UNIVERSIDAD DE CASTILLA - LA MANCHA

GUÍA DOCENTE

1. General information

Course:	PHYSICAL-CHEMISTRY II: INTRODUCTION TO QUANTUM CHE	**Code:**	57315
Type:	CORE COURSE	**ECTS credits:**	6
Degree:	398 - UNDERGRADUATE DEGREE PROGRAMME IN CHEMISTRY	**Academic year:**	2020-21
Center:	1 - FACULTY OF SCIENCE AND CHEMICAL TECHNOLOGY	**Group(s):**	20 23
Year:	2	**Duration:**	C2
Main language:	Spanish	**Second language:**	
Use of additional languages:	English	**English Friendly:**	Y
Web site:		**Bilingual:**	N

Lecturer: **BEATRIZ CABAÑAS GALAN** - Group(s): **20 23**

Building/Office	Department	Phone number	Email	Office hours
Edificio Marie Curie (primer piso)	QUÍMICA FÍSICA	926052042	beatriz.cabanas@uclm.es	Monday, Tuesday and Wednesday from 10 a.m. to 1 p.m.

Lecturer: **MARIA DEL PILAR MARTIN PORRERO** - Group(s): **20 23**

Building/Office	Department	Phone number	Email	Office hours
Marie Curie, 2ª planta	QUÍMICA FÍSICA	926052614	mariapilar.martin@uclm.es	Tuesday, Wednesday from 3:30 p.m. to 5:30 p.m. and Thursday and Friday from 12:30 p.m. to 1:30 p.m.

Lecturer: **LUCIA SANTOS PEINADO** - Group(s): **20 23**

Building/Office	Department	Phone number	Email	Office hours
Edifico Marie Curie/2.05	QUÍMICA FÍSICA	926052480	lucia.santos@uclm.es	Monday and Thursday 10.00h-12.00h Wednesday 18h-20h

2. Pre-Requisites

It is necessary to have studied the subjects of Mathematics, Physics and Fundamentals of Chemistry. It is recommended to have passed these subjects. In the subjects Fundamentals of Chemistry and Physics are introduce different aspects that will be developed in depth in this subject. The subject of Mathematics will provide some of the calculation tools that will be used in the treatment of Quantum Mechanics and the spectroscopy that is done in the subject of Physical Chemistry II.

3. Justification in the curriculum, relation to other subjects and to the profession

The objective of the subject is the study of matter from the atomic-molecular point of view using the tools provided by Quantum Mechanics and the study of molecular spectra. The 6 credit obligatory subject belongs to the module II: Fundamentals of Chemistry. This subject establishes the fundaments about the atomic and molecular structure and how to obtain atomic and molecular properties.The different points studied in this course will be developed in more depth in different subjects of the Degree in Chemistry.
Physical Chemistry II is an important subject for the future of the students since more than 50% of the GDP of the USA and the European Union is based on applications derived from Quantum Mechanics. It is a basic subject to deal with more complex issues in the field of Physical Chemistry such as the study of polyatomic molecules, chemical reactivity, statistical thermodynamics, etc.

4. Degree competences achieved in this course

Course competences

Code	Description
CB01	Prove that they have acquired and understood knowledge in a subject area that derives from general secondary education and is appropriate to a level based on advanced course books, and includes updated and cutting-edge aspects of their field of knowledge.
CB02	Apply their knowledge to their job or vocation in a professional manner and show that they have the competences to construct and justify arguments and solve problems within their subject area.
CB03	Be able to gather and process relevant information (usually within their subject area) to give opinions, including reflections on relevant social, scientific or ethical issues.
CB04	Transmit information, ideas, problems and solutions for both specialist and non-specialist audiences.
CB05	Have developed the necessary learning abilities to carry on studying autonomously
E08	Know the principles of quantum mechanics and their application to the structure of atoms and molecules
E14	Know and know how to apply the metrology of chemical processes, including quality management
E17	Develop the ability to relate to each other the different specialties of Chemistry, as well as this one with other disciplines (interdisciplinary character)
	Know the principles and theories of Chemistry, as well as the methodologies and applications characteristic of analytical chemistry,

G01	physical chemistry, inorganic chemistry and organic chemistry, understanding the physical and mathematical bases that require
G02	Be able to gather and interpret data, information and relevant results, obtain conclusions and issue reasoned reports on scientific, technological or other problems that require the use of chemical tools
G04	Know how to communicate, orally and in writing, the knowledge, procedures and results of chemistry, both specialized and non-specialized
T10	Ability to use specific software for chemistry at user level
T11	Ability to obtain bibliographic information, including Internet resources

