Course Outline

1) General

SCHOOL	SCIENCE		
DEPARTMENT	CHEMISTRY		
DEGREE	MASTER		
COURSE CODE	**18A6**	**SEMESTER**	**1**
COURSE TITLE	Topics of Inorganic chemistry		

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**
Lectures	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*	SPECIAL BACKGROUND, SKILL DEVELOPMENT
PREREQUISITE COURSES:	NO
COURSE AND EXAM LANGUAGE:	GREEK
IS THE COURSE OFFERED TO ERASMUS STUDENTS ?	IF NEEDED YES
COURSE WEBSITE (URL)	**https://eclass.uoa.gr/courses/CHEM254/**

(1) 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 course aims at describing a large range of methodologies currently applied in Inorganic Chemistry, with emphasis in the mechanisms of chemical reactions.
More specifically, during the course, the following topics are taught:
More specifically, in the context of this course, students are taught:

- Basic concepts of chemical kinetics.
- Mechanisms of substitution reactions of octahedral and square-planar complexes.
- Mechanisms of redox reactions.
- Marcus Theory for the electron-transfer reactions in biological systems.
- Photosynthetic H_2O-oxidation by the Mn_4CaO_5 center (OEC).
- Function of the metalloenzymes hydrogenase and nitrogenase.
- Transfer hydrogenation reactions. Definitions and general aspects.
- Main reaction mechanisms.
- Meerwein-Ponndorf-Verley (MPV) mechanism or direct hydrogen transfer.
- The hydridic route. The mono-and dihydride mechanisms.
- Mechanistic studies.
- Inner sphere hydrogen transfer with substrate coordination.
- Outer sphere hydrogen transfer with no substrate coordination.
- Factors that influence the whole process.
- Selected examples with different categories of organic ligands and transition metals.
- Asymmetric catalysis. Noyori type catalysts for the asymmetric reduction of various unsaturated substrates.
- Asymmetric transfer hydrogenation in the pharmaceutical and fragrance industries.
- Transfer hydrogenation reactions in cancer cells. A new approach to anticancer drug design.
- Alkene and alkyne metathesis reactions. The nature of the metal-carbon bonds, reaction mechanisms (steps, reactive intermediates) and catalytic systems, with emphasis on the structure/reactivity relationship and catalyst design.
- The most important industrial applications of olefin and alkyne metathesis reactions.
- Clusters with multiple metal-metal bonds. Nature and properties of metal-metal bonds. Applications of those clusters to catalytic metathesis

reactions. Mode of reactivity and comparison to analogous monometallic catalytic systems with respect to reactivity and selectivity.

Knowledge

- Knowledge and understanding of the basic principles of chemical kinetics.
- Knowledge and understanding of the mechanisms for substitution reactions in octahedral and square planar complexes.
- Knowledge and understanding of the mechanisms for redox reactions and biological electron-transfer reactions.
- Knowledge and understanding of the possibility to utilize the metalloenzymes Hydrogenase and Nitrogenase in the chemical industry (for instance bioelectrocatalytic synthesis of NH_3 from N_2).
- Knowledge and understanding of the basic concepts related to transfer hydrogenation reactions. Benefits in relation to the classic hydrogenation process are also discussed.
- Knowledge and understanding of the relevant mechanisms that describe the transfer hydrogenation process.
- Knowledge and understanding of a plethora of applications in chemical industry related to the transfer hydrogenation process.
- Knowledge and understanding of alkene and alkyne metathesis reactions, with emphasis on the structure/catalytic reactivity relationship and on the design of new catalytic systems.
- Knowledge and understanding of (a) the nature and properties of multiple metal-metal bonds; (b) how these affect the properties of the corresponding clusters; and, (c) the reactivity and selectivity of these clusters in metathesis reactions (also compared to those of mononuclear catalytic systems).

Skills

- Skills in the literature search of review and original research articles in fields related to this course.
- Skills in the oral presentation of specific topics of the course based on their literature survey.
- Skills in evaluating experimental data of chemical kinetics related to catalytic and biocatalytic reactions.
- Skills in employing the Protein Data Bank (PDB) and the PyMol software, for the investigation of the relationship between the structure and properties of redox metalloenzymes.
- Skills in the design of suitable catalysts for appropriate applications.
- Skills towards the in-situ investigation of transfer hydrogenation reactions metathesis reactions by means of absorption, vibration and NMR (e.g., ^{1}H, ^{31}P) spectroscopy.
- Skills in evaluating experimental data of the relevant catalytic processes. In situ reaction monitoring.

- Skills in employing the appropriate software required for catalyst characterization, such as NMR spectroscopy (^{1}H, ^{31}P) etc.

Abilities

- Ability to apply the knowledge gained in dealing with problems related to chemical kinetics.
- Ability in the interpretation of experimental data from the investigation of redox metalloproteins and metalloenzymes.
- Ability in the utilization of the existing knowledge in the field of redox metalloproteins for the design of novel biocatalysts.
- Ability to apply the knowledge gained in dealing with problems related to catalysis (e.g., selectivity, mechanism, catalyst design).
- Ability in the interpretation of experimental data obtained from *in situ* reaction monitoring.
- Ability to use knowledge gained in this and other courses in order to elucidate experimental data.
- Ability to use the appropriate software required for problems related to the fields of the course.

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	*Project planning and management*
Adaptation to new situations	*Respect for diversity and multiculturalism*
Decision making	*Respect for the environment*
Independent work	*Demonstrating social, professional and ethical responsibility and sensitivity to gender issues*
Teamwork	*Exercise criticism and self-criticism*
Working in an international environment	*Promotion of free, creative and inductive thinking*
Working in an interdisciplinary environment	*Other……….*
Generating new research ideas	

The course aims at equipping students with the following general skills:

- Search, analysis and synthesis of data and information, using the necessary technologies.
- Autonomous work.
- Group work.
- Ability to apply knowledge to problem solving.
- Generation of new research ideas.
- Work in an interdisciplinary environment.
- Promotion of free, creative and inductive thinking.
- Decision making.

