Universidade Vigo

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			
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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