5. Objectives or Learning Outcomes

Course learning outcomes

Description

Ability to understand and predict the behavior and reactivity of atoms and molecules from their structural characteristics, which can be determined from spectroscopic data or quantum chemical calculations

Ability to solve chemical problems applying the proper methodologies of physical chemistry

Dexterity in the handling of the main instrumental techniques used in physical chemistry and in the experimental determination of the structural, thermodynamic and kinetic properties of chemical systems

Additional outcomes

Ability to use scientific language correctly - Ability to seek to understand and use relevant bibliographic and technical information. - Develop the ability to work as a team in seminars and laboratory sessions.

6. Units / Contents

Unit 1: ORIGINS OF QUANTUM MECHANICS. Classical Theoretical Physics in the late 19th century. Radiation of the black body. Planck's hypothesis. Photoelectric effect. Compton effect. Atomic spectra. Atomic Bohr models. Insufficiency of this model. Correspondence principle. Wave-corpuscle duality. De Broglie's hypothesis. Heisenberg's uncertainty principle. Uncertainty relations of position-moment and time-energy.

Unit 2: BASIC ELEMENTS OF QUANTUM MECHANICS. Schrödinger wave equation. Hamiltonian operator. Stationary states. Interpretation of the wave function. Construction rules of quantum operators. Operator algebra. Quantum Mechanics postulates. Fundamental consequences of the postulates.

Unit 3: MECHANO-QUANTUM STUDY OF SOME SIMPLE SYSTEMS WITH LINEAR MOVEMENT Free particle. Particle in a one-dimensional box. Quantum numbers. Residual energy at the zero point. Particle in a three-dimensional box. Degenerate states. Potential barriers. Tunnel effect. One-dimensional harmonic oscillator. Comparison of classical and quantum results. Reduction of the two-particle problem to the one-particle problem

Unit 4: MOVEMENT IN A CENTRAL FIELD. The angular momentum in Quantum Mechanics. Spherical polar coordinates. Functions and values of the operators and. Spherical harmonics. Spatial quantization. Central force fields. System of two particles with a central potential. Rigid rotor. The hydrogen atom as a central force system. Solution of the radial equation for a coulomb potential. Hydrogen orbitals. Physical meaning. Representation. Probability distribution functions. Interaction with a magnetic field: spatial quantization Electronic spin.

Unit 5: POLYELECTRONIC ATOMS. Fundamental state of the He atom. Pauli's exclusion principle. Slater's determinants. Approximate methods for solving the Schrödinger equation. Method of variations. Theory of perturbations. Comparison of both methods for the fundamental state of the He atom. Angular momentum in polyelectronic atoms. Spectral terms corresponding to an electronic configuration. Hund's rule. Spin-orbit interaction. J-j coupling. Periodic system of the elements Aufbau principle Zeeman effect. Atomic spectra. Selection rules. Fine structure of the spectra.

Unit 6: ELECTRONIC STRUCTURE OF DIATOMIC MOLECULES. Molecular hamiltonian. Born-Oppenheimer's approximation. Hydrogen ion molecule. Molecular Orbital Method. OM-CLOA approximation and application to the hydrogen ion molecule Types and symmetry of OM. Potential energy curves. Treatment of the hydrogen molecule by the OM method. Interaction of configurations. Electronic configurations of homonuclear diatomic molecules Correlation diagrams. Molecular electronic terms. Treatment of the heteronuclear diatomic molecules by the OM method. Valence-binding method

Unit 7: MOLECULAR SPECTROSCOPY BASICS. Simplified treatment of the radiation-matter interaction by means of the time-dependent perturbation theory. Probability of transition. Dipolar moment of transition. Selection rules. Types of spectroscopy. Kinetics of radiation absorption and emission processes: Einstein's coefficients. Spontaneous emission. Mean radiant life time. Population inversion. Stimulated emission amplification. Lasers. Shape and width of lines. Lambert-Beer law.

