UNIVERSIDADE DA CORUÑA

Teaching Guide				
Identifying Data				2015/16
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	Canle López, Moisés Fernandez Perez, Maria Isabel Santaballa Lopez, Juan Arturo	E-mail	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	
Code	Study programme competences
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

Learning outcomes			
Learning outcomes	Study programme competences		
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 A7 A8 A9 A12 A14 A20 A21 A27	B1 B2 B3	C1 C2 C6 C8
Apply the fundamentals of the point group theory.	A1 A8 A14 A27	B1 B2 B3	C1 C2 C3 C6
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
Practical determination of spectra, their analysis and interpretation: structural and analytical (qualitative and quantitative).	A7 A12 A14 A16 A19 A20 A21 A23 A24 A26 A27	B1 B2 B3 B5 B6 B7	C1 C2 C3 C6 C7 C8

Understand and apply theoretical and practical aspects of photochemistry, as well as their basic implications in environmental processes.	A1 A8 A9 A12 A14 A15 A16 A19 A20 A21 A23 A24 A26 A27	B1 B2 B3 B5 B6 B7	C1 C2 C3 C6 C7 C8
Understand the theoretical and practical aspects involved in the diffraction methods, with special attention to the elucidation of cystal structures by X-ray diffraction.	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 and practical aspects of the laser action and its applications, with emphasis to Chemistry.	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

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

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 distorsion. Symmetric tops spectra. Asymmetric tops spectra. Molecular structure determination. Experimental aspects of microwave spectroscopy: Stark effect and dipole moment.
Vibrational spectroscopy	Diatomic molecules. Quantum harmonic oscillator approximation: energy levels. Anharmonicity. Empiric potentials. Selection rules. Dissociation energies. Rotation-vibration spectra. Polyatomic molecules. Classical treatment: normal modes & coordinates. Quantum mechanical approach: energy levels. Symmetry considerations. Selection rules. Group frequencies. Experimental techniques. Raman spectroscopy. Molecular polarizability & polarizabilty tensor. Rayleigh e Raman dispersion: classical treatment. Quantum approach. Pure rotation spectra. Vibration spectra. Experimental techniques.

Electronic spectroscopy	Diatomic molecules. Electronic states. Selection rules. Relative Intensities of Vibronic Transitions: Frank-Condon principle. Vibronic structure: progressions. Dissociation energy. 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. Photoelectron spectroscopy. Ionization processes. Experimental techniques. Ultraviolet photoelectron spectroscopy (UPS). X-ray photoelectron spectroscopy (XPS): chemical shift.
Fundamentals of Photochemistry	Fluorescence & Phosphorescence: Jablonski -Perrin diagram. The basic laws of photochemistry. Quantum yield. Quenching. Photochemical processes. Experimental techniques and applications.
Laser spectroscopy	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.
Magnetic resonance spectroscopies	Nuclear and electronic spin states: selection rules. Nuclear magnetic resonance spectroscopy (NMR). Chemical shift: contributions to the shielding factor. Fine structure splitting, coupling. Experimental aspects: Fourier transform. Relaxation processes. Electron spin resonance spectroscopy (ESR): fine and hyperfine structure. Experimental techniques and applications.
Diffraction methods	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.
Other spectroscopies and new trends in spectroscopy	Mössbauer spectroscopy. Introduction to non-linear spectroscopies. Applications. New trends.

Planning				
Methodologies / tests	Competencies	Ordinary class hours	Student?s personal work hours	Total hours
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	A24 A21 A20 A16 A15 A14 A12 A9 A8 A7 A1 A27 B1 B2 B3 C3 C6	2	4	6
Workbook	A1 A16 A23 A24 C6 C7 C8	0	6.5	6.5
Multiple-choice questions	A24 A21 A20 A16 A15 A14 A12 A9 A8 A1 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**

Laboratory practice Seminar Oral presentation Problem solving Simulation	To help student in the critical analysis of the lab and simulation results, in the improvement of the oral presentation, and, finally, in the search for the best personalized strategy in problem solving. Tutoring schedule will be decided at lecturers and students convenience. They take place at the lecturers' offices.

