Jagiellonian University

Faculty of Chemistry

# LIST OF COURSES

# CHEMISTRY

(5-year Master Program)

2007/8

- 1. Course code: A101
- 2. Title of the course: Principles of chemistry
- 3. **Tutor**: Prof. Roman Dziembaj
- 4. Teaching objectives:

Developing understanding and ability of using of fundamental laws and concepts of chemistry. Creating basis for studying of all disciplines of chemistry, especially inorganic, organic, analytical and physical chemistry. Equalizing level of students coming from different types of high schools. In laboratory students obtain many manual skills, learn about observation of experiments, drawing conclusions and their formulation in written reports.

### Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture and classes(i)

### Lecture

- 1. Course code: A101W
- 2. Type of course: lecture
- 3. Tutor: Prof. Roman Dziembaj
- 4. Number of hours: 45
- 5. Description of the course:

Stoichiometry and stoichiometric calculations, concentration of solutions. Ideal gas law, real gases, types of intermolecular interactions. Heat of chemical reactions, Hess law, enthalpy of formation, additivity of bond energy. Equilibrium of chemical reaction,  $\Delta G^0 = -RT \ln K$ , direction of spontaneous reactions, Le Chatelier principle. Brönsted acid and bases, dissociation of water, pH, hydrolysis, buffers, dissociation constant, protic solvents. Redox reactions, standard potentials, Nernst equation,  $\Delta G^0 = -nFE^0$ . Phase equilibria, Gibbs phase rule. First and second order kinetic equations, collision theory, Arrhenius equation, catalysts and inhibitors. Experimental basis of quantum theory. Schrödinger equation for hydrogen atom, quantum numbers, wavefunctions and their radial and angular parts, orbitals, spectrum of the hydrogen atom. Multielectron atoms, electron configurations – aufbau principle and exemptions, Slater rules, effective nuclear charge and electron energy in multielectron atoms. Molecular orbitals as linear combinations of atomic orbitals, homonuclear diatomic molecules, energy diagrams. Heteronuclear diatomic molecules, electronegativity, dipole moment, bond polarization. Hybridization  $sp^3$ , coordination tetrahedron, alkanes, isomers, conformers. Hybridization sp<sup>2</sup>, alkenes, cis-trans isomers, ozone molecules, delocalization of electrons, aromatic hydrocarbons. Symmetry of molecules, basic symmetry elements, optical isomers. Crystal lattice, hexagonal and regular unit cells. Electron bands, intrinsic and doped semiconductors, structural defects, nonstoichiometry. Lewis acids and bases, donor-acceptor bonds, hard and soft acid and bases, examples of coordination compounds, polyions, multicenter complexes.

- 6. Method of evaluation: written exam
- 7. **ECTS:** 3.5
- 8. Semester: winter
- 9. **Bibiography:**

Basic:

- 1. A. Bielański *Podstawy Chemii Nieorganicznej*, (wydanie V zmienione) rozdz. I-IV, V (§1 i 2), VI, VII, IX-XII, XIV (§1-5 oraz 10), XV (§1-3) PWN, Warszawa 2002
- 2. R. T. Morrison, R.M. Boyd *Chemia organiczna*, rozdz. I i XII, PWN, Warszawa 1990 i wydania późniejsze

Additional:

- 1. J. E. Wells Strukturalna chemia nieorganiczna, tłum. polskie, WNT, Warszawa 1993
- 2. R.T. Morrison, R.M. Boyd *Chemia organiczna*, PWN, Warszawa 1990 i wydania późniejsze
- 3. D.F. Shriver, P.W. Atkins i C.H. Langford *Inorganic Chemistry*, Oxford University Press, 1991
- 4. L. Jones i P. Atkins, *Chemia ogólna Cząsteczki, materie, reakcje,* PWN, Warszawa, 2004
- 5. F.A. Cotton, G. Wilkinson, D.L. Gaus *Chemia nieorganiczna podstawy*, PWN, Warszawa 1995

### PRINCIPLES OF CHEMISTRY

Hours:; credit: ; ECTS: semester: 1;entry conditions: student recruitment: SYM./-; maximal number of participants: 160/ - completing requirements:.

## Laboratory

- 1. Course code: A101L
- 2. Type of course:
- 3. Tutor: Dr Anna Reizer
- 4. Number of hours: 105 of laboratory practice
- 5. Description of the course:

Course content: Laboratory techniques; Preparative inorganic chemistry; Separation mixture (crystallization, fractional destination, extraction, sublimation); Chemical equilibrium in aqueous solution, pH, dissociation constant, equilibrium between acid-bases, solid-solution, buffers; Compound complexes; Redox reaction; Electrochemistry; Chemical kinetics; Elements of qualitative analysis cations and anions.

- 6. Method of evaluation: internal assessment
- 7. **ECTS**:
- 8. Semester: 1
- 9. **Bibiography:**
- Basic bibliogaphy:
- A. Reizer redakcja "Ćwiczenia z podstaw chemii i analizy jakościowej" skrypt Uniwersytetu Jagiellońskiego
- A. Bielański Podstawy Chemii Nieorganicznej (wydanie II poprawione) PWN Warszawa 1999 i wydania późniejsze

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- 1. Course code: A102
- 2. Title of the course: Mathematics
- 3. Tutor: Dr Marian Łoboda
- 4. **Teaching objectives:** Preparing for solving mathematical problems in physics and chemistry

## Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

## Lecture

- 1. Course code: A102W
- 2. Type of course: lecture
- 3. Tutor: Dr Marian Łoboda
- 4. Number of hours: 45
- 5. Description of the course:

Real sequences and series, tests for convergence, power series.

Limits and continuity of functions, elementary limits, properties of continuous functions.

Differential calculus of one variable functions, Taylor's formula, extremes.

Indefinite integrals, integration of some classes of functions.

Definite integrals, construction, properties, geometric applications, improper integrals.

Algebraic structures: groups, fields, vector spaces, linear operators.

Complex numbers, operations, functions.

- 6. Method of evaluation: writing exam
- 7. **ECTS:** 3,5
- 8. Semester: winter term
- 9. Bibiography:

## **Calculation classes**

- 1. Course code: A102C
- 2. Type of course: Calculation classes
- 3. Tutor: scientific workers of Department of Mathematics and Computer Science
- 4. Number of hours: 60
- 5. Description of the course: compatible with lectures
- 6. Method of evaluation: writing tests
- 7. ECTS: 5
- 8. Semester: winter term
- 9. Bibiography:

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- 1. Course code: A202
- 2. Title of the course: Mathematics
- 3. Tutor: Dr Marian Łoboda
- 4. **Teaching objectives:** Preparing for solving mathematical problems in physics and chemistry

## Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

### Lecture

- 1. Course code: A202W
- 2. Type of course: lecture
- 3. Tutor: Dr Marian Łoboda
- 4. Number of hours: 30
- 5. Description of the course: Matrices, operations, determinants, quadratic forms.

Systems of linear equations, Cramer's formula.

Elements of geometry, scalar and vector products, lines and planes in the space.

Functions of several variables: partial derivatives, total differentials, gradients, partial

derivatives and differentials of higher orders, local and conditional extremes.

Differential equations, methods of solving.

Multiple integrals, physical and geometrical applications.

Elements of probability.

- 6. Method of evaluation: writing exam
- 7. **ECTS:** 3.0
- 8. Semester: summer term
- 9. Bibiography:

## **Calculation classes**

- 10. Course code: A202C
- 11. Type of course: Calculation classes
- 12. Tutor: scientific workers of Department of Mathematics and Computer Science
- 13. Number of hours: 45

- 14. Description of the course: compatible with lectures
- 15. Method of evaluation: writing tests
- 16. **ECTS:** 3,5
- 17. Semester: summer term
- 18. Bibiography:

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- 1. Course code: A 103
- 2. Title of the course: Physics
- 3. Tutor: Prof. dr hab. Andrzej Szytuła
- 4. Teaching objectives:

The main aim of the course is to give basic knowledge of the fundamentals in mechanics. The lecture illustrates the theoretical and experimental character of physical science. Tutorials give familiarity with some of the mathematical methods used in physics. Physics Lab trains experimental problem-solving techniques including experimental error calculations.

## Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

## Lecture

- 1. Course code: A 103w
- 2. Type of course: lecture
- 3. Tutor: Prof. dr hab. Andrzej Szytuła
- 4. Number of hours: 30
- 5. Description of the course:

The topics of the lecture include basic concepts of mechanics, general motion of particles in three dimensions, particle dynamics including noninertial frames of reference, work and energy, the universal law of gravitation, systems of particles, motion of rigid bodies in three dimensions, collisions, dynamics of oscillating systems, mechanical waves, elasticity and acoustics.

A calculus-based approach is employed. The lecture is illustrated by numerous demonstrations.

- 6. Method of evaluation: test exam
- 7. **ECTS:** 3
- 8. Semester: winter
- 9. Bibiography:

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- 1. Course code: A203
- 2. Title of the course: Physics
- 3. Tutor: Professor Zbigniew Majka
- 4. Teaching objectives: Basic course in physics and mathematical method of physics. Calculation classes allow students to gain their abilities in using mathematical methods to describe phenomena. The goals of few laboratory exercises are teaching of physical quantity measurements, data analysis and the error evaluations.

## Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

### Lecture

- 1. Course code: A203W
- 2. Type of course: lecture
- 3. Tutor: Professor Zbigniew Majka
- 4. Number of hours: 30
- Description of the course: Static electric and magnetic fields. Field operators. Electric and magnetic fields in matter. Currents. Introduction to electrodynamics. Maxwell's equations. Electromagnetic waves and light. Elements of optics.
- 6. Method of evaluation: examination, test
- 7. **ECTS:** 3.0
- 8. Semester: summer
- 9. Bibiography:

D. J. Griffiths, Introduction to Electrodynamics, third edition, Prentice-Hall Co.,, 1989

## Laboratory

- 1. Course code: A203L
- 2. **Type of course:** laboratory
- 3. Tutor: Professor Andrzej Magiera
- 4. Number of hours: 30
- 5. Description of the course: Mechanics: mathematical pendulum, rotational motion law, determination of moment of inertia, determination of viscosity coefficient, suppressed pendulum; Heat: determination of water vaporization heat, ice melting heat, solid state and liquid specific heats; Electricity: determination of temperature coefficient of metal resistance, capacity of capacitors; Optics: determination of lens focal point, of emission spectra, of diffraction and interference on the gap, of wave length using diffractive net.
- 6. Method of evaluation: 6 exercises and exercise reports
- 7. **ECTS:** 2,5
- 8. Semester: summer
- 9. Bibiography:

## **Calculation classes**

- 1. Course code: A203C
- 2. Type of course: Calculation classes
- 3. Tutor: Department of Physics Staff
- 4. Number of hours: 30
- 5. Description of the course: Compatible to the lectures and laboratory
- 6. Method of evaluation: tests
- 7. **ECTS:** 2.5
- 8. Semester: summer
- 9. Bibiography:

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1. Course code: A204

- 2. Title of the course: Analytical Chemistry I
- 3. Tutor: dr Stanisław Walas
- 4. Teaching objectives:
- Instruction of the students about the fundamentals of qualitative, quantitative and instrumental analysis basing on knowledge acquired in the course of general chemistry.
- Acquaintance the students with selected analytical methods and necessary laboratory techniques on hand of individual work.
- Introduction to good laboratory practice, calculation, data handling and evaluation results uncertainty.

### Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

### Lecture

- 1. Course code: A204W
- 2. Type of course: lecture
- 3. Tutor: dr Stanisław Walas
- 4. Number of hours: 30
- 5. Description of the course:

General problems: the tasks and importance of analytical chemistry in science and technology. Outline of history. Basic concepts of analytical chemistry: sample, signal, analytical method and analytical process. Classification of analytical methods. Theory and practice of sampling. Sample pretreatment (decomposition and digestion, separation of the components). Introduction to qualitative analysis: identification and separation of selected ionic species in solution, group reagents. Sensitivity of analytical tests. The principles of qravimetry. Classification of gravimetric methods. The solubility and physical properties of analytical precipitates. Organic reagents used in gravimetry. Classification of volumetric methods: alkali– and acidimetry, precipitation analysis, complexometry, redoxometry. Primary and secondary standards. Advantages and disadvantages of titrimetric methods. Introduction to instrumental methods of analysis. The classical versus instrumental analysis. Calibration. Electrochemical methods. Ion-selective electrodes. Potentiometric analysis. Absorption of light by coloured solutions. Beer's law. Colorimetry and spectrophotometry.

interpretation of analytical data. Standard methods of analysis. Standards and reference materials.

- 6. **Method of evaluation:** multiple choice test examination. Students are allowed to sit the examination on condition that they have fulfilled all requirements of the laboratory and tutorials
- 7. **ECTS:** 3
- 8. Semester: 2
- 9. Bibiography:
- 1. A. Cygański, Chemiczne metody analizy ilościowej, Warszawa, WNT, 1999, wyd. 5
- 2. A. Rokosz, Wprowadzenie do chemii analitycznej, Kraków, UJ, 1980
- 3. J. Minczewski, Z. Marczenko, *Chemia analityczna*, t.1 i 2, Warszawa, PWN, 1985
- 4. W. Szczepaniak, Metody instrumentalne w analizie chemicznej, Warszawa, PWN, 1996

### Laboratory

- 1. Course code: A204L
- 2. Type of course: laboratory
- 3. Tutor: dr Jolanta Kochana
- 4. Number of hours: 105
- 5. Description of the course:

Gravimetric determination of one of the following cations: barium, iron, nickel. Calibration of volumetric glassware. Preparation and standardization of sodium hydroxide solution and determination of hydrochloric acid sample. Preparation and standardization of thiosulfate solution. Bromate titration of phenol. Iodimetric determination of hydrochloric acid. Complexometric determination of the total water hardness. Analysis of multicomponent samples: determination of H<sup>+</sup>, Mg<sup>2+</sup>, Na<sup>+</sup> with use of ion exchange resin. Separation ions of copper and iron and complexometric determination of copper with EDTA and spectrophotometric determination of trace amounts of iron(III) with thiocyanate. Analysis of real samples: determination of oxygen dissolved in water by Winkler's method. Titrimetric determination of acetic acid in commercial vinegar with visual and potentiometric end–point detection.

- 6. Method of evaluation: Results of the analytical process
- 7. **ECTS:** 6
- 8. **Semester:** 2
- 9. Bibiography:

- 1. A. Cygański, Chemiczne metody analizy ilościowej, Warszawa, WNT, 1999, wyd. 5
- 2. A. Rokosz, Wprowadzenie do chemii analitycznej, Kraków, UJ, 1980
- 3. J. Minczewski, Z. Marczenko, Chemia analityczna, t.1 i 2, Warszawa, PWN, 1985
- 4. W. Szczepaniak, Metody instrumentalne w analizie chemicznej, Warszawa, PWN, 1996
- 5. A. Cygański, B. Ptaszyński, J. Krystek, *Obliczenia w chemii analitycznej*, Warszawa, WNT, 2000

### **Tutorials**

- 1. Course code: A204K
- 2. **Type of course:** tutorials
- 3. Tutor: dr Stanisław Walas
- 4. Number of hours: 15
- 5. Description of the course:

The joining of the principal topics of lectures and laboratory exercises program. Connection of theoretical aspects of particular determinations with good laboratory practice. Broadening of understanding theory of applied methods.

- 6. Method of evaluation: multiple choice tests
- 7. **ECTS:** 1
- 8. Semester: 2
- 9. Bibiography:

## A205/A305 ORGANIC CHEMISTRY

Head:	Janusz Jamrozik PhD, DSc
Lecture:	45 hrs (2 semester) + 45 hrs (3 semester)
Seminar:	45 hrs (2 semester) + 45 hrs (3 semester)
Laboratory:	180 hrs (3 semester)
ECTS:	24.5 (3.5 lec + 3.5 sem + 3.5 lec + 3.0 sem + 11 lab)

### **Teaching objectives:**

The main purpose of teaching organic chemistry is providing students with a key to understanding chemistry of carbon compounds, showing that the knowledge of organic chemistry is necessary to understand principles of biology and medicine and to encourage them to study further these fascinating subjects.

At the end of the tutorial students should be able to solve problems, to think in an abstract way, to apply known solutions in new situations, to compare and interpret data, to present in a spoken and written manner the obtained results, to take part actively in discussions, to be prepared for a tem work.

During a laboratory practice, partly supervised and partly co-operative, students should learn: how to plan and carry our syntheses, multi-step processes and functional group protection strategies; how to use chemical literature (Beilstein, Chemical Abstracts, Current Contents); how to complete laboratory experiments safely (especially when flammable materials, bromine, cyanides and other toxic organic substances are used); how to protect the environment (knowledge of SDS). Additionally students gain a wide variety of manual skills, learn to observe experiments and to draw certain conclusions from them, and report experimental results in a written form (often with the help of word processors). Exercises teach how to tackle and solve problems and how to organises own time (students choose the sequence of exercises by themselves).

## **A205/A305lec** Lecture ECTS 7.0 (3.5 + 3.5)

#### Lecturer: Janusz Jamrozik PhD, DSc

Isomerism in organic chemistry: constitutional, stereoisomerism. Alkanes, cycloalkanes, alkenes, alkynes: preparation and reactivity. Radical substitution, addition to multiple bonds. Radical and carbo-cation structure and stability, carbo-cation rearrangements. Conjugated dienes, resonance. Alkyne electrophilic addition. Stereochemistry: stereogenic (chiral) centres. Enantiomers, diastereoisomers, meso compounds, racemic mixtures and their separation. Conformational analysis of cyclohexane. Aromatic compounds: aromaticity criterion. Resonance. Electrophilic substitutions. Isomerism of the polysubstituted aromatic compounds. Nucleophilic aromatic substitutions. Benzyne. Halogenation of alkylbenzene side chains, benzyl cation, anion, radical. Polycyclic aromatic hydrocarbons. Spectroscopy in structure determination of organic compounds. Alkyl halides: necleophilic substitutions SN1, SN2. Elimination reactions E1 and E2 – mechanism and stereochemistry. Alkohols, phenols, ethers and epoxides: synthesis and reactivity. Dehydration, conversion into alkyl halides, oxidation, reactions with metals, alkyl halides, phosphorus trihalides, acylation. Aldehydes and ketones: structure and properties of carbonyl group. Nucleophilic addition of: water, alcohols, amines and Grignard reagents to carbonyl compounds. Aldol condensation, Cannizzaro reaction, Wittig reaction. Carboxylic acids and their derivatives. Acidity. Synthesis of carboxylic acids and their reactivity. Formation of esters, acid chlorides, amides and acid anhydrides. Acyl substitution reactions. Carbonyl -substitution reactions: keto-enol tautomerism, -halogenation, alkylation and acylation of enolate ions. The application of acetoacetic and malonic esters in organic synthesis. Carbonyl condensation reactions: aldol reaction, Claisen condensation, Michael addition and similar reactions. Enamine 1H and 13C nuclear magnetic resonance: chemical shifts, intensity of signals, spin-spin couplings; determination of structural elements and their sequence in organic molecules. Ultraviolet and visible spectroscopy: spectra of species with conjugated bond system: dienes, enones and aromatic compounds. Colour of organic molecules. The scope and limitation of certain methods. Complementary usage of all the mentioned methods for structure elucidation of organic compounds.

Assessment: written exam

### A205/A305s Seminar ECTS 6.5 (3.5 + 3.0)

Tutorial is complementary to the lecture: Organic Chemistry and it emphasises problems that need student co-operation in small groups. The convincing examples are here stereochemistry taught with the help of molecular models or structure elucidation by means of spectroscopic methods. These problems are illustrated by many exercises solved during tutorials or suggested for student's own work. During tutorials, reaction mechanisms will be explained by various examples and many problems discussed that should lead to deeper understanding of a broad area of organic chemistry.

*Introduction.* The structure of organic molecules resulting from sp<sup>3</sup>, sp<sup>2</sup>, and sp hybridisation. Homolytic and heterolytic bond cleavage, acidity and basicity of organic compounds, nucleophilicity and electrophilicity of reagents, inductive and resonance effect. IUPAC rules of nomenclature including E/Z and R/S configuration. Types of organic reactions. The structure of carbocation, carboanion and radical.

*Stereochemistry*. Kinds of stereoisomerism. The specification of stereoisomers number and the relation between them. Configuration of stereogenic centres. Presentation of configuration on the plane. Molecular models. Conformation analyses of alkanes: ethane, butane, cyclohexane and its mono and disubstituted derivatives. Stereochemistry of halogen addition to the double bond, stereochemistry of SN1 and SN2. Monosaccharides: D configuration, anomers, epimers, anomeric effect. Disaccharides – explanation of their structure. Amino acids, configuration , L.

*Reaction mechanisms*. Substitution: radical, electrophilic, nucleophilic. Addition to the multiple bonds: electrophilic and nucleophilic. Elimination. Some factors having influence on reaction mechanism, mechanism competition, e.g. SN/E. Aldol condensation. Substituent effects in aromatic electrophilic substitution. Rearrangements.

*The outlines of organic synthesis planning*. Protecting groups, inter-conversion of functional groups, formation of carbon skeleton, multi-step syntheses, the way from product to starting material.

#### Application of spectroscopic methods for structure elucidation

Mass spectrometry: molecular formula and the presence of some elements (Cl, Br, S, I, F, N) in organic compounds; fragmentation pathways of basic classes of organic compounds.

Infrared spectroscopy: absorption bands characteristic for typical structural elements and functional groups; dependence of some group frequencies on conjugation.

<sup>1</sup>H and <sup>13</sup>C nuclear magnetic resonance: chemical shifts, intensity of signals, spin-spin couplings; determination of structural elements and their sequence in organic molecules.

Ultraviolet and visible spectroscopy: spectra of species with conjugated bond systems: dienes, enones and aromatic compounds. Colour of organic molecules.

The scope and limitations of certain methods. Complementary usage of all the mentioned methods for structure elucidation of organic compounds.

Assessment: graded credits

### A305lab Laboratory ECTS 11.0

Head: Dr. Bożena Kawałek

Goals: knowledge of basic techniques used in a preparative organic chemistry as well as some elements of organic analysis. Students get acquainted with the application of the following unit operations (some of them known from the Principles of Chemistry course) for the synthesis, separation, isolation, purification and identification of reaction products: crystallisation from organic solvent (the choice of a proper solvent included), distillations (simple, fractionated, steam and vacuum), the usage of a rotary evaporator, chromatographic techniques (thin layer – the choice of conditions included – and column chromatography), extraction with organic solvents, heating of reaction mixtures under reflux condenser, filtration under reduced pressure, drying of solvents, solutions and solids, determination of physical properties (melting and boiling points, refraction).

