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Faculty XXX

GENERAL SPECIFICATIONS

Subject Data

Name:
MÉTODOS ESTRUCTURALES EN QUÍMICA INORGÁNICA
English name:
STRUCTURAL METHODS IN INORGANIC CHEMISTRY

Code:	**Type:**
757509218	COMPULSORY

Hours:

	Total	**In class**	**Out class**
Time distribution	150	60	90

ECTS:

Standard group	**Small groups**			
	Classroom	**Lab**	**Practices**	**Computer classroom**
4.5	0	1.5	0	0

Departments:	**Knowledge areas:**
CHEMISTRY	INORGANIC CHEMISTRY
Year:	**Semester**
2023/24	FIRST

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TEACHING STAFF

Name:	E-mail:	Telephone
TOMÁS RODRÍGUEZ BELDERRAIN	trodri@dqcm.uhu.es	959219955

Others Data (Tutoring, schedule...)

Office Location: Research Center in Sustainable Chemistry (CIQSO) Robert H. Grubbs Building Second floor

HOUR	MONDAY	TUESDAY	WEDNESDAY	THURSDAY	FRIDAY
9:00-10:00	SMIC	SMIC	SMIC		
10:00-11:00					
11:00-12:00					
12:00-13:00					
13:00-14:00					
15:00-16:00					
16:00-17:00					
17:00-18:00			Tutorial	Tutorial	Tutorial
18:00-19:00			Tutorial	Tutorial	Tutorial

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SPECIFIC INFORMATION OF THE COURSE

1. Contents description:

1.1 In English:

This subject provides the student a fundamental knowledge about structural characterization of inorganic compounds and the application of different spectroscopic methods commonly used in Inorganic Chemistry.

1.2 In Spanish:

Esta asignatura proporciona al alumno un conocimiento fundamental sobre la caracterización estructural de compuestos inorgánicos y la aplicación de diferentes métodos espectroscópicos comúnmente utilizados en Química Inorgánica.

2. Background:

2.1 Situation within the Degree:

FOURTH YEAR

2.2 Recommendations

In order to join this course, it is highly recommended to have previously passed all the previous years subjects of Inorganic Chemistry, as well as "Structural Determination of Organic Compounds"

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3. Objectives (as result of teaching, or skills or abilities and knowledge):

The subject has been designed by a practical approach in order to provide the student a solid formation on the experimental methods of structural determination and their uses, which is essential for the formation of a Graduate in Chemistry.

4. Skills to be acquired

4.1 Specific Skills:

This subject will develop the knowledge that the student has previously acquired on the structural determination of chemical compounds.

4.2 General, Basic or Transversal Skills:

GENERAL SKILLS
CG1 - To develop and demonstrate learning skills and knowledge from their field of study, being able to apply them in their work, interpreting relevant data to make judgments on topics of various kinds, being able to transmit them to both a specialized and non-specialized audience.
SPECIFIC SKILLS
C2 - To know the main types of reactions and the main characteristics associated with each of them.
C4 – To know the main structural research techniques, including spectroscopy.
C10 – To know the structural aspects of chemical elements and their compounds, including stereochemistry.
C16 – To know the instrumental techniques and their applications.
Q1 - To show knowledge and understanding of essential facts, concepts, principles and theories related to chemistry.
Q2 – To apply the knowledge to the resolution of qualitative and quantitative problems according to models previously developed.
Q3 – To evaluate, interpret and synthesize chemical data and information.
Q4 – To recognize and carry out good practices in scientific and professional work.
Q6 – To handle and process, by computer, the chemical data and information.
P1 - To safely handle chemical materials, taking into account their physical and chemical properties, including any specific hazards associated with its use.
P2 - To carry out standard laboratory procedures involved in analytical and synthetic work, in relation with organic and inorganic systems.
P4 – To handle standard chemical instrumentation
P5 – To interpret data from observations and measurements in the laboratory in terms of their significance.

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5. Training Activities and Teaching Methods
5.1 Training Activities:
The course includes both lectures sessions in the classroom and practical in the laboratory, during which exercises are carried out on the topics covered in the theoretical lessons.

