of view and also its most outstanding properties. English Friendly subject: International students may request from the teachers: a) materials and bibliographic references in English, b) tutoring sessions in English, c) exams and assessments in English.			

Training and Learning Results

Code	
A2	Students have demonstrated knowledge and understanding in a field of study that builds upon their general secondary education, and is typically at a level that, whilst supported by advanced textbooks, includes some aspects that will be informed by knowledge of the forefront of their field of study
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
B1	Ability for auronomous learning
B3	Ability to manage information
B4	Ability for analysis and synthesis
C7	Distinguish the main types of chemical reactions and their characteristics
C15	Know the main techniques of structural research, including spectroscopy
C26	Perform correctly usual procedures in the laboratory, including the use of standard chemical instrumentation for synthetic and analytical work
D2	Capacity for teamwork

Expected results from this subject

Expected results from this subject	Training and Learning Results			
Define the global and steps thermodynamic stabilities constants and describe the chelated, macrocyclic and crypto effects.			C7	
Classify the ligands and the compounds of coordination, as well as recognize the presence of isomerism.	A2	B3	C15	
Deduce the spectroscopic term for the electronic configuration of a metal in a coordination compound.	A5		C15	
Construct and interpret a qualitative diagram of energies from molecular orbitals to octahedral complexes.	A5	B1		
Interpret the electronic spectra of the octahedral and tetrahedral complexes of transition metals and rationalize their magnetic behavior.		B3 B4	C15	
Describe the different types of substitution mechanisms and rationalize the different products obtained in substitution reactions of octahedral and plane-square complexes.		B3	C7	
Rationalize the thermodynamic stability of coordination compounds as a function of the oxidation state of the metal and the type of ligand.	A3	B3	C7	
Be that to carry out in the laboratory to preparation of any composed of coordination as well as to realize his structural determination			C26	D2
Describe the mechanisms of internal sphere and external sphere in the processes of electronic transfer in complexes.			C7	

Contents	
Topic	
Types of ligands.	Denticity of the ligands Functionality of the ligands
The coordination polyhedron	Number of coordination Geometry of coordination *Isomería. Nomenclature and indexes of coordination
The bond in coordination compounds(I)	Introduction to crystal field theory Octahedral complexes of weak field and strong field. Tetrahedral and Square-plane complexes
Thermodinamic properties of the coordination compounds	Stability constants and factors that affect them Chelate, macrocycle and criptate effects Irvin-Williams series Approximation of Pearson
The bond in coordination compounds(II)	Molecular orbital theory in octahedral complexes Metal-Ligand Interaction
Spectroscopic and magnetic properties of complex.	Energetic states. Rules of selection. General characteristics of the electronic spectra. Magnetic behaviour
Reaction mechanism in coordination compounds.	Substitution reactions in square-plane and octahedral complexes. Electronic transfer processes.
Practices of laboratory	Synthesis of transition metal coordination compounds. Characterization by means of different spectrocopic techniques Study of properties and catalysis applications

Planning			
	Class hours	Hours outside the classroom	Total hours
Seminars	24	36	60
Laboratory practical	14	14	28
Lecturing	24	24	48
Objective questions exam	2	0	2
Report of practices, practicum and external practices	0	12	12
Objective questions exam	0	0	0
*The information in the planning table is for guidance only and does not take into account the heterogeneity of the students.			

Methodologies	
	Description
Seminars	The seminar classes will be dedicated to the resolution of practical cases related with the subject as well as to the resolution of doubts or questions that arose in the development of each subject. It is also contemplated to carry out seminars in which aspects not taught in previous subjects but necessary for the course of the course will be addressed.
Laboratory practical	The laboratory practices will consist of 4 sessions of 3.5 hours attendance. The students will carry out different experiences in the laboratory and must make the corresponding laboratory book. Some of the experiences may require the previous study individually or by group.
Lecturing	In the theoretical kinds will present the fundamental aspects of the subjects

Personalized assistance	
Methodologies	**Description**
Seminars	During all the teaching period them/the students will be able to consult all type of doubts of the subject in schedule of tutorships or previous appointment.
Laboratory practical	The students will be able to consult to professors all type of doubts of the work in the practices of laboratory
Lecturing	During all the teaching period them/the students will be able to consult all type of doubts of the subject in schedule of tutorships or previous appointment.

Assessment			
	Description	Qualification	Training and Learning Results

Seminars	In the seminar sessions, students may be asked to solve simple questions that they must deliver at that time and that will serve for their evaluation. The score will only be taken into account if the score obtained in the global test is equal to or greater than 3 points out of 10.	15		C7 C15
Laboratory practical	The evaluation in the laboratory practices will have 10% regarding the laboratory notebook (it can be through a written test) and 5% to the behavior and skills by direct observation of the teacher. Students may also be asked to solve simple questions that they must deliver at that time and that will serve for their evaluation.	15	A2 A3	C26 D2
Lecturing	In the lecturing sesions, Students may also be asked to solve simple questions that they must deliver at that time and that will serve for their evaluation. The score will only be taken into account if the score obtained in the global test is equal to or greater than 3 points out of 10.	5	A3 B3 B4	C7 C15
Objective questions exam	There will be two short tests (1 hour) where the skills acquired at the time will be evaluated. The date and time of completion will appear in the academic schedule approved by the corresponding Faculty Board.	30		C7 C15
Objective questions exam	There will be a final test in which an overall evaluation of the subject will be made. The date and time of completion will appear in the academic schedule approved by the corresponding Faculty Board.	35		C7 C15 C26

Other comments on the Evaluation

Conditions that affect **any type of evaluation**:

- All written tests will include a set of questions on nomenclature and formulating simple inorganic compounds. If you do not achieve 90% of correct answers, the qualification of the corresponding test will not be considered in the corresponding evaluation.
- You can be requested, in person, from the student, the clarifications he deems appropriate regarding his/her answers in any of the written tests. Your answers may be considered in the evaluation of the test and modify its qualification.
- Laboratory practices are of an experimental nature and compulsory attendance at all sessions (Article 14 of the Regulation on Evaluation, Qualification and Quality of Teaching and the Student Learning Process of the University of Vigo). The evaluation of experimental skills will be carried out in the compulsory attendance sessions.
- The final grade of the students, if it is higher than 7 points out of 10, may be normalized so that the highest grade can be up to 10 points.

Conditions to qualify for **continuous evaluation**:

- Attendance at theoretical classes and seminars (Article 13 Evaluation regulation) and laboratory practices is mandatory
- The teacher must have a minimum of 80% of the deliverables proposed in the different face-to-face activities (exercises in theoretical classes and seminars or autonomous work exercises) in time and form at the end of the course.
- It is also mandatory for the student to take all the written tests planned to pass the subject.
- Failure to comply with any of these conditions implies the loss of the right to continuous evaluation.

Development of continuous evaluation:

- The specific competences of the subject related to the competences of the degree (CE7, CE15 and CE26) will be explicitly evaluated in exercises in the classroom and written tests. The basic, general and transversal competences will be evaluated implicitly in the qualification of the exercises.
- A score greater than or equal to 30% of the total value will be required in each of the written tests (short and final) and in the total sum of the grades of the deliverables, as well as 50% of the laboratory practices, so that the final grade has taking into account the rest of the evaluation elements (deliverables and short tests).
- In the case of not achieving any of the minimums, the report will include the weighted result of the tests and qualified exercises in which the criterion was achieved.
- Students who do not pass the subject at the end of the semester must take a written test in the closing period of the final evaluation in July. This test will have a value of 35% of the grade and will replace the results of the test at the end of the semester.
- The qualification of the deliverables (of the classroom activities) and short tests are not recoverable.

Global assessment
1) For non-compliance with the conditions for continuous evaluationIf the conditions for continuous assessment are not met, the student may take a test at the end of the semester where he/she must solve questions related to all the specific skills of the subject. If you have passed the CE26 competency (relating to laboratory practices) in the same course, this will be considered passed.2) Within the period determined by the Faculty of Chemistry, the student may request the overall assessment.
Respect for the final test:
It will be written and in each question, the learning outcome competence that is being evaluated will be identified. In that case:

- It will be necessary to obtain a minimum of 3 points out of 10 on average in the evaluation in those related to the CE7 and CE15 skills and 5 in those related to the CE26 skill (laboratory work skills) to pass the subject
- It will be necessary to obtain an overall grade equal to or higher than 5 out of 10 in that test to pass the subject and, in no case will the previous grades obtained during the semester be taken into account
- This test will be different in extension to the one carried out by those who opt for continuous evaluation, although it will be carried out on the same date.

Sources of information

Basic Bibliography

Bhatt, Vasishta, **Essentials of coordination chemistry [Recurso de Internet] : a simplified approach with 3D visuals**, Elsevier : Academic Press, 2016
Catherine E. Housecroft, Alan G. Sharpe ; traducción Pilar Gil Ruiz,, **Química inorgánica**, 2ª, Pearson Prentice Hall, 2006
Catherine E. Housecroft, Alan G. Sharpe, **Inorganic Chemistry**, 5ª, Harlow: Pearson Education, 2018

Complementary Bibliography

Ribas Gispert, Joan, **Coordination chemistry**, Wiley-VCH, 2008
Winter, Mark J., **D-block chemistry**, 2ª, Oxford University Press, 2015
Huheey, James E., **Inorganic chemistry : principles of structure and reactivity**, 4ª, New York : Harper Collins, 1993

Recommendations

Subjects that continue the syllabus

Inorganic Chemistry IV: Transition Metals and Solid State/V11G201V01309

Subjects that are recommended to be taken simultaneously

Physical Chemistry III: Quantum Chemistry/V11G201V01303

Subjects that it is recommended to have taken before

Inorganic chemistry I/V11G201V01204
Inorganic chemistry II/V11G201V01209

IDENTIFYING DATA

Organic Chemistry III: Concerted, Radical and Photochemical Reactions

Subject	Organic Chemistry III: Concerted, Radical and Photochemical Reactions			
Code	V11G201V01305			
Study programme	Grado en Química			
Descriptors	ECTS Credits	Choose	Year	Quadmester
	6	Mandatory	3rd	1st
Teaching language	#EnglishFriendly Spanish Galician			
Department				
Coordinator	Nieto Faza, Olalla			
Lecturers	Gómez Bouzó, Uxía Gómez Pacios, María Generosa Nieto Faza, Olalla Silva López, Carlos			
E-mail	faza@uvigo.es			
Web				
General description	This class will study radical, pericyclic and photochemical processes, using a mechanistic approximation with emphasis on selectivity. The teaching methodology is centered around problem-solving, and includes laboratory and molecular modeling practical work. Subject in the English Friendly program: International students can ask the instructors for a) learning materials and bibliography in English, b) personal attention in English at office hours and c) assignments and exams in English.			

