



## IDENTIFYING DATA

### Structural Determination

Subject	Structural Determination			
Code	V11G201V01206			
Study programme	Grado en Química			
Descriptors	ECTS Credits	Choose	Year	Quadmester
	6	Mandatory	2nd	2nd
Teaching language	#EnglishFriendly Spanish Galician			
Department				
Coordinator	Silva López, Carlos Valencia Matarranz, Laura María			
Lecturers	Pérez Lourido, Paulo Antonio Silva López, Carlos Valencia Matarranz, Laura María			
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Web				
General description	The subject devotes to the learning of the application of the methods but used in the structural determination of chemical substances. English Friendly subject: International students may request from the teachers: a) materials and bibliographic references in English, b) tutoring sessions in English, c) exams and assessments in English.			

### Training and Learning Results

Code	
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
A5	Students have developed those learning skills that are necessary for them to continue to undertake further study with a high degree of autonomy
B1	Ability for autonomous learning
B3	Ability to manage information
B4	Ability for analysis and synthesis
C1	Ability to know and understand essential facts, concepts, principles and theories related to Chemistry
C2	Use correctly chemical terminology, nomenclature, conversions and units
C3	Recognize and analyze chemical, qualitative and quantitative problems, proposing strategies to solve them through the evaluation, interpretation and synthesis of data and chemical information
C6	Know the basics and tools for resolution of analytical problems and characterization of chemical substances
C15	Know the main techniques of structural research, including spectroscopy
D1	Ability to solve problems

### Expected results from this subject

Expected results from this subject	Training and Learning Results		
New	A3 A5	B3	C1 C2 C6 C15
Analyze the information that can be obtained from spectroscopic techniques	A3	B1 B3 B4	C1 C6 C15

Describe the information that supply the distinct methods of X ray diffraction	A3	B3	C1 C6 C15	
Foretell the basic characteristics of a determined spectrum from a known substance	A3 A5	B3 B4	C2 C3	D1
Design the basic process to obtain structural information of a chemical substance.	A3 A4	B3 B4	C2 C3	D1
Resolve the molecular structure of a simple compound from the its spectra	A3 A4	B1 B3 B4	C2 C3	D1

## Contents

Topic	
Subject 1. Gathering of general data of a substance.	Analysis of combustion. Empirical formula. Qualitative analysis. Optical properties.
Subject 2. Methods of diffraction.	Applications and limitations of the technique.
Subject 3. Electronic and photoelectron spectroscopy.	Determination of chromophores.
Subject 4. Vibrational spectroscopy.	Determination of characteristic functional groups.
Subject 5. Mass spectrometry.	Determination of the molecular mass. Ionization methods. Isotopic patterns. Interpretation of the MS spectrum.
Subject 6. NMR spectroscopy.	<sup>1</sup> H and <sup>13</sup> C monodimensional experiments. Structural Information from the chemical shift. Dynamic NMR: chemical equilibrium. Noe experiment. Heteronuclear NMR.

## Planning

	Class hours	Hours outside the classroom	Total hours
Lecturing	12	26	38
Problem solving	24	70	94
Objective questions exam	2	7	9
Objective questions exam	2	7	9

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

## Methodologies

	Description
Lecturing	The theoretical sessions will be devoted to present the fundamentals of the techniques that are relevant to this subject
Problem solving	The sessions will be devoted to solve exercises or problems

## Personalized assistance

Methodologies	Description
Problem solving	Students will be able to consult with professors during the spring term

## Assessment

	Description	Qualification	Training and Learning Results	
Problem solving	In class students will be asked to solve a number of practical examples and exercises that will be graded.	20	A3	D1
Objective questions exam	There will be a test along the period of 2 h. of length that will include the Subjects 1-4.	40	A3 A4	D1
Objective questions exam	There will be a second test focused on MS, IR and NMR applied to the structural determination of organic compounds	40	A3 A4	D1

## Other comments on the Evaluation

To surpass the matter the student has to:

- Achieve a 5 (out of 10) of average on all the graded activities.
- Achieve a minimum of 4 in each one of the exams of objective questions.

In the case of not achieving these two conditions the final grade will be the mean of the two exam

A student that enrolls in 20% of the total work scheduled will be qualified in accordance with the valid legislation. In any case, the realization of any of the tests will imply a final grade. The students that do not pass the subject at the end of the term will have the opportunity to do a final test in July. The grade of such test will replace the grades of the written tests (hence it will weigh 80% of the final grade of the student, no more)

Students who do not pass the subject at the end of the semester must take an overall written test in the final evaluation closing period in July. This test will replace the results of the written tests. The qualification of the seminar tests, deliverables (of the face-to-face activities) and the work/project, etc., are not recoverable.

For students who renounce continuous assessment and opt for a global assessment, the first of the short tests will be equivalent to 40% of the final mark, and the second to the remaining 60%. Students who do not pass one or both of the short tests that are carried out during the semester must take the corresponding part in the July session.

**In order to guarantee a quality and individualized evaluation, any certifiable competence in this subject can be verified by means of an oral test, at any time before the final closing of the official records.**

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#### **Sources of information**

##### **Basic Bibliography**

##### **Complementary Bibliography**

Williams, D.H., Fleming, I., **Spectroscopic Methods in Organic Chemistry**, 6<sup>a</sup>, 2007

Hammond, Christopher, **The Basics of crystallography and diffraction**, 2009

Pavia, D.L., Lampman, G.M., Kriz, G.S., Vyvyan, J.R., **Introduction to Spectroscopy**, 5<sup>a</sup>, 2014

Pretsch, Ernő, **Structure determination of organic compounds : tables of spectral data**, 4a, Springer, 2009

Clayden, Jonathan, **Organic Chemistry**, 2a, 2012

Hesse, M, Meier, H, Zeeh, B., **Métodos espectroscópicos en Química orgánica**, 2a, Síntesis, 2005

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#### **Recommendations**