



Teaching Guide				
Identifying Data			2016/17	
Subject (*)	Química Física 2	Code	610G01017	
Study programme	Grao en Química			
Descriptors				
Cycle	Period	Year	Type	Credits
Graduate	2nd four-month period	Second	Obligatoria	6
Language	SpanishGalicianEnglish			
Teaching method	Face-to-face			
Prerequisites				
Department	Química Física e Enxeñaría Química 1			
Coordinador	Fernandez Perez, Maria Isabel	E-mail	isabel.fernandez.perez@udc.es	
Lecturers	Armesto Barbeito, Xose Luis Canle López, Moisés Fernandez Perez, Maria Isabel Santaballa Lopez, Juan Arturo	E-mail	xose.luis.armesto@udc.es moises.canle@udc.es isabel.fernandez.perez@udc.es arturo.santaballa@udc.es	
Web	moodle.udc.es/			
General description	This subject follows Physical Chemistry I, and deals with the knowledge, skills and competencies associated with the interaction of electromagnetic radiation, or particle beams, with matter, in terms of the key aspects of its structural characterization, and the basics of the corresponding analytical techniques.			

Study programme competences / results	
Code	Study programme competences / results
A1	Ability to use chemistry terminology, nomenclature, conventions and units
A7	Knowledge and application of analytical methods
A8	Knowledge of principles of quantum mechanics and atomic and molecular structure
A9	Knowledge of structural characteristics of chemical and stereochemical compounds, and basic methods of structural analysis and research
A12	Ability to relate macroscopic properties of matter to its microscopic structure
A14	Ability to demonstrate knowledge and understanding of concepts, principles and theories in chemistry
A15	Ability to recognise and analyse new problems and develop solution strategies
A16	Ability to source, assess and apply technical bibliographical information and data relating to chemistry
A19	Ability to follow standard procedures and handle scientific equipment
A20	Ability to interpret data resulting from laboratory observation and measurement
A21	Understanding of qualitative and quantitative aspects of chemical problems
A23	Critical standards of excellence in experimental technique and analysis
A24	Ability to explain chemical processes and phenomena clearly and simply
A26	Ability to follow standard laboratory procedures in relation to analysis and synthesis of organic and inorganic systems
A27	Ability to teach chemistry and related subjects at different academic levels
B1	Learning to learn
B2	Effective problem solving
B3	Application of logical, critical, creative thinking
B5	Teamwork and collaboration
B6	Ethical, responsible, civic-minded professionalism
B7	Effective workplace communication
C1	Ability to express oneself accurately in the official languages of Galicia (oral and in written)
C2	Oral and written proficiency in a foreign language
C3	Ability to use basic information and communications technology (ICT) tools for professional purposes and learning throughout life
C6	Ability to assess critically the knowledge, technology and information available for problem solving
C7	Acceptance as a professional and as a citizen of importance of lifelong learning

C8	Understanding role of research, innovation and technology in socio-economic and cultural development
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Learning outcomes			
Learning outcomes	Study programme competences / results		
Apply the fundamentals of the point group theory.	A1 A8 A14 A27	B1 B2 B3	C1 C2 C3 C6
Adquisition of knowledge on other spectroscopies, as well as to know the new trends in the field of the structural elucidation as well as that of the chemical analysis.	A1 A7 A8 A9 A12 A14 A15 A16 A19 A20 A21 A23 A24 A27	B1 B2 B3 B5 B6 B7	C1 C2 C3 C6 C7 C8
Understand the theoretical aspects of the different spectroscopy types, as well as the application to structural elucidation and the techniques of analysis.	A1 A7 A8 A9 A12 A14 A15 A20 A21 A27	B1 B2 B3	C1 C2 C6 C8
Understand the ways in which the electromagnetic radiation interacts with matter, and consequently the various types of spectroscopy, as well the analytical and structural information provided by them.	A1 A7 A8 A9 A12 A27	B1 B3	C1 C2 C3 C8
Understand the theoretical aspects of the absorption and emission processes of the electromagnetic radiation, with special attention to the role of the transition dipole moment.	A1 A7 A8 A9 A12 A27	B1 B2 B3	C1 C2 C3 C8