Training and Learning Results

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
A4	Students can communicate information, ideas, problems and solutions to both specialist and non-specialist audiences
B3	Ability to manage information
B4	Ability for analysis and synthesis
C18	Know the properties of aliphatic, aromatic, heterocyclic and organometallic compounds
C19	Know the main synthesic routes in organic chemistry, including the interconversions of functional groups and the formation of carbon-carbon and carbon-heteroatom bonds
C27	Demonstrate the ability to observe, monitor and measure chemical processes, by systematically and reliably recording them and presenting reports of the work done
C28	Interpret data derived from laboratory observations and measurements in terms of their meaning and relate them to the appropriate theory
D3	Ability to communicate in both oral and written form in Spanish and / or Galician and / or English

Expected results from this subject

Expected results from this subject	Training and Learning Results			
Know and apply the factors affecting the stability of organic radicals.	A3 A4	B3 B4	C18 C19	D3
Identify and understand the mechanisms of radical reactions and use this knowledge to propose strategies to either avoid or exploit them.	A3 A4	B3 B4	C18 C19	D3
Use the Woodward-Hoffmann rules to differentiate between allowed and forbidden reaction paths in pericyclic processes.	A3 A4	B3 B4	C18 C19	D3
Recognize the most common pericyclic mechanisms (electrocyclizations, cycloadditions, and sigmatropic and ene reactions) and use them in synthetic sequences.	A3 A4	B3 B4	C18 C19	D3
Predict the regio and stereoselectivity of pericyclic reactions.	A3 A4	B3 B4	C18 C19	D3
Understand the mechanisms of photochemical activation of organic molecules.	A3 A4	B3 B4	C18 C19	D3
Understand and apply the mechanisms of photochemical reactions: double bond isomerizations, photodissociations, photoreductions and pericyclic reactions.	A3 A4	B3 B4	C18 C19	D3

Perform pericyclic, radical and photochemical reactions and elaborate, separate and purify their products using common techniques.	A3 A4	B3 B4	C18 C19 C27 C28	D3
Use spectroscopic tools to establish the structure of organic compounds.	A3 A4	B3 B4	C18 C27 C28	D3
Use molecular modeling tools to study the properties of organic compounds and reaction mechanisms.	A3 A4	B3 B4	C18 C19 C27 C28	D3

Contents

Topic	
1. Reaction mechanisms	1.1. Reaction mechanism. Reaction profiles and transition state theory. 1.2. Reaction driving force. Frontier orbital theory. 1.3. Types of selectivity in organic transformations. 1.4. Mechanism classifications.
2. Radical reactions	2.1. Homolytic vs. heterolytic bond breaking. 2.2. Radical stability. 2.3. Chain reactions, alkane halogenation. 2.4. Radical polymerizations. 2.5. Radical reductions and reductive couplings. 2.6. Radical reactions in nature.
3. Pericyclic reactions	3.1. Woodward-Hoffmann rules. Orbital symmetry conservation and transition state aromaticity. Thermal and photochemical allowed and forbidden reactions. 3.2. Electrocyclizations. 3.3. Cycloadditions. Frontier orbital theory. 3.4. Sigmatropic and ene reactions.
4. Photochemical reactions	4.1. UV/vis spectra of organic molecules. Properties of excited states. 4.2. Photophysical processes: unimolecular deactivation, internal conversion, intersystem crossing, emission (fluorescence, phosphorescence). 4.3. Double bond isomerizations. 4.4. Photodissociations. 4.5. Photoreductions. 4.6. Pericyclic reactions. 4.7. Photochemical reactions in nature.
5. Laboratory work	Practical work on experiments related to the previous sections of the course. Synthesis, purification and characterization of organic compounds.
6. Molecular modeling	Use of computational chemistry tools to study the properties of organic molecules and reaction mechanisms associated to the previous sections of the course.

Planning

	Class hours	Hours outside the classroom	Total hours
Introductory activities	0	2	2
Flipped Learning	12	20	32
Problem solving	24	44	68
Laboratory practical	28	10	38
Mentored work	0	8	8
Problem and/or exercise solving	2	0	2

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

Methodologies

	Description
Introductory activities	Presentation of the course and instructors. Review of the syllabus and the structure of the course in the remote learning platform.
Flipped Learning	The interaction of the students with the materials available in the remote learning platform is expected, as is working on the activities proposed to prepare for class. Classroom time will be used to consolidate, review, clarify and apply the studied concepts.
Problem solving	Practical exercises and problems will be solved to apply the concepts developed in the flipped classroom sessions.

Laboratory practical	The students will perform in the laboratory basic techniques related to the synthesis, separation, purification and structural characterization of organic compounds. The work includes evaluation of risk, experiment planning and analysis of results. Molecular modeling techniques will be used to study the properties of organic compounds and selected reaction mechanisms. To be allowed in the laboratory, the student is required to perform a set of preliminary preparation tasks on the remote learning platform. The work will be carried out individually in 3.5 h sessions, and will be documented in a laboratory notebook. After the practical sessions, a paper will be prepared according to the instructions of the professors.
Mentored work	

Personalized assistance

Methodologies	Description
Flipped Learning	Continuous evaluation provides both instructors and students with feedback about the evolution of student learning and students' strengths and weaknesses. Although instructors can set tutorial appointments for students they deem at risk, it is expected that the students will take responsibility for they own learning and ask for help when needed. Students can request personalized support from the instructors at any time along the course, in order to solve any problem related to the subject, to review difficult concepts or to ask for help with the assignments. Tutorial sessions can be held through office hours in person or online, using the virtual campus. Personalized attention will also be provided through e-mail or the forums in the remote learning platform.
Problem solving	Problem-solving sessions in small groups facilitates personalized support to the student as soon as difficulties arise. As in the previous section, personalized attention will be provided in office hours, as well as through e-mail or forums in the remote learning platform.
Laboratory practical	In the laboratory sessions, most individual problems will be solved in class. As in the previous section, personalized attention will be provided in office hours, as well as through e-mail or forums in the remote learning platform.
Mentored work	

Assessment

	Description	Qualification	Training and Learning Results
Flipped Learning	Students must participate in class activities and interact with the contents planned in the online learning platform. The results of the tests and other online activities integrated in every lesson in the platform will be evaluated.	10	A3 B3 C18 D3 A4 B4 C19
Problem solving	Students must solve short questions, problems and exercises, actively participating in the seminar sessions and completing them with independent work. A series of assignments will be graded. The grading will take into account the correctness of the provided answers, the quality of argumentation and the presentation of the results.	15	A3 B3 C18 D3 A4 B4 C19
Laboratory practical	The competencies associated to the safe handling of chemicals, the assessment of risks in the laboratory and the planning and execution of experiments (both computational and in the laboratory) and the analysis of results, will be evaluated. For this, we will use the systematic observation of the student's work, the preliminary work, previous to the laboratory sessions, and the quality of the laboratory notebook and the assigned report. The laboratory work will get a PASS/FAIL grade. Attendance to laboratory sessions and a PASS grade in them is needed to pass this course. 10% of the final grade is associated to an assignment related to the practical sessions.	10	
Mentored work	The students will work on the elaboration of documents in different formats, associated to the contents of the course.	10	

Problem and/or exercise solving	There will be three exams, involving problems and exercises: 1. A test about the first sections of the subject (2 hours), associated to a 15% of the final grade. 2. A test about all the contents covered in the class (2 hours), associated to a 40% of the final grade. A minimum grade of 4.0 out of 10 is required for a global passing grade. 3. A written exam (0.5 hours) related to the experimental part of the subject, associated to a 10% of the final grade. A 4.0 grade (out of 10) in this test is required for a global passing grade.	55	A3 B3 C18 D3 A4 B4 C19 C27 C28

Other comments on the Evaluation

Students need to demonstrate complete mastery of a set of essential learning outcomes in order to pass the course.

In case there is doubt about the mastery of the course's learning outcomes by any student, further or complementary oral tests can be scheduled for a sound evaluation.

Student participation in any of the graded activities will result in the assignment of a grade in this course (the student will be considered "presentado"). Attendance to laboratory sessions, participation in exams and the handing out of assignments are considered graded activities in this context.

Students who have attended the course in previous academic years: Those evaluated with a PASS grade in the experimental part of the course, upon request, will be awarded a PASS grade in this part of the course this year. As a result, their attendance to the laboratory sessions will not be required. However, assignments and the written test associated to the experimental part are required to achieve the grades associated to the experimental contents of the course this year (20%).

In the 2ª Edición de la Convocatoria Ordinaria, the grades obtained by the student in the problem solving, flipped learning and laboratory practical parts will be kept. An exam covering all the theoretical contents of the subject will be proposed, with a qualification that will represent a 45% of the final grade. A written test covering the experimental work will also be administered, with a contribution of 10% to the final grade. A minimum grade of 4.0 out of 10 in each of these two tests is needed for a passing grade and the consideration of the other grading elements.