Organic synthesis experiments are ordered into seven groups which illustrate the following basic types of organic reactions explained earlier during lectures: addition and elimination, nucleophilic substitution, electrophilic aromatic substitution, nucleophilic aromatic substitution, reactions of carbonyl compounds, oxidation and reduction, synthesis of heterocyclic compounds and rearrangements.

Each student is obliged to perform the following experiments: twelve syntheses (at least one of each group), some of the as multi-step syntheses; one experiment based on literature data preceded by a short course on literature search (students are obliged to find in literature some methods of synthesis of a given compound, to choose the proper one, to discuss that problem with a tutor and, finally, to carry out the experiment); one experiment prescribed by a tutor,

fitting in level of difficulty student's ability and very often related to research done at the Department of Organic Chemistry.

Analytical part of laboratory practice concerns one sample analysed by means of classical chemical methods and another analysed by spectroscopy means.

Assessment: assessment of theoretical background for experiments, experimental results, written reports

## A409 ELEMENTS OF BIOCHEMISTRY

Head:Prof. Jerzy Silberring PhD, DScLecture:30 hrs (4 semester)ECTS:2.0

### **Teaching objectives:**

Basic components of living organisms (nucleic acids, proteins, oligosacharides, lipids) – structure, physicochemical properties and structure-function relationship.

### A409lec Lecture ECTS 2.0

Lecturer: Piotr Laidler PhD, DSc, Prof. Jerzy Silberring PhD, DSc

Assessment: written and test exams

Basic groups of compounds:

Nucleic acids. Structural elements of pro- and eukaryotic cells. Purine and pyrimidine bases, ribose and deoxyribose, nucleosides and nucleotides – their structure and physicochemical properties. DNA and RNA – differences in structure, physicochemical properties, denaturation. DNA – replication, mutation and repair. RNA – ribosiems (catalytic properties, transcription). Biosynthesis of protein – role of RNA, ribosomes, amino acids and their activation. Molecular basis of neoplasm processes. Application of molecular biology techniques – oligonucleotides, recombinanted DNA, PCR, transgenic animals. Proteins. Peptides – peptide bonding, peptide precursors , biologically active peptides, role of peptides in central nervous system. Simple and conjugated proteins – structure of I-IV order, denaturation – relationship between structure and function of proteins. Enzymes and their inhibitors – mechanism of activity (chymotrypsin), cholinesterase and conveterase of angiotensin and their inhibitors. Neuropeptides in alcohol and drug addiction. Participation of peptides in conduction of stimuli.

Carbohydrates. Monosacharides and disacharides – properties. Polisacharides – starch (amylose and amylopectin), glycogen, cellulose – structure and properties. Glycoproteins and their oligosacharide components. Role of carbohydrates in organism – energetic metabolism. Defects in carbohydrates transformations .

Lipides. Division of lipides. Biological films – structure and properties. Role of lipides in organism – basic transformations. Defects in lipdes transformations.

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- 2. Title of the course: Computer laboratory
- 3. **Tutor**: Dr. Habil. Janusz Mrozek
- 4. **Teaching objectives:** Teaching students processing of experimental data and editing laboratory reports using computer software for numerical calculations, computer text editors. Students should learn also how to use facilities provided by the computer network of Faculty of Chemistry.

### Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture and classes(i)

### Laboratory

- 1. Course code:
- 2. Type of course:
- 3. **Tutor:**
- 4. Number of hours:
- 5. Description of the course:

Teaching students processing of experimental data and editing laboratory reports using computer software for numerical calculations, computer text editors. Students should learn also how to use facilities provided by the computer network of Faculty of Chemistry including such set of standard operations like e.g. starting various types of sessions on workstations in student laboratories, logging in, changing passwords and operations on files and directories. Students shall also learn how to use software included into MS Office 2000 such as: Access, Excel, PowerPoint and Word for running basic calculations and preparing reports. Acquired knowledge and skills shall be useful both during the studies and in future work.

- 6. Method of evaluation: 3 tests during the course
- 7. **ECTS:** 2.0
- 8. Semester:winter
- 9. Bibiography:

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### Laboratory

- 1. Course code: A206
- 2. Type of course:
- 3. Tutor:

### 4. Number of hours:

### 5. Description of the course:

Using e-mail software and groupwork tools in MS Outlook, and other e-mail programs like e.g. pine, Pegasus Mail. Preparing presentations in MS PowerPoint Moving objects and data between programs of MS Office. Writing basic macroinstructions in MS Word and Excel.

- 6. Method of evaluation: 1 test at the end of the semester
- 7. **ECTS:** 1.0
- 8. Semester: summer
- 9. Bibiography:
  - 1. A. Eilmes, Word dla chemików, wyd. MIKOM 2001
  - 2. M. Pilch, Excel dla chemików, wyd. MIKOM 2001
  - 3. A. Michalak, PowerPoint dla chemików, wyd. MIKOM 2002
  - 4. Microsoft instruction manuals for MS Office
  - 5. opisy podstawowych poleceń systemów Windows NT i Linux
  - 6. on-line documentation for ssh, ftp, telnet i SMB

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- 1. Course code: A307
- 2. Title of the course: Physical Chemistry
- 3. Tutor: prof. dr hab. Maria Paluch

**4. Teaching objectives:** Student should master the basic issues of physical chemistry and gain the ability to apply laws describing physicochemical phenomena (on the basis of mathematical laws). Student should also acquaint with various research methods and maintenance of the equipment used in determination of various physicochemical values. Gaining the ability of interpretation and description of the experimental results and teamwork in the frame of students group

## Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

### Lecture

- 1. Course code: A307w
- 2. Type of course: Physical Chemistry
- 3. Tutor: prof. dr hab. Marek Wójcik, prof. dr hab. Maria Paluch

#### 4. Number of hours: 30 hours

5. Description of the course: (covers also course A407, which is a continuation of this course in the summer semester) Molecular spectroscopy: permanent and induced dipole moments, polarization, rotational and vibrational spectra of molecules, characteristics of electronic transitions - transition dipole moment, magnetic properties of molecules, nuclear magnetic resonance, electron spin resonance, mass spectrometry. First law of thermodynamics: parameters of state, functions of state, work, heat, internal energy, enthalpy, enthalpy of chemical reactions, bond energies, correlation of thermo-chemical data, Kirchhoff's law, relation between C<sub>v</sub> and C<sub>p</sub>, adiabatic change. Second law of thermodynamics: statistic and thermodynamic definition of entropy, Carnot cycle, Helmholtz and Gibbs functions, chemical potential. Phase transitions of simple mixtures: partial molar quantities, Gibbs-Duhem equation, Raoult's law and Henry's law, ebullioscopic and cryoscopic constants, osmosis. Real solutions: activity and activity constant, fugacity. Phase transitions in multicomponent systems: phase rule, liquid-liquid and liquid-solid diagrams, three-component systems. Equilibrium in chemical reations: equilibrium constants, dependence of equilibrium constant on temperature and pressure. Kinetics of chemical reactions: rate constants of chemical reactions, reaction order, half life time, stage determining rate of reaction, consecutive reactions, reversible, parallel and chain reactions. Molecularity of reactions, Lindemann mechanism. Temperature dependence of rate constant, activation energy and pre-exponential factor. Collision theory, active complex, transition state, entropy and enthalpy of activation.

Equilibrium in electrochemical systems: thermodynamical properties of ions and their definition from ideal behaviour, Debye-Hückel's theory of strong electrolytes, conductivity of electrolytes. Electrode processes, reversible electrodes, electrochemical calls, Nernst equation, electromotive force and its relation to thermodynamics of reaction in cells, diffusion potential, membrane potential and ion-selective electrodes, electrode's polarization, corrosion. Physical chemistry of surface phenomena: surface tension, adsorption at solid-gas, liquid-liquid and liquid-gas interface, adsorption isotherm, surface active compounds, properties of surface films, characterization of disperse systems.

- 6. Method of evaluation: written examination
- 7. ECTS: 2.5
- 8. Semester: winter
- 9. Bibiography:

#### **Calculation Classes**

- 1. Course code: A307c
- 2. Type of course: calculation classes
- 3. Tutor: dr Danuta Góralczyk
- 4. Number of hours: 15 hours
- 5. Description of the course: (covers also course A407, which is a continuation of this course in the summer semester) Application of the thermodynamic laws in thermochemical calculations. Application of the Clausius-Clapeyron equation to phase transitions. Liquid-vapour equilibrium in ideal and real systems. Calsulation of the equilibrium constant for reactions in gaseous phase, temperature dependence of equilibrium constant. Chemical kinetics, methods of determination of the order of reaction, effect of temperature on the reaction rate, Selected problems of molecular spectroscopy. Specific and equivalent conductivity of solutions of electrolytes, calculation of dissociation constants and solubility products on the basis of conductance values. Thermodynamics of reactions in cells, calculation of the mean ionic activity coefficients, equilibrium constant for redox reactions and solubility products on the basis of EMF values. Activation and diffusion overpotentials. Adsorption on the various interfaces, adsorption isotherms.

### 6. Method of evaluation: colloquia, oral answers

- 7. **ECTS:** 1.5
- 8. Semester: winter
- 9. Bibiography:

#### Laboratory

- 1. Course code: A307l
- 2. **Type of course:** laboratory
- 3. Tutor: dr Tadeusz Bieszczad
- 4. Number of hours: 45 hours
- 5. Description of the course: (covers also course A407, which is a continuation of this course in the summer semester) Thermochemistry. Partial volume. Gibb's phase rule. Distribution coefficient. Activity coefficient. Surface tension. Adsorption isotherms. Viscosity of solutions. Molecular weight of polymers. Critical micelle concentration. Chemical reactions rate. Catalytic reactions. Absorption spectroscopy. Quenching of fluorescence. Electric dipole moments. Conductivity of electrolytes. Ionic mobility. Transport numbers of ions. Galvanic cells. Electrolysis.
- 6. Method of evaluation: colloquia, exercises performance

- 7. **ECTS:** 3.5
- 8. Semester: winter
- 9. Bibiography:

**Tutorials** 

- 1. Course code: A307k
- 2. Type of course: tutorials
- 3. Tutor: dr Joanna Kowal
- 4. Number of hours: 15 hours

Description of the course: (covers also course A407, which is a continuation of this course in the summer semester) Basic principles of molecular spectroscopy. The first law of thermodynamics, thermochemistry. The second and the third law of thermodynamics. Partial molar quantities, chemical potential. Changes of state, the phase rule. Systems of one component, the Clapeyron-Clausius equation. Phase equilibria in solutions, phase diagrams. Thermodynamics of ideal and real solutions. Chemical equilibrium. Chemical kinetics, simple and complex reactions, collision theory of reactions in gas phases, the transition-state theory. Catalysis. Photochemistry. Electrochemistry, conductivity, transport numbers, the Debye-Huckel theory, electrodes and electrochemical cells, kinetics of electrochemical reactions, overpotential. Physical chemistry of surfaces, surface tension, adsorption isoterms. Electrical phenomena at interfaces. Colloidal solutions.

