FACULTAD DE
CIENCIAS QUÍMICAS

STRUCTURAL ORGANIC CHEMISTRY

COURSE GUIDE

BSc Chemistry

Academic Year 2025-2026

UNIVERSIDAD
COMPLUTENSE
MADRID

I.- IDENTIFICATION

COURSE NAME:	**Structural Organic Chemistry**
CREDITS (ECTS):	**6**
CHARACTER:	**Optative**
SUBJECT:	**Organic Chemistry**
MODULE:	**Advanced**
UNDERGRADUATE DEGREE:	**Bachelor's Degree (BS) in Chemistry**
SEMESTER/TERM:	**Second semester (fourth year)**
DEPARTMENT/S:	**Organic Chemistry**

LECTURER:

Group A		
Theory, seminar and tutorial	**Lecturer:** **Department:** **Office Number:** **e-mail:**	RAFAEL GÓMEZ ASPE Organic Chemistry QB-329-D rafaelgomez@quim.ucm.es

II.- OBJECTIVES

■ GENERAL OBJECTIVE

Introduce the student to the study of spectrum-structure correlation and the different applications of spectroscopic techniques.

It is also intended that the student:

- Acquire the appropriate and necessary knowledge that allows you to identify organic substances from a series of spectra or given spectroscopic data.
- Acquire enough knowledge to design the best way to deal with a specific problem of structural determination, knowing the information that each type of spectrum provides or contributes.
- Know the applications and limitations of the different spectroscopic techniques.

■ SPECIFIC OBJECTIVES

o Correlate the UV-Vis spectrum with the structure and recognize the different chromophores. Learn and know the management of tables.
o Correlate the IR-Raman spectrum with the different functional groups. Know the modifications in the spectrum that introduce the structural variations of the different functional groups.
o Correlate the NMR spectra of nuclei of organic interest: 1H, 13C, 19F and 31P with the structure. Interpret one- and two-dimensional spectra. Learn to use the tables.

o Correlate mass spectra and ionization systems. Recognize the molecular ion and isotopic satellites. Know the main fragmentations.

o Know and use spectroscopic databases, their management, applications and limitations. Use programs for the theoretical calculation of spectra.

o Consult and use the bibliography proposed for the development of the course.

III.- BACKGROUND KNOWLEDGE AND RECOMMENDATIONS

■ BACKGROUND KNOWLEDGE:

Structure and reactivity of the main functional groups. Stereochemistry. Notions of spectroscopy of organic molecules acquired in the Fundamental Module.

■ RECOMMENDATIONS:

It is recommended that students who enroll in this subject have previously completed and passed the subjects of Organic Chemistry I and Organic Chemistry II.

IV.- CONTENTS

■ BRIEF DESCRIPTION:

Spectroscopic techniques in the analysis of organic entities and methodology of structural determination. Mass spectrometry applied to the structural determination of organic compounds. The hydrocarbon skeleton: NMR-MS combinations. Determination of functional groups: combination of spectroscopic techniques. Advanced methods in NMR. Strategies in structural and configurational determination. Methodology/Procedure to apply spectroscopic information to structural determination. Emerging methods: applications to life sciences, food industry, gels, polymers and intermediate phases.

■ SYLLABUS:

PART 1: ULTRAVIOLET-VISIBLE SPECTROSCOPY (UV-Vis)

1- Chromophores, auxochromes and their interactions.
2- Olefins, polyenes, benzene and aromatic systems, unsaturated carbonyl compounds.
3- Examples of spectra and handling of Tables.

PART 2: INFRARED (IR) AND RAMAN SPECTROSCOPY

4- Characteristic absorptions of single and multiple links.
5- Variation of the frequency with the structure.
6- Raman spectroscopy.
7- Problems and applications.

PART 3: MASS SPECTROMETRY

8- Ionization and registration of the spectrum.
9- Molecular ion and isotopic satellites. Information. Management of tables. exact mass.
10- Main fragmentations.
11- Problems and applications.

PART 4: NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY

12- Introduction. Nuclei of interest in Organic Chemistry. Chemical shift for different nuclei.
13- Causes that modify the chemical displacement.
14- Homo and heteronuclear coupling.
15- Systems of increments for the estimation of displacements. Management of tables and simulation programs.
16- Two-dimensional homo and heteronuclear spectroscopy.
17- Problems and applications.