Unit 8: ROTATIONAL VIBRATION SPECTROSCOPY. Nuclear Schrodinger equation. Vibrational energy: Approxiation of the harmonic oscillator and corrections of the anarmonicity Morse potential. Rotational energy: approximation of the rigid rotor, rotation-vibration coupling and centrifugal distortion Internal energy of a diatomic molecule Fundamental vibrational state. Dissociation energy. Pure rotation spectra of diatomic molecules. Selection rules. Line intensities of the rotational spectra. Rotation-vibration spectra of diatomic molecules. Raman spectroscopy

Unit 9: ELECTRON SPECTROSCOPY. Energy of electronic levels. Selection rules. Vibrational structure of electronic transitions. Intensity of the vibrational bands is: Principle of Franck-Condon. Fine rotational structure of the electronic-vibrational bands. Obtaining the energy of dissociation. Extrapolation of Birge-Sponer Dissociation and predissociation. Fluorescence and phosphorescence.

Unit 10: LABORATORY PRACTICES : 1.- Representation of atomic and molecular orbitals with Matlab Rotation-vibration spectrocopy: IR spectrum of CO. 3.- Atomic emission spectroscopy. Atomic spectra: Hydrogen. Calculation of spectral terms of an alkaline metal. 4- UV-Visible absorption spectrum of a dye.

7. Activities, Units/Modules and Methodology

Training Activity	Methodology	Related Competences (only degrees before RD 822/2021)	ECTS	Hours	As	Com	Description
							Presential teaching where the theoretical concepts and resolution of standard exercises will be taught. (G1, G2, E8) The student will be given the best resources to prepare the teaching activities and will be encouraged to participate with suggestions, questions, etc. that may arise during their work in the classroom or during the personal work that each student has done outside the classroom. The student will have the material related to the subject in the Virtual Campus (Moodle) and on the website of the

Class Attendance (theory) [ON-SITE]	Lectures	E08 G01 G02	0.8	20	N	-	teachers of the subject. To teach the subject, both the blackboard and transparencies or Power Point presentations will be used. We will choose, in each case, the means that will allow the student to learn better the objectives previously proposed for this subject. Presential teaching where the theoretical concepts and resolution of standard exercises will be taught. (G1, G2, E8) The student will be given the best resources to prepare the teaching activities and will be encouraged to participate with suggestions, questions, etc. that may arise during their work in the classroom or during the personal work that each student has done outside the classroom. The student will have the material related to the subject in the Virtual Campus (Moodle) and on the website of the teachers of the subject. To teach the subject, both the blackboard and transparencies or Power Point presentations will be used. We will choose, in each case, the means that will allow the student to learn better the objectives previously proposed for this subject.
Study and Exam Preparation [OFF-SITE]	Self-study	E17 G01	2.6	65	N	-	The student will study the theoretical concepts presented in the master classes and will work on the problems proposed in the seminars
Workshops or seminars [ON-SITE]	Problem solving and exercises	E08 G01 G02 G04	0.6	15	N	-	Problem solving by the student, previously raised and guided by the teacher.
Laboratory practice or sessions [ON-SITE]	Practical or hands-on activities	E08 E14 E17 G02 G04 T10	0.48	12	Y	Y	Handling of laboratory material, use of basic techniques and operations, obtaining and analysing results (G2, G4, E8, E17, T7, T8, T10)
Problem solving and/or case studies [ON-SITE]	Problem solving and exercises	CB01 E08 G01 G02	0.16	4	Y	N	The student will autonomously solve a series of practical cases.
Other off-site activity [OFF-SITE]	Practical or hands-on activities	T11	0.4	10	Y	Y	Previous study and elaboration of reports related to the practical activities. Study after the realization of the missions
Computer room practice [ON-SITE]	Practical or hands-on activities	G01 G02 T10	0.12	3	Y	Y	The student will make a practical assumption using the methodology and appropriate software and guided by the teacher.
Study and Exam Preparation [OFF-SITE]	Self-study	E08 E14 G01	0.6	15	Y	N	
Progress test [ON-SITE]	Assessment tests	CB01 CB03 E08 G01 G02	0.12	3	Y	N	The student will solve a series of questions and perform exercises
Final test [ON-SITE]	Assessment tests	E08 G01	0.12	3	Y	Y	The student will study autonomously examples proposed in class
		Total:	**6**	**150**			
		Total credits of in-class work: 2.4					**Total class time hours: 60**
		Total credits of out of class work: 3.6					**Total hours of out of class work: 90**

As: Assessable training activity
Com: Training activity of compulsory overcoming (It will be essential to overcome both continuous and non-continuous assessment).