Understand the theoretical aspects that explain the intensity and the shape of the spectral lines, as well as be able to make predictions in concrete cases.	A1	B1	C1
	A7	B2	C2
	A8	B3	C6
	A9		C8
	A12		
	A14		
	A20		
	A21		
	A27		
	Understand the theoretical and practical aspects involved in the diffraction methods, with special attention to the elucidation of crystal structures by X-ray diffraction.	A1	B1
A7		B2	C2
A8		B3	C3
A9		B5	C6
A12		B6	C7
A14		B7	C8
A15			
A16			
A19			
A20			
A21			
A23			
A24			
A27			
Understand the theoretical and practical aspects of the laser action and its applications, with emphasis to Chemistry.	A1	B1	C1
	A7	B2	C2
	A8	B3	C3
	A9	B5	C6
	A12	B6	C7
	A14	B7	C8
	A15		
	A16		
	A19		
	A20		
	A21		
	A23		
	A24		
	A27		

Understand and apply theoretical and practical aspects of photochemistry, as well as their basic implications in environmental processes.	A1	B1	C1
	A8	B2	C2
	A9	B3	C3
	A12	B5	C6
	A14	B6	C7
	A15	B7	C8
	A16		
	A19		
	A20		
	A21		
	A23		
	A24		
	A26		
	A27		
Practical determination of spectra, their analysis and interpretation: structural and analytical (qualitative and quantitative).	A7	B1	C1
	A12	B2	C2
	A14	B3	C3
	A16	B5	C6
	A19	B6	C7
	A20	B7	C8
	A21		
	A23		
	A24		
	A26		
	A27		

Contents	
Topic	Sub-topic
Introduction to Spectroscopy	Electromagnetic radiation and matter. Resonant and non-resonant processes. Radiation-matter interaction: classical approach. Semi-classical approach: Einstein's coefficients and dipolar transition moment. Spontaneous emission. Selection rules. Spectra types. Intensities of spectral lines and population of the energy levels. Bouger-Lambert-Beer law. Width and shape of spectral lines. General aspects of instrumentation in spectroscopy: Fourier transform.
Symmetry & Chemistry	Symmetry elements and operations. Basic properties of point group symmetry. Point group representations: reducible and irreducible. Applications in Chemistry.
Rotation spectra	Molecular rotation: classical treatment. Classification of molecules. Diatomic and linear molecules spectra. Intensity of the transitions and energy levels population. Centrifugal distortion. Symmetric tops spectra. Asymmetric tops spectra. Molecular structure determination. Experimental aspects of microwave spectroscopy: Stark effect and dipole moment.



<p>Vibrational spectroscopy</p>	<p>Diatomic molecules. Quantum harmonic oscillator approximation: energy levels. Anharmonicity. Empiric potentials. Selection rules. Dissociation energies. Rotation-vibration spectra.</p> <p>Polyatomic molecules. Classical treatment: normal modes & coordinates. Quantum mechanical approach: energy levels. Symmetry considerations. Selection rules. Group frequencies. Experimental techniques.</p> <p>Raman spectroscopy. Molecular polarizability & polarizability tensor. Rayleigh e Raman dispersion: classical treatment. Quantum approach. Pure rotation spectra. Vibration spectra. Experimental techniques.</p>
<p>Electronic spectroscopy</p>	<p>Diatomic molecules. Electronic states. Selection rules. Relative Intensities of Vibronic Transitions: Frank-Condon principle. Vibronic structure: progressions. Dissociation energy.</p> <p>Polyatomic molecules. Estructure and electronic states. Selection rules. Spectra of simple molecules. Cromophores. Circular dicroism & rotatory optical dispersion. UV-VIS spectroscopy: experimental techniques & analytical applications.</p> <p>Photoelectron spectroscopy. Ionization processes. Experimental techniques. Ultraviolet photoelectron spectroscopy (UPS). X-ray photoelectron spectroscopy (XPS): chemical shift.</p>
<p>Fundamentals of Photochemistry</p>	<p>Fluorescence & Phosphorescence: Jablonski -Perrin diagram. The basic laws of photochemistry. Quantum yield. Quenching. Photochemical processes. Experimental techniques and applications.</p>
<p>Laser spectroscopy</p>	<p>The laser action. Laser types. Absorption and excitation spectroscopies: laser induced fluorescence. Raman spectroscopies. Multiphoton ionization spectroscopy: TOF detection. Femtosecond spectroscopy: applications in chemical reaction dynamics. Experimental techniques.</p>
<p>Magnetic resonance spectroscopies</p>	<p>Nuclear and electronic spin states: selection rules.</p> <p>Nuclear magnetic resonance spectroscopy (NMR). Chemical shift: contributions to the shielding factor. Fine structure splitting, coupling. Experimental aspects: Fourier transform. Relaxation processes.</p> <p>Electron spin resonance spectroscopy (ESR): fine and hyperfine structure. Experimental techniques and applications.</p>
<p>Diffraction methods</p>	<p>General aspects of diffraction. X-ray diffraction. Bragg & Laue conditions. The structure factor. Crystal structure determination. Fourier synthesis. The phase problem. Neutron diffraction. Electron diffraction in gases. Wierl function & radial distribution function. Experimental techniques and applications.</p>
<p>Other spectroscopies and new trends in spectroscopy</p>	<p>Mössbauer spectroscopy. Introduction to non-linear spectroscopies. Applications. New trends.</p>