The students desiring to opt-out of the continuous evaluation mode, need to attend the laboratory sessions and obtain a PASS in them, as well as obtaining a grade equal or higher than 5 out of 10 in the written test associated to the experimental part of the class (20% of the grade). On top of that, a grade equal or higher to 5 out of 10 is needed in a written exam covering all the contents of the course (80% of the grade).

Sources of information

Basic Bibliography

Eric V. Anslyn, Dennis A. Dougherty, **Modern physical organic chemistry**, University Science Books, 2006

Felix A. Carroll, **Perspectives on structure and mechanism in organic chemistry**, John Wiley, 2010

John Perkins, **Radical chemistry : the fundamentals**, Oxford University Press, 2000

Ian Fleming, **Pericyclic reactions**, Oxford University Press, 1999

Carol E. Wayne, Richard P. Wayne, **Photochemistry**, Oxford University Press, 1996

Steven M. Bachrach, **Computational organic chemistry**, John Wiley & Sons,, 2007

James W. Zubrick, **The Organic Chem Lab Survival Manual: a student's guide to techniques**, John Wiley & Sons, 2009

Jerry R. Mohrig ... [et al.], **Laboratory techniques in organic chemistry : supporting inquiry-driven experiments**, W.H. Freeman, 2014

Complementary Bibliography

Nicholas J. Turro, V. Ramamurthy, J.C. Scaiano, **Modern molecular photochemistry of organic molecules**, University Science Books, 2010

Ernö Pretsch, Philippe Buhlmann, Martin Badertscher, **Structure determination of organic compounds : tables of spectral data**, Springer,, 2009

Chemistry Libre Texts, **ChemistryLibre Texts**, ookshelves/Organic_Chemistry,

James Ashenhurst, **MasterOrganicChemistry**, https://www.masterorganicchemistry.com/,

Recommendations

Subjects that continue the syllabus

Organic Chemistry IV: Design of Organic Synthesis/V11G201V01310

Subjects that are recommended to be taken simultaneously

Physical Chemistry III: Quantum Chemistry/V11G201V01303

Subjects that it is recommended to have taken before

Structural Determination/V11G201V01206
Organic chemistry I/V11G201V01205
Organic chemistry II/V11G201V01210

Other comments

In this class, the student is expected to learn how to deftly manipulate a relevant number of new concepts in a short period of time. As a result, daily work and study is a must. The same applies to class attendance and active participation in all the proposed activities, including interaction with the materials available in the online platform or the reading of the designated documents before every in person session.

It is strongly advised to have passed Organic Chemistry I and II and Structural Determination or equivalent, since the concepts learnt in these classes will be required in this one.

The use of molecular models is heavily recommended, as one of the main difficulties of this course is the visualization of the three-dimensional structure of molecules.

A laboratory coat and notebook is needed for the laboratory sessions.

IDENTIFYING DATA				
Química analítica IV: Métodos cromatográficos e afins				
Subject	Química analítica IV: Métodos cromatográficos e afins			
Code	V11G201V01306			
Study programme	Grao en Química			
Descriptors	ECTS Credits	Choose	Year	Quadmester
	6	Mandatory	3	2c
Teaching language	Castelán			
Department	Química analítica e alimentaria			
Coordinator	Gago Martínez, Ana			
Lecturers	Costas Rodríguez, Marta Estévez Bastos, Pablo Gago Martínez, Ana Leao Martins, Jose Manuel			
E-mail	anagago@uvigo.es			
Web				
General description	Coñecementos básicos sobre as técnicas de separación e a súa aplicación na análise química. Aplicacións xerais.			

Resultados de Formación e Aprendizaxe	
Code	
A1	Que os estudantes saiban aplicar os seus coñecementos ó seu traballo ou vocación dunha forma profesional e posúan as competencias que adoitan demostrarse por medio da elaboración e defensa de argumentos e a resolución de problemas dentro da súa área de estudo
A4	Que os estudantes poidan transmitir información, ideas, problemas e solución a un público tanto especializado coma non especializado
B5	Capacidade de adaptarse a novas situacións e adoptar decisións
C6	Coñecer os fundamentos e ferrramentas habituais na resolución de problemas analíticos e na caracterización de substancias químicas
C26	Levar a cabo correctamente procedementos habituais no laboratorio, incluíndo o uso de instrumentación química estándar para o traballo sintético e analítico
D1	Capacidade para resolver problemas

Resultados previstos na materia				
Expected results from this subject	Training and Learning Results			
Describir os fundamentos e principios da *cromatografía de gases, identificar e saber seleccionar detectores en función das aplicacións analíticas.	A1 A4	B5		D1
Describir os fundamentos da *cromatografía e os seus principios	A1 A4	B5	C6	D1
Describir os fundamentos e principios da *cromatografía de líquidos, identificar e saber seleccionar detectores en función das aplicacións analíticas.	A1 A4	B5	C6	D1
Describir os fundamentos e principios da *electroforesis *capilar, identificar e saber seleccionar detectores en función das aplicacións analíticas.	A1 A4	B5	C6	D1
Describir os fundamentos e principios dos axustes das diferentes técnicas de separación á *espectrometría de masas e as súas aplicacións na análise química.	A1 A4	B5	C6	D1
Aplicacións prácticas e de laboratorio das diferentes técnicas de separación no ámbito da análise ambiental, alimentos ou outras aplicacións	A1 A4	B5	C6 C26	D1

Contidos	
Topic	
1- Introdución á *cromatografía	Antecedentes, evolución, definicións e clasificación das técnicas *cromatográficas, principios da *cromatografía, parámetros *cromatográficos, aspectos cualitativos e cuantitativos
2 - *Cromatografía de gases	Introdución, Clasificación e compoñentes instrumentais. Detectores (principios e selección). Estratexias de preparación de mostra previos á análise *cromatográfico, optimizacións *cromatográficas, *calibración e medida. Aplicacións.

3- *Cromatografía de líquidos	Introdución, Clasificación e compoñentes instrumentais. Detectores (principios e selección). Estratexias de preparación de mostra previos á análise *cromatográfico, optimizacións *cromatográficas, *calibración e medida. Aplicacións.
4- *Electroforesis *capilar	Introdución, Clasificación e compoñentes instrumentais. Detectores (principios e selección. Estratexias de preparación de mostra previos á análise *electroforético, optimizacións *electroforéticas, *calibración e medida. Aplicacións.
5- *Espectrometría de masas	Principios e conceptos básicos da *espectrometría de masas. Principios da *ionización. Sistemas de *ionización. *Analizadores de masas. Espectros de masas: interpretación.
6- Técnicas axustadas	Introdución e principios do axuste *GC-*MS, *LC-*MS e CE-*MS. *Interfaces. Aplicacións

Planificación

	Class hours	Hours outside the classroom	Total hours
Lección maxistral	24	21	45
Seminario	12	20	32
Prácticas de laboratorio	14	19	33
Obradoiro	0	22	22
Resolución de problemas e/ou exercicios	0	6	6
Exame de preguntas de desenvolvemento	2	10	12
*The information in the planning table is for guidance only and does not take into account the heterogeneity of the students.			

Metodoloxía docente

	Description
Lección maxistral	As clases maxistrais teñen unha duración de 50 minutos pretenden dar unha visión global e a nivel *introductorio sobre as técnicas de separación e a súa aplicación na análise. Os temas abordados nas clases teóricas poden estar acompañados de artigos científicos que poderán servir para ampliar os coñecementos abordados na clase teórica. A plataforma *Moodle utilizarase como ferramenta e recurso de comunicación entre o alumnado e os docentes.
Seminario	O obxectivo que se pretende alcanzar coa esta actividade pedagóxica é asentar os coñecementos e ampliar as competencias adquiridas nas clases maxistrais, explorando. Tanto nos seminarios, talleres como actividades de laboratorio farase un seguimento do traballo individual e/ou colectivo que estea a realizar os estudantes. Os estudantes disporán dos medios facilitados para dita atención personalizada (*tutorías presenciais, foros na plataforma *Moodle, correo electrónico, etc.).
Prácticas de laboratorio	As sesións de laboratorio están orientadas á aprendizaxe dunha serie de técnicas *cromatográficas que permitan a identificación e cuantificación de *analitos en diferentes matrices (contaminantes ambientais e alimentos, aditivos en alimentos, residuos farmacéuticos, etc.). A partir de experimentos de laboratorio preténdese aproximar os conceptos das clases maxistrais e casos prácticos dos seminarios á actividade práctica de laboratorio. Os estudantes deberán, de forma autónoma e en grupo, ser capaces de planificar e executar a actividade de laboratorio. A execución dos experimentos deberá ir acompañada con análises e organización datos. Cálculos, interpretación e discusión dos mesmos. Redacción adecuada e apropiada dos experimentos realizados.
Obradoiro	Formarían parte dunha actividade non presencial complementaria ás clases maxistrais, seminarios e de laboratorio. Os estudantes deberán resolver por si mesmos de forma autónoma, individualmente e/ou en grupos, un traballo de investigación e/ou *monografía escrito de temas relacionados cos contidos da materia.

Atención personalizada

Methodologies	Description
Lección maxistral	As clases maxistrais teñen unha duración de 50 minutos pretenden dar unha visión global e a nivel *introductorio sobre as técnicas de separación e a súa aplicación na análise. Os temas abordados nas clases teóricas poden estar acompañados de artigos científicos que poderán servir para ampliar os coñecementos abordados na clase teórica. A plataforma *Moodle utilizarase como ferramenta e recurso de comunicación entre o alumnado e os docentes.
Seminario	O obxectivo que se pretende alcanzar coa esta actividade pedagóxica é asentar os coñecementos e ampliar as competencias adquiridas nas clases maxistrais, explorando Tanto nos seminarios, talleres como actividades de laboratorio farase un seguimento do traballo individual e/ou colectivo que estea a realizar os estudantes. Os estudantes disporán dos medios facilitados para dita atención personalizada (*tutorías presenciais, foros na plataforma *Moodle, correo electrónico, etc.).

