COURSE DESCRIPTION

COURSE DETAILS

Title (of the course): **AMPLIACIÓN DE QUÍMICA INORGÁNICA**
Code: 100457
Degree/Master: **GRADO DE QUÍMICA** Year: 3
Name of the module to which it belongs: FUNDAMENTAL
Field: QUÍMICA INORGÁNICA
Character: OBLIGATORIA Duration: FIRST TERM
ECTS Credits: 6 Classroom hours: 60
Face-to-face classroom percentage: 40% Study hours: 90
Online platform: http://www.uco.es/moodle

LECTURER INFORMATION

Name: TIRADO COELLO, JOSE LUIS (Coordinator)
Department: QUÍMICA INORGÁNICA E INGENIERÍA QUÍMICA
Area: QUÍMICA INORGÁNICA
Office location: Edificio Marie Curie, primera planta
E-Mail: iq1ticoj@uco.es Phone: 957218637
URL web: www.uco.es/moodle

Name: ORTIZ JIMÉNEZ, GREGORIO FCO
Department: QUÍMICA INORGÁNICA E INGENIERÍA QUÍMICA
Area: QUÍMICA INORGÁNICA
Office location: Edificio Marie Curie, primera planta
E-Mail: q72maorg@uco.es Phone: 957218663
URL web: www.uco.es/moodle

PREREQUISITES AND RECOMMENDATIONS

Prerequisites established in the study plan

None specified.

Recommendations

The English language level must be at least B1.

INTENDED LEARNING OUTCOMES

CB4	Knowledge of a foreign language
CB6	Problem solving
CB10	Ability to study independently for continued professional development.
CE3	Principles and proceedures used in chemical analysis and in the characterisation of chemical compounds.
CE4	The main structural investigation techniques, including spectroscopy.
CE10	Structural aspects of chemical elements and their compounds, including stereochemistry
CE20	Study, properties and applications of the materials
CE21	The ability to show knowledge and understanding of the essential facts, concepts, principles, and theories relating to chemistry
CE22	The ability to apply knowledge to solve qualitative and quantitative problems according to previously developed models
CE23	Competency to evaluate, interpret and summarise Chemical data and information.
CE24	Ability to recognise and carry out good scientific practices.

COURSE DESCRIPTION

CE28	Ability to carry out standard laboratory procedures involved in analytical and concise work in relation with organic and inorganic systems.
CE31	Interpretation of data from previous observations and measurements in the laboratory in terms of their significance and the theories that support them

OBJECTIVES

- To understand and to know how to apply the experimental techniques commonly used in the structural determination of inorganic compounds.
- To acquire knowledge on the bonding, structure, reactivity and properties of inorganic solids.

CONTENT

1. Theory contents

Section 1. Experimental methods for determining the structure of inorganic compounds
Lesson 1. Theory of symmetry point groups. Operations, representations and character tables. Transformation of reducible representations into irreducible. The direct product. Application of the group theory to study vibrational spectroscopy. Symmetry of the normal modes. Fundamental levels and transitions. Selection rules in IR and Raman spectroscopies.
Lesson 2. Nuclear magnetic resonance (NMR) spectroscopy. Nuclear spin levels in the presence of a magnetic field. Resonance condition and instrumentation. Dynamic aspects. Applications to structural studies of inorganic molecules. Solid-state NMR. Magic angle spinning. Applications to the study of inorganic solids.
Lesson 3. Photoelectron spectroscopy. Instrumentation and radiation used. Auger spectroscopy. Calibration. Chemical information obtained. Intensity of photoelectrons. Study of the core levels. Chemical shift. Satellites and spin-orbit coupling. Studies of valence energy levels. Fine structure of the spectra.
Lesson 4. Crystal Systems. Bravais lattices. The 32 crystallographic point groups. Space group symmetry. Symmorphic and nonsymmorphic groups. International Tables of Crystallography. X-ray diffraction. Single crystal methods. The powder method. Structural determinations by powder X-ray and neutron diffraction. Rietveld refinement.
Lesson 5. Microscopy techniques. The transmission electron microscope. Sample Preparation. Fundamentals of image formation and interpretation. High-resolution electron microscopy. Electron diffraction. Scanning tunneling microscopy: instrumental and applications. Atomic force microscopy. AFM modes.
Section 2. Inorganic Solids
Lesson 6. Description and prediction of crystal structures based on packing of spheres. Close packed structures. Related structures: substitutions, interstitial positions, distortions and complex ions. Coordination polyhedra and connectivity. Relations with the crystallographic description.
Lesson 7. Bonding-structure relations. Ionic solids. Pauling postulates. Bond directionality. Mooser-Pearson diagrams. The equation of Phillips and Van Vechten. Covalent solids and dimensionality. Glasses: Zachariasen rules. Metals. Band theory and structures. Molecular solids: Kitaigorodskii theory. Hydrogen bonds and crystal structure. Water in crystals: Baur theory.
Lesson 8. Defects in solids. point defects. Thermodynamics of Shottky and Frenkel defects. Unidimensional defects: Edge and screw dislocations. The Burgers vector. Dislocation density. Two-dimensional defects: phase boundaries. High-angle and low-angle grain boundaries. Stacking faults. Three-dimensional defects: inclusions and pores. Nonstoichiometric solid. Vacancies and interstices. Defect assimilation: vacancies and clusters. Defects elimination: Crystallographic shear structures. Misfit structures.
Lesson 9. Reactivity and synthesis of solids. Phase diagrams and phase rule. Reconstructive or displacive polymorphic transformations. Solid-solid reactions. Interdiffusion. Kirkendall effect. Solid-gas reactions. Oxidation. Thermal decomposition.
Lesson 10. Properties of inorganic solids. Mechanical properties. Hardness and microstructure. Magnetic properties: Ferro-, ferri- and antiferro-magnetism. Curie-Weiss and Neel laws. Electrical properties. Superconductors. Optical properties. Solid-state laser.

