COURSE DATA

DATA SUBJECT

Code: 44705
Name: Advanced organic chemistry
Cycle: Master's Degree
ECTS Credits: 4
Academic year: 2025-26

STUDY (S)

Degree	Center	Acad. year	Period
2226 - Master's degree in Organic Chemistry	Facultat de Química	1	Annual

SUBJECT-MATTER

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

COORDINATION

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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 / LEARNING OUTCOMES

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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.

Be able to access to information tools in other areas of knowledge and use them properly.

Competencias de gestión tales como la capacidad para la planificación y gestión de tiempo y recursos, así como para dirigir y tomar decisiones.

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

Poseer habilidades sociales, un buen nivel de comunicación oral y escrita, así como capacidad para trabajar en equipo y con personas de diferentes procedencias.

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.

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.

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.

DESCRIPTION OF CONTENTS

1. Structure and bonding

Theories of chemical bonding. Molecular orbital theory. π-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. Light.

Excited states. Characterization of excited states. Absorption. Properties of excited states. The fate of excited states

7. Reactivity of excited states.

Introduction: energy transfer and electron transfer. Kinetic aspects. Thermodynamic aspects. Theoretical models. Marcus theory of electron transfer reactions

8. Irradiation sources.

Optical properties of glassware. Filters. Further irradiation devices: light emitting diodes (LEDs). Further irradiation devices: Organic light emitting diodes (OLEDs). Comparison of different irradiation sources

9. Photochemistry and nanotechnology.

History of nanomaterials. Unique properties of nanomaterials. Metal nanoparticles. Semiconductor nanoparticles: Quantum dots. Semiconductor nanoparticles: Titanium dioxide

10. Organic photoredox catalysis.

Basis of photoredox catalysis. Metal photocatalysts. Metal-free photocatalysts. Photocatalysis for the formation of C-C bonds

11. Environmental applications of photocatalysis.

Advanced Oxidation Processes (AOPs). Organic photocatalysts. Titanium dioxide. Photo-Fenton. Preparation and characterization of photocatalysts for environmental applications

WORKLOAD

PRESENCIAL ACTIVITIES

Activity	Hours
Theory	20,00
Seminar	20,00

Total hours	**40,00**

NON PRESENCIAL ACTIVITIES

Activity	Hours
Attendance at other activities	0,00
Individual or group project	0,00
Independent study and work	50,00
Preparation of lessons	0,00
Preparation for assessment activities	10,00
Resolution of case studies	0,00
Total hours	**60,00**

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:

1) written exam (70%):

The exam will be held within the period established in the course organization and the specific date will be agreed between the teacher and the students. If a second call is required, the date will also be agreed between the students involved and the teacher.

The exam will be adjusted to the following modality: traditional style exam of both theoretical and problem

questions related to the subject. These questions and problems will force the student to relate different aspects that appear in different topics of the subject or also, if the teacher considers it appropriate, in different subjects of the area.

2) Direct evaluation of the teacher (30%):

20% of the grade will come from the direct evaluation of the teacher in the theoretical, problem and tutorial classes, as well as any other activity scheduled by the teacher. This evaluation will take into account aspects such as class attendance (**the teacher will establish whether or not attendance at classes is mandatory**), study work and interventions in the discussions that arise during the classes. At the discretion of the teacher, follow-up exercises may be proposed, the grade of which will contribute to the final grade in this section.

3) Qualification

The final grade will be the average of the marks obtained in each of its sections (Photochemistry and Physical Organic Chemistry, both parts make an identical contribution to the overall computation). The minimum grade of a section to access the average is 4.5. To pass the subject, the average grade must be greater than or equal to 5.

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

REFERENCES

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