PART 5:

18- Joint problems of complete structural elucidation of organic molecules.

V.- COMPETENCES

■ GENERAL:

The general competences of the degree, CG1, CG2, CG3, CG4, CG7, CG8, CG11 and CG13, are collected, in this module, in the following (CG-MA: General Competences of the Advanced Module):

CG1-MA1: Recognize and value chemical processes in daily life.

CG2-MA1: Assess the importance of Chemistry and its impact on industrial and technological society.

CG2-MA2: Relate interdisciplinary areas in full expansion, and become aware of the importance that interdisciplinary research has in the advancement of Science.

CG3-MA1: Demonstrate a base of knowledge and skills with which you can continue your studies in specialized areas of Chemistry or in multidisciplinary areas.

CG4-MA1: Capture the specific knowledge of each subject in the universal scientific language, understood and shared interdisciplinary.

CG7-MA1: Apply theoretical and practical knowledge to solve problems in Chemistry and select the most appropriate method to solve them.

CG8-MA1: Evaluate research and detailed studies in the field of Chemistry.

CG11-MA1: Manage instrumentation for analysis, synthesis, and structural investigations.

CG13-MA1: Develop good scientific measurement and experimentation practices.

- **SPECIFIC:**

In addition to the general and transversal competences of the module, the specific competences of the title, CE14, CE15, CE16 and CE30, are developed, for this subject, in the following (CEMAQO: Specific Competences of the Advanced Module of the subject Advanced Organic Chemistry):

CE14-MAQO4: Recognize the chemical structure of organic and organometallic molecules and relate it to their spectroscopic or spectrometric properties.

CE14-MAQO5: Distinguish the specific structural information that spectroscopic techniques can provide in the study of different matrices.

CE14-MAQO6: Design the structural analysis procedure required by a specific problem sample.

- **GENERIC:**

The transversal competences of the title, CT1, CT2, CT3, CT4, CT5, CT7, CT8, CT11 and CT12 are collected, in this module, in the following (CT-MA: Transversal Competences of the Advanced Module):

CT1-MA1: Prepare and write reports and reports of a scientific and technical nature.
CT2-MA1: Teamwork.
CT3-MA1: Learn to make decisions when faced with a real practical problem.
CT4-MA1: Select the most appropriate method to solve a problem.
CT5-MA1: Consult, use and analyze any bibliographical source.
CT5-MA2: Manage bibliography and specialized databases, and resources accessible through the Internet.
CT7-MA1: Use computer programs that serve, in the world of Chemistry, to calculate, design, simulate, approximate, and predict.
CT8-MA1: Communicate in Spanish using the most common audiovisual media.
CT11-MA1: Develop autonomous work.
CT12-MA1: Develop sensitivity towards environmental issues and environmental preservation.

VI.- RESULTADOS DEL APRENDIZAJE

Once this course has finished, the student must be able to:

– Identify the structural information that each spectroscopic technique provides.

– Recognize the advantages and disadvantages of using each of the techniques studied for a given molecule based on its structure.

– Identify chromophores and auxochromes.

– Identify functional groups through IR spectroscopy.

– Identify the skeletal structural elements provided by MRI

– Identify molecular peaks, presence of certain polyisotopic atoms and fragments and their applications to structural determination.

– Elucidate the total structure of an organic molecule from a series of spectra.

VII. – WORKING HOURS DISTRIBUTED BY ACTIVITY

Actividad	Presential (hours)	Personal work (hours)	Credits (hours)
Presential classes	22,5	37,5	2,4 (60)
Seminars & problems	22,5	37,5	2,4 (60)
Tutorials/Guided work	4	6	0,4 (10)
Preparation of activities and exams	6	14	0,8 (20)
Total	**55**	**95**	**6 (150)**

VIII.- METHODOLOGY

A mixed methodology based on cooperative learning, collaborative learning and self-learning will be followed. The face-to-face activities of the subject are structured in expository or master classes of theory, seminar classes, tutorials and directed activities.