8. Evaluation criteria and Grading System

Evaluation System	Continuous assessment	Non-continuous evaluation*	Description
Progress Tests	30.00%	0.00%	Two 1.5 hour written tests during class time to evaluate the learning of the contents taught in the classes and seminars
Final test	30.00%	80.00%	A comprehensive global written examen will be done to evaluate learning in theory and problems.
Laboratory sessions	20.00%	20.00%	Participate actively in the practical laboratory classes. The skill acquired in the handling of the different systems will be valued, as well as the adequate elaboration of the proposed questionnaires for these practical activities and the laboratory notebook.
			To make a continuous evaluation on knowledge based on the

Assessment of active participation	20.00%	0.00%	resolution and exposition of the proposed problems, resolution of test and other types of activities that are proposed.
Total:	**100.00%**	**100.00%**	

According to art. 4 of the UCLM Student Evaluation Regulations, it must be provided to students who cannot regularly attend face-to-face training activities the passing of the subject, having the right (art. 12.2) to be globally graded, in 2 annual calls per subject , an ordinary and an extraordinary one (evaluating 100% of the competences).

Evaluation criteria for the final exam:

Continuous assessment:

The student will take into account the following clarifications:

- Passing both tests gives the option of not having to take the final test. To do so, it will be necessary to pass each of them with a minimum point score of 5. They can be compensated as long as the student has at least a 4 in one of them and 7 in the other.

- Attendance at the laboratory sessions is obligatory. As well as the delivery of the memory of the work done in the laboratory.

Non-continuous evaluation:

The final test note will contribute to 80 % of the subject note and the remaining 20 % will be the laboratory note.
The final test will be different from the one carried out for the continuous evaluation, since 100% of the competences must be evaluated.

Specifications for the resit/retake exam:

In the extraordinary exam, the mark obtained in the laboratory practice classes of the ordinary exam will be kept and a global exam of the subject will be carried out, which will be passed with a 5/10.

Specifications for the second resit / retake exam:

The same methodology will be followed as for the extraordinary call.

9. Assignments, course calendar and important dates

Not related to the syllabus/contents

Hours	**hours**

Unit 1 (de 10): ORIGINS OF QUANTUM MECHANICS. Classical Theoretical Physics in the late 19th century. Radiation of the black body. Planck's hypothesis. Photoelectric effect. Compton effect. Atomic spectra. Atomic Bohr models. Insufficiency of this model. Correspondence principle. Wave-corpuscle duality. De Broglie's hypothesis. Heisenberg's uncertainty principle. Uncertainty relations of position-moment and time-energy.

Activities	**Hours**
Class Attendance (theory) [PRESENCIAL][Lectures]	2
Study and Exam Preparation [AUTÓNOMA][Self-study]	4
Workshops or seminars [PRESENCIAL][Problem solving and exercises]	1
Progress test [PRESENCIAL][Assessment tests]	.11
Final test [PRESENCIAL][Assessment tests]	.11

Unit 2 (de 10): BASIC ELEMENTS OF QUANTUM MECHANICS. Schrödinger wave equation. Hamiltonian operator. Stationary states. Interpretation of the wave function. Construction rules of quantum operators. Operator algebra. Quantum Mechanics postulates. Fundamental consequences of the postulates.

Activities	**Hours**
Class Attendance (theory) [PRESENCIAL][Lectures]	2
Study and Exam Preparation [AUTÓNOMA][Self-study]	9
Workshops or seminars [PRESENCIAL][Problem solving and exercises]	1.5
Progress test [PRESENCIAL][Assessment tests]	.1
Final test [PRESENCIAL][Assessment tests]	.1

Unit 3 (de 10): MECHANO-QUANTUM STUDY OF SOME SIMPLE SYSTEMS WITH LINEAR MOVEMENT Free particle. Particle in a one-dimensional box. Quantum numbers. Residual energy at the zero point. Particle in a three-dimensional box. Degenerate states. Potential barriers. Tunnel effect. One-dimensional harmonic oscillator. Comparison of classical and quantum results. Reduction of the two-particle problem to the one-particle problem

Activities	**Hours**
Class Attendance (theory) [PRESENCIAL][Lectures]	2
Study and Exam Preparation [AUTÓNOMA][Self-study]	9
Workshops or seminars [PRESENCIAL][Problem solving and exercises]	1.5
Problem solving and/or case studies [PRESENCIAL][Problem solving and exercises]	1
Progress test [PRESENCIAL][Assessment tests]	.3
Final test [PRESENCIAL][Assessment tests]	.3

Unit 4 (de 10): MOVEMENT IN A CENTRAL FIELD. The angular momentum in Quantum Mechanics. Spherical polar coordinates. Functions and values of the operators and. Spherical harmonics. Spatial quantization. Central force fields. System of two particles with a central potential. Rigid rotor. The hydrogen atom as a central force system. Solution of the radial equation for a coulomb potential. Hydrogen orbitals. Physical meaning. Representation. Probability distribution functions. Interaction with a magnetic field: spatial quantization Electronic spin.