## 5. Method of evaluation: colloquia, oral answers

### 6. **ECTS:** 1.5

- 7. Semester: winter
  - 1. Bibiography: A. Atkins, Chemia fizyczna, PWN, Warszawa 2000
  - 2. K. Pigoń, Z. Ruziewicz, Chemia fizyczna, PWN, Warszawa 2005
  - 3. Praca zbiorowa Chemia fizyczna, PWN, Warszawa 1980
  - 4. L. Sobczyk, A. Kisza, Chemia fizyczna dla przyrodników, PWN, Warszawa 1975
  - 5. G.M. Barrow, Chemia fizyczna, PWN, Warszawa 1976
  - 6. M. Sonntag, Koloidy, PWN, Warszawa 1982
  - 7. J. Koryta, J. Dvořak, V. Bohačkowa, Elektrochemia, PWN, Warszawa 1980
  - 8. T. Bieszczad, M. Boczar, D. Góralczyk, Ćwiczenia laboratoryjne z chemii fizycznej, UJ, Kraków 1995
  - 9. H. Buczak, D. Góralczyk, M. Jaskuła, J. Kosacz, Zbiór przykładów i zadań z chemii fizycznej, UJ, Kraków 1995
  - 10. A. Adamson, Zadania z chemii fizycznej, PWN, Warszawa 1978

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- 1. Course code: A407
- 2. Title of the course: Physical Chemistry
- 3. Tutor: prof. dr hab. Maria Paluch
- 4. Teaching objectives: Student should master the basic issues of physical chemistry and gain the ability to apply laws describing physicochemical phenomena (on the basis of mathematical laws). Student should also acquaint with various research methods and maintenance of the equipment used in determination of various physicochemical values. Gaining the ability of interpretation and description of the experimental results and teamwork in the frame of students group

## Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture and classes(i)

## Lecture

- 1. Course code: A407w
- 2. Type of course: Physical Chemistry
- 3. Tutor: prof. dr hab. Marek Wójcik, prof. dr hab. Maria Paluch
- 4. Number of hours: 30 hours
- 5. Description of the course: Continuation of the course A307
- 6. Method of evaluation: written examination
- 7. ECTS: 3.0
- 8. Semester: summer
- 9. Bibiography:

**Calculation Classes** 

- 1. Course code: A407c
- 2. Type of course: calculation classes
- **3 Tutor: dr Danuta Góralczyk**
- 4. Number of hours: 30 hours
- 5. Description of the course: Continuation of the course A307
- 6. Method of evaluation: colloquia, oral answers
- 7. ECTS: 1.5

- 8. Semester: summer
- 9. Bibiography:

## Laboratory

- 1. Course code: A407l
- 2. Type of course: laboratory
- 3. Tutor: dr Tadeusz Bieszczad
- 4. Number of hours: 90 hours
- 5. Description of the course: Continuation of the course A307
- 6. Method of evaluation: colloquia , exercises performance
- 7. ECTS: 3.5
- 8. Semester: summer
- 9. Bibiography:

## **Tutorials**

- 1. Course code: A407k
- 2. Type of course: tutorials
- 3. Tutor: dr Joanna Kowal
- 4. Number of hours: 15 hours
- 5. Description of the course: Continuation of the course A307
- 5. Method of evaluation: colloquia, oral answers
- 6. ECTS: 1.5
- 7. Semester: summer
  - 1. Bibiography: A. Atkins, Chemia fizyczna, PWN, Warszawa 2000
  - 2. K. Pigoń, Z. Ruziewicz, Chemia fizyczna, PWN, Warszawa 1980
  - 3. Praca zbiorowa Chemia fizyczna, PWN, Warszawa 1980
  - 4. L. Sobczyk, A. Kisza, Chemia fizyczna dla przyrodników, PWN, Warszawa 1975
  - 5. G.M. Barrow, Chemia fizyczna, PWN, Warszawa 1976
  - 6. M. Sonntag, Koloidy, PWN, Warszawa 1982
  - 7. J. Koryta, J. Dvořak, V. Bohačkowa, Elektrochemia, PWN, Warszawa 1980
  - 8. T. Bieszczad, M. Boczar, D. Góralczyk, Ćwiczenia laboratoryjne z chemii fizycznej, UJ, Kraków 1995
  - 9. H. Buczak, D. Góralczyk, M. Jaskuła, J. Kosacz, Zbiór przykładów i zadań z chemii fizycznej, UJ, Kraków 1995
  - 10. A. Adamson, Zadania z chemii fizycznej, PWN, Warszawa 1978

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**1.Course code**: A 308 w

**2.Title of the course:** INORGANIC CHEMISTRY OF THE MAIN GROUP ELEMEMNTS.

**3.Tutor**: Dr hab Alicja Drelinkiewicz

**4.Teaching objectives:** the objective of this course is inorganic chemistry of the main group elements

## Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture and classes(i)

## Lecture

- 1. Course code: A 308 w
- 2. Type of course: lecture
- 3. Tutor: Dr hab Alicja Drelinkiewicz
- 4. Number of hours: 30

## 5. Description of the course:

History of inorganic chemistry, genesis, discovery and distribution of the elements, Mendeleev's periodic table of elements, periodic properties of atoms, ionization energy, electron affinity, covalent and ionic radii, electronegativity, effective nuclear charge, role of valence and inner electrons, inert "s" pair effect, role of  $\pi$ -bonds, molecular  $\pi$  and  $\delta$  orbitals from p and d orbitals. General trends in main group chemistry, Hydrogen, isotopes, hydride ion, hydrides, hydrogen bond, hydrogen bridges. The noble gases, compounds. Bonding in molecules, formal charge, molecular orbitals, hybrid orbitals, VSEPR model, predicting the structure and reactivity of molecules, electronegativity and atomic size effects, polar molecules. The s-block metals, characterization of s-block elements (1 and 2 group, chemical properties, the crystalline structure of binary compounds,, ionic crystal lattice energy, p-block elements (nonmetals, semiconductors, metals), the boron, carbon, nitrogen, oxygen and halogens groups elements, general characterization and reactivity. Methods of recovery of elements and their applications

- 6. Method of evaluation: written exam
- 7. **ECTS:** 2.5
- 8. Semester:winter
- 9. **Bibiography:**

A. Bielański, Podstawy Chemii Nierganicznej, PWN Warszawa 2002

F.A. Cotton, G. Wilkinson, Chemia Nierganiczna, podstawy PWN Warszawa 1995

P.A. Cox, Krótkie Wykłady Chemia Nierganiczna, PWN Warszawa 2003

T. Senkowski, Z. stasicka, Zarys Struktury Elektronowej Atomów i Cząsteczek, Skrypt Uczelniany Uniwersyteteu Jagiellońskiego Kraków 1982

A.F. Williams, Chemia Nierganiczna, Podstawy Teoretyczne, PWN Warszawa 1986

D.F. Shriver, P.W. Atkins, C.H. Langford, Inorganic Chemistry, Oxford University Press, Oxford 1994

N.N. Greenwood, A. Earnshaw, Chemsitry of the Elements, Pergamon Press, Oxford 1986 S.F.A. Kettle, Fizyczna Chemia Nierganiczna, PWN Warszawa 1999

## Seminar

- 1. Course code: A 308
- 2. Type of course: S
- 3. **Tutor:**
- 4. Number of hours: 15
- 5. **Description of the course:** extention of the problems presented in the lecture, formal charge, molecular sahape in terms of molecular orbitals, VSEPR model, predicting a shape of molecules
- 6. Method of evaluation: oral examination
- 7. **ECTS:** 1,5
- 8. Semester: winter
- 9. **Bibiography:** the same as for the lecture

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- 1. Course code: A408
- 2. Title of the course: Inorganic Chemistry
- 3. Tutor: prof.dr hab.Barbra Sieklucka

## 4. Teaching objectives:

Introduce the discipline of inorganic chemistry. Presentation of the descriptive, systematic chemistry of the s, p , d and f elements, basic principles and elements of structure and reactivity. Classes of inorganic compounds. Acquiring elucidation inorganic chemistry problems skills. Developing laboratory skills. Introduction to the important techniques of

synthesis and study of the reactivity of inorganic and coordination compounds in the context of inorganic experiments. Developing the skills of reporting the results and their interpretation...

## Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

## Lecture

- 1. Course code: A408
- 2. **Type of course:** lecture (w)
- 3. Tutor: Prof.dr hab.Barbara Sieklucka
- 4. Number of hours: 30
- 5. Description of the course: Coordination chemistry. Inorganic chemistry of dand f-block metals. Coordination compounds. Constitution. Representative ligands and nomenclature. Symmetry of molecules. Application of symmetry (polarity, chirality, symmetry of orbitals). Isomerism. Bonding and electronic structure. Crystafield theory. Ligand-field splitting parameters. Spectrochemical series of linands and metal ions. Simple interpretation of electronic spectra. Weak-field and strong-field limits. Magnetic properties. Jahn-Teller effect. Ligand-field theory. Thermodynamics of complex formation: coordination equilibrium, the Irving-Williams series, Hard and soft transition metals and ligands. Chelate and macrocyclic effects. Redox potentials, Latimer diagrams. Self-assembly and metal-templated reactions. Mechanisms of substitution and redox reactions. The d-block metals. Occurrence and recovery. Oxidation states and Frost diagrams. Typical oxidation states and typical compounds. Oxygen and oxygen compounds as the ligands. Aqua-, hydroxo- and oxo-complexes. Mononuclear oxo complexes. Polyoxometalates. Metal-metal bonded compounds and clusters. Metal sulfides and sulfide complexes. Noble metals. Group 12 metals. dmetal organometallic chemistry. Electron counting and oxidation states. d-block carbonyls. Anologs of carbonyls compounds – complexes with other  $\pi$ -acceptor ligands (dinitrogen and nitrogen monoxide). Other organometallic compounds. Metallocenes. The f-block metals.
- 6. Method of evaluation: written exam
- 7. **ECTS:** 3.0
- 8. Semester: summer
- 9. Bibiography:

- 1. A.Bielański, Podstawy Chemii nieorganicznej, Wyd.5, PWN 2003.
- 2. F.A.Cotton, G.Wilkinson, P.L.Gaus, Chemia nieorganiczna. Podstawy, PWN 1995.
- 3. S.F.A.Kettle, Fizyczna chemia nieorganiczna, PWN 1999.
- 4. D.F.Shriver, P.W.Atkins, T.L.Overton, J.P.Rourke, M.T.Weller, and F.A.Armstrong, Inorganic Chemitry, 4th Ed., OUP 2006.

5. J.E.Huheey, E.A.Keiter, R.L.Keiter, Inorganic Chemistry. Principles of Structure and Reactivity, 4th Ed., HarperCollins 1994.

## Classes

- 1. Course code: A408
- 2. Type of course: classes
- 3. Tutor: prof.dr hab.B.Sieklucka
- 4. Number of hours: 15
- 5. Description of the course: in accordance with the lecture
- 6. Method of evaluation: written credit
- 7. **ECTS:** 1.5
- 8. Semester: summer
- 9. Bibiography:
- 1. A.Bielański, Podstawy Chemii nieorganicznej, Wyd.5, PWN 2003.
- 2. F.A.Cotton, G.Wilkinson, P.L.Gaus, Chemia nieorganiczna. Podstawy, PWN 1995.
- 3. S.F.A.Kettle, Fizyczna chemia nieorganiczna, PWN 1999.
- 4. D.F.Shriver, P.W.Atkins, T.L.Overton, J.P.Rourke, M.T.Weller, and F.A.Armstrong, Inorganic Chemitry, 4th Ed., OUP 2006.
- 5. J.E.Huheey, E.A.Keiter, R.L.Keiter, Inorganic Chemistry. Principles of Structure and

Reactivity, 4th Ed., HarperCollins 1994.