5.2 Teaching Methods::
Master classes related to the theoretical and practical contents (problems) of the subject, using teaching resources such as slides, computerized presentations and videos. The practical laboratory classes (compulsory attendance) will be aimed at the student acquiring skills in the developing their deductive, communicative, teamwork and analytical skills. Tutored seminars on problem solving and practical cases. Test and resolution of theoretical-practical questions. Self-assessment exercises on the contents of the subject.
5.3 Development and Justification:
The knowledge acquired in each unit will be evaluated by the different activities of the subject: the theoretical exam, laboratory work and the academic activities, which help to make a continuous evaluation of the student.

6. Detailed Contents

Unit 1. Determining Structures. How and why?. Introduction to Spectroscopy: The electromagnetic spectrum. Interaction of matter with electromagnetic radiation: General characteristics. Time scales. Selection rules.The absorption and emission spectra. Spectrometers and Resolution.
Unit 2. Electronic Spectroscopy. Basic Concepts. The technique: ultraviolet-visible spectrophotometry. Spectrophotometers. Cells. Spectrophotometric method. Electronic spectra. Overview. Ligand field transitions. Orgel diagrams. Tanabe-Sugano diagrams. Selection rules. Charge transfer bands.
Unit 3. Vibrational Spectroscopy. Introduction: Molecular vibrations. IR and Raman spectrophotometers. Selection rules.
Symmetry and vibrational spectroscopy. Frequency of functional groups and ligands.
Unit 4. The Basics of NMR (I). Atomic nucleus and nuclear spin. Magnetic alignment. Transitions. Sensitivity. The origin of the NMR signal. The precession of the nuclear spin. System perturbation. Detection of the NMR signal. Pulse sequence. Free Induction Decay (FID). Signal/noise ratio. NMR spectrometers: CW spectrometers and FT-NMR spectrometers.
Unit 5. The Basics of NMR (II). Scalar coupling. Types of scalar coupling. First order systems. Spin decoupling. Examples with heteronuclei. Chemical and magnetic equivalence. Second order systems. Coupling constants. Carbon -13 NMR.
Unit 6. Two Dimensions Nuclear Magnetic Resonance (2D NMR). 2D experiments. Introduction. Representation of 2D NMR spectra. Types of 2D NMR experiments: COSY, TOCSY, HETCOR, HSQC, HMQC and HMBC, INADEQUATE, 2DJ Experiments. The "NOE" effect. 2D Experiments based in the NOE effect: NOESY.
Unit 7. Dynamic NMR Spectroscopy. Dynamic Process Exchange. Fluxionality. Variable temperature spectra. The Eyring equation. Examples.
Unit 8. Relaxation and NMR of nuclei with I> 1/2. Relaxation Phenomena. T1 and T2. Measurement of T1. Metal hydrides. NMR of nuclei with I> 1/2. Spin coupling.
Unit 9. Electronic Spin Resonance. Basics of ESR. Proportionality factor. Hyperfine interaction. Relative intensity. Examples. Summary
Unit 10. Practical Examples.

7. Bibliography

7.1 Basic Bibliography:

1) E. A. V. EBSWORTH, D. W. H. RANKIN, S. CRADOCK, "Structural Methodsin Inorganic Chemistry", Blackwell Scientific Publications, 1987.
2) D. W. H. Rankin, Norbert Mitzel, Carole Morrison "Structural Methods inMolecularInorganic Chemistry" Wiley; 1 edition
(April 1, 2013)
3) R. Macomber "A Complete Introduction to Modern NMR Spectroscopy JohnWiley & Sons Inc (Jan 8, 1998)
4) J. W. AKITT, "NMR and Chemistry", 2nd Ed., Chapman and Hall, 1983.
5) A. K. Brisdon "Inorganic Spectroscopic Methods (Oxford Chemistry Primers)"Oxford University Press (Jun 18, 1998)
6) Housecroft, Catherine, "Inorganic Chemistry" Oxford University Press, 1999.ISBN:0-19-850103-X
7) "Inorganic Chemistry, 5th ed.", Duward F. Shriver, Peter W. Atkins, Tina Overton, Jonathan Rourke; W. H. Freeman, 2009
8) Joseph P. Hornak, "The Basics of NMR" https://www.cis.rit.edu/htbooks/nmr/bnmr.htm.

