Course Outline

1) General

SCHOOL	SCIENCE		
DEPARTMENT	CHEMISTRY		
DEGREE	MASTER		
COURSE CODE	**18A5**	**SEMESTER**	**1**
COURSE TITLE	Inorganic Structure and Reactivity		

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*	GENERAL 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/CHEM237/**

(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 aim of the course is to disseminate knowledge about a wide range of modern methodologies used in structure analysis and its correlation with the activity of inorganic compounds and materials.

More specifically, in the context of this course, students are taught:

- Symmetry and Structure: Molecules' Imaging software.
- What is the -Z matrix and how can we create it. Elements of symmetry. Point groups. Intermolecular forces: dipole - dipole, hydrogen bonding, ion - dipole, ion or dipole ion - induced dipole, induced dipole - induced dipole.
- Electronegativity as an indicator of chemical reactivity: Definitions.
- Examples of semiconductors and nanomaterials: Correlation of structure and reactivity.
- Theories and models about the structure of inorganic solids: bond-valence
- model. Correlation of valence bond with physical properties and chemical reactivity.
- Computational study of structure and reactivity.
- Fundamentals of X-ray crystallography.
- The Cambridge crystallographic database: Usage, capabilities and applications in the design of new crystalline solids.
- Metal-Organic Frameworks - porous crystalline solids: correlation of structure- topology with reactivity and properties as well as their applications in the industry.
- Zero-field splitting in paramagnetic systems with $S > 1/2$ and methods of
- determining its axial (D) and rhombic (E) component.
- Structure and magnetic properties in mononuclear complexes with single ion magnet behavior (SIMs).
- Principles for the design of novel SIMs.

Knowledge

- Knowledge and understanding of the basic principles of crystallography.
- Knowledge and understanding of Metal-Organic Frameworks, the way they are synthesized, the structure and topology of their networks as well as their properties and applications and the correlation of their structure with their properties.

- Knowledge and understanding of the use of the Cambridge crystallographic database, its capabilities and its applications.
- Knowledge and understanding of the prediction of chemical activity based on structural characteristics of molecular structures (symmetry, bond strength, molecular valence orbitals, etc.), their electrical properties (atomic charges, electronegativity, etc.) and intermolecular interactions.
- Knowledge and understanding of the concept of zero-field splitting in paramagnetic systems with $S > ½$, as well as its consequencers in their magnetic behavior.
- Investigation of the relationship between the structure and the magnetic properties of mononuclear single molecule magnets (SIMs).
- Knowledge of the basic principles for the design of novel SIMs.

Skills

- Skills in evaluating basic results of crystallography.
- Skills in designing and using appropriate synthetic methods for Metal-Organic Frameworks.
- Skills in analyzing the crystal structures and the underlying networks of Metal-Organic Frameworks and relating these to their properties.
- Skills in using the Cambridge crystallographic database.
- Skills in using molecular design programs and measuring the structural features of molecules.
- Skills in predicting the structure of inorganic solids using the bond-valence model.
- Skills in the literature search of original and review articles in the field of molecular magnetism.
- Skills in employing the Cambridge strucrural database for the investigation of the relationship between the structure and the properties of SIMs.
- Skills in the presentation by the students in their class, of the results of their literature survey in matters related with the structural and magnetic properties of SIMs.

Abilities

- Ability to apply the knowledge gained by the students in dealing with problems related to crystallography.
- Ability to interpret experimental data from the synthesis of Metal-Organic Frameworks and relate them to their structures and their underlying networks.
- Ability to use the Cambridge crystallographic database and correlate crystal structures with the properties of the corresponding compounds.
- Ability to design molecules in 3-D with the help of computer programs and measure their structural characteristics.
- Ability to predict the structure of inorganic solids with the help of the bond-valence model.

- Ability in the interpretation of experimental data from the investigation of the structural and magnetic properties of SIMs.
- Ability in the utilization of the existing knowledge in the field of molecular magnetism for the design of novel SIMs.

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

Symmetry and Structure: Molecules' Imaging software. What is the -Z matrix and how can we create it. Elements of symmetry. Point groups. Intermolecular forces: dipole - dipole, hydrogen bonding, ion - dipole, ion or dipole ion - induced dipole, induced dipole - induced dipole. Electronegativity as an indicator of chemical reactivity: Definitions. Examples of semiconductors and nanomaterials: Correlation of structure and reactivity. Theories and models about the structure of inorganic solids: bond-valence model. Correlation of valence bond with physical properties and chemical reactivity. Computational study of structure and reactivity. Fundamentals of X-ray crystallography. The Cambridge crystallographic database: Usage, capabilities and applications in the design of new crystalline solids. Metal-Organic Frameworks - porous crystalline solids: correlation of structure-topology with reactivity and properties as well as their applications in the industry. Zero-field splitting in paramagnetic systems with $S > 1/2$ and methods of determining its axial (D) and rhombic (E) component. Structure and Magnetic Properties in mononuclear complexes with single ion magnet behavior (SIMs). Basic principles for the design of novel SIMs.

(3) TEACHING AND LEARNING METHODS – EVALUATION

LECTURES' DELIVERY *In person, distance, etc..*	In person

USE OF INFORMATION AND COMMUNICATIONS TECHNOLOGIES *Use of I.C. T. in Lectures, Laboratory Exercises, Communication with students*	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.
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), PaperWriting 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: 78 Unguided study: 62 Paper writing: 50 Study preparation: 10 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.*	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.

(4) RECOMMENDED BIBLIOGRAPHY

- https://www.ccdc.cam.ac.uk/Community/educationalresources/
- W. Massa, Crystal Structure Determination, Springer-Verlag, 2004. ISBN 978-3-642-05841-7
- S. Kaskel (ed), The Chemistry of Metal–Organic Frameworks, Synthesis, Characterization, and Applications, Wiley, 2016. ISBN 978-3-527-33874-0

- Bond Valences, Editors I. David Brown, Kenneth R. Poeppelmeier, Series Title Structure and Bonding, DOIhttps://doi.org/10.1007/978-3-642-54968-7, Publisher Springer Berlin, Heidelberg, eBook Packages Chemistry and Materials Science, Chemistry and Material Science (R0), Copyright Information Springer-Verlag Berlin Heidelberg 2014, Hardcover ISBN978-3-642-54967-0, Softcover ISBN978-3-662-51076-6, eBook ISBN978-3-642-54968-7
- L. Pauling, The Nature of the Chemical Bond, Cornell Univ., USA, 3rd ed., 1960.
- M. Feng, M. L. Tong, Chem. Eur. J., 2018, **24**, 7574-7594.
- J. Krzystek, J. Telser, Dalton Trans., 2016, **45**, 16751-16763.
- J. M. Frost, K. L. M. Harriman and M. Murugesu, Chem. Sci., 2016, **7**, 2470-2491.