In-person theoretical classes: these classes will be expository and in them the epigraphs indicated in the course program as in-person classes will be developed orally, which will allow the student to obtain a global and comprehensive vision of it. Use will be made of the blackboard and PowerPoint presentations. At the end of the topic, new proposals can be made that allow the interrelation of contents already studied with those of the rest of the subject or with other subjects. Prior to the exhibition, all the material presented necessary for the follow-up of the classes will be available to the students on the Virtual Campus.

Seminar classes: the objective will be to apply the acquired knowledge to a set of questions/exercises. To do this, students will be provided with a collection of exercises. The teacher will explain some typical exercises (which will be indicated as such in the statement) and the rest will be solved by the students as personal work. Some of the questions will be related to aspects not described in the theoretical development of the subject, so that students can use the knowledge acquired to justify the facts raised in them.
In this subject, the part devoted to problems is fundamental. Once the student has acquired the necessary knowledge, the problems will be solved and exposed by the students. For particularly difficult problems, groups of two or three students will be formed in charge of solving them.

Face-to-face tutorials/Directed Activities: four face-to-face tutorial sessions will be scheduled on exercises related to the subject's agenda. In the first tutorial sessions, the

teacher will review and correct, if applicable, the solutions proposed by the students, will resolve any doubts and difficulties that have arisen in solving the proposed exercises and will guide the students to the correct solution of the exercises that were poorly planned or resolved. In the later ones the solutions of the proposed exercises will be definitively reviewed, and the last doubts and difficulties will be resolved.

IX.- BIBLIOGRAPHY

There are very few works on the structural determination of organic compounds translated into Spanish. The student can find different monographs in English and German. A specific textbook will not be followed, but perhaps the most complete and general work is:

GENERAL TEXTBOOKS:

- Hesse, M.; Meier, H. y Zeeh, B.: *"Métodos espectroscópicos en Química Orgánica"*, 2ª edición, Editorial Síntesis 2005, ISBN: 84-7738-522-X
- Silverstein, R.M.; Webster, F.X.; Kiemble, D.: *"Spectrometric Identification of Organic Compounds"*, 8ª ed., John Wiley & Sons, 2015.
- Fleming, I.; Williams, D.: *"Spectroscopic Methods in Organic Chemistry"*, 7ª ed., Springer Nature Switzerland, 2019.

SPECTROSCOPY TABLES

- Pretsch, E.; Bühlmann, P.; Affolter, C.; Herrera, A. y Martínez R.: "*Determinación estructural de compuestos orgánicos*", Elsevier-Masson 2002, ISBN13: 978844581215-0.
- Pretsch, E.; Bühlmann, P; Badertscher, M. "*Structure Determination of Organic Compounds"* Springer 2009. ISBN 978-3-540-93809-5.

THEORY AND PROBLEMS TEXTBOOKS

- Field, L. D., Sternhell, S. y Kalman, J. R.: "*Organic Structures from Spectra"*, 6ª edición, Wiley 2020, ISBN: 978-1-119-52480-9.
- Field, L. D.; Li, H.L.; Magill, A.M.: *"Organic Structures from 2D NMR Spectra"*, John Wiley & Sons, Chichester, 2015.
- Randazzo, A. *"Guía Práctica para la interpretación de espectros de RMN. Ejercicios para la determinación estructural de pequeñas moléculas orgánicas"*. Loghia 2018, ISBN: 978-88-95122-44-1.
- Blay, G., Pedro, J.R.: *"200 Problemas de Determinación Estructural de Compuestos Orgánicos"*, Visión Libros 2010, ISBN: 978-84-9983-993-6.

MONOGRAPHIES

UV-Vis spectroscopy:

- Thomas, M.: *"Ultraviolet and Visible Spectroscopy"*, Analytical Chemistry by Open Learning, John Wiley & Sons, Chichester, 1996.

Infrared/Raman spectroscopy:

- Günzler, H. y Gremlich, H-U.: "*IR Spectroscopy*", Wiley 2002, ISBN: 3-527-28896-1.

- Stuart, B.; George, B.; McIntyre, P.: *"Modern Infrared Spectroscopy"*, Analytical Chemistry by Open Learning, John Wiley & Sons, Chichester, 1998.
- Socrates, G.: *"Infrared and Raman Characteristic Group Frequencies. Tables and Charts"*, John Wiley & Sons, Chichester, 2005.

