



Teaching Guide

Teaching Guide				
Identifying Data				2020/21
Subject (*)	Physical Chemistry 2	Code	610G01017	
Study programme	Grao en Química			
Descriptors				
Cycle	Period	Year	Type	Credits
Graduate	2nd four-month period	Second	Obligatory	6
Language	SpanishGalicianEnglish			
Teaching method	Face-to-face			
Prerequisites				
Department	Química			
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.			
Contingency plan	<p>1. Modifications to the contents Without changes.</p> <p>2. Methodologies *Teaching methodologies that are maintained - Simulation (included into the assessment) - Multiple choice test (included into the assessment) ? Tutoring *Teaching methodologies that are modified - Lectures (on-line teaching) - Lab work (on-line teaching) (included into the assessment) ? Seminars (on-line teaching) (included into the assessment) - Final exam (on-line) (included into the assessment)</p> <p>3. Mechanisms for personalized attention to students ? e-mail: daily, to ask questions and to follow proposed activities. ? Moodle: daily, depending on student needs. ? Teams: also to make inquiries, request and carry out virtual meetings to resolve doubts and monitor the proposed activities.</p> <p>4. Modifications in the evaluation Without changes. *Evaluation observations:</p> <p>5. Modifications to the bibliography or webgraphy No changes will be made. They already have related materials in MOODLE and / or in the corresponding Class Notebook (Office365).</p>			

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

Learning outcomes			
Learning outcomes	Study programme competences / results		
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 in molecular spectroscopy.	A1 A8 A14	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 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



Understand the theoretical and practical aspects involved in photoelectronic spectroscopy.	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 basic theoretical and practical aspects of photochemistry: fluorescence and phosphorescence, Perrin-Jablonski diagram.	A1	B1
A8		B2	C2
A9		B3	C3
A12		B5	C6
A14		B6	C7
A15		B7	C8
A16			
A19			
A20			
A21			
A23			
A24			
A26			
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		

Contents

Topic	Sub-topic
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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. 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	Classification of molecules. Diatomic and linear molecules spectra. Intensity of the transitions and energy levels population. Centrifugal distortion. Molecular structure determination. Experimental aspects of microwave spectroscopy: Stark effect and dipole moment.
Vibration- rotation spectrum	Diatomic molecules. Quantum harmonic oscillator approximation: energy levels. Anharmonicity. Empirical 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 & polarizability tensor. Rayleigh and Raman dispersion: classical treatment. Quantum approach. Pure rotation spectra. Rotation-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. Structure and electronic states. Selection rules. Spectra of simple molecules. Chromophores. 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.
Principles of Laser Operation	The laser action. Laser types. Absorption and excitation spectroscopies: laser induced fluorescence. Raman spectroscopies.
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. 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.
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Planning				
Methodologies / tests	Competencies / Results	Teaching hours (in-person & virtual)	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	13	21
Problem solving	A1 A14 A15 A21 A27 B2 C6	9	14	23
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	5.5	7.5
Simulation	A1 A7 A8 A9 A12 A14 A15 A16 A20 A21 A24 B1 B2 B3 C3 C6	2	5	7
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	4	4
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.
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 on-line multiple choice tests and/or completion of other on-line activities by the corresponding deadlines.	15
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
Seminar	A1 A8 A9 A12 A14 A15 A16 A20 A21 A24 A27 B1 B2 B3 B5 B7 C1 C2 C6 C7 C8	Active participation	10
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



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
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Assessment comments

Knowledge, the ability of:

critical thinking, synthesis, comparison, processing, concepts application and originality of the student will be assessed. Grading system. 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 Attendance. It is strongly suggested the attendance at all activities. Attendance at all laboratory sessions is mandatory. Non attendance implies not pass, fail with zero over ten, the subject.

First opportunity. At least a grade of 4.5 over ten 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 4.5 over ten 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 4.5 over ten.

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 4.5 over ten is not obtained in each of the two parts of the final exam and lab work and/or a grade below 4.5 over ten in the rest of each assessable activities. In both opportunities, a final grade of five over ten is required to pass the subject. The final grade is calculated by considering all assessable activities and applying the weights indicated above. Matrícula de Honor (MH). An extra exam will be carried out in case of the number of student students, eligible for Matrícula de Honor, 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. No presentado grade. Students who have participated in scheduled assessment activities whose sum is less than 50% of the final mark will be graded as no presentado, except they achieved a mark of five over ten in the lab work. Next academic courses. As regard to next academic courses, everything starts again with the new course, but the lab work if it was graded with five over ten. Such exemption, if it is offered, must be requested by the student within the established term. Part-time students and those exempted from attending classes. Previous criteria also apply, 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 by electronic means. Complement in doctorate studies. The mark will be PASS or FAIL.

Sources of information



Basic	<ul style="list-style-type: none">- Atkins, Peter W. (2014). Atkins' Physical Chemistry. Oxford : Oxford University Press- Atkins, Peter W. (2008). Química física. Buenos Aires : Médica Panamericana- Luis Carballeira Ocaña & Ignacio Pérez Juste (2008). Problemas de Espectroscopía Molecular . Oleiros : Netbiblo- Levine, Ira N. (2004). Físicoquímica. Madrid : McGrawhill <p>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.</p>
Complementary	<ul style="list-style-type: none">- Andrew Gilbert & Jim Baggott (1991). Essentials of molecular photochemistry.. Oxford ; Boston : Blackwell Scientific Publications- 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. New York : Dover- P. R. Griffiths (2007). Fourier transform infrared spectrometry. . John Wiley & Sons- 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- 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- T. N. Mitchell (2004). NMR--from spectra to structures: an experimental approach. Berlin: Springer- B. Metin (2005). Basic ¹H-and ¹³C-NMR spectroscopy. Amsterdam : Elsevier- Françoise Hippert et al. (2006). Neutron and x-ray spectroscopy. Dordrecht : Springer- R. Jenkins (1996). Introduction to X-ray powder diffractometry. New York : John Wiley & Sons- (2005). International tables for crystallography. Volume A, Space-group symmetry. Dordrecht : Springer- 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. New York : Springer- J. Michael Hollas (2004). Modern Spectroscopy. Hoboken (New Jersey) : John 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.. Chichester : John Wiley and Sons- Carol E. Wayne & Richard P. Wayne (1996). Photochemistry. Oxford : Oxford University Press- Ooi, Li-ling (2010). Principles of x-ray crystallography. Oxford : Oxford University Press- http://www.spectroscopynow.com/ () . .- http://photobiology.info/ () . .- 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/ () . .- http://www.ch.ic.ac.uk/local/symmetry () . .

Recommendations

Subjects that it is recommended to have taken before



Mathematics 1/610G01001

Mathematics 2/610G01002

Physics 1/610G01003

Physics 2/610G01004

Biology/610G01005

Geology/610G01006

General Chemistry 1/610G01007

General Chemistry 2/610G01008

General Chemistry 3/610G01009

Chemistry Laboratory 1/610G01010

Analytical Chemistry 1/610G01011

Physical Chemistry 1/610G01016

Inorganic Chemistry 1/610G01021

Organic Chemistry 1/610G01026

Chemistry, Information and Society/610G01031

Subjects that are recommended to be taken simultaneously

Chemistry Laboratory 2/610G01032

Subjects that continue the syllabus

Physical Chemistry 3/610G01018

Experimental Physical Chemistry/610G01019

Advanced Physical Chemistry/610G01020

Final Dissertation/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.

(*)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.