Universitat Autònoma de Barcelona

2019/2020

Supramolecular Chemistry and Molecular Recognition

Code: 103294
ECTS Credits: 5

Degree	Type	Year	Semester
2501922 Nanoscience and Nanotechnology	OB	3	1

Contact

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Use of Languages

Principal working language: catalan (cat)
Some groups entirely in English: No
Some groups entirely in Catalan: Yes
Some groups entirely in Spanish: No

Teachers

Carles Jaime Cardiel
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Prerequisites

It is recommended to have passed and passed the 2nd year subjects "Chemistry of the Elements", "Organic Chemistry" and "Thermodynamics, Kinetics and Phase Transformations"

Although the classes are in Catalan, much of the material that the student will have to work as well as the main bibliographic sources are written in English. Therefore, good knowledge of this language is recommended.

Objectives and Contextualisation

In this subject, the students will learn the basis of in Supramolecular Chemistry, which will allows them to recognize molecular recognition phenomena from a chemical point of view and to understand the processes involved in the formation of self-assembled supramolecular structures.

The specific objectives of this subject are:

· To introduce the concept of Supramolecular Chemistry, to study the chemical interactions on which it is based and know the main methods of characterization and manipulation of the supramolecular complexes.

· To apply the basics of Supramolecular Chemistry to the understanding of the processes of molecular recognition both at a chemical and biological level.

· To use the basics of Supramolecular Chemistry to interpret the formation of self-assembled supramolecular structures.

Competences

- Adapt to new situations.
- Apply the concepts, principles, theories and fundamental facts of nanoscience and nanotechnology to solve problems of a quantitative or qualitative nature in the field of nanoscience and nanotechnology.
- Apply the general standards for safety and operations in a laboratory and the specific regulations for the use of chemical and biological instruments, products and materials in consideration of their properties and the risks.
- Communicate clearly in English.
- Communicate orally and in writing in ones own language.
- Demonstrate knowledge of the concepts, principles, theories and fundamental facts related with nanoscience and nanotechnology.
- Handle the standard instruments and materials of physical, chemical and biological testing laboratories for the study and analysis of phenomena on a nanoscale.
- Interpret the data obtained by means of experimental measures, including the use of computer tools, identify and understand their meanings in relation to appropriate chemical, physical or biological theories.
- Learn autonomously.
- Manage the organisation and planning of tasks.
- Obtain, manage, analyse, synthesise and present information, including the use of digital and computerised media.
- Operate with a certain degree of autonomy.
- Propose creative ideas and solutions.
- Reason in a critical manner
- Recognise and analyse physical, chemical and biological problems in the field of nanoscience and nanotechnology and propose answers or suitable studies for their resolution, including when necessary the use of bibliographic sources.
- Recognise the terms used in the fields of physics, chemistry, biology, nanoscience and nanotechnology in the English language and use English effectively in writing and orally in all areas of work.
- Resolve problems and make decisions.
- Show sensitivity for environmental issues.
- Work correctly with the formulas, chemical equations and magnitudes used in chemistry.
- Work on the synthesis, characterisation and study of the properties of materials on a nanoscale from previously established procedures.

Learning Outcomes

1. Adapt to new situations.
2. Apply the acquired theoretical contents to the explanation of experimental phenomena.
3. Communicate clearly in English.
4. Communicate orally and in writing in ones own language.
5. Correctly handle standard instruments and materials of physics and chemistry laboratories in nanoscience and nanotechnology.
6. Correctly observe protocols for using instrumentation, reagents and chemical waste in laboratories related to the subject.
7. Critically evaluate experimental results and deduce their meaning.
8. Describe the basics of self-assembly and recognise self-assembly in amphiphilic molecules.
9. Describe the concept of solubility and the variables that affect it.
10. Describe the recognition processes of ions and molecules.
11. Design simple supramolecular entities.
12. Distinguish the different methods for characterising supramolecular complexes.
13. Draft and present reports on the subject in English.

14. Identify supramolecular interactions and the most characteristic molecular recognition processes in biological systems.
15. Interpret and rationalise the results obtained in the laboratory in processes related with physics and chemistry in nanoscience and nanotechnology.
16. Interpret texts in English on aspects related with the physics and chemistry of nanoscience and nanotechnology.
17. Learn autonomously.
18. Manage the organisation and planning of tasks.
19. Obtain, manage, analyse, synthesise and present information, including the use of digital and computerised media.
20. Operate with a certain degree of autonomy.
21. Perform bibliographic searches for scientific documents.
22. Perform studies to characterise the electronic, thermal, optical, magnetic and mechanical properties of nanomaterials
23. Perform synthesis, separation and basic analysis procedures in a nanoscience and nanotechnology laboratory
24. Predict the supramolecular interactions of organic molecules and in biological systems
25. Propose creative ideas and solutions.
26. Rationalise the results obtained in the laboratory in terms of physical magnitudes and their relation with the observed physical phenomena.
27. Reason in a critical manner
28. Recognise supramolecular entities formed by self-assembly of amphiphilic molecules (micelles, vesicles or membranes)
29. Recognise the risks for the health and environment associated with the manipulation of chemicals and material compounds in general.
30. Recognise the terms used in topics related to nanoscience, nanotechnology and society.
31. Resolve problems and make decisions.
32. Resolve problems with the help of the provided complementary bibliography.
33. Show sensitivity for environmental issues.
34. Work correctly with the formulas, chemical equations and magnitudes used in chemistry.

Content

1. Introduction to Supramolecular Chemistry.

Supramolecular systems. Supra molecular forces (van der Waals, hydrogen, ion-ion, ion-dipole, dipole-dipole, ion-π, π-π, hydrophobic). Relationship between strength and directionality. Coordination chemistry: metallic centers and ligands. Basic concepts in supramolecular chemistry: host-guest systems and self-assembling; association constants and selectivity; complementarity, preorganization and cooperativity.

