



IDENTIFYING DATA

Structural Determination

Subject	Structural Determination			
Code	V11G200V01501			
Study programme	(*)Grao en Química			
Descriptors	ECTS Credits	Choose	Year	Quadmester
	6	Mandatory	3rd	1st
Teaching language	Spanish Galician			
Department				
Coordinator	Álvarez Rodríguez, Rosana			
Lecturers	Álvarez Rodríguez, Rosana Castro Fojo, Jesús Antonio Rodríguez de Lera, Angel			
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Web				
General description	The subject devotes to learning the application of the methods used in the structural determination of chemical compounds			

Competencies

Code	
A1	Students have demonstrated knowledge and understanding in a field of study that builds upon their general secondary education, and is typically at a level that, whilst supported by advanced textbooks, includes some aspects that will be informed by knowledge of the forefront of their field of study
A2	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
A3	Students have the ability to gather and interpret relevant data (usually within their field of study) to inform judgments that include reflection on relevant social, scientific or ethical issues
A4	Students can communicate information, ideas, problems and solutions to both specialist and non-specialist audiences
C4	Demonstrate knowledge and understanding of essential facts, concepts, principles and theories: Basics and tools for solving analytical problems and characterization of chemical substances
C8	Demonstrate knowledge and understanding of essential facts, concepts, principles and theories: main techniques for structural determination, including spectroscopy
C12	Demonstrate knowledge and understanding of essential facts, concepts, principles and theories: structural features of chemical elements and their compounds, including stereochemistry
C19	Apply knowledge and understanding to solve basic problems of quantitative and qualitative nature
C20	Evaluate, interpret and synthesize data and chemical information
C24	Recognize and analyze new problems and plan strategies to solve them
D1	Communicate orally and in writing in at least one of the official languages of the University
D3	Learn independently
D4	Search and manage information from different sources
D5	Use information and communication technologies and manage basic computer tools
D7	Apply theoretical knowledge in practice
D8	Teamwork
D9	Work independently
D12	Plan and manage time properly
D13	Make decisions
D14	Analyze and synthesize information and draw conclusions
D15	Evaluate critically and constructively the environment and oneself
D16	Develop an ethical commitment

Learning outcomes

Expected results from this subject	Training and Learning Results		
Describe the fundamental concepts of the methods for structural elucidation	A1	C4 C8 C12	
Analyse the information that the different methods offer on the molecular structure elucidation, and understand their advantages and limitations.	A2 A3	C8 C12 C20	D3 D4 D7 D8 D9 D14
Predict the basic features of a given spectrum for a particular compound.	A2 A3	C4 C8 C12 C20	D3 D4 D7 D9 D14
Design the rational process to obtain key structural information of a chemical compound.	A2 A3	C4 C8 C24	D3 D4 D7 D9 D13 D14
Determine the molecular structure of a simple compound from the analysis of its spectroscopic data (IR, UV, MS, NMR, etc.).	A2 A3 A4	C4 C8 C12 C19 C20	D1 D3 D4 D5 D7 D9 D12 D14 D16
Understand the information provided by the different methods of X-ray diffraction.	A2 A3	C4 C12	D3 D4 D9 D13 D14 D15 D16
Observe the presence of defects and disorder in solids.	A1	C4	

Contents

Topic	
Chapter 1. Obtaining general data of a chemical compound.	Combustion Analysis: empirical formula. Qualitative analysis. Point and space symmetry Optical Properties.
Chapter 2. Electronic and photoelectronic spectroscopy.	Determination of the chromophore groups. Effect of conjugation. Study of the valence shell MOs.
Chapter 3. Structural determination of crystalline samples.	Applications and limitations of the diffractometric techniques in structural determination. Three-dimensional determination of the molecular structure. Defects and disorders in crystalline solids.
Chapter 4. NMR Spectroscopy.	Monodimensional experiments of ^1H and ^{13}C Structural information from the chemical shift. Dynamic NMR: equilibria in solution. Two-dimensional experiments. Homo- and Heteronuclear Correlation spectroscopy.
Chapter 5. Vibrational Spectroscopy.	Determination of the presence of characteristic functional groups. Other applications in structural determination.
Chapter 6. Mass Spectrometry.	Determination of the molecular mass. Ionisation techniques. Detection methods. Fragmentation reactions. Isotopic patterns. Interpretation of the mass spectra.

Planning			
	Class hours	Hours outside the classroom	Total hours
Master Session	13	26	39
Troubleshooting and / or exercises	24	48	72
Practical tests, real task execution and / or simulated.	3	15	18
Jobs and projects	1	20	21

*The information in the planning table is for guidance only and does not take into account the heterogeneity of the students.

Methodologies	
	Description
Master Session	The theoretical classes will be devoted to the presentations of the basis of the different techniques that are most relevant for the interpretation of the data from the structural point of view (relationships between spectra and structures).
Troubleshooting and / or exercises	The classes of small groups will be devoted to solve exercises or problems that allow at the end of each chapter to obtain appropriate information of the corresponding techniques.