Prácticas de laboratorio	As sesións de laboratorio están orientadas á aprendizaxe dunha serie de técnicas *cromatográficas que permitan a identificación e cuantificación de *analitos en diferentes matrices (contaminantes ambientais e alimentos, aditivos en alimentos, residuos farmacéuticos, etc.). A partir de experimentos de laboratorio preténdese aproximar os conceptos das clases maxistrais e casos prácticos dos seminarios á actividade práctica de laboratorio. Os estudantes deberán, de forma autónoma e en grupo, ser capaces de planificar e executar a actividade de laboratorio. A execución dos experimentos deberá ir acompañada con análises e organización datos. Cálculos, interpretación e discusión dos mesmos. Redacción adecuada e apropiada dos experimentos realizados.

Tests	**Description**
Resolución de problemas e/ou exercicios	Formarían parte dunha actividade complementaria ás clases maxistrais, seminarios e de laboratorio. Os estudantes deberán resolver por si mesmos de forma autónoma, individualmente e/ou en grupos, exercicios prácticos relacionados cos contidos da materia.
Exame de preguntas de desenvolvemento	O exame das preguntas de desenvolvemento terá unha duración máxima de tres horas. Nela incluiranse preguntas relacionados cos temas impartidos na materia.

Avaliación

	Description	Qualification	Training and Learning Results			
Seminario	Realizarase un seguimento do traballo individual e/ou colectivo desenvolvido polos estudantes, os cales disporán dos medios facilitados para unha atención personalizada (*tutorías presenciais, foros na plataforma *Moodle, correo electrónico, etc.). A nota mínima a alcanzar neste apartado deberá ser de 4 puntos (nunha cualificación global sobre 10)	25	A1		C6	D1
Prácticas de laboratorio	Realizarase un seguimento do traballo individual e/ou colectivo do traballo desenvolvido en lle laboratorio podendo requirirse a presentación dun informe ou resolución de cuestións expostas no Laboratorio. A nota mínima a alcanzar neste apartado deberá ser de 4 puntos (nunha cualificación global sobre 10)	15	A1		C6 C26	D1
Resolución de problemas e/ou exercicios	Realizarase unha proba curta dunha hora de duración con data establecida no *cronograma definido pola Facultade. É unha proba de carácter non *eliminatorio e permite ao alumno facer o seu seguimento de estudo na materia. Os seus contidos estarán relacionados coa materia impartida na materia.	20	A1		C6	D1
Exame de preguntas de desenvolvemento	O exame (proba longa), estará constituída por contidos impartidos nas clases maxistrais, actividades desenvolvidas nos seminarios, talleres e laboratorio. Terá a duración de tres horas. É requisito alcanzar un valor mínimo de 4 puntos (nunha cualificación global sobre 10)	40	A1 A4	B5	C6 C26	D1

Other comments on the Evaluation

Dado que las actividades de formación y evaluación continua programadas dentro de las Prácticas de Laboratorio y del Estudio de casos (incluida en el seguimiento de la actividad de seminarios) están diseñadas para formar al alumnado en habilidades y competencias directamente relacionadas con el ejercicio de la profesión en el campo del Análisis Químico, por ello la asistencia y participación del alumnado en ambas actividades evaluables es OBLIGATORIA, de tal manera que la ausencia o no realización injustificada de estas actividades impedirá superar la materia. Por lo tanto, considerando el carácter teórico-práctico de la asignatura y los resultados de formación y aprendizaje que se persiguen alcanzar con ambas metodologías, el alumnado que opte por la Modalidad de Evaluación Global Final también deberá realizar OBLIGATORIAMENTE estas actividades.

Para SUPERAR la materia será necesario alcanzar una calificación GLOBAL FINAL de 5,0 (sobre 10), una vez sumadas las calificaciones ponderadas obtenidas en las componentes evaluables de la asignatura y descritas con detalle en esta sección de evaluación. Muy Importante, PARA PODER SUPERAR LA MATERIA (poder sumar las calificaciones obtenidas en cada actividad evaluable), es OBLIGATORIO alcanzar una nota mínima de 4,0 (sobre 10) en cada una de las actividades evaluables mencionadas anteriormente (Pruebas cortas, Prueba final, Prácticas de laboratorio y Seminarios). Los alumnos que no cumplan este requisito en la primera oportunidad, serán calificados en el acta con la nota más alta alcanzada en las partes suspensas, y deberán repetir en la segunda oportunidad (convocatoria de Julio) la prueba relativa a la parte o partes en las que no hayan alcanzado el 4,0. Lógicamente, los alumnos que se encuentren en esta situación conservarán la nota de la/s parte/s superada/s (≥4,0) en primera oportunidad.

En la segunda oportunidad de evaluación, tal como fue ya descrito, es OBLIGATORIO alcanzar como mínimo una calificación de 4.0 (sobre 10) en todas las partes objeto de recuperación.

Los alumnos que optan por la modalidad **evaluación global final,** deberán tener en cuenta que las actividades de contenido práctico (seminarios y Prácticas de laboratorio) son de carácter obligatorio, por lo que la evaluación de dichas actividades, se realizará independientemente de la evaluación final.

ATENCIÓN: El alumno que desee optar por la modalidad EVALUACIÓN FINAL deberá informar y entregar un documento escrito y firmado a los docentes responsables de la materia durante las dos primeras semanas desde el inicio de la docencia de la materia correspondiente.

En la presentación de la materia, así como en la pagina de la Facultad de Química disponen de las fechas para las actividades de evaluación.

Bibliografía. Fontes de información

Basic Bibliography

Luis María Polo Díez, **Fundamentos de la cromatografía**, 1ª Ed., Dextra Editorial S.L, 2015

A. Braithwaite and J.F. Smith,, **Chromatographic Methods,**, 1ª Ed, Springer, Dordrecht, 1999

Phillipe Schmitt Kopplin, **Capillary Electrophoresis: Methods and Protocols**, 2ª Ed, Humana Press, 2016

Complementary Bibliography

Chhabil Dass,, **Fundamentals of Contemporany Mass Spectrometry,**, 1ª Ed., Wiley-Interscience,, 2010

Recomendacións

Subjects that are recommended to be taken simultaneously

Química analítica III: Métodos eletroanalíticos e separacións/V11G201V01302

Subjects that it is recommended to have taken before

Química analítica I: Principios de química analítica/V11G201V01202

Química analítica II: Métodos ópticos de análise/V11G201V01207

IDENTIFYING DATA

Physical Chemistry IV: Molecular Structure and Spectroscopy

Subject	Physical Chemistry IV: Molecular Structure and Spectroscopy			
Code	V11G201V01307			
Study programme	Grado en Química			
Descriptors	ECTS Credits	Choose	Year	Quadmester
	6	Mandatory	3rd	2nd
Teaching language	Spanish Galician			
Department				
Coordinator	Flores Rodríguez, Jesús Ramón			
Lecturers	Flores Rodríguez, Jesús Ramón Giráldez Martínez, Jesús Mandado Alonso, Marcos			
E-mail	flores@uvigo.es			
Web	http://https://moovi.uvigo.gal/			
General description	In the present subject Quantum Mechanics is applied to the study of molecules and the fundamentals of molecular spectroscopy. First, the Born-Oppenheimer approximation is introduced and the concept of potential energy surface presented, so a relatively detailed study of the rotation and vibration-rotation spectroscopies can later be done. The molecular orbital (MO) and valence bond (VB) methods for the analysis of the electronic structure of molecules are presented, so that of simple molecules can be studied and some basic aspects discussed. The concepts needed for studying the electron and photoelectron spectroscopies are, therefore, given. The most important computational methods for the study of the electronic structure, which form the basis of Computational Chemistry, are also presented in a simple way. The analysis of the spectroscopic methods includes the fundamentals of the magnetic resonance techniques, which is done from a theoretical perspective, as well as those of some other methods, including those based on the use of the laser. The theoretical developments studied in this subject rely on the fundamentals of Quantum Mechanics and the models for translation, vibration and rotation as presented in Química Física III: Química Cuántica. The introduction to Group Theory provided in that subject is completed in the present one by the first theme. Some elements of Statistical Mechanics are used to analyze the intensity and width/shape of the spectral lines for instance. By its theoretical and experimental contents, it provides some support to Química Física V: Cinética Química.			

