



## Teaching Guide

Identifying Data					2023/24
Subject (*)	Supramolecular Chemistry	Code	610509107		
Study programme	Mestrado Universitario en Investigación Química e Química Industrial (Plan 2020)				
Descriptors					
Cycle	Period	Year	Type	Credits	
Official Master's Degree	2nd four-month period	First	Optional	3	
Language	SpanishGalician				
Teaching method	Face-to-face				
Prerequisites					
Department	Departamento profesorado másterQuímica				
Coordinador	Brea Fernández, Roberto Javier	E-mail	roberto.brea@udc.es		
Lecturers	Brea Fernández, Roberto Javier Esteban Gomez, David Mosquera Mosquera, Jesús	E-mail	roberto.brea@udc.es david.esteban@udc.es j.mosquera1@udc.es		
Web					
General description	<p>A Química Supramolecular é unha materia imprescindible no módulo de "Química Sintética", que permite comprender a natureza das interaccións intermoleculares, e analizar as posibles implicacións que éstas poden chegar a ter, tanto desde o punto de vista estrutural, como de reactividade en procesos catalíticos e estereoselectivos.</p> <p>Os contidos tratados na materia profundizan en moitos dos aspectos presentados en diferentes materias do módulo, e resultan un complemento necesario para facer fronte aos contidos de materias dos módulos de "Química Biolóxica", "Nanomateriais e Novos Materiais" e de "Técnicas Analíticas Avanzadas".</p> <p>Unha vez cursada, o alumnado terá adquirido os coñecementos básicos relacionados coa Química Supramolecular, como ferramenta na construción de sistemas complexos a partir de unidades perfectamente definidas, e das interaccións que os gobernan, tanto para a súa aplicación en distintas áreas de investigación como para entender diferentes procesos industriais tales como a catálise, xelificación, solubilización de sistemas complexos, etc.</p>				

## Study programme competences

Code	Study programme competences
A1	Define concepts, principles, theories and specialized facts of different areas of chemistry.
A3	Innovate in the methods of synthesis and chemical analysis related to the different areas of chemistry
A7	Operate with advanced instrumentation for chemical analysis and structural determination.
A8	Analyze and use the data obtained independently in complex laboratory experiments and relating them with the chemical, physical or biological appropriate techniques, including the use of primary literature sources
B2	Students should apply their knowledge and ability to solve problems in new or unfamiliar environments within broader (or multidisciplinary) contexts related to their field of study.
B3	Students should be able to integrate knowledge and handle complexity, and formulate judgments based on information that was incomplete or limited, include reflecting on social and ethical responsibilities linked to the application of their knowledge and judgments.
B4	Students should be able to communicate their conclusions, and the knowledge and the reasons that support them to specialists and non-specialists in a clear and unambiguous manner
B7	Identify information from scientific literature by using appropriate channels and integrate such information to raise and contextualize a research topic
B9	Demonstrate ability to analyze, describe, organize, plan and manage projects
B10	Use of scientific terminology in English to explain the experimental results in the context of the chemical profession
B11	Apply correctly the new technologies to gather and organize the information to solve problems in the professional activity.
C1	CT1 - Elaborar, escribir e defender publicamente informes de carácter científico e técnico
C3	CT3 - Traballar con autonomía e eficiencia na práctica diaria da investigación ou da actividade profesional.
C4	CT4 - Apreciar o valor da calidade e mellora continua, actuando con rigor, responsabilidade e ética profesional.
C5	CT5 - Demostrar unha actitude de respecto polas opinións, valores, comportamentos e prácticas doutros



Learning outcomes			
Learning outcomes	Study programme competences		
Use chemical terminology, nomenclature, conventions, and units.	AC1	BC4 BC10	CC1
Acquire the basic knowledge related to Supramolecular Chemistry.	AC3 AC8	BC2 BC7 BC11	
Understand the relationship between the structure of chemical compounds and the formation of super and supramolecules through processes of molecular recognition and self-assembly.	AC7 AC8	BC2 BC3	
Understand Supramolecular Chemistry as a tool for the construction of complex systems from perfectly defined units and its application in different areas of research.	AC3 AC8	BC2 BC3 BC7	CC3 CC4
Interpret the data from experimental observations and the use of the various experimental techniques used in their characterization.	AC7 AC8	BC2 BC3 BC7 BC9 BC11	CC1 CC3 CC5