## Laboratory

- 10. Course code: A408 L
- 11. Type of course: laboratory
- 12. Tutor: dr R.Gryboś
- 13. Number of hours: 90
- 14. Description of the course:

Practical classes on selected topics of inorganic chemistry. Coordination equilibrium in solution. Isomerism of coordination compounds and rate of isomerisation. Reactivity of coordination compounds. Photochemical properties of coordination compounds. Redox properties of inorganic compounds. Selected topics on solid state inorganic chemistry: nonstoichiometric compounds, defects, and catalytic properties.

15. Method of evaluation: performed practical classes, written credit

16. ECTS: 7

17. Semester: summer

## 18. Bibiography:

1. A.Bielański, Podstawy Chemii nieorganicznej, Wyd.5, PWN 2003.

2. F.A.Cotton, G.Wilkinson, P.L.Gaus, Chemia nieorganiczna. Podstawy, PWN 1995.

3. S.F.A.Kettle, Fizyczna chemia nieorganiczna, PWN 1999.

4. D.F.Shriver, P.W.Atkins, T.L.Overton, J.P.Rourke, M.T.Weller, and F.A.Armstrong, Inorganic Chemistry, 4th Ed., OUP 2006.

5. J.E.Huheey, E.A.Keiter, R.L.Keiter, Inorganic Chemistry. Principles of Structure and Reactivity, 4th Ed., HarperCollins 1994.

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- 1. Course code: A410
- 2.Title of the course: Crystal Chemistry
- 3.Tutor: Prof. dr hab. Stanisław Hodorowicz

## 4. Teaching objectives:

The aim of the course is to acquaint the students with the basic knowledge of crystallography including such problems as long-distance ordered phases – lattice theory – symmetry (point groups and space groups); diffraction methods; principles of crystal structure analysis with the special emphasis on crystal chemistry; crystal growth, real crystals; polymorphism; phase transitions; introduction to crystal physics.

## Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

## Lecture

- 1. Course code: A410w
- 2. Type of course: lecture(w)
- 3. Tutor: Prof. dr hab. Stanisław Hodorowicz
- 4. Number of hours: 30

### 5. Description of the course:

Crystals as the ordered phases: the order range in various states of matter, mesomorphous phases. Geometric crystallography: point symmetry (crystal families and crystal systems, geometrical classes), lattice symmetry (Bravais systems, choice of the unit cell) and Bravais lattices, space groups. Structural crystallography: diffraction methods in structure determination (X-ray diffraction, neutron diffraction and electron diffraction) – kinematics theory principles (Laue, Bragg and Ewald approach, factors determining the intensity of diffracted beam), outline of X-ray structure analysis and application in chemistry. Crystal genesis: crystallization processes (nucleation and growth), techniques of crystal growing, real crystals (defects, quasi-crystals, modulated phases (commensurate and incommensurate)), polymorphism, phase transitions. Crystal chemistry: classification of crystal structures, the character of interatomic interactions (metallic, ionic, covalent, coordination, van der Waals and hydrogen bonds). Crystal physics: physical property of crystal, tensorial description, classes of general point groups, Neumann principle.

- 6. Method of evaluation: multi-choice test
- 7. **ECTS:** 3.0
- 8. Semester: summer
- 9. **Bibliography:**
- 1. J. Chojnacki., *Elementy krystalografii chemicznej i fizycznej*, III wyd. Warszawa PWN 1973
- 2. T. Penkala, Zarys krystalografii, III wyd. Warszawa PWN 1983
- 3. A.F. Wells, Strukturalna chemia nieorganiczna, Warszawa WNT 1993
- 4. Z. Bojarski, M. Gigla, K. Stróż, M. Surowiec, *Krystalografia, podręcznik* wspomagany komputerowo, Warszawa PWN 1996
- 5. J.P. Glusker, K.N. Trueblood, Zarys rentgenografii kryształów, PWN Warszawa 1977

## **Tutorials**

- 1. Course code: A410k
- **2. Type of course:** tutorials(k)
- 3. Tutor: Prof. dr hab. Stanisław Hodorowicz together with assistants and PhD students
- **4. Number of hours:** 30
- 5. Description of the course: The subject area of the tutorials is consistent with the progress

of the lecture.

- 6. Method of evaluation: written tests
- 7. ECTS: 2.5
- 8. Semester: summer
- **10. Bibliography:**

- 1. J. Chojnacki., *Elementy krystalografii chemicznej i fizycznej*, III wyd. Warszawa PWN 1973
- 2. Z. Bojarski, H. Habla, M. Surowiec, *Materiały do nauki krystalografii*, Warszawa PWN 1986
- 3. Z. Bojarski, M. Gigla, K. Stróż, M. Surowiec, *Krystalografia, podręcznik* wspomagany komputerowo, Warszawa PWN 1996
- 4. J.P. Glusker, K.N. Trueblood, Zarys rentgenografii kryształów, PWN Warszawa 1977
- 5. International Tables for Crystalography, Vol. A. Dordrecht: Kluwer Academic Publishers, 1996

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- 1. Course code: A511
- 2. Title of the course: Analytical Chemistry II
- 3. Tutor: dr Stanisław Walas
- 4. Teaching objectives:
- to make the students familiar with the main problems and methods of advanced analytical chemistry,
- to transfer the general analytical knowledge and skills in the area complementary to this of the subject "Analytical Chemistry I",
- to equip students with the knowledge and skills they need in order to be able to do research in analytical laboratories,
- to equip students with the knowledge and skills enabling them the employment in any units of analytical profile
- Students are allowed to participate in the course on condition that they have fulfilled

requirements of ANALYTICAL CHEMISTRY I.

### Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture

and classes(i)

## Lecture

- 1. Course code: A511W
- 2. Type of course: lecture
- 3. Tutor: dr Stanisław Walas
- 4. Number of hours: 30
- 5. Description of the course:

Instrumental analysis vs. classical analysis; classification of the methods of instrumental analysis; essence and general rule of the methods of instrumental analysis; analytical

procedure; methods of the sample digestion; optimization of the analytical conditions; analytical calibration; matrix and interference effects; calibration methods; absolute analysis; advanced methods of the sample separation; automation of the analytical procedure; qualitative instrumental analysis; quantitative trace analysis; two- and multicomponent analysis; speciation analysis; local and surface analysis; estimation methods of accuracy and precision of the analytical results; statistical analysis of the analytical results. Problems are presented in respect of the applicability of the main methods of spectrometric, electrochemical, chromatographic, thermometric.

- 6. **Method of evaluation:** multiple choice test examination. Students are allowed to sit the examination on condition that they have fulfilled all requirements of the laboratory
- 7. **ECTS:** 8
- 8. Semester: 5
- 9. Bibiography:
- 1. W. Szczepaniak, Metody instrumentalne w analizie chemicznej, PWN, Warszawa 1996
- 2. J. Minczewski, Z. Marczenko, Chemia analityczna t. III, PWN, Warszawa 1985
- 3. A. Cygański, Metody spektroskopowe w chemii analitycznej, WNT Warszawa 1997
- 4. A. Cygański, Podstawy metod elektroanalitycznych, WNT Warszawa 1999

### Laboratory

- 1. **Course code:** A511L
- 2. **Type of course:** laboratory
- 3. **Tutor:** dr Małgorzata Herman
- 4. Number of hours: 60
- 5. **Description of the course:**

Acquaintance with the most important theoretical and practical issues of instrumental analysis e.g.: qualitative instrumental analysis, analytical calibration, examination and elimination of interference effect, sample digestion, instrumental separation of sample components, speciation analysis, flow injection analysis, application of instrumental techniques to the titration end-point detection, analytical optimization. Familiarization with the selected techniques of spectral, electrochemical and chromatographic analysis.

- 6. Method of evaluation: internal regulation considering written tests and reports
- 7. **ECTS:**
- 8. Semester: 5
- 9. **Bibiography:** 
  - 10. W. Szczepaniak, Metody instrumentalne w analizie chemicznej, PWN, Warszawa 1996
  - 11. J. Minczewski, Z. Marczenko, Chemia analityczna t. III, PWN, Warszawa 1985
  - 12. A. Cygański, Metody spektroskopowe w chemii analitycznej, WNT Warszawa 1997
  - 13. A. Cygański, Podstawy metod elektroanalitycznych, WNT Warszawa 1999

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- 1. Course code:
- 2. Title of the course: Informatics
- 3. Tutor: Dr. Habil. Janusz Mrozek

4. **Teaching objectives:** Teaching students techniques of coding simple numerical algorithms in C and Fortran and computing using freeware packages for symbolic and numerical computing as well as packages for visualization of data

## Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

laboratory

- 1. Course code:
- 2. **Type of course:**
- 3. Tutor: Dr. Habil. Janusz Mrozek
- 4. Number of hours: 30

5. **Description of the course:** Implementing numerical algorithms using programming langauages: Fortran and C, using various options of the compilers. Program structure, keywords, data types, commands, functions and subroutines. Using computer libraries. Integrated packages for numerical (Scilab) and symbolic (Maple and Mathematica) calculations 2- and 3D graphics using Gnuplot and Xmgr.

6. **Method of evaluation:** Three tests during the semester (X1-X3) and one final test X4 common for all students test końcowy (X4) – final score:  $X = 0.50^{*}(X1 + X2 + X3) + 0.50^{*}X4$ 

- 7. **ECTS:** 2.0
- 8. Semester: winter
- 9. **Bibiography:**

1. Handbook: skrypt J. Mrozek, A. Eilmes, M. Pilch, *Programowanie prostych algorytmów w językach Fortran i C* (in Polish) (to be published).

2. instruction manuals for Scilab, Gnuplot i Xmgrace packages

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- 1. Course code: A513
- 2. Title of the course: Theoretical chemistry (small course)
- 3. Tutor: Professor Piotr Petelenz

4. **Teaching objectives:** The student is expected: 1. to acquire the understanding of basic mechanisms operative in the micro-world (with particular emphasis on the physics of molecules) and of their relation to the macroscopic picture; 2. to learn the basic concepts of quantum mechanics, quantum chemistry, statistical mechanics and statistical thermodynamics.

## Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

### Lecture

1.Course code: A513W

- 2. Type of course: lecture
- 3. Tutor: Professor Marek Pawlikowski, Professor Piotr Petelenz
- 4.Number of hours: 30

5.**Description of the course:** Elements of theoretical mechanics: Newtonian, Lagrangian and Hamiltonian formalisms; generalized coordinates, normal vibrations. Classical statistical mechanics: phase spaces, canonical ensemble (other ensembles briefly mentioned), Maxwell-Boltzmann distribution, energy equipartition. Principles of quantum mechanics: postulates (Hilbert space), stationary states, simple applications (particle in a box, harmonic oscillator, rigid rotor, hydrogen atom).

6.Method of evaluation: written + oral exam (jointly, after completing A613)

- 7.ECTS: 5.0 (jointly with A613)
- 8.Semester: winter term

9.Bibiography:

### Classes

- 10. Course code: A513n
- 11. Type of course: classes

- 12. Tutor: Professor Marek Pawlikowski, Professor Piotr Petelenz
- 13. Number of hours: 30
- 14. Description of the course: According to the description of the lectures
- 15. Method of evaluation: written tests
- 16. ECTS: 2.5
- 17. Semester: winter term
- 18. Bibiography:

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- 1. Course code: A613 (continuation of A513)
- 2. Title of the course: Theoretical chemistry (small course)
- 3. Tutor: Professor Piotr Petelenz
- 4. Teaching objectives: The student is expected: 1. to acquire the understanding of basic mechanisms operative in the micro-world (with particular emphasis on the physics of molecules) and of their relation to the macroscopic picture; 2. to learn the basic concepts of quantum mechanics, quantum chemistry, statistical mechanics and statistical thermodynamics.

## Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

## Lecture

- 1. Course code: A613W
- 2. Type of course: lecture
- 3. Tutor: Professor Marek Pawlikowski, Professor Piotr Petelenz
- 4. Number of hours: 15
- 5. Description of the course: Quantum statistical mechanics: indistinguishability of quantum particles, ideal boson gas, ideal fermion gas (Pauli exclusion principle, electrons in metals). Statistical thermodynamics: application of spectroscopic data. Interacting many-electron systems: variational principle, Ritz method, secular equations, one-electron approximation and self-consistent field theory, correlation

energy. Elements of the quantum-mechanical theory of molecules: Born-Oppenheimer approximation and conditions of its applicability (potential energy surfaces, qualitative description of the Jahn-Teller effect), MO method (localized and delocalized orbitals, hybridization), SCF theory for molecules and limits of its applicability (basic methodological principles of *ab initio* and semi-empirical calculations), configuration interaction.

- 6. Method of evaluation: written + oral exam (jointly with A613)
- 7. **ECTS:** 5.0 (jointly with A513)
- 8. Semester: summer term
- 9. Bibiography:

#### Classes

- 1. Course code: A613N
- 2. Type of course: classes
- 3. Tutor: Professor Marek Pawlikowski, Professor Piotr Petelenz
- 4. Number of hours: 15
- 5. Description of the course: According to the description of the lectures
- 6. Method of evaluation: written tests
- **7. ECTS:** 1,5
- 8. Semester: summer
- 9. Bibiography:

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- 1. Course code: A514 (first part; continued as A614)
- 2. **Title of the course:** Theoretical chemistry ("large course"?)
- 3. Tutor: prof dr hab. Roman Nalewajski
- 4. Teaching objectives: (for both parts)

Introduction of basic notions of theoretical mechanics, statistical physics and quantum mechanics. Pointing out relationships between microscopic and macroscopic description. Presentation of basic methods of quantum mechanics and their application to the description of structure and dynamics of chemical systems

## Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture and classes(i)

## Lecture

- 1. Course code: A514W
- 2. Type of course: Lecture
- 3. Tutor: Marek Frankowicz
- 4. Number of hours:
- 5. Description of the course:

Elements of theoretical mechanics: Newton, Lagrange and Hamilton formalisms. Elements of theory of dynamical systems. Phase space and Liouville equaltion. Statistical ensembles: microcanonical, canonical, grand canonical. Maxwell-Boltzmann distribution.

Thermodynamical fluctuations. Quantum statistics. Statistical thermodynamics: molecular partition functions. Non-ideal gases. Simulation methods.

- 6. Method of evaluation: written exam
- 7. **ECTS:** 9.0 (together with A614)
- 8. Semester:winter
- 9. Bibliography:
  - 1. H. Buchowski, Elementy termodynamiki statystycznej, WNT, Warszawa 1998
  - 2. K. Gumiński, P.Petelenz, *Elementy chemii teoretycznej*, PWN, Warszawa 1989
  - 3. A. Maczek, Statistical Thermodynamics, Oxford Chemistry Primers, Vol. 58, 1998
  - 4. D. Stauffer, H.E.Stanley, Od Newtona do Mandelbrota, WNT, Warszawa 1996

## **Tutorials**

- 1. Course code: A514k
- 2.**Type of course:** tutorials

3.Tutor:

- 4.Number of hours: 30
- 5. Description of the course: same as lecture A514W
- 6.Method of evaluation:

7.**ECTS:** 2.5

8.Semester:winter

## 9.Bibliography:

- 1. H. Buchowski, *Elementy termodynamiki statystycznej*, WNT, Warszawa 1998
- 2. K. Gumiński, P.Petelenz, Elementy chemii teoretycznej, PWN, Warszawa 1989

- 3. A. Maczek, Statistical Thermodynamics, Oxford Chemistry Primers, Vol. 58, 1998
- 4. D. Stauffer, H.E.Stanley, Od Newtona do Mandelbrota, WNT, Warszawa 1996

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- 1. **Course code**: A515, A615
- 2. Title of the course: PRINCIPLES OF THE CHEMICAL TECHNOLOGY
- 3. Tutor: Prof. Roman Dziembaj, PhD, DSc
- 4. **Teaching objectives:** The Principles of Chemical Technology is an integrated course addressed to the students who already learned principles of inorganic, organic, physical and analytical chemistry together with those of mathematics and physics. The aim of the course is to provide students of university chemistry studies with minimum knowledge of industrial chemistry as well as of application of chemistry in various technological processes. Hence, rather large part of the course consists of laboratories and seminars.

#### **Description of the unit included in the course:**

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

### Lecture

- 1. Course code: A 515 W
- 2. Type of course: lecture
- 3. Tutor: Prof. Roman Dziembaj, PhD, DSc
- 4. Number of hours: 15+15
- 5. Description of the course: Essentials of the industrial chemistry, related to the process scale-up. Mass transport physics of flow, divergence between real and ideal systems, flow resistance, empirical parameters, technical solutions. Heat transport types, physical laws, real and ideal systems, empirical parameters, technical solutions. Theory of similarity as a tool of process engineer, modelling of technological processes. Kinetics of mass transport diffusion processes, phenomena on the phase boundary (adsorption, absorption, distillation, drying), porous systems, suspensions. Separation of mixtures unit operations. Chemical reactors chemical kinetics in ideal and real

systems, types of chemical reactors, diffusion restraints, catalytic reactors. Detailed description of some chosen groups of technological processes. Biotechnology – enzymatic reactions, biological treatment of waste waters, renewable sources of energy. Chemical technology in environment protection and regeneration – recycling, wasteless technologies.

- 6. Method of evaluation: examination
- 7. **ECTS:** 1,5+1,5
- 8. Semester: winter/summer
- Bibiography: [1] E. Bortel, H. Koneczny, "Zarys technologii chemicznej", [2] Wykład;
   [3] R. Gayer, Z. Matysikowa, "Zbiór zadań z technologii Chemicznej";

### Laboratory

- 1. Course code: A 515 L
- 2. Type of course: laboratory
- 3.Tutor: dr Marian Piasecki, dr Andrzej Cichocki, dr Andrzej Kochanowski, dr Marcin Molenda

4.Number of hours: 30

**Description of the course:** Students conduct laboratory experiments on diffusion operations (distillation, rectification), heat transport, hydrodynamics (flows, filtration sedimentation) and polymerisation.

5.Method of evaluation: tests before lab, execution of experiment, report

6.**ECTS:** 3

7.Semester: summer

**Bibiography:** [1] E. Bortel, H. Koneczny, "Zarys technologii chemicznej",[2] Wykład; [3] R. Gayer, Z. Matysikowa, "Zbiór zadań z technologii Chemicznej";

8.plus skrypt do cwiczen

#### **Calculation classes**

1. Course code: A 515 C

2. Type of course: calculation classes

3.Tutor: dr Marcin Molenda

4.Number of hours: 15

5. **Description of the course:** Students solve problems on hydrodynamics (mass transport, flow continuity, flow resistance, criteria numbers, sedimantation, filtration), theory of
similarity, heat transport (heat transport processes, heat exchangers) and diffusion operations (drying, distillation, rectification).

- 6. Method of evaluation: tests
- **7. ECTS:** 1,5
- 8. Semester: winter
- **9. Bibiography:** [1] Wykład; [2] R. Gayer, Z. Matysikowa, "Zbiór zadań z technologii Chemicznej"; [3] E. Bortel, H. Koneczny, "Zarys technologii chemicznej".

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- 1. Course code: A516
- 2. Title of the course: Molecular Spectroscopy
- 3. Tutor: prof. dr hab. Leonard M. Proniewicz
- 4. **jTeaching objectives:** The course provides an introduction to fundamentals and applications of molecular spectroscopy in chemistry. Students acquaint with principles of molecular spectrometric methods, their theory, methodology, instrumentation and applications in analysis and molecular structure determination. Students gain knowledge and skills in practical aspects of molecular spectroscopy methods, among others things: applications, advantages and disadvantages of particular methods in solution of typical problems, techniques of sample preparation, operation of equipment and interpretation of obtained results for simple molecules.

## Description of the unit included in the course:

## Lecture

- 1. Course code: A516w
- 2. Type of course: lecture
- 3. Tutor: prof. dr hab. Marek Pawlikowski, prof. dr hab. Marek Wójcik, prof. dr hab. Leonard M. Proniewicz
- 4. Number of hours: 34
- 5. Description of the course: Group theory and background of molecular spectroscopy. Symmetry operations, symmetry point groups, categories, discreet and continuous groups, invariance of Hamiltonian, linear space, linear independence of vectors, basis, operators and their unitary representations, reducible and irreducible representations,

characters, Great Orthogonality Theorem and its consequences, direct product of representations, projection operators, crystal (Ligand) field theory. Fundamentals of molecular spectroscopy: character of electromagnetic radiation and its features, spectrum of electromagnetic radiation, forms of molecular energy, thermal radiation and the Planck law, interaction between electromagnetic radiation and matter: absorption, spontaneous and induced emissions (Einstein coefficients), transition probability and selection rules, continuous and discreet spectra. Optical molecular spectroscopy: rotational spectra (energy levels of the rigid rotor, selection rules, model of the non-rigid rotor), vibrational-rotational and vibrational spectroscopy (infrared absorption, normal and resonance Raman scattering, non-linear Raman effects – energy levels of harmonic and anharmonic oscillators, permanent and induced dipole moments, polarizability and polarizability of radiation, selection rules, categories of normal modes), UV-VIS electronic, electronic-vibrational and electronic-vibrational-rotational spectra (the Jabłoński diagram, selection rules, vibronic transitions - Franck-Condon principle), time-resolved spectroscopy. Magnetic properties of matter (moment of momentum and magnetic moment of electrons and nuclei, selection rules of the spin absorption, the magnetic resonance), electron paramagnetic resonance EPR (paramagnetic centers, spinspin coupling, anisotropy of the spectral splitting factor) and nuclear magnetic resonance NMR (the nucleus shielding, chemical shift, spin-spin coupling), EPR and NMR relaxation processes. Electron spectroscopies: UV photoelectrons (UPS), Auger electron (AES) and X-ray photoelectrons (XPS or ESCA). Mössbauer spectroscopy. Mass spectrometry.

## 6. Method of evaluation: written exam

7. ECTS: 2.5

#### 8. Semester: winter

**Bibiography:** A. Cotton, *Teoria grup*, PWN, Warszawa, 1973; P.W. Atkins, *Molekularna mechanika kwantowa*, PWN, Warszawa, 1974; J.M. Janik (red.), *Fizyka chemiczna*, PWN, Warszawa, 1989; J. Twardowski (red.), *Biospektroskopia*, PWN, Warszawa, 1989-1990, tom 1-5; J. Konarski, *Teoretyczne podstawy spektroskopii molekularnej*, PWN, Warszawa, 1991; Z. Kęcki, *Podstawy spektroskopii molekularnej*, PWN, Warszawa, 1992; W. Demtröder, *Spektroskopia laserowa*, PWN, Warszawa, 1993; K. Małek, L.M. Proniewicz (red.), *Zastosowanie metod spektroskopii i spektrometrii molekularnej w analizie strukturalnej*,

Wydawnictwo UJ, Kraków, 2005; J. Sadlej, *Spektroskopia Molekularna*, WNT, Warszawa 2002; M. Pawlikowski, M. Pilch, *Spektroskopia molekularna*, skrypt (w przygotowaniu).

