



## 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<br>Spanish<br>Galician                                                                                                                                                                                                                                                                                                                  |           |      |            |
| Department          |                                                                                                                                                                                                                                                                                                                                                          |           |      |            |
| Coordinator         | Silva López, Carlos<br>Valencia Matarranz, Laura María                                                                                                                                                                                                                                                                                                   |           |      |            |
| Lecturers           | Pérez Lourido, Paulo Antonio<br>Silva López, Carlos<br>Valencia Matarranz, Laura María                                                                                                                                                                                                                                                                   |           |      |            |
| E-mail              | carlos.silva@uvigo.es<br>qilaura@uvigo.es                                                                                                                                                                                                                                                                                                                |           |      |            |
| Web                 |                                                                                                                                                                                                                                                                                                                                                          |           |      |            |
| General description | The subject devotes to the learning of the application of the methods but used in the structural determination of chemical substances.<br>English Friendly subject: International students may request from the teachers:<br>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<br>A5                      | B3             | C1<br>C2<br>C6<br>C15 |
| Analyze the information that can be obtained from spectroscopic techniques | A3                            | B1<br>B3<br>B4 | C1<br>C6<br>C15       |

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

## Contents

| Topic                                                 |                                                                                                                                                                                                   |
|-------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Subject 1. Gathering of general data of a substance.  | Analysis of combustion.<br>Empirical formula.<br>Qualitative analysis.<br>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.<br>Ionización methods.<br>Isotopic patterns.<br>Interpretation of the MS spectrum.                                                                           |
| Subject 6. NMR spectroscopy.                          | <sup>1</sup> H and <sup>13</sup> C monodimensional experiments.<br>Structural Information from the chemical shift.<br>Dynamic NMR: chemical equilibrium.<br>Noe experiment.<br>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 br 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<br>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<br>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, Sintesis, 2005

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#### Recommendations