Contents	
Topic	Sub-topic
Topic 1.- Basic Principles. Weak bond forces: types and properties.	Basic definitions. Relationship between structure, supramolecular reactivity and properties. Types and properties of noncovalent bonding forces involved in supramolecular processes
Topic 2.- Molecular recognition: molecular receptors.	Molecular recognition: definition. Principles for receiver design. Modes of study receptor-substrate interactions.
Topic 3.- Supramolecular protein systems: enzymatic catalysis and enzyme design.	Secondary and tertiary structure of proteins. Basis of activity and specificity of enzymes. Principles for the design of enzymes.
Topic 4.- Molecular self-assembly: Nanotubes, molecular capsules and other systems.	Properties and characteristics of molecular self-assembly processes. Implications in biological processes. Main nanostructures obtained through this type of process: design and properties.
Topic 5.- Applications of Supramolecular Chemistry: Transport, catalyst, dynamic combinatorial chemistry, sensors, molecular machines and self-replicating systems. Applications in nanotechnology.	Introduction to applications. Molecular transport. Catalysis. Dynamic combinatorial chemistry. Designs of molecular machines. Self-replicating systems. Applications to nanotechnology
Topic 6.- Liquid crystals. Classifications, properties and applications.	Introduction, self-organization and self-assembly. Liquid crystals: Generalities. Liquid crystals formed by non-covalent interactions. Other soft materials.
Topic 7.- Chemistry of Supramolecular Coordination.	Generalities in supramolecular processes guided by coordination chemistry. cyclic oligomers. Molecular boxes. Interchained architectures (rotaxanes and catenanes). Helicates.
Topic 8.- Supramolecular Organometallic Chemistry.	Basic concepts and principles. Intermolecular bonds, types of bonds present in organometallic supramolecular chemistry. Organometallic receptors and their substrate/receptor complexes. Self-assembly processes through the different types of organometallic bonds (dative, pi interactions, hydrogen bonds, etc).

Planning				
Methodologies / tests	Competencies	Ordinary class hours	Student?s personal work hours	Total hours
Guest lecture / keynote speech	A1 A3 A7 B10 C4	12	12	24
Problem solving	A1 B2 B3 B7 B10 C3	4	12	16



ICT practicals	A8 B2 C1 C3	2	3	5
Seminar	A1 A3 A7 A8 B2 B3 B7 B10 B11 C1 C3	1	1.5	2.5
Supervised projects	A1 A3 A7 B3 B7 B10 B11 C1	1	5.5	6.5
Oral presentation	A1 A3 A7 B4 B9 B10 B11 C1 C5	1	5	6
Mixed objective/subjective test	A1 A3 A7 B10 C4	2	11	13
Personalized attention		2	0	2

(\*)The information in the planning table is for guidance only and does not take into account the heterogeneity of the students.

Methodologies	
Methodologies	Description
Guest lecture / keynote speech	Theoretical classes. Expositive classes (use of blackboard, computer, cannon), complemented with the tools of virtual teaching.
Problem solving	Resolution of practical exercises (problems, multiple choice questions, interpretation and processing of information, evaluation of scientific publications, etc.)
ICT practicals	Practices carried out in the computer room. Use of specialized computer programs and the Internet. Online teaching support (Virtual Campus).
Seminar	Seminars carried out with the Master's own teaching staff, or with invited professionals from the company, the administration or from other universities. Interactive sessions related to the different subjects with debates and exchange of opinions with the students.
Supervised projects	Carrying out work, both individually and in groups, on scientific topics related to the different subjects of the Master.
Oral presentation	Oral presentation of works, reports, etc., including debate with teachers and students.
Mixed objective/subjective test	Completion of the different tests to verify the acquisition of both theoretical and practical knowledge and the acquisition of skills and attitudes.

Personalized attention	
Methodologies	Description
Problem solving Supervised projects Guest lecture / keynote speech ICT practicals	<p>The proposed teaching methodology is based on the work of the student, who becomes the main person in charge of their educational process. In order to get the best performance from its effort, and to guide the student in this process and determine to what extent the student is reaching the objectives proposed in each thematic unit, problem-solving sessions and practical cases will be held. These will allow students to be guided and ensure that they reach the competencies associated with the subject. Likewise, this orientation will be reinforced through individual interviews that will be held during the teacher's tutoring hours and/or at the most convenient times for the students. Obviously, and apart from these tutorials proposed by the teacher, students may attend tutorials at their own request as many times as they wish and at the times that are most convenient for them.</p> <p>It should be noted that during the master sessions participation in debate rounds related to the content covered in each unit will be encouraged.</p> <p>The hours of personalized attention will serve to clarify the fundamental concepts of the subject, as well as to resolve individual issues presented in seminars, lectures, and practices.</p> <p>Those students who take advantage of the regime of "recognition of part-time dedication and academic exemption from attendance" according to the regulations of the UDC, will have specific attention that will be specified in the following aspects:</p> <ul style="list-style-type: none"> <li>- These students will have, at their own request and at a time to be agreed, tutorial help for the preparation of the contents that will be worked on in the practical laboratory classes, as well as in the seminars.</li> <li>- Similarly, and when requested, these students will receive additional tutorial help for guidance and resolution of doubts.</li> </ul>