7.2 Additional Bibliography:
Paul Callaghan lectures on the principles of NMR and MRI: http://www.magritek.com/support/videos/ Introduction to NMR Spectroscopy https://www.youtube.com/watch?v=TJhVotrZt9I Organometallic HyperTextBook http://www.ilpi.com/organomet/

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8. Systems and Assessment Criteria

8.1 System for Assessment:

Final exam
Laboratory classes
Other activities (exercises, questionnaires ...).

8.2 Assessment Criteria and Marks:

8.2.1 Examinations Convocatory I

The grades will have the following relative value:
- 70% will correspond to the mark obtained in the final exam. The exam will consist of theoretical-practical questions and problems. If the student chooses to make the partial exam, a minimum mark of 5 must be obtained in order to be evaluated just of the second part of the subject in the final exam. If the student does not pass the partial exam, he/she will be examined about the contents of the entire program. The final exam will be divided in two blocks: the first part of the subject corresponding to the partial exam, and the second to the rest of the program. It will be necessary to obtain a minimum of 5 points in each of the parts each part to be able to make the average grade, otherwise way, the global grade will be "fail". In the case that both parts are above 5 points, the exam grade will be the result of the both marks average, and it will represent 70% of the final grade of the subject.
- 20% will correspond to the mark of the laboratory work. Attendance at practical laboratory classes is mandatory. The day of the final exam, a test about the laboratory will be carried out, which will correspond to 20% of the total grade. This number will only be added to the total if a mark of 5 is achieved in the previous block.
- 10% will correspond to the grade of the other activities (exercises, questionnaires ...). This mark will be only will added to the total grade if a mark of 5 is achieved in the final exam.

8.2.2 Examinations Convocatory II

The grades will have the following relative value:
-80% will correspond to the mark obtained in the exam. The exam will consist of theoretical-practical questions and problems.
- 20% will correspond to the mark of the laboratory test. The mark will only be added to the total if a 5 is achieved in the theoretical exam.

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8.2.3 Examinations Convocatory III
The grades will have the following relative value: -80% will correspond to the mark obtained in the exam. The exam will consist of theoretical-practical questions and problems. - 20% will correspond to the mark of the laboratory test. The mark will only be added to the total if a 5 is achieved in the theoretical exam.

8.2.4 Extraordinary Convocatory

The grades will have the following relative value:
-80% will correspond to the mark obtained in the exam. The exam will consist of theoretical-practical questions and problems.
- 20% will correspond to the mark of the laboratory test. The mark will only be added to the total if a 5 is achieved in the theoretical exam.

8.3 Single Final Evaluation:

The student must communicate to the professor, within the period established by the evaluation regulations, his willingness to be evaluated by the single evaluation method, filling the request that the Faculty or the professor himself will send him. Once the corresponding documentation is delivered, the student will be able to be evaluated by this system. The remaining 20% will be obtained from a practical test. The grade obtained in the final exam of the subject will account for 80% of the grade for the subject. The exam will consist of theoretical-practical questions and problems

9. Indicative weekly teaching organization:

Date	Large groups	Small Group	Evaluable tests and/or activities	Content
		Laboratory		
Week Sept 11	3	0	Face-to-face classes related to the theoretical and practical contents (problems) of the subject, using didactic resources such as presentations and videos.	Units 1 and 2
Week Sept 18	3	0		Unit 2
Week Sept 25	3	0		Unit 2
Week Oct 2	3	0		Unit 3
Week Oct 9	3	0		Units 3 and 4
Week Oct 16	3	0		Unit 4
Week Oct 23	3	0		Units 4 and 5
Week Oct 30	3	0		Unit 5
Week Nov 6	3	0		Unit 6
Week Nov 13	3	0		Unit 7

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Week Nov 20	3	0		Units 7 and 8
Week Nov 27	3	0		Unit 8
Week Dec 4	3	0		Unit 8
Week Dec 11	3	0		Units 8 and 9
Week Dec 18	3	15 (5 x 3 days)		Unit 9 and lab
TOTAL	**45**	**15**		