Personalized attention	
Methodologies	Description
Troubleshooting and / or exercises	Students may consult any doubt with the teaching staff of the subject in mentoring time.
Tests	Description
Jobs and projects	Students may consult any doubt with the teaching staff of the subject in mentoring time. In addition, students will be called individually or in small groups for mentoring of the work proposed.

Assessment		Qualification	Training and Learning Results
	Description		
Troubleshooting and / or exercises	In the different classes (lectures, seminars) the students will be given handouts with problems and/or exercises that will be used for their evaluation. Learning outcomes: (1). Describe the fundamental concepts of the methods for structural determination. (2). Analyse the information that, on the molecular structure, provide the different methods and understand their main limitations. (3). Predict the basic features of a particular spectrum for a given compound. (4). Describe the information supplied by the different methods of X-ray diffraction.	20	A1 C4 D7 A2 C8 D8 A3 C12 D13 C19 D15 C20 C24
Practical tests, real task execution and / or simulated.	There will be two short tests of about 2 hour duration in which the students will be asked to obtain structural information from experimental data (spectra and other physical data). The first tests covers chapters 1-3 (10% of qualification), and the second chapter 4 (20% of qualification). Learning outcomes: (1). Analyse the information that, on the molecular structure, provide the different methods and understand their main limitations. (2). Predict the basic features of a particular spectrum for a given compound. (3) Design the basic process to obtain a particular structural information of a compound. (4). Solve the molecular structure of a simple compound from its spectra (UV, IR, MS, NMR, X-Ray, etc). Further, there will be a final test that covers all chapters (30% of qualification)	60	A1 C8 D3 A2 C12 D7 A3 C19 A4 C20 C24
Jobs and projects	The students will carry out a small project proposed by the professors of multidisciplinary spectroscopic nature. The results will be presented as a written report. Learning outcomes:(1). Solve the molecular structure of a simple compound from its spectra (UV, IR, MS, NMR, X-Ray, etc).	20	A1 C4 D1 A2 C8 D4 A3 C12 D5 A4 C19 D9 C20 D12 C24 D14 D16

Other comments on the Evaluation

To pass the course the students must handle the professor the following material:

- A minimum of 80% of the handouts and homework proposed in the seminar classes.

- All the short tests.

- The final report.

To pass the course at the end of the quarter the students will be required to get a minimum of 5 points (on the basis of 10) in the final mark. Besides, it is indispensable to obtain in the evaluation of the different parts of the course the following minima:

- 30% of the total value in each one of the short tests.
- 40% of the total value in the group of the handouts.
- 30% of the total value in the final test.

In the event the minima is not reached, the student record will show the balanced mark of the short tests.

For students that complete less than 20% of the total work scheduled, the records will not show, in agreement with the current legislation and, the quotation NOT PRESENTED. In any case, the presentation to one of the short tests, will imply the qualification of the course.

The students that fail at the end of the quartet will have to pass a final exam at the end of the academic year (June, July). Said proof will replace the results of the final tests. A minimum of 30% of the total value of the exam will be required to pass the course. The qualifications of the handouts and the project report are non-recoverable. In case the minima established in each part is not reached, the qualification will be FAILED. Once the minima is passed a global mark equal or higher than 5.0 (on the basis of 10) will be required to pass the course.

The final qualification of the students that pass the course will be normalised to 10 points.

Sources of information

Basic Bibliography

Complementary Bibliography

Williams, D.H., Fleming, I., **Spectroscopic Methods in Organic Chemistry**, 6^a,

Hammond, Christopher, **The Basics of crystallography and diffraction**,

Pavia, D.L., Lampman, G.M., Kriz, G.S., Vyvyan, J.R., **Introduction to Spectroscopy**, 5^a,

Pretsch, Ernő, **Structure determination of organic compounds : tables of spectral data**, 4a,

Clayden, Jonathan, **Organic Chemistry**, 2a,

Recommendations

Subjects that it is recommended to have taken before

Geology: Geology/V11G200V01205

Chemistry: Chemistry I/V11G200V01105

Chemistry: Chemistry 2/V11G200V01204

Numerical methods in chemistry/V11G200V01402

Physical chemistry I/V11G200V01303

Physical chemistry II/V11G200V01403

Inorganic chemistry I/V11G200V01404

Organic chemistry I/V11G200V01304

Other comments

The students have to remember that to reach the competitions of the matter is indispensable to have purchased previously the following results of learning:

- ☐ Determination of the formal state of oxidation of a tie it to me inside a compound
- ☐ Structures of the main functional groups in organic chemistry
- ☐ Representation by means of structures of Lewis of organic substances
- ☐ three-dimensional Structure of the organic substances in accordance with the model of orbital hybrid
- ☐ Representation of reactions by means of diagrams of arrows
- ☐ basic Concepts of spectroscopy