ΠΕΡΙΓΡΑΜΜΑ ΜΑΘΗΜΑΤΟΣ

(1) General Information

School	Science		
DEPARTMENT	CHEMISTRY		
DEGREE	MASTER		
COURSE CODE	**18A4**	**SEMESTER**	**Winter**
COURSE TITLE	**Inorganic Synthesis and Analysis**		

INDEPENDENT TEACHING ACTIVITIES *in the case that the credits are awarded to separate parts of the course e.g. Lectures, Laboratory Exercises, etc. If the credits are awarded uniformly for the entire course, enter the weekly teaching hours and total credits*	**TEACHING HOURS PER WEEK**	**CREDITS**
Theory	6	8
Add lines if necessary. The teaching organization and methods used are described in detail in (d).		

COURSE TYPE *general background, special background, general knowledge specialization, skill development*	GENERAL BACKGROUND, GENERAL KNOWLEDGE SPECIALISATION
PREREQUISITE COURSES:	INORGANIC CHEMISTRY III
COURSE AND EXAM LANGUAGE:	GREEK
IS THE COURSE OFFERED TO ERASMUS STUDENTS?	OFFERED IF REQUESTED
COURSE WEBSITE (URL)	**https://eclass.uoa.gr/courses/CHEM249/**

(1) LEARNING OUTCOMES

LEARNING OUTCOMES
LEARNING OUTCOMES *The learning outcomes, specific knowledge, skills and abilities of an appropriate level that the students will acquire after the successful completion of the course are described.* *Consult Appendix A* *• Description of the Level of Learning Outcomes for each course of study according to the Qualifications Framework of the European Higher Education Area* *• Descriptive Indicators for Levels 6, 7 & 8 of the European Qualifications Framework for Lifelong Learning and Annex B* *• Comprehensive Guide to writing Learning Outcomes*

The purpose of the course is to provide MSc students with a more in-depth knowledge of inorganic chemistry and its extension and application to related themes of the subject (organometallic chemistry, metal nanoparticles, quantum dots, structure-reactivity relations, X-ray crystallography, aspects of f-block chemistry). The goal is to provide students with new knowledge and instill novel methodological approaches and tools, so that they can specialize in varied aspects/facets (either basic or applied) of the inorganic chemistry discipline. These learning outcomes will be achieved *via* the combination of (i) providing face to face lectures on new material and on methodology (ii) practice in tackling problems in chemical synthesis (stoichiometric or catalytic) and analysis (liquid or solid phase) as well as introducing the students to elastic X-ray scattering data modeling to answer synthesis and analysis problems and (iii) access to and extensive use of original research articles (research led teaching) as well as of teaching material either in the form of subject reviews or textbooks.

Upon successful completion of the course, the students will be able to:

1. Understand and explain qualitatively the factors influencing σ- and π- interactions between the donor atom and the transition metal especially in the case of certain coordination geometries
2. Understand hard-soft acid theory, its connection to molecular orbital theory and its application in the synthesis of coordination compounds
3. Compare, contrast, and classify different types of ligands based on the type of the donor atom and its electronic structure
4. Distinguish non-innocent ligands and their role in redox phenomena and processes in coordination complexes
5. Comprehend the participation of non-innocent ligands in determining the geometry of complexes as well as their contribution to their excited states
6. Predict the geometries and structural properties of metal complexes based on the electronic properties of the metal centre and the ligands
7. Provide a rational choice of ligands to target a specific synthetic goal
8. Understand and rationalize synthetic routes and applications (catalytic or not, laboratory or industrial scale) where transition metal complexes are present
9. Suggest methods of analysis and characterization based on the nature and the properties of coordination compounds (complexes?)
10. Comprehend the factors influencing the synthesis of nanomaterials and quantum dots
11. Explain and analyse the properties of nanoparticles originating from their dependence on the metal ion
12. Comprehend phenomena such as plasmonic resonance, hyperthermia, phototherapy, as well as the optical properties of quantum dots as a result of the electron-hole relationship
13. Comprehend and explain the dependence of properties on the size of the nanoparticles
14. Make use of bibliography and literature to explore/interrogate and ultimately answer problems and questions related to the course
15. Understand Bragg's law and its importance in crystallography, especially in the resolution of data
16. Comprehend the role of symmetry in X-ray crystallography and how it influences data collection; more specifically what are centrosymmetric, non-centrosymmetric and chiral space groups and what are the symmetry elements both in space and point groups
17. Comprehend what is the atomic and structural scattering factor
18. Have an understanding of the statistical factors describing whether an elastic X-ray scattering data collection and the modelling of the derived periodic electron density is good or not

19. Describe the lanthanide contraction and its effect
20. To calculate the magnetic properties of lanthanide ions and their complexes
21. To describe the differences between actinides and lanthanides

