VNIVERSITAT DE VALÈNCIA

Course Guide
44705 Advanced organic chemistry

COURSE DATA

Data Subject	
Code	44705
Name	Advanced organic chemistry
Cycle	Master's degree
ECTS Credits	4.0
Academic year	2024 - 2025

Study (s)

Degree	Center	Acad. year	Period
2226 - Master's degree in Organic Chemistry	Faculty of Chemistry	1	Annual

Subject-matter

Degree	Subject-matter	Character
2226 - Master's degree in Organic Chemistry	1 - Advanced organic chemistry	Obligatory

Coordination

Name	Department
DEL POZO LOSADA, CARLOS	325 - Organic Chemistry

SUMMARY

The Physical Organic Chemistry (2 credits) together with fotochemistry (2 credits) constitute the subject Advanced Organic Chemistry. This topic provide a deep understanding in different aspects of the organic chemistry previously studied, with the aim to place students in conditions to be able to deal with more complex aspects of organic chemistry, specially those interesting for the chemical and pharmaceutical industry.

In this subject, the knowledge of the chemical bonding will be enhanced, together with the theoretical study of pecicyclic reactions, including electrocyclic, cycloaddition and sigmatropic rearrangement reactions. Additionally, pertubations theory will be studied as a tool to explain the selectivity of the reactions

PREVIOUS KNOWLEDGE

Relationship to other subjects of the same degree

There are no specified enrollment restrictions with other subjects of the curriculum.

Other requirements

Knowledege of physical organic chemistry at graduate level.

COMPETENCES (RD 1393/2007) // LEARNING OUTCOMES (RD 822/2021)

2226 - Master's degree in Organic Chemistry

- Students should apply acquired knowledge to solve problems in unfamiliar contexts within their field of study, including multidisciplinary scenarios.
- Students should be able to integrate knowledge and address the complexity of making informed judgments based on incomplete or limited information, including reflections on the social and ethical responsibilities associated with the application of their knowledge and judgments.
- Students should communicate conclusions and underlying knowledge clearly and unambiguously to both specialized and non-specialized audiences.
- Students should demonstrate self-directed learning skills for continued academic growth.
- Students should possess and understand foundational knowledge that enables original thinking and research in the field.
- Use different presentation formats (oral, written, slide presentations, boards, etc.) to communicate knowledge, proposals and positions.
- Be able to access to information tools in other areas of knowledge and use them properly.
- Saber participar en debates y discusiones, dirigirlos y coordinarlos y ser capaces de resumirlos y extraer de ellos las conclusiones más relevantes y aceptadas por la mayoría.
- Poseer habilidades sociales, un buen nivel de comunicación oral y escrita, así como capacidad para trabajar en equipo y con personas de diferentes procedencias.
- Competencias de gestión tales como la capacidad para la planificación y gestión de tiempo y recursos, así como para dirigir y tomar decisiones.
- Ser capaces de valorar la necesidad de completar su formación científica, en lenguas, en informática, asistiendo a conferencias o cursos y/o realizando actividades complementarias, autoevaluando la aportación que la realización de estas actividades supone para su formación integral.
- Afianzar y profundizar en aquellos temas relacionados con la estereoquímica de las moléculas orgánicas y la descripción del enlace químico.
- Alcanzar un conocimiento profundo de los aspectos teóricos de las reacciones pericíclicas.

- Conocer los fundamentos de las reacciones fotoquímicas, en especial de los compuestos orgánicos, y sus aplicaciones en síntesis.

LEARNING OUTCOMES (RD 1393/2007) // NO CONTENT (RD 822/2021)

The final aims of this subject are the following:

- The acquisition of a deep knowledge in organic chemistry in aspects previously studied, placing the students in conditions to face more complex aspects of the organic chemistry.

- The knowledge of some aspects of applied organic chemistry interesting for the chemical and pharmaceutical industry.

More specifically, the main objectives of this subject are the following:

- Enhance the knowledge of some topics related with the stereochemistry of organic molecules and the description of chemical bonding.

- Enhance the knowledge of the physic-chemical aspects of organic reactions.

- To reach a better understanding of some theoretical aspects of pericyclic reactions and its synthetic applications.

- Design, selection and/or development products and chemical processes efficiently (ODS 7) that minimize their impact in the environment (ODS 14 and 15), taking advantage of the alternative row materials and generating the minor amount of residues possible (ODS 11)

DESCRIPTION OF CONTENTS

1. Structure and bonding

Theories of chemical bonding. Molecular orbital theory. -Conjugation. Hyperconjugation. Localized molecular orbitals. Non-covalent interactions. Stereoelectronic effects. Conformations

2. Perturbation theory

Chemical reactivity: perturbation theory. The Salem-Klopman equation. Reactive intermediates. Ionic, radical and pericyclic reactions.