Planning

Methodologies / tests	Competencies / Results	Teaching hours (in-person & virtual)	Student?s personal work hours	Total hours
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Guest lecture / keynote speech	A1 A7 A8 A9 A12 A14 A27 B1	19	28.5	47.5
Laboratory practice	A1 A7 A9 A12 A14 A15 A16 A19 A20 A21 A23 A24 A26 A27 B1 B2 B3 B5 B7 C6	10	12.5	22.5
Seminar	A1 A8 A9 A12 A14 A15 A16 A20 A21 A24 A27 B1 B2 B3 B5 B7 C1 C2 C6 C7 C8	8	12	20
Problem solving	A1 A14 A15 A21 A27 B2 C6	9	13.5	22.5
Oral presentation	A1 A7 A8 A9 A12 A14 A15 A16 A20 A21 A24 A27 B2 B3 B5 B6 B7 C1 C2 C3 C6 C7 C8	2	5	7
ICT practicals	A1 A16 A27 B5 B7 C3 C6	0	4	4
Simulation	A1 A7 A8 A9 A12 A14 A15 A16 A20 A21 A24 B1 B2 B3 C3 C6	2	4	6
Workbook	A1 A16 A23 A24 C6 C7 C8	0	6.5	6.5
Multiple-choice questions	A1 A8 A9 A12 A14 A15 A16 A20 A21 A24 A27 B1 B2 B3 B5 B7 C1 C2 C3 C7 C8	0	3	3
Mixed objective/subjective test	A1 A8 A9 A12 A14 A15 A16 A20 A21 A24 B1 B2 B3 B5 B7 C1 C2 C3 C6 C7 C8	3	7	10
Personalized attention		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	
Methodologies	Description
Guest lecture / keynote speech	Classical lecture format with audiovisual aids. Main theoretical features of each topic will be presented. Students participation is encouraged.
Laboratory practice	Lab work to apply on the theoretical concepts and to acquire the experimental skills associated with them.
Seminar	This activity will take place in small groups. The aim is to gain insight and to deepen in the lecture topics based on the active participation of students.
Problem solving	Practical application, numerical and conceptual, of the theoretical knowledge.
Oral presentation	One of the experiments carried out in the lab, selected by the lecturer, must be orally presented and discussed.
ICT practicals	The aim is to promote students effective learning through practical exercises by using information and communication technologies (ICT).
Simulation	Spectra simulation and the corresponding critical analysis to deepen the key concepts. Activity in small groups at the computers room.
Workbook	Readings to gain insight in the theoretical concepts.



Multiple-choice questions	Throughout the course there will be, using the Moodle learning platform, a series of tests to assess learning of concepts, skills, competencies and skills associated with the subject.
Mixed objective/subjective test	Combination of different types of questions: multiple choice, short answer, essay, etc. and numerical problems. Knowledge, reasoning, and critical thinking will be assessed.

Personalized attention

Methodologies	Description
Simulation Problem solving Seminar	<p>To look for a deeper understanding of the subject content, mainly spectroscopic applications, and to find the best personalized strategy in problem solving.</p> <p>Tutoring schedule will be decided at lecturers and students convenience. The plan is to have four sessions, fifteen minutes each, during the term. They take place at the lecturers' offices.</p> <p>Part-time students and those exempted from attending classes must attend personally to, at least, at one tutoring session per seminar in time schedule agreed between lecturer and student. This is complemented by the use of e-tutoring.</p>