Cognizance outcomes

1. Comprehension and understanding of the unifying trends implicit to the periodic table and their function in inorganic/organometallic chemistry; use of qualitative molecular orbitals in the study of inorganic and organometallic complexes
2. Systematic knowledge of ligands used in inorganic chemistry and related disciplines (organometallic chemistry/homogeneous catalysis)
3. Comprehension of the role of non-innocent ligands in redox phenomena
4. Selected applications whose core lies in the choice of the right transition metal as well as the design of the ligands
5. Solving and modelling of molecular structures of small molecules from diffraction experiments
6. Theoretical background to enable them to make better use of the new X-ray diffractometers at NKUA
7. Lanthanides and actinides in synthesis, catalysis and small molecule activation

Skills

1. Ability to approach/assess/tackle problems in the specific areas of inorganic chemistry, covered in the syllabus of the
2. Ability to devise rational synthetic routes and use analytical methods and techniques in inorganic chemistry.
3. Ability to extrapolate and assess the role of ligand scaffolds and metal centres in various applications using experimental data originating from various analytical techniques
4. Ability to categorise and appropriately choose the right synthetic methodology to access nanoparticles based on their desired properties
5. Ability to use analytical techniques, perform data processing and assess results in order to derive, understand, explain and extrapolate structure-reactivity
6. Ability to use software packages for the solution and modelling and refinement of molecular structures from X-ray diffraction data
7. Ability to comprehend and perform/collect the best possible data from an single crystal X-ray diffraction experiment.

General Skills

Taking into account the general skills that the graduate must have acquired (as stated in the Diploma Appendix and listed below) which of the following is/are the course aimed at?.

Reearch, analysis and synthesis of data and information, using the necessary technologies
Adaptation to new situations
Decision making
Independent work
Teamwork
Working in an international environment
Generating new research ideas
Demonstrating social, professional and ethical responsibility
Promotion of free, creative and inductive thinking

Promotion of free, creative and inductive thinking
Explore/Search/Investigate, analyse and combine data
Adapting to new situations
Teamwork
Independent/autonomous work
Generating and pursuing new research ideas and avenues
Work in an international environment

(2) COURSE CONTENT

The cource focuses on:

1. Hard-Soft acid-base theory, its connection with molecular orbitals and its role in the synthesis of coordination complexes
2. What is a non-innocent ligand
3. Role of non-innocent ligands in redox phenomena and their involvement in the excited states of complexes.
4. Non-innocent ligands in inorganic chemistry, energy and materials applications and methods of their analysis.
5. Construction of qualitative molecular orbital diagrams (σ-and π-interactions) in the following geometries: octahedral (C.N. 6), tetragonal (C.N. 4), tetragonal pyramid (C.N. 5), trigonal (C.N. 3), linear (C.N. 2). Discussion of factors influencing them and how these alter based on periodic trends across the periodic table.
6. Valence electron counting in transition metal complexes either taking into account or not π-interactions between the metal centre and the ligand
7. Isoelectronic and isolobal analogy in the periodic table with emphasis on transition metal complexes.
8. Donor-ligands explicitly forming multiple bonds with transition metals (oxo-, imido-, nitrido-, alkylidenes and alkylidines, N-heterocyclic carbenes) and study of these interactions.
9. Donor ligands bearing multiple bonds with transition metals and their spectator or non-spectator nature depending on the electronic structure of the metal centre they are coordinated to.
10. The electronic structure of carbenes and N-heterocyclic carbenes. Their complexes with metals and examples of their reactivity (stoichiometric and catalytic).
11. Experimental methods for the study of electronic and steric characteristics of ligands.
12. Design and ligand architecture (bi/multi-dentate, tripodal, pincer, macrocyclic). Synergy between ligand and metal centre in reactivity.
13. Nitrogen reduction catalysed by well-defined, structurally characterised transition metal complexes to demonstrate the afore-mentioned principles.
14. Synthetic avenues towards nanoparticles (sol-gel, hydrothermal, microwaves, autoclave, electrochemical, Ostwald maturation, thermal decomposition)
15. Classification of mono and dimetallic nanoparticles (a) alloys, (b) diametallics, (c) subclusters, (d) core-shell, (e) core-multi-shell, (g) multiple cores covered by a shell
16. Choice and design of conditions to furnish nanoparticles with desired attributes (magnetic, plasmonic, thermal)
17. Applications of metal nanoparticles in biological and non-biological systems.
18. Nanoparticles in diagnostic applications.
19. Plasmonic resonance and other properties of nanoparticles (phototherapy and hyperthermia).
20. Properties of quantum dots.
21. Instrumentation of X-ray diffractometers(X-ray sources and their operation, photon detectors, goniometer types).
22. Crystal systems, crystal lattices and their description with lattice points and planes.
23. Miller indices and reciprocal space.
24. Space groups, point groups and symmetry elements in crystal lattices.
25. Disadvantages and shortcomings of X-ray diffraction.
26. The position of the lanthanides in the periodic table.
27. Electronic structure of the lanthanides and the f-orbitals.
28. Russel-Saunders coupling and magnetism.
29. Lanthanide organometallic chemistry – the zero-oxidation state.
30. The actinides uranium and thorium, mineral extraction, and applications.
31. Small molecule activation and electro-catalysis.