2. Characterization and manipulation of supramolecular systems.

X-ray diffraction. Mass spectrometry. Spectroscopic techniques (UV-vis, IR, NMR). Electrochemical techniques. Electrochemical and photochemical manipulation of supramolecular systems.

3. Complexation and molecular recognition.

Recognition of cations, anions and neutral molecules. Association constants. Stoichiometry. Applications.

4. Self-assembly and self-organization.

Concept of self-assembly and self-organization. Self-assembling based on intermolecular interactions (amphiphilic molecules). Self-assembling based on coordination in metal centers (helicates, racks, ladders, grids). Mechanical self-assembling (rotaxanes, catenanes, knots).

5. Supramolecular interactions and molecular recognition in biological systems. Biological structures and processes based on supramolecular interactions: nucleotides and DNA; peptides and proteins; lipids and membranes; virus.

LAB EXPERIMENTS

Experiment 1. Determination of critical micelle concentration by means of conductivity measurements

Experiment 2. Characterization of the inclusion complex between cyclodextrin and phenolphthalein by means of UV-vis spectroscopy

Experiment 3. Synthesis and characterization of an anion-binding host

Methodology

Students will have to develop different types of activities throughout this course:

a) Guided activities: Theoretical classes and exercises will be held in the classroom. On the other hand, students will also carry out laboratory experiments consisting of the synthesis and / or characterization of supramolecular systems.
All the materials needed for these activities will be found in the space of the course on the Virtual Campus.

b) Supervised activities: Tutorial classes would be done in order to monitor one of the assessment activities that students must work on, which consists in reading, understanding and writing a scientific article related to the subject.

c) Autonomous activities: Students will have to study the contents of the course, solve problems, prepare laboratory experiments, summarize and present a scientific article.

Activities

Title	Hours	ECTS	Learning Outcomes
Type: Directed			
Laboratory teaching	14	0.56	1, 17, 4, 23, 18, 15, 16, 5, 33, 20, 25, 26, 27, 22, 29, 31, 34, 6
Problems and Exercices	8	0.32	1, 2, 7, 4, 9, 8, 10, 11, 12, 14, 16, 24, 25, 27, 28, 13, 32, 34
Theoretical classes	22	0.88	2, 7, 9, 8, 10, 11, 12, 14, 16, 19, 24, 27, 28
Type: Supervised			
Tutorial classes	1	0.04	4, 21, 18, 16, 19, 31, 34
Type: Autonomous			
Exercices	14	0.56	1, 2, 17, 7, 11, 21, 18, 14, 16, 20, 24, 25, 27, 28, 32, 31
Laboratory	25	1	2, 17, 7, 12, 21, 18, 14, 16, 19, 20, 24, 25, 27, 28, 13, 34
Preparation of laboratory experiments	2.75	0.11	18, 16, 33, 19, 20, 29
Self study	33	1.32	17, 9, 8, 10, 11, 12, 18, 14, 16, 19, 20, 24, 27, 28

Assessment

The evaluation of the students will be realized by means of several evidences:

Written exams: There will be two midterm exams throughout the course, one in the middle and the other at the end of the semester.
Each of these exams will have a weight of 35% on the final grade. If the average mark of these two exams is less than 5,
a final exam will be required at the end of the semester (as long as 2/3 assessment tasks have been passed), which will include the contents of the whole course, and the mark will equal 70% of the total (i will replace the partial exams).
In order to do the final exam the student will have to appear in both partial sessions. Students who want to improve
their mark may also be present at the final exam; If the mark of this exam is greater than the average of the two partial exams,
then the final exam will equal 70% of the final. Otherwise, the exam grades will correspond to the average of the partial exam
grades and the final exam mark.

Laboratory: Laboratory experiments will be evaluated by carrying out a small written test at the end of the last practice session,
which will be equal to 10% of the final mark of the subject.

Written work on a scientific article: The students will be distributed in groups of 3-5 students
and each of these groups will be assigned a subject related to the contents of the subject.
Students will have to look for a scientific article focused on this topic, read it, analyze it and prepare a presentation
in the English language that will be evaluated. This activity will have a weight of 20% on the final grade of the subject.

In order to pass the subject, students must have:

1) An average grade of exams exceeding 5.

2) An average grade over 5.

3) Have attended the three practice sessions in the laboratory. In the event of having completedless than one third of the evaluable evidence
of the course and / or having failed in an unjustified manner in any of the practice sessions in the laboratory, the students will be evaluated as "not presented".

Assessment Activities

Title	Weighting	Hours	ECTS	Learning Outcomes
Laboratory	10	0.25	0.01	1, 2, 17, 7, 3, 4, 11, 21, 18, 14, 16, 19, 20, 24, 25, 27, 30, 28, 13, 32, 31, 34
Presentation of a scientific paper	20	2	0.08	1, 17, 4, 23, 18, 15, 16, 5, 33, 20, 25, 26, 27, 22, 29, 30, 31, 34, 6
Writting Exams	70%	3	0.12	1, 2, 7, 4, 9, 8, 10, 11, 12, 14, 20, 24, 25, 27, 30, 28, 32, 31

Bibliography

- J.W. Steed, D.R. Turner, K. Wallace, *Core Concepts in Supramolecular Chemistry and Nanochemistry* , Wiley, Chichester, 2007.
- P.D. Beer, P.A. Gale, D.K. Smith, *Supramolecular Chemistry*, Oxford University Press (Oxford Chemistry Primers), New York, 1999.
- J.W. Steed, P.A. Gale, *Supramolecular Chemistry: from Molecules to Nanomaterials*, Wiley, Chichester, 2012.