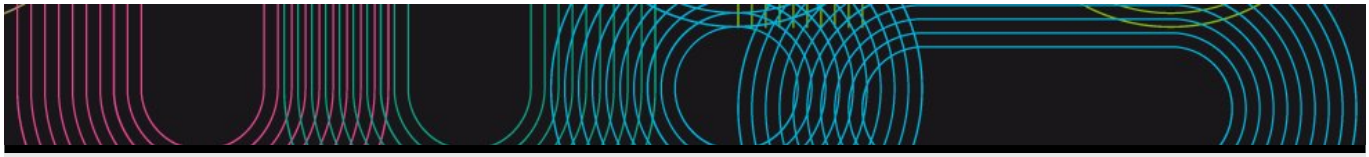

IDENTIFYING DATA				
Physical chemistry II				
Subject	Physical chemistry II			
Code	V11G200V01403			
Study programme	(*)Grao en Química			
Descriptors	ECTS Credits	Choose	Year	Quadmester
	9	Mandatory	2nd	2nd
Teaching language	Spanish Galician			
Department				
Coordinator	Mosquera Castro, Ricardo Antonio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

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

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

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

Contents

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

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

Planning

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

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

Methodologies

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

Laboratory practises	Completion of laboratory or computational chemistry practices under the supervision of a teacher in an autonomous way. Lab practices will be done by pairs in sessions of 3,5 hours. With advance enough, students will have in the TEM@ platform guide notes for the practices together with all the additional neccessary material. Guide notes will present the essential elements to realise the experimental or computational practices, as well as the fundamental theoretical points and further data treatment. After practice completion, in the terms set by the teacher, it will be necessary to deliver the corresponding report, elaborated following the guidelines given by the teacher.
Autonomous troubleshooting and / or exercises	For each one of the subjects, some problems or other works to be solved by the student and delivered to the teacher in due time will be proposed.

Personalized attention

Methodologies	**Description**
Master Session	In tutorial sessions, the teacher may solve in an individual and more personal way those doubts of the students that can arise along the course in any one of its parts (theory lessons, seminars, laboratory practice and the several types of autonomous activities to realise).
Seminars	In tutorial sessions, the teacher may solve in an individual and more personal way those doubts of the students that can arise along the course in any one of its parts (theory lessons, seminars, laboratory practice and the several types of autonomous activities to realise).
Laboratory practises	In tutorial sessions, the teacher may solve in an individual and more personal way those doubts of the students that can arise along the course in any one of its parts (theory lessons, seminars, laboratory practice and the several types of autonomous activities to realise).
Autonomous troubleshooting and / or exercises	In tutorial sessions, the teacher may solve in an individual and more personal way those doubts of the students that can arise along the course in any one of its parts (theory lessons, seminars, laboratory practice and the several types of autonomous activities to realise).
Tests	**Description**
Long answer tests and development	In tutorial sessions, the teacher may solve in an individual and more personal way those doubts of the students that can arise along the course in any one of its parts (theory lessons, seminars, laboratory practice and the several types of autonomous activities to realise).
Reports / memories of practice	In tutorial sessions, the teacher may solve in an individual and more personal way those doubts of the students that can arise along the course in any one of its parts (theory lessons, seminars, laboratory practice and the several types of autonomous activities to realise).
Short answer tests	In tutorial sessions, the teacher may solve in an individual and more personal way those doubts of the students that can arise along the course in any one of its parts (theory lessons, seminars, laboratory practice and the several types of autonomous activities to realise).
Multiple choice tests	In tutorial sessions, the teacher may solve in an individual and more personal way those doubts of the students that can arise along the course in any one of its parts (theory lessons, seminars, laboratory practice and the several types of autonomous activities to realise).
Practical tests, real task execution and / or simulated.	In tutorial sessions, the teacher may solve in an individual and more personal way those doubts of the students that can arise along the course in any one of its parts (theory lessons, seminars, laboratory practice and the several types of autonomous activities to realise).

Assessment

	Description	Qualification	Training and Learning Results
Laboratory practises	This mark comprises the effort and the attitude, the skills and the competitions developed by the student during the realisation of the laboratory practices.	ata 10,0	C3 D1 C6 D4 C8 D5 C19 D6 C20 D7 C21 D8 C22 D12 C27 D13 C28 D14 D15

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

Other comments on the Evaluation

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

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

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

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

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

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

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

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

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

Sources of information

ATKINS, P. W.; DE PAULA, J., **Química Física**, 8ª edición,
BERTRÁN, J.; BRACHANDELL, V.; MORENO, M.; SODUPE, M., **"Química Cuántica"**, 2ª edición,
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- **ATKINS P. W., FRIEDMAN R.S., "Molecular Quantum Mechanics" (5ª Edición). Oxford University Press. (2011).**
- **LEVINE I.N., "Química Cuántica" (5ª ed.), Prentice Hall (2001).**
- **LEVINE I.N., "Quantum Chemistry" (7ª ed.), Pearson (2014).**
- **LEVINE I.N., "Fisicoquímica" (5ª ed.), McGraw Hilll (2004).**
- **REQUENA A., ZÚÑIGA J., "Espectroscopía", Pearson Prentice Hall (2004).**

Libros de problemas:

- **CARBALLEIRA OCAÑA L., PÉREZ JUSTE I., "Problemas de Espectroscopía Molecular", Netbiblo (2008).**
- **LEVINE I.N., "Problemas de Fisicoquímica" (5ª ed.), McGraw Hilll (2005).**

Libros de prácticas:

- **GARLAND C.W., NIBLER J.W., SHOEMAKER D.P., "Experiments in Physical Chemistry" (7ª ed.), McGraw-Hill (2003).**
- **FORESMAN J.B., FRISH A., "Exploring Chemistry with Electronic Structure Methods: a guide to using Gaussian" (2ª ed.), Gaussian Inc (1996).**

Recommendations

Subjects that are recommended to be taken simultaneously

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

Subjects that it is recommended to have taken before

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