Training and Learning Results

Code	
A1	Students can apply their knowledge and understanding in a manner that indicates a professional approach to their work or vocation, and have competences typically demonstrated through devising and sustaining arguments and solving problems within their field of study
A5	Students have developed those learning skills that are necessary for them to continue to undertake further study with a high degree of autonomy
B1	Ability for auronomous learning
B2	Organization and planning capacity
B4	Ability for analysis and synthesis
C2	Use correctly chemical terminology, nomenclature, conversions and units
C4	Use computer tools properly to obtain information, process data, perform computational calculations and calculate matter properties
C14	To know the principles of quantum mechanics and its application in the description of the structure and properties of atoms and molecules
C15	Know the main techniques of structural research, including spectroscopy
D1	Ability to solve problems

Expected results from this subject

Expected results from this subject	Training and Learning Results			
To apply the group theory in the context of the chemistry	A1 A5		C4	D1
To formulate the molecular Hamiltonian taking into account the Born-Oppenheimer approximation and to know about potential energy surfaces	A1 A5	B4	C2 C4 C14	D1
To describe the MO and VB methods and to apply the MO method to simple molecules.	A1 A5	B1 B2 B4	C2 C4 C14	D1

To describe some important computational methods and apply them to molecular electronic structure calculations.	A1 A5	B1 B2 B4	C2 C4 C14	D1
To apply the basic concepts of molecular spectroscopy.	A1 A5	B1 B2 B4	C2 C4 C14 C15	D1
To interpret distinct types of molecular spectra (microwave, infrared and visible-ultraviolet) in order to obtain structural information.	A1 A5	B1 B2 B4	C2 C4 C14 C15	D1
To describe the foundations of resonance spectroscopies	A1 A5	B1 B2 B4	C2 C4 C14 C15	D1

Contents	
Topic	
Subject I. The Group Theory in Chemistry.	1. Matrix representations. 2. Character tables. Degeneracy. 3. Basis functions. 4. Direct product representations. 5. Vanishing integrals. 6. Symmetry adapted linear combinations and projection operators. 7. Group Theory and Quantum Chemistry.
Subject II. Molecular electronic structure I.	1. The molecular hamiltonian: the Born-Oppenheimer approximation. 2. Potential energy surfaces. 3. The hydrogen molecule ion H2+: the MO method. 4. The hydrogen molecule H2: the VB method 5. Comparison of the MO and VB methods. 6. The validity of the Born-Oppenheimer approximation.
Subject III. Molecular electronic structure II.	1. Electronic configurations and electronic terms in diatomic molecules. 2. The effect of the spin-orbit interaction. 3. Electron density and bond polarity. 4. The MO and VB methods applied to diatomic molecules. 5. Polyatomic molecules: classification of the electronic states. 6. Application of the MO method to simple polyatomic molecules. 7. Electron population analysis. 8. Localized MOs. 9. Molecules with conjugate bonds: the sigma-pi separation. The free electron MO method. 10. The Hückel MO method. 11. Electron delocalization and aromatic stability. 12. Application of the VB method to polyatomic molecules: types of hybridization. 13. Resonance.
Subject IV. Electronic structure and Computational Chemistry.	1. The Hartree-Fock SCF method applied to molecules. 2. Basis functions in molecular calculations. 3. The Roothaan-Hall and Pople-Nesbet equations. 4. Limitations of the Hartree-Fock SCF method. 5. Post-Hartree-Fock methods. 6. Density Functional Theory (DFT). 7. Relativity in molecular calculations. 8. Semi-empirical methods.
Subject V. Interaction of the electromagnetic radiation with matter and molecular spectroscopy.	1. Interaction of the electromagnetic radiation with matter. 2. Diffusion. 3. Absorption: transition moments and selection rules. 4. The Lambert-Beer law. 5. Broadening of the spectral lines. 6. Raman effect. 7. Laser. 8. Fourier transform. 9. General aspects of the experimental techniques

Subject VI. Molecular rotation and rotational spectroscopies.	1. The polyatomic rigid rotor: results of the classical and quantum treatments. 2. Rotational spectra. 2.1. Selection rules, populations and line intensities 2.2. Stark effect. 2.3. Hyperfine structure and nuclear quadrupole moment. 2.4. Molecules with non-zero electronic angular momentum. 2.5. Type-l doubling. 3. Microwave spectroscopy (MW) and its applications. 4. Rotational Raman spectra. 5. Obtaining the molecular geometry from the rotational constants. 6. Nuclear spin and rotational states.
Subject VII. Molecular vibration and vibrational spectroscopies.	1. Vibration in diatomics. 2. Anharmonicity, vibration-rotation interaction and centrifugal distortion. 3. Vibration and vibration-rotation spectra in diatomic molecules. 4. Line intensity and nuclear spin. 5. Vibration in polyatomic molecules. 6. Vibration-rotation spectra in polyatomic molecules. 7. Analysis based on the symmetry: IR and Raman activities. 8. Anharmonicity and potential energy surfaces. 9. Normal modes with more than a minimum.
Subject VIII. Electronic spectra.	1. Electronic spectra. 2. Diatomic molecules. 2.1 Selection rules. 2.2 Franck-Condon principle and fine structure. 2.3 Dissociation and predissociation. 3. Electronic spectra in polyatomic molecules. 4. Fluorescence and phosphorescence. 5. Non-radiative transitions. 6. Photoelectron spectroscopies 7. Optically active molecules. Circular dicroism. 8. Laser techniques.
Subject IX. Resonance spectroscopies	1. Introduction. 2. Foundations of the RMN and RSE spectroscopies : Chemical shift. 3. Interpretation of the shielding constants. 4. Interpretation of the fine structure. 5. RMN and nuclear exchange processes. 6. RMN for the solid state. 7. Foundations of the pulse techniques and spin relaxation. 8. RSE spectroscopy: hyperfine structure. 9. Quadrupole resonance spectroscopy. 10. Mössbauer spectroscopy.

Planning

	Class hours	Hours outside the classroom	Total hours
Lecturing	23	57.6	80.6
Problem solving	12	26.4	38.4
Laboratory practical	14	14	28
Objective questions exam	2	0	2
Objective questions exam	1	0	1

*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 basic aspects of each topic and description of those to be addressed in the seminars. Discussion of the specific issues raised by students. The student will be provided with the necessary study material to follow the lessons through the Moovi (Moodle) platform.
Problem solving	Solution to numerical problems and theoretical questions as well as test-type exercises. Numerical and theoretical problems will be solved by the teacher in the seminars with the participation of the students. The results will be analyzed and interpreted. On a voluntary basis, the student may solve some of these exercises in the seminar, with the assistance of the teacher and the participation of the other students. They may, voluntarily as well, present a written resolution to an exercise and debate it with the teacher in tutoring time.

Laboratory practical	Every student is expected to perform a well-balanced set of experiments which exemplifies and develops the basic topics. The experiments will be carried out by couples of students for agility. Scripts describing every experiment, references to bibliography and instructions for the use of computers, programs and instrumentation, as well as others related to laboratory safety, will be made available as needed. The student must produce the figures and do the necessary calculations to obtain the final results, as well as analyze and discuss them.

Personalized assistance

Methodologies	Description
Lecturing	The student may raise specific questions in the lectures and ampler ones in the teacher's tutoring time.
Problem solving	The solution to the exercises will be discussed with the students in connection with the development of the theoretical aspects. The additional questions students may raise will be answered during the teacher's tutoring time.
Laboratory practical	The practical problems or doubts the students may raise regarding the theoretical foundation of the experiments, their development or the key aspects of the calculations needed to obtain the result will be discussed during the practical sessions. Additional issues may be addressed in tutoring hours.
Tests	**Description**
Objective questions exam	Any doubts regarding the exams, in particular those related to their scope and configuration, will be clarified. In the case of the short exams, the solutions to the exercises will be briefly presented and discussed in a seminar after the short exam. During tutoring hours, the answers provided by the student will be discussed with him/her at his/her request.

Assessment

	Description	Qualification	Training and Learning Results
Problem solving	The resolution of one or more exercises by the student and their presentation in the seminar will be rated. Short tests taken in the seminar will be rated as well. In both cases on a voluntary basis. The weight in the global grade lies between 0-10%.	10	A1 B1 C2 D1 A5 B2 C4 B4 C14 C15
Laboratory practical	Lab practices are compulsory. They will be rated by the assessment of their development (5%) as well as by that of the corresponding practice reports (15%), one per practice. Those reports have to be elaborated individually, must contain tables, figures and graphics and the calculations needed to obtain the results, as well as an analysis of them. Students must upload them to the Moovi platform before the deadline.	20	A1 B1 C2 D1 A5 B2 C4 B4 C14 C15
Objective questions exam	For the written exams the subject is divided into two parts (I and II), which have a relative weight of 50% in the mark. The written exams consist in the resolution of questions and problems. First short exam ("Primera prueba corta", Part I). Voluntary. It will take place by about half of the lecturing period. If its mark is equal or greater than 5 points over 10, part I will be considered as passed by the student. If it is lower than 5 but equal or greater than 3.75, it may represent 50% of the mark of part I, the other 50% coming from part I of the Final Exam, if that leads to improvement; otherwise the latter prevails. Its weight on the global mark depends on the results of other items and lies in the range: 0-40%.	35	A1 B1 C2 D1 A5 B2 C14 B4 C15

Objective questions exam	Second short exam (Part II). Voluntary. It will take place near the end of the lecturing period. Independently of the mark, the students must take part II in the Final Exam (see below). Its mark is only valid for calculating an average for part II with corresponding mark of the Final Exam, not independently of the latter. It may represent 25% of part II if that leads to an improvement, otherwise the mark obtained for part II in the Final Exam will prevail. Its weight on the global mark, depending on that other sections is: 0-10%. Final Exam. Compulsory. It will take place shortly after the lecturing period (May/June). Those students who have not passed the first short exam (mark>=5) will have to take all the exercises. Those who passed it can still take the exercises of part I to improve the corresponding mark. Its weight on the global mark depends on that of other sections and lies within 26.5%-80%. The combined mark of the exams (not including the tests of the first item) has to be of at least 3.75 on the 10-point scale for the subject to be passed. The lab practices and the final exam are compulsory. See also the second and third points of the next section (Other Comments on the Evaluation) The assessment rules of the second call (late June or early July) to those students who have not passed the subject, are given in the first point of the next section.	35	A1 B1 C2 D1 A5 B2 C14 B4 C15

Other comments on the Evaluation

- In the *second-opportunity evaluation* ("July's exam") the corresponding Final Exam is also compulsory, otherwise the mark will be the same as in the first opportunity. In any case, the mark cannot be lower than that of the first-opportunity evaluation. Lab practices represent 20% of the mark. The marks corresponding to "Problem Solving", second short exam and also that of the first short exam if >= 3.75, will be kept and used to calculate the average by the weights given in the last section, but only if their use gives a higher grade. Otherwise the mark of the Final Exam, including all exercises, will prevail, being 80% of the global grade.
- The average mark corresponding to the exams, third and fourth items of the last section, has to be >=3.75 on a 10 point scale for the other items to be considered in the global average. Such global average must be >=5 on the 10 point scale for the subject to be passed. Lab Practices and the Final Exam are compulsory.
- Taking two or more tests or presenting one exercise (Problem Solving), or attending one Lab session or any of the short exams, makes it impossible to get "No Presentado" as a grade.

