DETAILS OF THE SUBJECT

Title: 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% **Non-contact hours:** 90
Online platform: http://www.uco.es/moodle

TEACHER INFORMATION

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SPECIFICS OF THE SUBJECT

REQUIREMENTS AND RECOMMENDATIONS

Prerequisites established in the study plan

None.

Recommendations

None specified.

SKILLS

CB4
CB6
CB10
CE3
CE4
CE10
CE20
CE21
CE22
CE23
CE24
CE28
CE31

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. Theoretical content

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 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

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

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*

Not on-site activities

Actividad	Total
Bibliographic consultations	*10*
Exercises	*15*
Finding information	*10*
Problems	*15*
Self-study	*40*
Total hours:	90

WORK MATERIALS FOR STUDENTS

Dossier
Exercises and problems
Manual of the subject

Clarifications:

La plataforma e-learning contendrá la guía docente, así como información detallada sobre los temas de teoría, presentaciones, enlaces a páginas de interés, ejercicios y problemas y sus soluciones, y resultados de las pruebas de evaluación. Así mismo, será una herramienta valiosa de comunicación entre alumnos y profesorado.

EVALUATION

Skills	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 subject

What is the weight of the attendace in the final grade ?:

Active attendance in seminars problems = 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.

General clarifications on evaluation and methodological adaptation for part-time students:

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*

Aclaraciones generales sobre las evaluaciones parciales, calificación mínima para eliminar materia y período de validez:

General clarification of the partial evaluations, to remove material and minimum period of validity rating:

Three Continuous Evaluation Tests (CET) of certain groups of subjects of theory and seminars related problems will be carried out through the term:

CET1: Items 1 and 2

CET2: Issues 3-5

CET3: Issues 6-8

Students who pass some of these CET need not being reconsidered for those parts at the end of the course in January.

The examination of the teaching unit in January must be done by all students to grade lessons 9 and 10 and any CET that was not passed.

The following calls will have a single agenda for items 1 to 10 for all participants.

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

- Performing activities

Clarifications:

Visit to advanced instrumental techniques (SCAI)

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	0	0
5# Week	0	0	2	1
6# Week	0	2	2	1
7# Week	0	2	2	1
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	0	0
13# Week	0	2	2	1
14# Week	0	2	2	1
15# Week	1	2	0	0
Total hours:	*5*	*28*	*18*	*9*