Assessment

Methodologies	Competencies / Results	Description	Qualification
Simulation	A1 A7 A8 A9 A12 A14 A15 A16 A20 A21 A24 B1 B2 B3 C3 C6	Critical analysis of the simulation exercises.	10
Multiple-choice questions	A1 A8 A9 A12 A14 A15 A16 A20 A21 A24 A27 B1 B2 B3 B5 B7 C1 C2 C3 C7 C8	Answer to online multiple choice tests by the corresponding deadlines.	10
Oral presentation	A1 A7 A8 A9 A12 A14 A15 A16 A20 A21 A24 A27 B2 B3 B5 B6 B7 C1 C2 C3 C6 C7 C8	<p>Content</p> <p>Verbal skills</p> <p>Non-verbal skills</p> <p>Ability to answer questions on the presentation.</p>	10
ICT practicals	A1 A16 A27 B5 B7 C3 C6	Participation in on-line activities (files uploads and downloads, forums, WIKI, conceptual maps, ...).	5
Seminar	A1 A8 A9 A12 A14 A15 A16 A20 A21 A24 A27 B1 B2 B3 B5 B7 C1 C2 C6 C7 C8	<p>Exercises preparation</p> <p>Attendance and active participation</p>	10
Laboratory practice	A1 A7 A9 A12 A14 A15 A16 A19 A20 A21 A23 A24 A26 A27 B1 B2 B3 B5 B7 C6	<p>Operational aspects.</p> <p>Lab notebook.</p> <p>Critical analysis of the lab results</p> <p>Written report</p>	15
Mixed objective/subjective test	A1 A8 A9 A12 A14 A15 A16 A20 A21 A24 B1 B2 B3 B5 B7 C1 C2 C3 C6 C7 C8	Final exam with two parts. One, the theoretical one (50%) which includes multiple choice questions, short answer and/or essay type, and, second, the numerical problems part (50%).	40



Assessment comments



Knowledge, the ability of: critical thinking, synthesis, comparison, processing, concepts application and originality of the student will be assessed. Attendance at all laboratory sessions is mandatory. Non attendance implies not pass (0) the subject.

The Spanish grading system will be used as follows:

Spanish Grade

Definition

ECTS Grade

Definition

10

Matrícula de Honor

A+

Top Qualification

9 -10

Sobresaliente

A

Highest 10%

7 ? 8.9



Notable

B

Next 20%

5 ? 6.9

Aprobado

C-D

Next 65%

0 ? 4.9

Suspenso

FX-F

Not Pass

First opportunity: a least a grade of four and a half (4.5) over ten (10) in each of the two parts of the final exam and lab work is required to take into consideration the rest of the assessable activities.

Second opportunity: activities subject to assessment graded below four (4) over ten (10) must be delivered again -but those related to seminars and lab sessions-, as well as redo the part(s) of the final exam with a mark below four and a half (4.5).

In both opportunities, in spite of getting a mark of five or above, over ten, by using the weighted average, the final mark will be 4.5 if a least a grade of four and a half (4.5) over ten (10) is not obtained in each of the two parts of the final exam and lab work and/or a grade below four (4) over ten (10) in the rest of each assessable activities.

Notice that, in both opportunities, a final grade of five (5) is required to pass the subject. The final grade is calculated by considering all assessable activities and applying the weights indicated above.

Students who have participated in scheduled assessment activities, but the mixed objective/subjective test, whose sum is less than 20% of the final mark will be graded as non attendance.

An extra exam will be carried out in case of the number of student students, eligible for Matrícula de Honor (MH), is greater than the number of allowed MHs.

Students assessed in the second opportunity could also be eligible for Matrícula de Honor if the maximum allowed number of MHs has not been fully covered in the first opportunity.

Finally, as regard to next academic courses, everything starts again with the new course.

If this topic is used as formation complement in doctorate studies the mark will be PASS or FAIL.

Previous criteria also apply to part-time students and those exempted from attending classes in both opportunities, but those related to attending and participating in seminars. In this case students will have available seminar activities which must be delivered/uploaded as timely indicated in MOODLE or by e-mail.