Sources of information

Basic Bibliography

Atkins, P.W.; de Paula, J.; Keeler, J., **Atkins Physical Chemistry**, 11th, Oxford University Press, 2018

Levine, I. N, **Physical Chemistry**, 6th ed., McGraw Hill, 2009

Complementary Bibliography

Levine, I. N, **Quantum Chemistry**, 7th, Pearson, 2014

Hollas, J.M., **Modern Spectroscopy**, 4th, Wiley, 2004

Levine, I.N., **Molecular Spectroscopy**, 1st ed., John Wiley & Sons, 1975

Banwell, C. N., **Fundamentals of Molecular Spectroscopy**, 4th, McGraw-Hill, 1994

Requena, A. ; Zúñiga, J., **Espectroscopía**, 1, Pearson, 2004

Gil Criado, M.; Núñez Barriocanal, J.L., **Espectroscopía Molecular**, 1, Garceta, 2018

Bernath, P.J., **Spectra of Atoms and Molecules**, 4th, Oxford University Press, 2020

Atkins, P. W. ; Friedman, R., **Molecular Quantum Mechanics**, 4th ed., Oxford University Press, 2005

Atkins, P. W., **Quanta : a handbook of concepts**, 2nd ed., Oxford University Press, 1991

Recommendations

Subjects that are recommended to be taken simultaneously

Physical Chemistry V: Chemical Kinetics/V11G201V01308

Subjects that it is recommended to have taken before

Physical chemistry I: Chemical thermodynamics/V11G201V01203

IDENTIFYING DATA				
Physical Chemistry V: Chemical Kinetics				
Subject	Physical Chemistry V: Chemical Kinetics			
Code	V11G201V01308			
Study programme	Grado en Química			
Descriptors	ECTS Credits	Choose	Year	Quadmester
	6	Mandatory	3rd	2nd
Teaching language	#EnglishFriendly Spanish			
Department				
Coordinator	Bravo Díaz, Carlos Daniel			
Lecturers	Bravo Díaz, Carlos Daniel Cepero Rodríguez, Elizabeth Giráldez Martínez, Jesús Losada Barreiro, Sonia			
E-mail	cbravo@uvigo.es			
Web				
General description	International students may request from the teachers: a) materials and bibliographic references in English, b) tutoring sessions in English, c) exams and assessments in English.			

Training and Learning Results	
Code	
A1	Students can apply their knowledge and understanding in a manner that indicates a professional approach to their work or vocation, and have competences typically demonstrated through devising and sustaining arguments and solving problems within their field of study
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
B1	Ability for auronomous learning
B4	Ability for analysis and synthesis
C12	Know the kinetics of chemical change, including catalysis and reaction mechanisms
C27	Demonstrate the ability to observe, monitor and measure chemical processes, by systematically and reliably recording them and presenting reports of the work done
C28	Interpret data derived from laboratory observations and measurements in terms of their meaning and relate them to the appropriate theory
D1	Ability to solve problems

Expected results from this subject	Training and Learning Results			
Define with precision, all the basic concepts in Chemical Kinetics, and know the different methods of data analysis to obtain speed equations. Be able to carry out the analysis of kinetic data, including those of complex reactions and relate them to the reaction mechanisms. Explain the fundamental hypotheses of the different theories on chemical change, as well as the results and limitations of each of them (Collision Theory and Transition State Theory and know how to apply them as a tool in the analysis of kinetic results). Describe the different types of catalysis, explain the mechanism of catalyzed reactions, and apply it to specific cases. Know how to particularize said kinetic-formal treatment to the different types of catalysis. Describe the basis of the different experimental techniques available for the study kinetics of chemical reactions.	A1 A3 A5	B1 B4	C12 C27 C28	D1

Contents	
Topic	
Statistical thermodynamics	Introduction to the Statistical Thermodynamics. Configurations. Function of molecular partition. Canonical community. Thermodynamic functions. Constants of balance.
Kinetical theory of the gases	Foundations of the kinetical theory of the gases. Collisions and surfaces. Effusion.

Kinetical formal.	Rates of chemical reactions and rate equations. Orders of reactions, half-lives, elementary steps, molecularity. Analysis of kinetic data. Kinetic analysis of some complex reactions. Mechanisms. Effects of temperature.
Experimental methods in Kinetical Chemical	Transformation of the rate equations. Conventional techniques for slow reactions. Relaxation methods to study fast reactions.
Theoretical interpretation of the speed of reaction.	Collision theory for bimolecular reactions. Transition state theory.
*Catálisis	Catalysis. Homogeneous, acid-base, enzymatic, and heterogeneous catalysis.
Kinetical *electródica	Electrode-solution interface. Steps of an electrodic process. Galvanic cells. Overpotentials. Butler-Volmer and Tafel equations. Corrosion. Experimental techniques.

Planning

	Class hours	Hours outside the classroom	Total hours
Lecturing	24	0	24
Seminars	12	60	72
Laboratory practical	14	11	25
Objective questions exam	2	16	18
Essay questions exam	0	3	3
Problem and/or exercise solving	0	6	6
Essay questions exam	0	3	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	Exposition delivered before an audience or class, especially for instruction or to set forth some subject of the course. The students have to develop the ideas and topics delivered after lectures.
Seminars	meeting for giving and discussing information, and that will mostly be employed to solve previously proposed problems and/or exercices to commplement lectures theoretical classes
Laboratory practical	Practical activities developed in laboratories related to topics of the course

Personalized assistance

Methodologies	**Description**
Seminars	Resolution of doubts on the proportionate explanations in classes. These queries will be able to attend also by telematic means (email, videoconference, forums of *FaiTIC, ...),previous application through an email.
Lecturing	Resolution of doubts on the proportionate explanations in classes. During all the educationalperiod the students will be able to consult all type of doubts related with the matter. Thesequeries will be able to attend by telematic means (email, videoconference, forumsof *FaiTIC, ...), previous application through an email.
Laboratory practical	In the schedule of *Tutorías of the professor will resolve of form *individualizada and more personalthose doubts of the students that can arise along the course during the realisation of thepractices of laboratory or the preparation of the corresponding reports. These queriesalso will be able to attend by telematic means (email, videoconference, forums of*FaiTIC, ...), previous application through an email.
Tests	**Description**
Problem and/or exercise solving	In the schedule of *Tutorías of the professor will resolve of form *individualizada and more personalthose doubts of the students that can arise along the course during the realisation of thepractices of laboratory or the preparation of the corresponding reports. These queriesalso will be able to attend by telematic means (email, videoconference, forums of*FaiTIC, ...), previous application through an email.
Essay questions exam	The examination will make , in the time that stipulate , on the contents of the subject and will be able to *contenter theoretical questions like practices (problems).

Assessment

	Description	Qualification	Training and Learning Results
Seminars	Examination / short proof	15	A1 C12 D1 A5 C28

Laboratory practical	It marks here, together with the effort and the attitude, the *destrezas and the competitions developed pole student during the realization of the distinct practices. Also it will value the quality of the summary of #each of the practices as well as it of the memory that will have to deliver to it finalize all they (memory of practical). The delivery of the summaries to it finalize each practical, the memory of practices, and the assistance the sessions of practices is MANDATORY and, therefore, is not possible to approve the subject in the case of not to have realized *alguna of them.	15	A1 A3 A5	C12 C27 C28	D1
Essay questions exam	Examination of theory - questions/*cuestions developmental	35	A1 A5	C12 C28	D1
Essay questions exam	*Examen Practical - development of exercises that can be numerical the theorists	35	A1 A5	C12 C28	D1

Other comments on the Evaluation

- On the date indicated for the exams there will be two tests, one theoretical (35%) and another practical (practical exercises, 35%).

- In the second and subsequent exams, the teacher may opt for this scheme or another set, corresponding to a score of 70% of the overall grade.

Attendance at practices, and the delivery of the corresponding reports (summary of each practice and memory of which indicated) is MANDATORY. An unjustified fault will mean a direct failure in the subject and have to do them again the following year. More than three (3) justified absences will mean the suspense of the subject and that they have to be done again in the following course.

Attendance at master classes and seminars is highly recommended.

The score of the laboratory part will have to be equal to or greater than 5.0 (scale 0-10). The minimum grade REQUIRED in each of the development exams will be 3.8 (on a scale 0-10) so that it can be averaged with the scores of the other sections. There is no minimum grade in the control exams / short tests. The overall average score must be equal to or greater than 5.0 (scale 0-10).

Sources of information

Basic Bibliography

I. N. Levine, **Química Física**,
P. W. Atkins, J. De Paula, **Physical Chemistry**, 10,

Complementary Bibliography

T. Engel, P. J. Reid, **Physical Chemistry**,
K. J.. Laidler, **Chemical Kinetics**,
S. Senent, **Química Física II, 3ª Ed.**,
M. E. Robson, **Chemical Kinetics**,

Recommendations

Subjects that it is recommended to have taken before

Physics: Physics 2/V11G201V01107
Mathematics: Mathematics 2/V11G201V01108
Physical chemistry I: Chemical thermodynamics/V11G201V01203
Physical Chemistry II: Surfaces and Colloids/V11G201V01208
Physical Chemistry III: Quantum Chemistry/V11G201V01303

IDENTIFYING DATA

Inorganic Chemistry IV: Transition Metals and Solid State

Subject	Inorganic Chemistry IV: Transition Metals and Solid State			
Code	V11G201V01309			
Study programme	Grado en Química			
Descriptors	ECTS Credits	Choose	Year	Quadmester
	6	Mandatory	3rd	2nd
Teaching language	Spanish			
Department				
Coordinator	García Fontán, María Soledad			
Lecturers	Carballo Rial, Rosa García Fontán, María Soledad			
E-mail	sgarcia@uvigo.es			
Web				
General description	The first part of the subject focuses on the structural study and the structure/properties relationship of inorganic solids. In the second part of the subject, the most relevant aspects of the Chemistry of Transition Metals and their derivatives, such as coordination compounds, are addressed. Experiments on the synthesis and characterization of coordination compounds and inorganic solids will be carried out in the laboratory.			