(3) TEACHING AND LEARNING METHODS – EVALUATION

DELIVERY OF LECTURES
in person, distance etc.

In person delivery

USE OF INFORMATION AND COMMUNICATIONS TECHNOLOGIES
Use of I.C. T. in Lectures, Laboratory Exercises, Communication with students

Face to Face teaching:

- powerpoint
- Additional education material (slides) uploaded to e-class platform.

Communicating with students:

- Use of the e-class platform as a supplementary tool for teaching as well as disseminating to students important information (announcements, information and messages, teaching material and documents, user groups, etc).
- E-mail.
- Webex platform for online meetings

TEACHING ORGANIZATION
The teaching style and methods are described in detail.
Lectures, Seminars, Laboratory Exercises, Field Exercises, Literature Study & Analysis, Tutorial, Internship (Placement), Clinical Exercises, Art Workshop, Interactive Teaching, Educational Visits, Study Preparation (Project), Paper Writing Assignments, Artistic Creation, etc. etc.

The student's study hours for each learning activity as well as unguided study hours according to ECTS principles are listed

Activity	*Semester workload*
Lectures	39
Lectures to group of students	39
Un-guided study	28
Literature essay (*project*) – critical analysis of scientific literature, essay writing and presentation	50
Assessment preparation	40
Assessment	4
Total	200

STUDENT EVALUATION
Description of the evaluation process

Assessment Language, Assessment Methods, Formative or Deductive, Multiple Choice Test, Short Answer Questions, Essay Development Questions, Problem Solving, Written Assignment, Report / Report, Oral Examination, Public Presentation, Laboratory Work, Clinical Patient Examination, Artistic Interpretation, Other / Others

Explicitly defined evaluation criteria are mentioned, and if and where they are accessible by students.

Student evaluation takes place in Greek and consists of

- Written exam assessment consisting of answering critical questions and problems.
- Literature (bibliographic) essay (referred to as *project*); assessment based on the quality of the written essay as well as its presentation to their peers and lecturers.

Final Mark Calculation for the course:
The final mark is determined by the final exam (60%) and the literature essay (40%) (with the assessment criteria outlined above)

(4) RECOMMENDED BIBLIOGRAPHY- SCIENTIFIC LITERATURE - TEXTBOOKS

-Recommended Literature and Textbooks:

- "Synthesis and technique in inorganic chemistry: a laboratory manual". Girolami, G.S., Rauchfuss, T.B., 3rd ed., 1999, University Science Books, ISBN: 0935702482.
- ' Advanced Inorganic Chemistry', Cotton, Wilkinson, Murillo, Bochman, 6th Ed., John Wiley & Sons, 1999
- E.I. Stiefel, 'Dithiolene Chemistry: Synthesis, Properties, and Applications', progress in Inorganic chemistry, editor K.D. Karlin, Volume 52, 2004 Wiley
- Jean, Y. Molecular Orbitals of the Transition Metals Oxford University Press, Oxford 2005 ISBN 0 19 853093 5

- Nugent W. A.; Mayer J. M. Metal-Ligand Multiple Bonds, Wiley Interscience, New York 1988.
- Kim, S; Loose, F.; Chirik, P. J.Beyond Ammonia: Nitrogen−Element Bond Forming Reactions with Coordinated Dinitrogen
- R. Ferrando, J. Jellinek, R. L. Hohnston, “Nanoalloys: from theory to applications of alloy clusters and nanoparticles”, Chemical Reviews, (2008), 108 (3), 845-910
- P. Sronoi, Y.T. Chen, V. Vittur, M.D. Marquez, T. Randall Lee, “Bimetallic Nanoparticles: Enhanced Magnetic and Optical Properties for Emerging Biological Applications”, Applied Sciences (2018), 8(7), 1106
- R. A. Sperling, W. J. Parak, “Surface modification, functionalization and bioconjugation of colloidal inorganic nanoparticles”, Philosophical Transactions of the Royal Society A, (2010), 368, 1333–1383
- A. Zaleska-Medynska, M. Marchelek, M. Diak, E. Grabowska, “Noble metal-based bimetallic nanoparticles: the effect of the structure on the optical, catalytic and photocatalytic properties”, Advances in Colloid and Interface Science, (2016), 229, 80–10
- Crystal Structure Determination William Clegg, Oxford Chemistry Primers, Oxford University Press ISBN 978-0-19-855901-6
- LANTHANIDE AND ACTINIDE CHEMISTRY, Simon Cotton, John Wiley & Sons, Ltd, ISBN-13: 978-0-470-01005-1
- Tutorial on the Role of Cyclopentadienyl Ligands in the Discovery of Molecular Complexes of the Rare-Earth and Actinide Metals in New Oxidation States William J. Evans *Organometallics* 2016, **35**, 3088–3100
- Research papers from referred journals of the field but also of general chemical interest Inorganic Chemistry, Angew. Chem., Dalton transactions etc