Sources of information

Basic	<p>Atkins, Peter W. (2014). Atkins' Physical Chemistry. Oxford : Oxford University PressLuis Carballeira Ocaña & Ignacio Pérez Juste (2008). Problemas de Espectroscopía Molecular . Oleiros : NetbibloAtkins, Peter W. (2008). Química física. Buenos Aires : Médica PanamericanaAdemás das fontes indicadas neste apartado, e no seguinte, poderán suxerirse na plataforma de teleformación MOODLE,outras que ó longo do curso se consideren interesantes.</p>
Complementary	<p>http://www.spectroscopynow.com/.http://jersey.uoregon.edu/vlab/PlankRadiationFormula/index.html.http://photobiology.info/.http://www.pol-us.net/ASP_Home/index.html.P. R. Griffiths (2007). Fourier transform infrared spectrometry. John Wiley & Sonshttp://nobelprize.org/nobel_prizes/.http://www.johnkyrk.com/photosynthesis.html.http://micro.magnet.fsu.edu/optics/timeline/people/jablonski.html.http://ozonewatch.gsfc.nasa.gov/.http://www.nist.gov/.S. F. A. Kettle (2007). Symmetry and structure : readable group theory for chemists. John WileyD. C. Harris (1989). Symmetry and spectroscopy an introduction to vibrational and electronic spectroscopy. DoverAndrew Gilbert & Jim Baggott (1991). Essentials of molecular photochemistry. Oxford ; Boston : Blackwell Scientific PublicationsG. Socrates (2005). Infrared and raman characteristic group frequencies tables and charts. John Wiley & SonsA. M. Ellis (2005). Electronic and photoelectron spectroscopy fundamentals and case studies. Cambridge University PressFotoquímica (inglés) (). http://web.mac.com/titoscaiano/Research_in_Scaianos_labs/teaching_movies.html.J. R. Albani (2007). Principles and applications of fluorescence spectroscopy. Oxford : BlackwellC. Gell (2006). Handbook of single molecule fluorescence spectroscopy. Oxford University PressHelmet H. Telle, Angel Gonzalez Ureña, Robert J. Donovan (2007). Laser chemistry : spectroscopy, dynamics and applications. West Sussex : John Wiley & SonsH. H. Telle (2007). Laser chemistry : spectroscopy, dynamics and applications. John Wiley & SonsT. N. Mitchell (2004). NMR--from spectra to structures: an experimental approach. SpringerB. Metin (2005). Basic ¹H-and ¹³C-NMR spectroscopy . ElsevierFrançoise Hippert et al. (2006). Neutron and x-ray spectroscopy. Dordrecht : SpringerR. Jenkins (1996). Introduction to X-ray powder diffractometry. John Wiley & Sons(2005). International tables for crystallography. Dordrecht : Springer(2005). International tables for crystallography brief teaching edition of volume A : space-group symmetry. Dordrecht : SpringerWikipedia - Español (). http://es.wikipedia.org/wiki/Wikipedia.Wikipedia - inglés (). http://en.wikipedia.org/wiki/Wikipedia.I. N. Levine (2004). Fisicoquímica 5ª edición. McGraw-HillAlberto Requena Rodríguez & José Zúñiga Román (2004). Espectroscopia . Pearson Educación, S.A.Víctor Luaña, V. M. García Fernández, E. Francisco & J. M. Recio (2002). Espectroscopía molecular. Universidad de Oviedo, Servicio de PublicacionesJ. R. Lakowicz (2006). Principles of fluorescence spectroscopy. SpringerJ. Michael Hollas (2004). Modern Spectroscopy. J. Wiley & SonsAlberto Requena & José Zúñiga (2007). Química Física : problemas de espectroscopia : fundamentos, átomos y moléculas diatómicas. Madrid : Pearson EducaciónJ. Keeler (2010). Understanding NMR spectroscopy.Carol E. Wayne & Richard P. Wayne (1996). Photochemistry. Oxford Chemistry Primers, 39http://www.ch.ic.ac.uk/local/symmetry/.Ooi, Li-ling (2010). Principles of x-ray crystallography. Oxford University Presshttps://moodle.udc.es/.</p>

Recommendations

Subjects that it is recommended to have taken before



Matemáticas 1/610G01001

Matemáticas 2/610G01002

Física 1/610G01003

Física 2/610G01004

Biología/610G01005

Xeoloxía/610G01006

Química 1/610G01007

Química 2/610G01008

Química 3/610G01009

Química 4/610G01010

Química Analítica 1/610G01011

Química Física 1/610G01016

Química Inorgánica 1/610G01021

Química Orgánica 1/610G01026

Química, Información e Sociedade/610G01031

Subjects that are recommended to be taken simultaneously

Laboratorio de Química/610G01032

Subjects that continue the syllabus

Química Física 3/610G01018

Experimentación en Química Física/610G01019

Química Física Avanzada/610G01020

Traballo de fin de Grao/610G01043

Other comments

<p class="MsoNormal" align="justify">It is strongly recommended to study regularly the theoretical concepts explained in the lectures, and, at the same time, to answer the questions and to solve the numerical problems proposed along the course.<?xml:namespace prefix =" o" ns ="

"urn:schemas-microsoft-com:office:office" /></p><p class="MsoNormal" align="justify">Handouts should never replace the recommended reference material.</p>

<p class="MsoNormal" align="justify">It could be very HELPFUL the use of the tutorships to clarify doubts and to deepen the knowledge associated with the subject.</p>

<p align="justify">&nbsp;</p>

(*)The teaching guide is the document in which the URV publishes the information about all its courses. It is a public document and cannot be modified. Only in exceptional cases can it be revised by the competent agent or duly revised so that it is in line with current legislation.