3. Electrocyclic reactions

Electrocyclic reactions. Conrotatory and disrotatory ring closures. Correlation diagrams: selection rules. Frontier orbitals. Aromatic transition state approach.

4. Cycloadditions

Cycloadditions. Selection rules. Diels-Alder reactions: regio and stereoselectivity. 1,3-Dipolar cycloadditions.

5. Sigmatropic rearrangements

Sigmatropic rearrangements. [1,j]-Sigmatropic rearrangement of hydrogen. [1,j]-Sigmatropic rearrangement of alkyl groups. [3,3]-Claisen and Cope rearrangements. [2,3]-Sigmatropic rearrangements. Ene reactions.

6. Photoredox catalysis

Synthetic applications of visible-light photoredox catalysis. C-C and C-heteroatom (B, O, N, P, S, F, Cl, Br, I) bond formation reactions. Mechanistic considerations

7. Excited states

Static and dynamic properties of excited states. Radiative and non-radiative transitions. Energy transfer processes. Charge transfer processes.

8. Experimental techniques

Light sources. Photochemical reactors. Wavelength selection.

9. Photochemistry of the carbonyl group

Introduction. Norrish type I reaction. Hydrogen abstraction. Norrish type II reaction. Paterno Buchi reaction.

10. Photochemistry of alkenes

Introduction. E/Z Isomerization. Di-p-methane rearrangement. Sigmatropic and carbene-mediated rearrangements.

11. Photochemistry of aromatic compounds

Introduction. Ring isomerization. Photoadditions. Photocycloadditions. Photodimerization. Photosubstitution. Side chain reactions.

12. Photochemistry of nitrogen compounds

Imines. Iminium salts. Oxides and related compounds. Nitrite esters. Nitrocompounds. Azocompounds. Diazocompounds. Azides

13. Photooxygenation

Reactive oxygen species. Oxygenation with triplet oxygen. Oxygenation with singlet oxygen. Oxygenation with oxygen radical anion.

WORKLOAD

ACTIVITY	Hours	% To be attended
Theory classes	20,00	100
Seminars	20,00	100
Study and independent work	40,00	0
Preparation of evaluation activities	20,00	0
TOTAL	**100,00**	

TEACHING METHODOLOGY

The subject is formulated in a manner that the student is the principal actor of its own learning. From the beginning of the course, students will have the whole didactic material necessary.

The employed methodology will combine master classes, discussion and analysis of selected examples and practical cases, together with the use of audiovisual methods and other electronic resources.

The teaching will be structured in the following manner:

• Master classes (in person): In these classes the basic concepts of the physical organic chemistry will be introduced. Theoretical themes will be imparted, developing the contents of the program.

• Seminars (in person).- Seminars will be dedicated to the resolution of problems and questions with an active participation of the students. The discussion of scientific articles related to the themes will be also performed.

• Written assignment.- In those assignments, the professor will proposed themes related, normally found in scientific publications.

EVALUATION

The assessment of student learning will be performed in a continuous manner for the teacher throughout the course, and it will contain the following points:

● **Direct assessment of the professor:** 20% of the final grade will come from the direct evaluation of the professor both in theoretical and practical classes. In this evaluation, some different aspects will be considered. Among them, we outlined the following:

- Attendance and participation in the discussions

- Progress in the use of the proper language of the field.

- Problem resolution and question proposal

- Critic spirit

- presentation of the exercices.

● **Written exams.** 80% of the final grade will come from the grades obtained in those written exams

- in person examination (traditional style) with both theoretical and practical questions of contents related to the subject. The nature of those questions and problems will force the students to connect several aspects that come from different themes of the subject, or if the teacher considers it convenient, from different subjects.

- Not in person exams. The teacher will give to the students directly or by electronic mail, a series of questions that the students have to complete, either individually or in group, depending on the decision of the teacher. In any case, the answers will be sent to the teacher again in person or by electronic mail, in the period previously stipulated.

REFERENCES

Basic

- Principles of Molecular Photochemistry: An Introduction, N.J. Turro, J.C. Scaiano, V. Ramamurthy, University Science Books, 2009.
- Modern Molecular Photochemistry of Organic Molecules, N.J. Turro, J.C. Scaiano, V. Ramamurthy, University Science Books, 2010.
- CRC Handbook of Organic Photochemistry and Photobiology (2 volúmenes), 3rd Edition, Editado por A. G. Griesbeck, M. Oelgemöller y F. Getti, CRC Press, 2012.

Additional

- Glosario de Términos Usados en Fotoquímica. Comisión de Fotoquímica de la IUPAC, 1996. Universitat Autònoma de Barcelona. Servei de Publicacions Bellaterra, 1999.