## **Tutorials**

- 1. Course code: A516k
- 2. Type of course: tutorials
- 3. Tutor: prof. dr hab. Leonard M. Proniewicz
- 4.Number of hours: 56
- 5.Description of the course: a) Group theory and its application in chemistry. Analysis of vibrational (classification of vibrational states and normal coordinates, symmetry in characteristic vibrations, determination of mode activity using the character tables) and electronic spectra (construction of molecular orbitals and symmetry of poly-electron functions). b) Infrared absorption (IR). c) Normal and resonance Raman scattering spectroscopy (NR i RR). d) Electronic spectroscopy (UV-VIS). e) Electron paramagnetic resonance spectroscopy (EPR). f) Nuclear magnetic resonance spectroscopy (NMR). g) Mass spectrometry (MS). b-g.: apparatuses and their advantages and disadvantages, techniques of sample preparation, measurement techniques, standard compounds, structural analysis of simple and complex spectra, qualitative analysis of mixtures, analysis of the band shape, application of the particular spectroscopic methods in various science disciplines.

6.Method of evaluation: the average grade of seven tutorial topics

7.ECTS: 5

8.Semester: winter

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- 1. Course code: A616
- 2. Title of the course: Molecular Spectroscopy

#### 3. Tutor: prof. dr hab. Leonard M. Proniewicz

**Teaching objectives:** The aim of this course is the practical acquaintance with the basic spectroscopic methods. Students gain knowledge and skills in practical aspects of molecular

spectroscopy methods, among others things: applications, advantages and disadvantages of particular methods in solution of typical problems, techniques of sample preparation, operation of equipment and interpretation of obtained results for simple molecules.

## **Description of the unit included in the course:**

## Laboratory

- 1. Course code: A616l
- 2. Type of course: laboratory
- 3. Tutor: prof. dr hab. Leonard M. Proniewicz
- 4. Number of hours: 30
- 5. Description of the course: The lab includes an acquaintance with construction and operation of various spectrometers, sample preparation, execution of measurements and analyses of obtained spectra. Experiments are carried out for following spectroscopic methods: Infrared, Electronic, Conventional and Resonance Raman Scattering, Electron Spin Resonance, Nuclear Magnetic Resonance and Mass Spectrometry.
- 6. Method of evaluation: the average grade of seven lab topics
- 7. **ECTS:** 3.5

## 8. Semester: summer

Bibiography: K. Małek, L.M. Proniewicz (red.), Zastosowanie metod spektroskopii i spektrometrii molekularnej w analizie strukturalnej, Wydawnictwo UJ, Kraków, 2005; A. Cotton, Teoria grup, PWN, Warszawa, 1973; P.W. Atkins, Molekularna mechanika kwantowa, PWN, Warszawa, 1974; J.M. Janik (red.), Fizyka chemiczna, PWN, Warszawa, 1989; J. Twardowski (red.), Biospektroskopia, PWN, Warszawa, 1989-1990, tom 1-5; J. Konarski, Teoretyczne podstawy spektroskopii molekularnej, PWN, Warszawa, 1991; Z. Kęcki, Podstawy spektroskopii molekularnej, PWN, Warszawa, 1992; W. Demtröder, Spektroskopia laserowa, PWN, Warszawa, 1993; J. Sadlej, Spektroskopia Molekularna, WNT, Warszawa 2002; M. Pawlikowski, M. Pilch, Spektroskopia molekularna, skrypt (w przygotowaniu).

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## 1. Course code: B501

## 2. Title of the course: Physical chemistry II

## 3. Tutor prof. dr hab. Jan Najbar

4. Teaching objectives: Basic physico-chemical models and their application for interpretation of properties of solutions, macromolecules, surface layers and colloids. Modern advances in instrumentation. Molecular aspects of dynamics of chemical reactions and transport phenomena.

## Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

#### Lecture

- 1. Course code: B501w
- 2. Type of course: lecture
- Tutor: : prof. dr hab. Maria Paluch, prof. dr hab. Jan Najbar, prof. dr hab. Marek Wójcik
- 4. Number of hours: 30 hours
- 5. Description of the course: Macromolecules and colloids: molecular, kinetic and electric properties; light scattering and rheology; thermodynamics of surface systems, surface films; molecular interactions and interactions between colloid particles. Tunneling, atomic force and near field fluorescence microscopies. Electric and magnetic properties of matter: liquid state, dielectric polarization and relaxation, solvation of ions and molecules, magnetic moments and magnetization. Kinetics and dynamics of chemical reactions: medium control of the reaction rates, relaxation of excited electronic states, laser techniques and their applications is chemistry, properties of transient species, transition states in elementary chemical transformations, photochemical processes; polymerization kinetics, catalysis and chemical oscillations. Conversion and accumulation of energy. Sonochemistry and radiochemistry Thermodynamics of irreversible processes and transport phenomena.
- 6. Method of evaluation: oral examination
- 7. ECTS: 2.5
- 8. Semester: winter
- 9. Bibiography:
- 1. A. Scheludko, Chemia koloidów, NT, Warszawa 1969

- 2. H. Sonntag, Koloidy, PWN, Warszawa 1982
- 3. A.W. Adamson, Chemia fizyczna powierzchni, PWN, Warszawa 1963
- 4. P.W. Atkins, Chemia fizyczna, Wydawnictwo Naukowe PWN, Warszawa 2000

P. Suppan, Chemia i światło, Wydawnictwo Naukowe PWN, Warszawa 1997

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- 1. **Course code**: B 502
- 2. Title of the course: Crystal Chemistry II
- 3.**Tutor**: prof. dr hab. Barbara Oleksyn
- 4. Teaching objectives:

The lectures aim at acquainting the students, who specialize in organic and biological chemistry, with elements of X-ray structure analysis of organic single crystals, especially of biologically active compounds. Special importance is assigned to the results of the crystal structure analysis and their role in determination and understanding the three-dimensional geometry of organic molecules and the structure – reactivity relationships. The students have opportunity to get knowledge of using crystal data contained in the crystallographic and chemical publications and in databases.

## Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture

and classes(i)

## Lecture

- 1. Course code: B 502 w
- 2. Type of course: lecture
- 3. Tutor: prof. dr hab. Barbara Oleksyn
- 4. Number of hours: 15
- 5. Description of the course:

Aims of the crystal structure analysis of organic compounds, its application to determination of the constitution, conformation, and absolute configuration of molecules and of their mutual interactions. Reminding the principles of the description of crystal structure as ordered arrays of molecules. Diffraction of X-rays on single crystals. Experimental methods of obtaining the diffraction pattern and its interpretation: phase problem and methods of its solution. Refinement of the obtained structure model. Information about molecular structure and intermolecular interactions gained from the crystal structure analysis: estimation of precision and accuracy of the obtained structure parameters. Examples of chemical problem solutions using results of crystal structure analysis of single crystals (on the base of recent publications in the field of organic chemistry).

- 6. Method of evaluation: writing test
- 7. **ECTS:** 1.5
- 8. Semester: winter
- 9. **Bibłiography:** 
  - J.P. Glusker, M. Lewis, M. Rossi, *Crystal Structure Analysis for Chemists and Biologists*, VCH, New York 1994
  - Selected papers published in Acta Crystallographica

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## Opis ogólny kursu:

(Cele dydaktyczne wypełnia się w stosunku do kursów obowiązkowych oznaczonych A i B)

- 1. Kod kursu: B503
- 2. Nazwa kursu: Crystallography II introduction to X-ray structure analysis of proteins
- 3. Osoba prowadząca: dr hab. Krzysztof Lewiński
- 4. **Cele dydaktyczne:** To develop the competence of the student to understand and apply results of protein crystallography.

## Opis jednostki wchodzącej w skład kursu.

np. wykład (w), ćwiczenia(n), laboratorium (l), konwersatorium (k), seminarium (s),

ćwiczenia rachunkowe (c), wykład + ćwiczenia (i)

# Wykład

- 1. Kod kursu: (powtórzyć poprzedni + odpowiednia literka)
- 2. Rodzaj zajęć: (z listy powyżej)
- 3. Prowadzący przedmiot:
- 4. Liczba godzin:

**Tematyka zajęć:** Protein crystallization: factors influencing solubility of proteins, crystallization methods, seeding. X-ray radiation sources, synchrotrones, diffractometers, low temperature experiments. Diffraction, relationship between the crystal structure and diffraction pattern. Methods of solving crystal structure: haevy atom method, multiple izomorphous replacement (MIR), multiwavelength anomalous diffraction (MAD), molecular replacement (MR), direct methods. Interpretation of electron density maps. Refinement and validation of protein structure, resolution, R and R<sub>free</sub>. Protein Data Bank.

- 5. Sposób zaliczenia: test
- 6. Liczba punktów ECTS: 2
- 7. Semestr: (zimowy, letni, zimowy/letni) summer

Literatura: J.P. Glusker, K.N. Trueblood, Zarys rentgenografii kryształów, PWN, 1997.;

D. Blow, Outline of Crystallography for Biologists, Oxford University Press, 2004.

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- 1. Course code: B504
- 2. **Title of the course:** CRYSTAL CHEMISTRY II (An Introduction to Crystal Structure Analysis)
- 3. Tutor: dr hab. Katarzyna Stadnicka
- 4. Teaching objectives:

Introducing students to the kinematics of X-ray diffraction on single crystals and to modern experimental methods; methods of phase problem solution and structural parameters refinement; discussion of the crystal structure analysis results such as the absolute structure, geometry of chemical units (e.g. molecules) and their mutual packing in the 3D space, conclusions concerning the type of interactions in the crystalline phases.

## Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

#### Lecture

- 1. Course code: B504w
- 2. **Type of course:** lecture(w)
- 3. Tutor: dr hab. Katarzyna Stadnicka
- 4. Number of hours: 15
- 5. Description of the course:

The basis of the kinematics theory of X-ray diffraction by single crystals: atomic scattering factor and structure factor; preliminary crystal data: unit cell parameters and lattice symmetry, Laue class, space group, determination of the number of molecules in the unit cell; methods of diffracted beams intensities collection – single crystal diffractometers; data processing; phase problem solution: Patterson methods (e.g. heavy atom method), isomorphic replacement methods, direct methods; structural parameters refinement: Fourier synthesis, difference Fourier synthesis, non-linear least-squares method; criteria for structural model reliability: absolute structure, features of the final difference Fourier map, residual indices; results of crystal structure analysis: atomic bond lengths, the values of valence angles and torsion angles, configuration and conformation of the molecules, mutual packing of the chemical units and intermolecular interactions (directional, like hydrogen bonds, and non-directional).

- 6. **Method of evaluation:** test or answering 11 questions concerning a crystallographic paper supplied
- 7. **ECTS:** 1.5
- 8. Semester: winter
- 9. Bibliography:
  - 1. J.P. Glusker, K.N. Trueblood, Zarys rentgenografii kryształów, PWN, 1977;
  - 2. P. Luger, Rentgenografia strukturalna monokryształów, PWN, 1989;
  - 3. Fundamentals of Crystallography, Giacovazzo (ed.), Oxford University Press, 1992;
  - 4. M.M. Woolfson, An Introduction to X-ray Crystallography, Cambridge University Press, 1997.

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## **Course code:** B505

Lecture ECTS 1,5

Introduction to Structural Analysis of Polycrystalline Materials.