## Assessment

Methodologies	Competencies	Description	Qualification
Mixed objective/subjective test	A1 A3 A7 B10 C4	The mixed test will be carried out in the calendar agreed by the Faculty Board of each center. Its objective is to obtain an evaluation of the level of knowledge and skills reached by the student, as well as to assess the student's ability to relate them and to obtain an overview of the subject.	65
Problem solving	A1 B2 B3 B7 B10 C3	Carrying out the activities associated with solving the problem sets provided by the teacher, submitting assignments and discussing the results in the seminar session corresponding to each topic.	10
Oral presentation	A1 A3 A7 B4 B9 B10 B11 C1 C5	Public presentation of the supervised work carried out by each student followed by a debate in which all the students will participate in order to establish knowledge and resolve specific doubts about the content presented.	5
Supervised projects	A1 A3 A7 B3 B7 B10 B11 C1	Elaboración de un trabajo crítico de revisión centrado en un artículo de investigación relacionado con los sistemas estudiados y descritos en una unidad temática. Éste se proporcionará con la suficiente antelación, y para su elaboración el/la estudiante se apoyará en tutorías de orientación con profesor que lo supervise.	10
Guest lecture / keynote speech	A1 A3 A7 B10 C4	In the master sessions the contents of the corresponding topics will be introduced, highlighting the most important aspects, focusing particularly on those fundamental concepts and/or those that are more difficult for students to understand.	5
Seminar	A1 A3 A7 A8 B2 B3 B7 B10 B11 C1 C3	Training activity of an eminently practical nature designed with the objective of influencing those aspects of the subject that are more difficult to understand	2.5
ICT practicals	A8 B2 C1 C3	Carrying out activities related to the structural characterization of supramolecular systems and the thermodynamic and/or kinetic study of the equilibria that these usually present in solution, using different software and computer support commonly used in these analyses.	2.5

## Assessment comments



The evaluation of this subject will be done through a continuous evaluation methodology that includes a final exam. Access to the exam is conditioned by the participation of students in face-to-face teaching activities (problem-solving seminars, debate, supervised work and associated oral presentation and practices through ICT), for which attendance and participation must be at least of 80%. In any case, it will be mandatory to attend at least one of the two scheduled follow-up tutorials.

The student must review the theoretical concepts introduced in the different topics using the reference manual and summaries. The degree of success in solving the proposed exercises will provide a measure of the student's preparation to face the final exam of the subject. Those students who encounter significant difficulties when working on the proposed activities must attend interviews during the teacher's tutoring hours so that the latter can analyze the problem and help resolve said difficulties. It is very important when preparing for the exam to solve some of the exercises that appear at the end of each of the chapters of the reference manual.

The professor will verify the attendance to the sessions according to the official attendance control system established in the University (or in its case Center) in which the student is enrolled. Absences must be documented justified.

The weighting of the continuous assessment and the final exam will be based on the percentages indicated in the table included in this section.

The professor will analyze with those students who do not successfully pass the evaluation process, and who so wish, the difficulties encountered in learning the contents of the subject. Likewise, it will provide them with all that additional material (questions, exercises, exam models, etc.) that contributes to reinforce the learning of the subject. As established by the "Rule that regulates the dedication to the study of undergraduate students at the UDC" (Art.3.b and 4.5) and the "Rules for assessment, review and claim of qualifications for undergraduate and university master's studies (Art. 3 e 8b), students with recognition of part-time dedication and academic exemption from assistance must be able to participate in a training methodology and associated teaching activities that allow them to achieve the training objectives and the competences of the subject. These students will be able to participate in a personalized system of orientation and evaluation tutorials that will serve, on the one hand, to guide the student's autonomous work and keep track of their progression during the course; and on the other, to assess the degree of competency development achieved.