Mass spectrometry:

- Lee, T. E.: "*A Beginner's guide to Mass Spectral interpretation*"**,** Wiley 1998, ISBN: 0-471-97629-6.
- Gross, J.H.: "*Mass Spectrometry",* Springer 2017, ISBN: 978-3-319-54397-0.

Nuclear Magnetic Resonance spectroscopy:

- H. Friebolin, *"Basic One- and Two-Dimensional NMR Spectroscopy"*, Wiley-VCH 2011, ISBN: 978-3-52732782-9.
- Günther, H.: *"NMR Spectroscopy"*, 3ª ed., Wiley-VCH, Weinheim, 2013.

Students will be provided with a series of web page addresses where they can find databases in the form of different spectra of numerous organic substances, glossaries of terms used in each type of spectroscopy and on-line courses with proposed and solved problems.

X.- ASSESSMENT PROCEDURE

For the final evaluation, participation in the different proposed activities is mandatory.

The student's academic performance and the final grade for the subject will be computed, in a weighted manner, based on the percentages shown in each of the aspects listed below. All grades will be based on the absolute score out of 10 points, and in accordance with the scale established in RD 1125/2003. This criterion will be maintained in all calls.

The qualifications of the activities planned for the evaluation of the subject will be communicated to the students sufficiently in advance before the completion of the final exam so that they can adequately plan the study of this or other subjects.

In any case, the minimum period of seven days between the publication of the qualifications and the date of the final exam of the subject will be respected.

■ WRITTEN EXAMS:

Final examen:	**60%**
The knowledge acquired will be assessed by means of a final exam to which all students must take. The exam will consist of theoretical questions on the application of concepts learned during the course and problem solving.	
Evaluated competences:	
All generic, specific and transversal competences.	

■ PERSONAL WORK AND DIRECTED ACTIVITIES

Questions and problems:	**40%**
The evaluation of the individual learning work carried out by the student will be carried out by solving questions and problems. The student's skill in solving the proposed problems and exercises and their knowledge of theoretical aspects will be valued. Active attendance and participation in classes is included in this evaluation. Evaluated Competences: All generic, specific and transversal competences.	

■ EXTRAORDINARY JULY EXAM

Exam:	**60%**
The continuous evaluation of the course will be taken into account in the extraordinary call. The exam of said call will have a value of 60% to which the marks obtained in the continuous assessment of the semester will be added.	
Evaluated competences:	
All generic, specific, and transversal competences.	

SCHEDULE

TOPIC	ACTIVITY	HOURS	GROUPS	START	END
PART 1 UV-Vis	Lectures & seminars	6	1	1st week	
PART 2 IR	Lectures & seminars	6	1	2nd week	4th week
PART 3 RMN	Lectures & seminars	15	1	5th week	8th week
PART 4 Mass Spectrometry	Lectures & seminars	8	1	9th week	10th week
PART 5 Mix problems	Lectures & seminars	10	1	11th week	14th week
PART 6	Lectures & tutorials*	4	1	15th week	

* The programming of the tutorials depends on the global planning of all the subjects of the course.

SUMMARY OF THE ACTIVITIES								
Teaching Activity	**Asociated Competences**	**Profesor´s duty**	**Student´s duty**	**Grading**	**P**	**NP**	**Total**	**C**
Lectures	All generic, specific and transversal competences	Preparation of the material Presentation of theoretical concepts	Pre-class preparation and note taking	Qualification of answers made in writing to questions made about theoretical concepts	22,5	37,5	60	
Problems and seminars	All generic, specific and transversal competences	Preparation of the material Application of theoretical concepts to the resolution of practical cases	Pre-class preparation note taking Troubleshooting Formulation of questions and doubts	Qualification of the proposed problems Qualification of the development of the methodology for structural determination Qualification of the proposal of structures Qualification of the proposal of spectroscopic techniques to be used for the best determination of the structure	22,5	37,5	60	40%
Tutoríals	All generic, specific and transversal competences	Preparation of controls, resolution of doubts and special problems	Realización de controles Formulación de preguntas y dudas	Grading of exams	4	6	10	
Exams	All generic, specific and transversal competences	Proposal, supervision and correction of the exam. student grading	Preparación y realización del examen	Grading of exams	6	14	20	60%
P : Presential; NP: non presential (autonomous work); C: grading								