Activities	**Hours**
Class Attendance (theory) [PRESENCIAL][Lectures]	3
Study and Exam Preparation [AUTÓNOMA][Self-study]	10
Workshops or seminars [PRESENCIAL][Problem solving and exercises]	3
Progress test [PRESENCIAL][Assessment tests]	.35
Final test [PRESENCIAL][Assessment tests]	.35

Unit 5 (de 10): POLYELECTRONIC ATOMS. Fundamental state of the He atom. Pauli's exclusion principle. Slater's determinants. Approximate methods for solving the Schrödinger equation. Method of variations. Theory of perturbations. Comparison of both methods for the fundamental state of the He atom. Angular momentum in polyelectronic atoms. Spectral terms corresponding to an electronic configuration. Hund's rule. Spin-orbit interaction. J-j coupling. Periodic system of the elements Aufbau principle Zeeman effect. Atomic spectra. Selection rules. Fine structure of the spectra.

Activities	**Hours**
Class Attendance (theory) [PRESENCIAL][Lectures]	3
Study and Exam Preparation [AUTÓNOMA][Self-study]	10
Workshops or seminars [PRESENCIAL][Problem solving and exercises]	3

Progress test [PRESENCIAL][Assessment tests]	.35
Final test [PRESENCIAL][Assessment tests]	.35

Unit 6 (de 10): ELECTRONIC STRUCTURE OF DIATOMIC MOLECULES. Molecular hamiltonian. Born-Oppenheimer's approximation. Hydrogen ion molecule. Molecular Orbital Method. OM-CLOA approximation and application to the hydrogen ion molecule Types and symmetry of OM. Potential energy curves. Treatment of the hydrogen molecule by the OM method. Interaction of configurations. Electronic configurations of homonuclear diatomic molecules Correlation diagrams. Molecular electronic terms. Treatment of the heteronuclear diatomic molecules by the OM method. Valence-binding method

Activities	Hours
Class Attendance (theory) [PRESENCIAL][Lectures]	2
Study and Exam Preparation [AUTÓNOMA][Self-study]	8
Workshops or seminars [PRESENCIAL][Problem solving and exercises]	2
Progress test [PRESENCIAL][Assessment tests]	.35
Final test [PRESENCIAL][Assessment tests]	.3

Unit 7 (de 10): MOLECULAR SPECTROSCOPY BASICS. Simplified treatment of the radiation-matter interaction by means of the time-dependent perturbation theory. Probability of transition. Dipolar moment of transition. Selection rules. Types of spectroscopy. Kinetics of radiation absorption and emission processes: Einstein's coefficients. Spontaneous emission. Mean radiant life time. Population inversion. Stimulated emission amplification. Lasers. Shape and width of lines. Lambert-Beer law.

Activities	Hours
Class Attendance (theory) [PRESENCIAL][Lectures]	2
Study and Exam Preparation [AUTÓNOMA][Self-study]	5
Workshops or seminars [PRESENCIAL][Problem solving and exercises]	1
Progress test [PRESENCIAL][Assessment tests]	.25
Final test [PRESENCIAL][Assessment tests]	.2

Unit 8 (de 10): ROTATIONAL VIBRATION SPECTROSCOPY. Nuclear Schrodinger equation. Vibrational energy: Approxiation of the harmonic oscillator and corrections of the anarmonicity Morse potential. Rotational energy: approximation of the rigid rotor, rotation-vibration coupling and centrifugal distortion Internal energy of a diatomic molecule Fundamental vibrational state. Dissociation energy. Pure rotation spectra of diatomic molecules. Selection rules. Line intensities of the rotational spectra. Rotation-vibration spectra of diatomic molecules. Raman spectroscopy

Activities	Hours
Class Attendance (theory) [PRESENCIAL][Lectures]	2
Study and Exam Preparation [AUTÓNOMA][Self-study]	5
Problem solving and/or case studies [PRESENCIAL][Problem solving and exercises]	2
Progress test [PRESENCIAL][Assessment tests]	.6
Final test [PRESENCIAL][Assessment tests]	.6

Unit 9 (de 10): ELECTRON SPECTROSCOPY. Energy of electronic levels. Selection rules. Vibrational structure of electronic transitions. Intensity of the vibrational bands is: Principle of Franck-Condon. Fine rotational structure of the electronic-vibrational bands. Obtaining the energy of dissociation. Extrapolation of Birge-Sponer Dissociation and predissociation. Fluorescence and phosphorescence.