The dispensation percentage will be established in a first interview with the students, once their personal situation is known. In this way, a schedule will be established for the orientation tutorials, and the number of problem-solving workshops that must be evaluated using this methodology will be determined. Once known, their number will be weighted over the total of them and the number of tutorials in which these students must participate will be set. All of them will be preset with the students based on their availability, according to the content schedule of the subject and specifying the deadlines for delivery of the different material likely to be evaluated (problems and questions bulletins). This material will be previously delivered through the Moodle platform according to the schedule agreed in the initial tutorial. During the tutorial sessions, aspects associated with both the contents of the subject and the joint review of the work delivered will be dealt with, as well as small evaluation tests to check if the students continue to take advantage of these activities.

Grading implications of plagiarism: The fraudulent completion of any exercise or test of the student for the evaluation of the subject will be subject to disciplinary

responsibilities, as stated in the Regulations for Evaluation, Review and Claim of University Degree and Master's Degree Qualifications (Article 11) and in the Statute of the UDC Student Body (Article 35, point 3): "Failed grade in the call in which the offense is committed: the student will be graded with "Fail" (numerical grade 0) in the corresponding call of the academic year, both the fault occurs both on the first opportunity and on the second. For this, their qualification will be modified in the first opportunity record if necessary".

## Sources of information

<b>Basic</b>	<ul style="list-style-type: none"><li>- J.-M. Lehn (1995). Supramolecular Chemistry. VCH, New York</li><li>- P. A. Gale, J. W. Steed (2012). Supramolecular Chemistry: From molecules to nanomaterials. Wiley and Sons Ltd. (Vol.1 - 2)</li><li>- J. W. Steed, J. L. Atwood (2009). Supramolecular Chemistry 2nd Ed. Wiley and Sons</li><li>- I. Haiduc, F. T. Edelman (2008). Supramolecular Organometallic Chemistry. Wiley-VCH</li></ul>
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<b>Complementary</b>	<ul style="list-style-type: none"><li>- K. Ariga, T. Kunitake (2006). Supramolecular Chemistry: Fundamentals and Applications. Springer-Verlag</li><li>- R. Ungaro, E. Dalcanale (1999). Supramolecular Science: Where it is and where it is going. Kluwer, Dordrecht</li><li>- J. L. Atwood et al. (1996). Comprehensive Supramolecular Chemistry. Pergamon</li><li>- V. Balzani, M. Ventura, A. Credi (2003). Molecular Devices and Machines. Wiley-VCH</li><li>- K. Gloe (2005). Macrocyclic Chemistry. Current Trends and Future Perspectives. Springer</li><li>- D. F. Shriver, H. D. Kaesz, R. D. Adams (2008). The Chemistry of Metal Cluster Complexes. VCH Publishers</li><li>- N. Rodríguez-Vázquez, A. Fuertes, M. Amorín, J. R. Granja (2016). Bioinspired Artificial Sodium and Potassium Channels. Springer International Publishing Switzerland</li></ul>
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<b>Recommendations</b>
<b>Subjects that it is recommended to have taken before</b>
Selection and validation of Analytical methodologies/610509101
Industrial Processes and Sustainability/610509104
Techniques of Characterization of Materials and Bionterphases/610509102
Advanced Structural Determination/610509103
Supervised Training Activities/610509105
<b>Subjects that are recommended to be taken simultaneously</b>
Applied Coordination Chemistry/610509110
Chemistry of Biomolecules/610509115
Fluorescence Spectroscopy and Photochemistry /610509108
Metals in Biological Processes/610509314
<b>Subjects that continue the syllabus</b>
Practical Academic Training/610509136
Master Thesis/610509139
<b>Other comments</b>



Gender perspective:- According to the different applicable regulations for university teaching, the gender perspective must be incorporated in this matter (non-sexist language will be used, a bibliography of authors of both sexes will be used, intervention in class of male and female students...)- Work will be done to identify and modify prejudices and sexist attitudes and the environment will be influenced to modify them and promote values of respect and equality.- Situations of discrimination based on gender must be detected and actions and measures to correct them will be

proposed.&nbsp;@font-face

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Program

To achieve an immediate sustainable environment and comply with point 6 of the "Environmental Declaration of the Faculty of Sciences (2020)", the documentary works carried out in this subject:

a.- They will

be requested mainly in virtual format and computer support.

b.- If done

on paper:

- Plastics

will not be used.

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Double-sided prints will be made.

- Recycled

paper will be used.

- The realization of drafts will be avoided.





(\*)The teaching guide is the document in which the URV publishes the information about all its courses. It is a public document and cannot be modified. Only in exceptional cases can it be revised by the competent agent or duly revised so that it is in line with current legislation.