Training and Learning Results

Code	
A2	Students have demonstrated knowledge and understanding in a field of study that builds upon their general secondary education, and is typically at a level that, whilst supported by advanced textbooks, includes some aspects that will be informed by knowledge of the forefront of their field of study
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
B1	Ability for auronomous learning
B3	Ability to manage information
B4	Ability for analysis and synthesis
C8	Know the characteristic properties of the elements and their compounds, including the relations between groups and their variations in the periodic table
C9	Know the structural aspects of chemical elements and their compounds, including stereochemistry
C26	Perform correctly usual procedures in the laboratory, including the use of standard chemical instrumentation for synthetic and analytical work
D2	Capacity for teamwork

Expected results from this subject

Expected results from this subject	Training and Learning Results			
Recognize and predict the main structural types of solids and their implications for physical and chemical properties.	A2 A3	B1 B3 B4	C8	
List and recognize the types of defects in crystals and their effect on the properties of the solid.	A2		C9	
Identify non-stoichiometric compounds.	A2		C9	
Recognize the effect of the addition of impurities on the color and optical properties of some inorganic solids.	A3	B3	C9	
Identify the main methods of preparation of inorganic solids.	A3		C8	
Describe how transition metals can be obtained from their natural resources and differentiate the behavior between the elements of the first, second and third transition series.	A2 A3	B3 B4	C8 C9	
Predict the reactivity of metal halides and oxides and coordination compounds based on the bond and oxidation state of the metal.	A2 A3	B3 B4	C8 C9	
Rationalize the thermodynamic stability of coordination compounds depending on the oxidation state of the metal and the type of ligand.	A2 A3	B3 B4	C8 C9	
Carry out in the laboratory the preparation, characterization and study of some physical and chemical properties of the main structural types of solids as well as other derivatives of transition metals.	A2 A3	B3 B4	C8 C9 C26	D2

Contents	
Topic	
1. Introduction and fundamentals.	(*)Importancia tecnolóxica dos sólidos . Clasificación de sólidos. Formulación de sólidos inorgánicos incorporando información estrutural. Polimorfismo, pseudomorfismo, politipismo
2. Structural rationalization.	(*)Empaquetamento de esferas. Representacións poliédricas Regras de Pauling. Regra da conectividade
3. Structure of solids.	(*)Principais tipos estruturais e a súa implicación na xeración de propiedades útiles dos sólidos
4. Perfect and imperfect crystals and their properties.	(*)Tipos de defectos Defectos puntuais. Consecuencias da presenza de defectos nas propiedades dos sólidos. Condutividade. Propiedades ópticas.
5. Solid preparation methods.	(*)Método cerámico. Química branda. Síntese en altas presión.Formación de sólidos a partir de gases e de líquidos.
6. Chemistry of metals in groups 3 and 4.	(*)Obtención e usos. Estados de oxidación máis frecuentes. Compostos representativos do titanio: haloxenuros, óxidos e óxidos mixtos. Compostos de coordinación.
7. Chemistry of group 5 metals.	(*)Obtención e usos. Estados de oxidación máis frecuentes. Compostos representativos do vanadio: haloxenuros, óxidos e oxoanións. Compostos de coordinación.
8. Chemistry of group 6 metals.	(*)Obtención e usos. Estados de oxidación máis frecuentes. Compostos representativos do cromo: haloxenuros, óxidos e oxoanións. Compostos de coordinación.
9. Chemistry of group 7 metals.	(*)Obtención e usos. Estados de oxidación máis frecuentes. Compostos representativos do manganeso: haloxenuros, óxidos e oxoanións. Compostos de coordinación. Bioinorgánica do manganeso e tecnecio
10. Chemistry of group 8 metals.	(*)Obtención e usos. Estados de oxidación máis frecuentes. Compostos representativos do ferro: óxidos e óxidos mixtos. Compostos de coordinación. Bioinorgánica do ferro.
11. Chemistry of group 9 metals.	(*)Obtención e usos. Estados de oxidación máis frecuentes. Compostos representativos do cobalto: haloxenuros e óxidos. Compostos de coordinación. Bioinorgánica do cobalto.
12. Chemistry of group 10 metals.	(*)Obtención e usos. Estados de oxidación máis frecuentes. Compostos representativos do níquel: haloxenuros e óxidos e compostos de coordinación. Bioinorgánica do platino.
13. Chemistry of group 11 metals.	(*)Obtención e usos. Estados de oxidación máis frecuentes. Compostos representativos do cobre: haloxenuros e óxidos e compostos de coordinación. Bioinorgánica do cobre e ouro.
Chemistry Practices of Compounds transition metais (4 sessions).	(*)Preparación e caracterización de compostos de metáis do bloque d
Inorganic Solids Practices (4 sessions).	(*)Preparación e estudo das propiedades dalgúns sólidos inorgánicos.

Planning			
	Class hours	Hours outside the classroom	Total hours
Lecturing	24	31	55
Laboratory practical	28	14	42
Seminars	12	12	24
Objective questions exam	2	9	11
Objective questions exam	0	18	18
*The information in the planning table is for guidance only and does not take into account the heterogeneity of the students.			

Methodologies	
	Description
Lecturing	(*)As clases teóricas adicaránse a presentar os aspectos fundamentáis dos temas.
Laboratory practical	(*)Realizaranse prácticas de laboratorio nas que se aplicarán os coñecementos teóricos adquiridos. As prácticas realizaranse en 8 sesións de 3,5 horas e os alumnos deberán reflectir e interpretar o observado no correspondente caderno de laboratorio.
Seminars	(*)As clases de seminario adicaranse á resolución de casos prácticos relacionados coa materia así como á resolución de dudas ou cuestións que surxan no desenvolvemento de cada tema. Contemplase tamén realizar seminarios nos que se abordarán aspectos non impartidos en materias anteriores pero necesarios para a marcha do curso.

Personalized assistance	
Methodologies	**Description**
Lecturing	
Laboratory practical	
Seminars	

Assessment			
	Description	Qualification	Training and Learning Results
Laboratory practical	(*)A asistencia ás clases prácticas presenciais é obrigatoria. A avaliación nas prácticas de laboratorio constará dun 10% de resolución de cuestións sinxelas e un 5% baseado no comportamento e destreza por observación directa do/a profesor/a. A puntuación soamente será considerada na proba longa conséguese unha cualificación igual ou superior a 3 puntos sobre 10.	15	A2 B3 C8 D2 A3 B4 C9 C26
Seminars	(*)Nas sesións de seminario pediráselles aos/*as estudantes a resolución de cuestións sinxelas que deberán entregar nese momento e que servirán para a súa avaliación. A puntuación soamente será considerada si na proba longa conséguese unha cualificación igual ou superior a 3 puntos sobre 10.	15	B1 C8 B3 C9 B4
Objective questions exam	(*)Haberá dúas probas curtas no cuadrimestre onde se avaliarán as competencias relacionadas cos temas. A puntuación soamente será considerada na proba longa si conséguese unha cualificación igual ou superior a 3 puntos sobre 10. A data e hora de realización é público e consta na programación académica aprobada na Xunta de Facultade correspondente.	30	B3 C8 B4 C9
Objective questions exam	(*)Haberá unha proba final na que se fará unha avaliación global da materia. A puntuación da proba soamente será considerada si conséguese na proba de *formulación un 9 sobre 10. A data e hora de realización é público e consta na programación académica aprobada na Xunta de Facultade correspondente.	40	B3 C8 B4 C9

Other comments on the Evaluation

Sources of information

Basic Bibliography

A. R. West, **Solid State Chemistry and its applications,**, 2, Wiley, 2014

L. Smart, E. Moore, **Solid State Chemistry. An introduction**, CRC, 2012

C. E. Housecroft y A. G. Sharpe.,, **Inorganic Chemistry,**, 5, Pearson, 2018

Complementary Bibliography

Winter, Mark J., **D-block chemistry, 1994**, Oxford University Press, 1994

Atkins, Peter, **Inorganic Chemistry,**, Willey-VCH, 2008

N.N. GREENWOOD , A. EARNSHAW, **Chemistry of the Elements**, 2, Butterwoth Heinemann, 1997

Recommendations

Subjects that it is recommended to have taken before

Structural Determination/V11G201V01206

Inorganic chemistry I/V11G201V01204

Inorganic chemistry II/V11G201V01209

Inorganic Chemistry III: Coordination Chemistry/V11G201V01304

IDENTIFYING DATA				
Organic Chemistry IV: Design of Organic Synthesis				
Subject	Organic Chemistry IV: Design of Organic Synthesis			
Code	V11G201V01310			
Study programme	Grado en Química			
Descriptors	ECTS Credits	Choose	Year	Quadmester
	6	Mandatory	3rd	2nd
Teaching language	#EnglishFriendly Spanish			
Department				
Coordinator	Álvarez Rodríguez, Rosana			
Lecturers	Álvarez Rodríguez, Rosana Gómez Pacios, María Generosa Rodríguez de Lera, Angel Sánchez Sanz, Irene			
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Web				
General description	In this subject, all previous knowledge of Organic Chemistry subjects will be integrated, in particular with regard to organic synthesis and its consequences in the creation of new elements. stereogenic. To do this, we will use the tools of retrosynthetic analysis, with special attention to the analysis of synthetic proposals that pass with selectivity (chemo, regio and stereoselectivity). English Friendly program subject: Foreign students may request from the teaching staff: a) material and bibliographic references for the follow-up of the subject in English, b) attend tutorials in English, c) tests and evaluations in English.			

