# Universida<sub>de</sub>Vigo

### Subject Guide 2017 / 2018

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Learning outcomes	D16 Develop	an ethical commitment			
	Learning ou	itcomes			

Expected results from this subject		Tr	Training and Learning Results		
Describe the fundamental concepts of the metho	ds for structural elucidation	A1	C4 C8 C12		
Analyse the information that the different method 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	r a particular compound.	A2 A3	C4 C8 C12 C20	D3 D4 D7 D9 D14	
Design the rational process to obtain key structur	ral information of a chemical compound.	A2 A3	C4 C8 C24	D3 D4 D7 D9 D13 D14	
Determine the molecular structure of a simple co data (IR, UV, MS, NMR, etc.).	mpound from the analysis of its spectroscopic	A2 A3 A4	C4 C8 C12 C19 C20	D1 D3 D4 D5 D7 D9 D12 D14 D16	
Understand the information provided by the diffe	rent methods of X-ray diffraction.	A2 A3	C4 C12	D3 D4 D9 D13 D14 D15 D16	
Observe the presence of defects and disorder in s	solids.	A1	C4		
Contents					
Topic Chapter 1. Obtaining general data of a chemical compound. Chapter 2. Electronic and photoelectronic	Combustion Analysis: empirical formula. Qualitative analysis. Point and space symmetry Optical Properties. Determination of the chromophore groups.				
spectroscopy.	Effect of conjugation. Study of the valence shell MOs.				
Chapter 3. Structural determination of crystalline samples.	<ul> <li>Applications and limitations of the difractometric techniques in structural determination.</li> <li>Three-dimensional determination of the molecular structure.</li> <li>Defects and disorders in crystalline solids.</li> </ul>				
Chapter 4. NMR Spectroscopy.	Monodimensional experiments of 1H and 13C Structural information from the chemical shift. Dynamic NMR: equilibria in solution. Two-dimensional experiments. Homo- and Heteronuclear Correlation spectrose				
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. lonisation techniques. Detection methods. Fragmentation reactions. lsotopic 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 guid	dance only and does no	ot take into account the het	erogeneity 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 are most relevant for the interpretation of the data from the structural point of view (relationships between spectra and structures).			
Troubleshooting and / or The classes of small groups will be devoted to solve exercises or problems that allow at the end of exercises 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			
	Description	Qualificatio	on Training and Learning Results
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.		A1 C4 D7 A2 C8 D8 A3 C12 D13 C19 D15 C20 C24
Practical tests, real task execution and , or simulated.	•		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, 6ª,	
Hammond, Christopher, The Basics of crystallography and diffraction,	
Pavia, D.L., Lampman, G.M., Kriz, G.S., Vyvyan, J.R., Introduction to Spectroscopy, 5ª,	
Pretsch, Ernö, 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 I/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

 $\hfill\square$  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