2. Practical contents

There will be a collection of exercises and problems in units related to the theoretical content, discussion and resolution being the basis of Guided Activities included in section Seminars. Three hours in total, 2 h of problems and 1 h tutorials will be ascribed to each unit.
The summary of the contents of these units is the following:
- Symmetry elements of and point groups
- Character Tables and IR and Raman spectroscopy
- NMR and XPS
- Space Groups
- X-ray diffraction
- Visit and use of large scientific instruments
- Bonding-structure relationships
- Defects in solids
- Reactivity and properties of solids

COURSE DESCRIPTION

METHODOLOGY

General clarifications on the methodology. (optional)

The goal of the lectures is the presentation to the students of the different theoretical contents specified in the course syllabus, which is included in this Teaching Guide. The presentations contain a series of knowledge adequately structured to constitute the basis for further study of each of the topics of the syllabus. This lecture tool is not intended to establish fixed limits for each subject or a unique development of its contents. Rather, it should enhance and facilitate the subsequent work of the student, indicating the main lines to follow in understanding the subject matter and showing the most important connections between the different lessons on the agenda. Additionally, an important contribution of the lectures should be pointing to the most useful literature for each of the program sections. The use of ancillary techniques in the exhibition, videos and dimensional models of molecules and crystal lattices, will be very useful to facilitate understanding.
Classes dedicated to practical contents involve the development of seminar activities and tutorials. The seminar will overcome the limitations inherent to the lectures, being able to develop a new and more interactive approach to the subject under study. In addition, specific details not included in the lectures in order to not obscure the fundamental principles that must be transmitted, can be examined in more detail in the seminars. The application of the basic principles to a wide range of real problems will also be developed. Moreover, tutoring students is a great opportunity to answer those questions that have not been solved based on the literature assigned to the subject, through direct contact with the teacher.

Methodological adaptations for part-time students and students with disabilities and special educational needs

Methodological adaptations for students to follow part-time shall be conducted in accordance with the regulations of the center and the casuistry of students.
The criteria for students of second and subsequent enrollment in relation to practical activities and assessment methodology are the same as for students of first registration.

Face-to-face activities

Activity	Large group	Medium group	Total
Assessment activities	5	-	*5*
Lectures	28	-	*28*
Seminar	-	18	*18*
Tutorials	-	9	*9*
Total hours:	***33***	***27***	***60***

Off-site activities

Activity	Total
Activities	*15*
Exercises	*15*
Information search	*10*
Reference search	*10*
Self-study	*40*
Total hours:	**90**

WORK MATERIALS FOR STUDENTS

Dossier
Exercises and activities
Coursebook

Clarifications:

The e-learning platform will contain the teaching guide, as well as detailed information on theory topics, presentations, links to Interest, exercises and problems and their solutions, and results of evaluation tests. It will also be a valuable communication tool between students and professors.

COURSE DESCRIPTION

EVALUATION

Intended learnig outcomes	Tools		
	Oral tests	Problem solving	Short answer tests
CB10	x		
CB4		x	x
CB6			x
CE10	x	x	
CE20	x		x
CE21		x	x
CE22	x	x	x
CE23		x	
CE24	x		x
CE28	x		x
CE3	x		x
CE31	x	x	x
CE4		x	
Total (100%)	**20%**	**20%**	**60%**
Minimum grade.(*)	**4**	**4**	**4**

(*) Minimum grade necessary to pass the course

Method of assessment of attendance:

Participación activa en seminarios y problemas = 1.