Assessment			
Methodologies	Competencies	Description	Qualification
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
Laboratory practice	A1 A7 A9 A12 A14 A15 A16 A19 A20 A21 A23 A24 A26 A27 B1 B2 B3 B5 B7 C6	Operational aspects. Lab notebook. Critical analysis of the lab results Written report	15
Seminar	A1 A8 A9 A12 A14 A15 A16 A20 A21 A24 A27 B1 B2 B3 B5 B7 C1 C2 C6 C7 C8	Exercises preparation Attendance and active participation	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	Content Verbal skills Non-verbal skills Ability to answer questions on the presentation.	10
ICT practicals	A1 A16 A27 B5 B7 C3 C6	Participation in on-line activities (files uploads and downloads, forums, WIKI, conceptual maps, ...).	5
Simulation	A24 A21 A20 A16 A15 A14 A12 A9 A8 A7 A1 A27 B1 B2 B3 C3 C6	Critical analysis of the simulation exercises.	10
Multiple-choice questions	A24 A21 A20 A16 A15 A14 A12 A9 A8 A1 A27 B1 B2 B3 B5 B7 C1 C2 C3 C7 C8	Answer to online multiple choice tests by the corresponding deadlines.	10

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. Alternatively, student can opt for a four hours lab work examination.

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 (4) 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 five (5) must be delivered again -but those related to seminar-, as well as redo the part(s) of the final exam with a mark below four (4).

In both oportunities, 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 (4) over ten (10) is not obtained in each of the two parts of the final exam and lab work.

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 no more than 50% of the scheduled assessment activities 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.

Sources of information	
Basic	- Atkins, Peter W. (2014). Atkins' Physical Chemistry. Oxford : Oxford University Press - Luis Carballeira Ocaña & Ignacio Pérez Juste (2008). Problemas de Espectroscopía Molecular . Oleiros : Netbiblo - Atkins, Peter W. (2008). Química física. Buenos Aires : Médica Panamericana - (). https://moodle.udc.es/. Además das fontes indicadas neste apartado, e no seguinte, poderán suxerirse na plataforma de teleformación MOODLE, outras que ó longo do curso se consideren interesantes.

Complementary	- (). 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 & Sons - (). http://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 Wiley - D. C. Harris (1989). Symmetry and spectroscopy an introduction to vibrational and electronic spectroscopy. Dover - Andrew Gilbert & Jim Baggott (1991). Essentials of molecular photochemistry. Oxford ; Boston : Blackwell Scientific Publications - G. Socrates (2005). Infrared and raman characteristic group frequencies tables and charts. John Wiley & Sons - A. M. Ellis (2005). Electronic and photoelectron spectroscopy fundamentals and case studies. Cambridge University Press - Fotoquímica (inglés) (). http://web.mac.com/titoscaiano/Research_in_Scaianos_labs/teaching_movies.html. - J. R. Albani (2007). Principles and applications of fluorescence spectroscopy. Oxford : Blackwell - C. Gell (2006). Handbook of single molecule fluorescence spectroscopy. Oxford University Press - Helmet H. Telle, Angel Gonzalez Ureña, Robert J. Donovan (2007). Laser chemistry : spectroscopy, dynamics and applications. West Sussex : John Wiley & Sons - H. H. Telle (2007). Laser chemistry : spectroscopy, dynamics and applications. John Wiley & Sons - T. N. Mitchell (2004). NMR--from spectra to structures: an experimental approach. Springer - B. Metin (2005). Basic ^{1}H-and ^{13}C-NMR spectroscopy . Elsevier - Françoise Hippert et al. (2006). Neutron and x-ray spectroscopy. Dordrecht : Springer - R. 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 : Springer - Wikipedia - Español (). http://es.wikipedia.org/wiki/Wikipedia. - Wikipedia - inglés (). http://en.wikipedia.org/wiki/Wikipedia. - I. N. Levine (2004). Fisicoquímica 5ª edición. McGraw-Hill - Alberto 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 Publicaciones - J. R. Lakowicz (2006). Principles of fluorescence spectroscopy. Springer - J. Michael Hollas (2004). Modern Spectroscopy. J. Wiley & Sons - Alberto Requena & José Zúñiga (2007). Química Física : problemas de espectroscopia : fundamentos, átomos y moléculas diatómicas. Madrid : Pearson Educación - J. Keeler (2010). Understanding NMR spectroscopy. - Carol E. Wayne & Richard P. Wayne (1996). Photochemistry. Oxford Chemistry Primers, 39 - (). http://www.ch.ic.ac.uk/local/symmetry/. - Ooi, Li-ling (2010). Principles of x-ray crystallography. Oxford University Press - (). https://moodle.udc.es/.

Recommendations
Subjects that it is recommended to have taken before

Matemáticas 1/610G01001
Matemáticas 2/610G01002
Física 1/610G01003
Física 2/610G01004
Bioloxía/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
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. Handouts should never replace the recommended reference material. It could be very HELPFUL the use of the tutorships to clarify doubts and to deepen the knowledge associated with the subject.