Activities	Hours
Class Attendance (theory) [PRESENCIAL][Lectures]	2
Study and Exam Preparation [AUTÓNOMA][Self-study]	5
Workshops or seminars [PRESENCIAL][Problem solving and exercises]	2
Problem solving and/or case studies [PRESENCIAL][Problem solving and exercises]	1
Progress test [PRESENCIAL][Assessment tests]	.65
Final test [PRESENCIAL][Assessment tests]	.65

Unit 10 (de 10): LABORATORY PRACTICES : 1.- Representation of atomic and molecular orbitals with Matlab Rotation-vibration spectrocopy: IR spectrum of CO. 3.- Atomic emission spectroscopy. Atomic spectra: Hydrogen. Calculation of spectral terms of an alkaline metal. 4- UV-Visible absorption spectrum of a dye.

Activities	Hours
Laboratory practice or sessions [PRESENCIAL][Practical or hands-on activities]	12
Other off-site activity [AUTÓNOMA][Practical or hands-on activities]	10
Computer room practice [PRESENCIAL][Practical or hands-on activities]	3
Study and Exam Preparation [AUTÓNOMA][Self-study]	15

Global activity

Activities	hours
Workshops or seminars [PRESENCIAL][Problem solving and exercises]	15
Study and Exam Preparation [AUTÓNOMA][Self-study]	65
Class Attendance (theory) [PRESENCIAL][Lectures]	20
Laboratory practice or sessions [PRESENCIAL][Practical or hands-on activities]	12
Other off-site activity [AUTÓNOMA][Practical or hands-on activities]	10
Final test [PRESENCIAL][Assessment tests]	2.96
Computer room practice [PRESENCIAL][Practical or hands-on activities]	3
Progress test [PRESENCIAL][Assessment tests]	3.06
Study and Exam Preparation [AUTÓNOMA][Self-study]	15
Problem solving and/or case studies [PRESENCIAL][Problem solving and exercises]	4
Total horas:	150.02

10. Bibliography and Sources

Author(s)	Title/Link	Publishing house	Citv	ISBN	Year	Description
A, Requena y J. Zuñiga	Espectroscopia	Pearson Educación	Madrid	84-205-3677-6.	2004	
P. Atkins, J. de Paula	Physical Chemistry 8th ed	Oxford University Press	Oxford U.K	0-19-870072-5	2006	Hay diferentes ediciones

I. N. Levine (traduccion A, Requena et al.)	Quimica Cuantica 5 th ed.	Prentice Hall	Madrid	84-205-3096-4.	2005
N. B . Sing	Physical Chemistry	New Age International	Nueva Delhi	9788122424034. 97881	2009
	http://eds.b.ebscohost.com/eds/detail/detail?vid=1&sid=fc96fcc9-0f40-41ac-8b90-f9ff8318d12b%40pdc-v-sessmgr03&bdata=Jmxhbmc9ZXMmc2l0ZT1lZHMtbGl2ZQ%3d%3d#AN=307445&db=nlebk				
A. Requena y J. Zúñiga	Química Física: Problemas de Espectroscopia	Prentice Hall	Madrid	8483223678	2007
I.N. Levine	Problemas de Fisico Química	Mc Graw Hill		84-481-9833-6	2005
I.N. Levine, Vol. 2	Fisicoquímica	McGraw-Hill	Madrid	84448106172	2004
J . Bertrán Rusca y col	Química Cuántica	Sintesis	Madrid	84-7738-742-7	2002
L.E. Bailey y M:D.Troitiño	la Quimica Cuantica en 100 problemas.	UNED	Madrid	9788476654637	2004
P.W. Atkins	Fisicoquímica	Panamerica	Madrid	9789500612487	2008
G. R. Mortimer	Physical Chemistry	Academic Press	San Diego USA	9780125083454. 97800	2000