General clarifications on instruments for evaluation:
The whole group will be evaluated by grading Continuous Evaluations Tests (CET) and final exam, which include a short-answers exam (60% of the final grade), and problem solving (20%). The practice lessons group will also be assessed continually by grading attendance (10%) and oral tests (10%) in seminar sessions.
To achieve this latter aspect, the following rubric will be used:
Participation
Advanced: The student offers himself voluntarily to solve the exercise on the board.
Proficient: The student participates when prompted by the teacher.
Unsatisfactory: The student offers resistance to participate in the seminar.
Behavior
Advanced: The student shows interest and actively involves in the seminar.
Proficient: The student remains silent; he shows interest but does not participate.
Unsatisfactory: The student is absent and / or annoying to the seminar.
Development Exercise
Advanced: The student clearly set out the exercise.
Proficient: The student is limited to writing the result mechanically.
Unsatisfactory: Student doubts and babbles during the course of the exercise.
Validity of results
Advanced: The student reaches the correct result.
Proficient: The student needs a little help, but correctly solves the exercise.
Unsatisfactory: The student does not complete the exercise and / or reaches incorrect results.
Discussion
Advanced: The student responds decisively to the questions put to him.
Proficient: The student doubts, but finally responds appropriately.
Unsatisfactory: The student does not know how to answer the questions.

COURSE DESCRIPTION

Clarifications on the methodology for part-time students and students with disabilities and special educational needs:
Adaptations assessment for students to follow part-time shall be conducted in accordance with the regulations of the center and the casuistry of students.
The criteria for students of second and subsequent enrollment in relation to practical activities and assessment methodology are the same as for students of first registration.

Qualifying criteria for obtaining honors: *Según normativa de la UCO*

BIBLIOGRAPHY

1. Basic Bibliography:

Adams, D.M. Sólidos inorgánicos: introducción a los conceptos de la química estructural en estado sólido, Alhambra, (1986).
Callister, W.D. Introducción a la ciencia e ingeniería de los materiales, Reverté (2007).
Cotton, F.A. La teoría de grupos aplicada a la química. Limusa Mexico (1991).
Housecroft, C.E. Química Inorgánica. Pearson-Prentice Hall (2006).
Shriver, D.F., Atkins, P.W. y C.H. Langford Química Inorgánica. Reverté (2004).

2. Further reading:

Akitt, J.W. NMR and Chemistry. Chapman. N.Y: (1992).
Bermudez Polonio, J. Métodos de difracción de rayos X. Ciencia y Técnica (1981).
Burns, G. y Glazer A.M. Space gropups for solid state scientists. Academic (1978).
Cox, P.A., The Electronic Structure and Chemistry of Solids. Oxford Univ. Press. Oxford. (1987).
Drago, R.S. Physical methods for Chemists. Saunders N.Y. (1992).
Hull, D. Introduction to Dislocations. Pergamon. N.Y. (1975).
Hyde, B.G. y Andersson, S. Inorganic Crystal Structures. Wiley. N.Y. (1989).
OKeefe, M. y Navrotsky, A. (eds.). Structure and Bonding in Crystals. Academic. N.Y. (1981).
Rao, C.N.R. y Gopalakrishnan, J. New directions in solid state chemistry. Cambridge Univ. Press. Londres (1986).
Schmalzried, H. Solid State Reactions. Verlag. N.Y. (1971).
Tilley, R.J.D. Defect Crystal Chemistry. Blackie. N.Y. (1987).
Tilley, R. Understanding Solids. Wiley, N.Y. (2004).
Wells, A.F. Structural Inorganic Chemistry. Clarendon. Oxford. (1975). 4 ed.
West, A.R. Solid State Chemistry and Its Applications. Wiley. N.Y. (1984).

COORDINATION CRITERIA

- Tasks performance

Clarifications:

Visit to advanced instrumental techniques (SCAI)

COURSE DESCRIPTION

SCHEDULE

Period	Activity			
	Assessment activities	Lectures	Seminar	Tutorials
1# Week	0	2	0	0
2# Week	0	2	0	0
3# Week	0	2	2	1
4# Week	0	2	2	1
6# Week	0	2	2	1
7# Week	0	2	0	0
8# Week	2	2	0	0
9# Week	0	2	2	1
10# Week	0	2	2	1
11# Week	0	2	2	1
12# Week	2	2	2	1
13# Week	0	2	0	0
14# Week	0	2	2	1
15# Week	1	2	2	1
Total hours:	***5***	***28***	***18***	***9***

The methodological strategies and the evaluation system contemplated in this Course Description will be adapted according to the needs presented by students with disabilities and special educational needs in the cases that are required.