Training and Learning Results	
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
B3	Ability to manage information
B4	Ability for analysis and synthesis
C15	Know the main techniques of structural research, including spectroscopy
C19	Know the main synthesic routes in organic chemistry, including the interconversions of functional groups and the formation of carbon-carbon and carbon-heteroatom bonds
C27	Demonstrate the ability to observe, monitor and measure chemical processes, by systematically and reliably recording them and presenting reports of the work done
C28	Interpret data derived from laboratory observations and measurements in terms of their meaning and relate them to the appropriate theory
D2	Capacity for teamwork

Expected results from this subject	Training and Learning Results		
Recognize structural elements in organic molecules	A3 A5	B3 B4	C19 C28
Propose retrosynthetic sequences of target molecules	A3 A5	B3 B4	C19 C28
Analyze alternative retrosynthetic proposals	A3 A5	B3 B4	C19 C28
Design selective synthetic sequences of target molecules	A3 A5	B3 B4	C19 C28
Assess the use of efficient structural simplification transformations	A3 A5	B3 B4	C19 C28
Properly manage interconversions between functional groups and protecting groups.	A3 A5	B3 B4	C19 C28
Study the reactions that can provide selectivity and its mechanisms	A3 A5	B3 B4	C19 C28

Apply in the laboratory, rigorously, the corresponding safety rules,as well as the proper treatment of the waste	A3		C15 C27 C28	D2
Write in the notebook laboratory, rigorously, the experiments carried out.		B4	C27 C28	
Perform the synthesis of an organic molecule using a selective stepwise synthesis	A3 A5	B3 B4	C15 C27 C28	D2

Contents	
Topic	
1. Design of the Organic Synthesis. Analysis retrosynthetic.	1.1. Target-oriented synthesis 1.2. The principles of retrosynthetic analysis 1.3. Strategic selection criteria 1.4. General principles of reactivity. Natural and unnatural polarity. 1.5 Selectivity. Basic concepts 1.6 Retrosynthetic strategies
2. Strategies based on transforms I. Selection of disconnections	2.1. C-X disconnections of monofunctional compounds 2.2. C-X disconnections of difunctional compounds (1, n) 2.3. C-C disconnections of monofunctional compounds 2.4. C-C disconnections of difunctional compounds (1, n) 2.5. Aromatic Compound Disconnections
3. Strategies based on functional groups I. Interconversion	3.1. Interconversion of functional groups. Oxidation levels 3.2. Functional group interconversion reactions 3.3. Oxidation reactions 3.4. Reduction reactions
4. Strategy based on functional groups II. Protective groups in Organic synthesis	4.1. Description of the protecting groups. 4.2. Sensitive to acid, basic, fluoride, oxidizing agents and reducing agents. 4.3. Selection of protecting groups
5. Strategy based on transfroms II. Disconnection of unsaturated compounds	5.1. Stereoselective synthesis of olefins. Csp2 = Csp2 disconnections 5.2. Palladium catalyzed reactions. Csp2-Csp2, Csp2-Csp, Csp-Ar and Ar-X (X = O, N) disconnections.
6. Strategy based on stereochemical	6.1. Description of stereochemistry. Chirality and descriptors. Topicity 6.2. Stereochemistry of chemical reactions. Product selectivity. Simple and induced diastereoselectivity.
7. Strategies based on molecular topology. Disconnection of cyclic compounds	7.1. Retrosynthetic analysis using topological strategies 7.2 Isolated ring retrosynthesis 7.3. Spiro ring retrosynthesis 7.4. Fused Ring Retrosynthesis 7.5. Bridging ring retrosynthesis
Experimental Section. The synthetic milestone of design and discovery of organic compounds with therapeutic applications.	4 sessions

Planning			
	Class hours	Hours outside the classroom	Total hours
Lecturing	24	24	48
Seminars	24	24	48
Laboratory practical	14	16	30
Essay questions exam	2	10	12
Essay questions exam	2	10	12
*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 material of the subject will be available on the Moovi platform in advance. The teaching staff will present, in a clear and structured way, the most relevant aspects of the subject assigned to each master session.
Seminars	The aspects discussed during the lectures will be worked on by solving the exercises proposed by teachers. In addition,using the Moovi platform, students will have the opportunity to work on the subject by solving additional exercises that will be evaluated.

Laboratory practical	The laboratory work will be developed in 4 sessions of 3.5h. During the synthesis, they will have to write the laboratory notebook, rigorously and clarity, which will be delivered at the end of the practices. In addition, the students will carry out a questionnaire about the experiments carried out in the laboratory, through the Moovi platform.

Personalized assistance

Methodologies	Description
Lecturing	The teaching staff will dedicate the necessary time to answer the questions of the students related to the subject of the course
Seminars	The teaching staff will dedicate the necessary time to answer the questions of the students about the exercises and problems solved in the seminar sessions, as well as those proposed in the Moovi platform
Laboratory practical	The teaching staff will dedicate the necessary time to answer the questions of the students related to retrosynthetic analysis of the target molecule and sequence design synthetic During the laboratory sessions, the faculty will supervise the development of the experiments proposed by students as well as compliance with security rules.
Tests	**Description**
Essay questions exam	
Essay questions exam	

Assessment

	Description	Qualification	Training and Learning Results
Seminars	The resolution of additional exercises and problems will be valued which are will be carried out through the Moovi platform. Learning outcome: - Recognize structural elements in organic molecules. - Propose retrosynthetic sequences of proposed molecules -Analyze alternative retrosynthetic proposals - Design selective synthetic sequences of target molecules . - Assess the use of efficient transformations of structural simplification. - Properly manage interconversions between functional groups and protecting groups. - Know the reactions that can provide selectivity and their mechanisms.	15	A3 B3 C15 A5 B4 C19
Laboratory practical	1. It is mandatory to carry out the laboratory practices 2. It will be valued: 2.1. The laboratory notebook (20% of practical qualification), structural analysis (25% of practical qualification), reaction mechanisms (20% of practical qualification), safety data sheets (10% of practical qualification) and questions about IUPAC nomenclature (15% of practical qualification) 2.2. Resolution of questions about work experimental, carried out in the laboratory, through the Moovi platform (10% of practical qualification)) 3. To achive the experimental sessions it is mandatory to have achived each one of the evaluated parts Learning outcome: All	25	A3 B3 C15 D2 A5 B4 C19 C27 C28

Essay questions exam	The following tests will be carried out throughout the subject: Two short tests (1h long; 10%) Learning outcome: - Recognize structural elements in organic molecules. - Propose retrosynthetic sequences of proposed molecules -Analyze alternative retrosynthetic proposals - Design selective synthetic sequences of target molecules . - Assess the use of efficient transformations of structural simplification. - Properly manage interconversions between functional groups and protecting groups. - Know the reactions that can provide selectivity and their mechanisms. Therefore, the qualification from the remaining sections will only be added when the score obtained in the sum of the written tests is equal to or greater than two points and a half.	20
Essay questions exam	A long written test (2h long; 40%) will be carried out throughout the subject: To achive the subject, students must obtain a minimum of 50% in all the written tests (proof of short answer and long answer test). Learning outcome: - Recognize structural elements in organic molecules. - Propose retrosynthetic sequences of proposed molecules -Analyze alternative retrosynthetic proposals - Design selective synthetic sequences of target molecules . - Assess the use of efficient transformations of structural simplification. - Properly manage interconversions between functional groups and protecting groups. - Know the reactions that can provide selectivity and their mechanisms. Therefore, the qualification from the remaining sections will only be added when the score obtained in the sum of the written tests is equal to or greater than two points and a half.	40

Other comments on the Evaluation

1. The participation of the students in any of the evaluation activities of the subject will imply that they acquire the condition of presented, therefore, they will be assigned a grade.

2. These activities are: attendance at laboratory sessions, completion of short tests and delivery of a minimum of 25% of the proposed exercises through the Moovi platform.

3. In addition, students may choose to be evaluated by a **single test** at the end of the semester and not by continuous evaluation. To do this, they will have to communicate it, in writing, to the subject coordinator at the beginning of the semester. In this case, the final evaluation will be 25% the laboratory work and 75% the single test .

June Assessment:

To achieve the subject it is mandatory to obtain a qualification equal or greater than 5 points in both of the evaluated parts, experimental and theoretical works.

July assessment:

1. The score obtained by students on the course: maximun of 4 points (2.5 points for laboratory practices and 1.5 points for exercise)

2. Written test: maximun 6 points.

Additional information:

1. The students who achieve the laboratory practices, in the previous course, will not have to do the laboratory work again.2. Serious conceptual mistakes, will mean the assignment of new activities aimed at solvent learning problems as soon as possible
3. For the correct performance of the laboratory practices, it is recommended to attend tutorial session in advance to

laboratory attendance

Sources of information

Basic Bibliography

Clayden, J.; Greeves, N.; Warren, S., **Organic Chemistry**, 2nd, Oxford University Press, 2012

Starkey, S., **Introduction to strategies for organic synthesis**, 1119347246, 2nd, Wiley, 2018

Complementary Bibliography

Warren, S.; Wyatt, P., **Organic Synthesis the Disconnection Approach**, 2nd, Wiley, 2011

Sunjic, V.; Perokovic, V. P., **Organic Chemistry from Retrosynthesis to Asymmetric Synthesis**, 1st, Springer, 2016

Recommendations

Subjects that it is recommended to have taken before

Chemistry: Chemistry Lab I/V11G201V01105
Chemistry: Chemistry Lab II/V11G201V01110
Chemistry: Chemistry 1/V11G201V01104
Chemistry: Chemistry 2/V11G201V01109
Structural Determination/V11G201V01206
Organic chemistry I/V11G201V01205
Organic chemistry II/V11G201V01210
Organic Chemistry III: Concerted, Radical and Photochemical Reactions/V11G201V01305