(2) COURSE CONTENT

Basic concepts of chemical kinetics and the experimental techniques employed to kinetically study chemical reactions. Types of mechanisms taking place in substitution reactions of octahedral and square-planar complexes, as well as in redox reactions. Description and application of the Marcus Theory for electron transfer reactions in biological systems. The conclusions of the experimental investigations are exploited to elucidate the function of significant bioinorganic catalysts, such as the photosynthetic H_2O-oxidizing Oxygen-Evolving-Complex (Mn_4CaO_5), as well as the metalloenzymes hydrogenase and nitrogenase. The possibility of utilizing the latter metalloenzymes in the chemical industry (e.g. for the synthesis of NH_3 by bioelectrocatalysis) is considered.

"Transfer hydrogenation" reactions, as an attractive alternative to standard hydrogenation, are described, along with the two main mechanisms that have been proposed. These are classified into the direct hydrogen transfer and the hydridic route. Mechanistic studies performed have revealed two types of catalysts that operate through the monohydride mechanism, the inner- sphere (with substrate coordination) and the outer-sphere mechanisms. The major factors that influence the whole process of "transfer hydrogenation" are also presented. Furthermore, selected examples with different categories of organic ligands and transition metals are presented. The general aspects of asymmetric transfer hydrogenation including the seminal work of Noyori's type catalysts for the asymmetric reduction of various unsaturated substrates is commented. The asymmetric transfer hydrogenation reaction is an important process in the pharmaceutical and fragrance industries. Therefore, selected examples from the chemical industry are given. Finally, a recent report about the application of transfer hydrogenation reactions in cancer cells is described. The latter is a new approach to anticancer drug design.

Olefin and alkyne metathesis reactions. Catalytic systems, with emphasis on the structure/reactivity relationship and catalyst design, are discussed. The most important industrial applications of those reactions are also presented. Clusters with multiple metal-metal bonds. The nature and the properties of the metal-metal bonds are discussed. Applications of those clusters to catalyticmetathesis reactions are presented. The reactivity of the catalytic systems is examined and compared to analogous monometallic and catalytic systems with respect to reactivity and selectivity.

(3) TEACHING AND LEARNING METHODS – EVALUATION

<table>
<tr><td>LECTURES' DELIVERY
In person, distance, etc..</td><td>In person</td></tr>
<tr><td>USE OF INFORMATION AND COMMUNICATIONS TECHNOLOGIES
Use of I.C.T. in Lectures, Laboratory Exercises, Communication with students</td><td>In Teaching:
• Presentations with multimedia content (power point)
In Communication with students:
• Support the learning process through the e-class electronic platform (announcements, information, messages, documents, user groups, etc.).
• Email.</td></tr>
<tr><td>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</td><td><table><tr><th>Activity</th><th>Semester workload</th></tr><tr><td>Lectures</td><td>78</td></tr><tr><td>Unguided study</td><td>62</td></tr><tr><td>Paper writing</td><td>50</td></tr><tr><td>Study preparation</td><td>10</td></tr><tr><td>Total</td><td>200</td></tr></table></td></tr>
<tr><td>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.</td><td>The evaluation of the course takes place in Greek and includes:
• written exam that includes multiple choice questions, short development of theoretical issues, judgment, as well as problem solving
• evaluation of the bibliographic work, evaluation of the presentation of the bibliographic work</td></tr>
</table>

(4) RECOMMENDED BIBLIOGRAPHY

- *Inorganic Chemistry*, C.E. Housecroft and A.G. Sharp, 4th Edition, Pearson Education Limited, 2012 (Chapter 26). ISBN 978-0-273-74275-3.
- Winkler, J.R. and Gray, H.B., Electron flow through metalloproteins, *Chem. Rev*., 2014, 114, 3369-3380. doi:10.1021/cr4004715.
- Page, C.C, Moser, C.C., Dutton, P.L., Mechanism for electron transfer within and between proteins, *Cur. Opin. Chem. Biol.*,2003, 7, 551-556. doi: 10.1016/j.cbpa.2003.08.005.
- Wang D, Astruc D., The Golden Age of Transfer Hydrogenation, *Chem. Rev*. 2015, 115, 6621-6686. doi: 10.1021/acs.chemrev.5b00203.
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- Noyori R., Asymmetric Catalysis: Science and Opportunities (Nobel Lecture), *Angew. Chem. Int. Ed.,* 2002, 41, 2008-2022. doi: 10.1002/1521-3773(20020617)41:12<2008::AID-ANIE2008>3.0.CO;2-4.
- Schrock, R.R., Multiple metal-carbon bonds for catalytic metathesis reactions (Nobel Lecture), *Angew. Chem. Int. Ed.* 2006, 45, 3748-3759.doi: 10.1002/anie.200600085.
- Grubbs, R.H., Olefin-metathesis catalysts for the preparation of molecules and materials (Nobel Lecture), *Angew. Chem. Int. Ed.* 2006, 45, 3760-3765. doi: 10.1002/anie.200600680.
- Ivin, K.J., Mol, J.C., Olefin Metathesis and Metathesis Polymerization; Academic Press: Cambridge, MA, USA, 1997. ISBN: 9780123770455.
- Dragutan, V., Streck, R., Catalytic Polymerization of Cycloolefins: Ionic, Ziegler-Natta and Ring-Opening Metathesis Polymerization; Elsevier: Amsterdam, the Netherlands, 2000. ISBN: 9780080528625 (e-book).