Lecturer: dr hab. Wieslaw Lasocha

Teaching aims:

Description of the steps of the Structural Analysis of Crystalline Materials, Introduction to the phase problem, Fourier's Map calculations and direct methods. Limits in the process of structural analysis of polycrystalline materials, discussion of the importance of crystallographic research in chemistry, catalysis, materials science.

Course description:

Determination of the conditions of powder diffraction measurement carried out for structural analysis of polycrystalline materials. Basis of structural analysis of mono- and polycrystalline materials: Phase problem, Patterson method, direct methods. Application of Rietveld method to the refinement of a structure model. Analytical and metric aspects of the received results – significance of structural analysis in chemistry of new materials. Literature:

- 1.Z. Bojarski, M. Gigla, K. Stróż, M. Surowiec, *Krystalografia, podręcznik wspomagany komputerowo*, PWN, Warszawa 1996
- 2.P. Luger, Rentgenografia strukturalna monokryształów, PWN Warszawa 1989
- 3.C. Giacovazzo, Direct Phasing in Crystalography, Oxford University Press, 1998

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## 1.Course code: B606

## 2. Title of the course: Inorganic Chemistry II

3. Tutor: prof.dr hab.B.Sieklucka/ prof.dr hab.G.Stochel/ prof.dr hab./Z.Sojka

## 4. Teaching objectives:

Presentation of contemporary inorganic chemistry in the field of coordination chemistry, bioinorganic chemistry and chemistry of solid state by building upon the introductory and descriptive material in Inorganic Chemistry course. Developing the skills of solving the problems related to vigorous nature of contemporary inorganic chemistry.

## Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

## Lecture

- 1. Course code: B606
- 2. Type of course: lecture
- 3. Tutor: prof.dr hab.B.Sieklucka/ prof.dr hab.G.Stochel/ prof.dr hab./Z.Sojka
- 4. Number of hours: 30
- 5. Description of the course:

#### Electronic spectra and magnetism of coordination compounds. Magnetic molecular

**materials.** (10h) Spectroscopic terms. Ligand-field transitions: weak and strong-field limits, tanabe-Sugano diagrams, the nepheloauxetic series. Charge-transfer transitions. Selection rules and intensities.Electronic spectra of f-block metals. Magnetic properties of coordination compounds.The different forms of bulk magnetism.Curie-Weiss law. Paramagnetism of coordination compounds of d- and f-block metals. Ferro-, antiferro- and ferri-magnetism. Mechanisms of spin coupling. Spin-crossover systems. Magnetic molecular materials.

- 6. Method of evaluation: written exam
- 7. **ECTS:** 3.0
- 8. Semester: summer
- 9. Bibiography:
- 1. A.Bielański, Podstawy Chemii nieorganicznej, Wyd.5, PWN 2003.
- 2. F.A.Cotton, G.Wilkinson, P.L.Gaus, Chemia nieorganiczna. Podstawy, PWN 1995.
- 3. S.F.A.Kettle, Fizyczna chemia nieorganiczna, PWN 1999.
- 4. D.F.Shriver, P.W.Atkins, T.L.Overton, J.P.Rourke, M.T.Weller, F.A.Armstrong, Inorganic Chemistry, 4th Ed., OUP 2006.

5. J.E.Huheey, E.A.Keiter, R.L.Keiter, Inorganic Chemistry. Principles of Structure and Reactivity, 4th Ed., HarperCollins 1994.

- 6. S.J.Lippard, J.M.Berg, Podstawy chemii bionieorganicznej, PWN Warszawa 1998
- 7. J.Dereń, J. Haber, R. Pampuch, Chemia Ciała Stałego, PWN Warszawa 1977
- 8. A. F.Wells, Strukturalna Chemia Nieorganiczna, WNT, Warszawa 1993
- 9. R.Zallen, Fizyka Ciał Amorficznych, PWN, Warszawa 1994

10. S.Mrowec, Defekty Struktury i Dyfuzja Atomów w Kryształach Jonowych, PWN Warszawa 1974

11. N.B.Hannay, Chemia Ciała Stałego, PWN Warszawa 1972

#### Classes

- 1. Course code: B606
- 2. Type of course: classes

- Tutor: prof.dr hab.Barbara Sieklucka/prof.dr hab.Grażyna Stochel/prof.dr hab.Zbigniew Sojka
- 4. Number of hours: 15
- 5. Description of the course: in accordance with the lecture
- 6. Method of evaluation: written credit
- 7. **ECTS:** 1.5
- 8. Semester: summer
- 9. Bibiography:
- 1. A.Bielański, Podstawy Chemii nieorganicznej, Wyd.5, PWN 2003.
- 2. F.A.Cotton, G.Wilkinson, P.L.Gaus, Chemia nieorganiczna. Podstawy, PWN 1995.
- 3. S.F.A.Kettle, Fizyczna chemia nieorganiczna, PWN 1999.
- 4. D.F.Shriver, P.W.Atkins, T.L.Overton, J.P.Rourke, M.T.Weller, F.A.Armstrong, Inorganic Chemistry, 4th Ed., OUP 2006.
- 5. J.E.Huheey, E.A.Keiter, R.L.Keiter, Inorganic Chemistry. Principles of Structure and Reactivity, 4th Ed., HarperCollins 1994.
- 6. S.J.Lippard, J.M.Berg, Podstawy chemii bionieorganicznej, PWN Warszawa 1998
- 7. J.Dereń, J. Haber, R. Pampuch, Chemia Ciała Stałego, PWN Warszawa 1977
- 8. A. F.Wells, Strukturalna Chemia Nieorganiczna, WNT, Warszawa 1993
- 9. R.Zallen, Fizyka Ciał Amorficznych, PWN, Warszawa 1994
- 10. S.Mrowec, Defekty Struktury i Dyfuzja Atomów w Kryształach Jonowych, PWN Warszawa 1974
- 11. N.B.Hannay, Chemia Ciała Stałego, PWN Warszawa 1972

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- 5. Course code: B607W
- 6. Title of the course: 2ND PHYSICS
- 7. Tutor: Professor Andrzej Bałanda
- 8. **Teaching objectives:** Instructing of listeners with introduction to the theory of relativity and with grounds of physics of smaller objects from the atom. The student should acquire knowledge referring to basic information about elementary particles and chosen issues of nuclear physics.

## Description of the unit included in the course:

- 10. Course code: B607W
- 11. **Type of course:** lecture(w)
- 12. Tutor: Professor Andrzej Bałanda
- 13. Number of hours: 30 h

**Description of the course:** Relativity of the movement: relativity of the movement and adding the speed, measurements of the speed of the light, simultaneity of events, the spacetime continuum, the Lorentz transformation and the transformation of the speed, the interval and calibration curves, the dilatation of the time and the counterwork of the distance, twins' paradox. Relativistic dynamics: relativistic speed, total energy, the association of energy and speed. Accelerating of particles to big energy. The laboratory setup and the setup of the center of the mass. Introduction to the physics of elementary particles. Methods of detection of particles, detection of basic particles. Positronium and energy of his states, the description of states by means of quantum numbers, classification of states. The model of quarks and the classification light hadrons. The scattering and nuclear reactions. Elements of nuclear physics. The measuring of parameters describing basic properties of atomic nucleus. The semiempirical model of atomic nucleus. Elements of the shell and deformed models. Decays of the atomic nucleus. Splitting of the atomic nucleus and obtaining nuclear energy. Nucleosynthesis and her astrophisical aspects..

- 14. Method of evaluation: control of presence on the lecture; test
- 15. **ECTS:** 2.5
- 16. Semester: summer
- 17. Bibiography:

A.Bałanda, Fizyka dla chemików, skrypt UJ, Kraków 1990

D. Halliday, R. Resnick, J. Walker, *Podstawy fizyki*, in particular vol. 5, PWN, Warszawa 2003

A.K.Wróblewski, J.A.Zakrzewski, *Wstęp do fizyki*, t.1, PWN Warszawa 1976 and subsequent editions

V. Acosta, C.L.Cowan, B.J. Graham, *Podstawy fizyki współczesnej*, PWN Warszawa 1987 and subsequent editions

A. Bałanda, Statystyczne metody opracowań pomiarów, PWSZ Nowy Sącz, 2002

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- 1. Course code: B608
- 2. Title of the course: Advanced methods in physical chemistry
- 3. Tutor dr hab. Marek Mac
- 4. **Teaching objectives:** To get acquainted with the modern methods applied in physical chemistry. Development of learning in the student team- arrangement of the experimental plan, discussion of the strategy of the realization of the project, carrying out the experiment, discussion and preparation of the appropriate form of the results presentation. Usage of the computer techniques in calculations and presentation of experimental results.

# Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

## Laboratory

- 1. Course code: B608l
- 2. Type of course: laboratory
- 3. Tutor: : dr hab. Marek Mac
- 4. Number of hours: 30 hours
- 5. Description of the course: Method of the range: estimation of the report and results presentation Equilibrium vapour-liquid in two-component systems, estimation of the activity coefficients from the solubility measurements, estimation of the critical micelle concentration (CMC) of the ionic surfactants in the presence of strong electrolyte, influence of electric polarization on the course of chemical reaction, Broensted salt effect, estimation of the transport number of ions in electrolyte, nanovoltaic sun battery, factor analysis of spectroscopic data.

## 6. Method of evaluation: evaluation of the report and of the oral presentation of results

- 7. ECTS: 3.0
- 8. Semester: summer

Bibiography: P.W. Atkins, Chemia fizyczna, PWN, Warszawa 2000

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## Course code: Ca01

Title of the course: Flow Analysis

Tutor: Prof. dr hab. Paweł Kościelniak

## **Teaching objectives:**

- a) To transform knowledge from the field of the flow analysis with special attention to its application aspects.
- b) To indicate the place and role of the flow analysis in analytical chemistry.

## Description of the unit included in the course:

Lecture

## **Course code: Ca01w**

Type of course: lecture

Tutor: Prof. dr hab. Paweł Kościelniak

## Number of hours: 15

**Description of the course:** Origin, review, characteristics and comparison of techniques in flow analysis. Design and operation mode of flow systems. Theoretical basis, basic features and parameters of flow analysis (with special attention to flow injection analysis). Control of chemical reactions. Dilution methods. Methods of the sample preconcentration and separation. Calibration procedures. Realization of multicomponent analysis and speciation analysis. Application of chemometrics methods to data analysis. Tendencies and perspectives of the flow analysis development.

Method of evaluation: examination

## **ECTS:** 1,5

## Semester: winter

## **Bibiography:**

 a) B. Karlberg, G.E. Pacey, "Wstrzykowa analiza przepływowa dla praktyków", WNT, Warsaw 1994.  b) M. Trojanowicz, "Automatyzacja w analizie chemicznej", chapter 4., WNT, Warsaw 1992.

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Course code: Ca03

Title of the course: Analytical Chemistry III Tutor: prof. dr hab. Andrzej Parczewski Teaching objectives:

# Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture

and classes(i)

Lecture

Course code: Ca03

**Type of course:** lecture (w)

Tutor: prof. dr hab. Andrzej Parczewski

Number of hours: 45

## **Description of the course:**

Classification of the instrumental methods of analysis; atomic absorption spectrometry; atomic emission spectrometry; basic concepts and definitions and the methods of analytical data handling; molecular spectrometry (UV/VIS/IR); X-rays spectrometry; electroanalytical methods of analysis; potentiometry, voltametric techniques, amperometric titrations, electroseparation, coulometry, conductance methods; mass spectrometry; radiochemical methods; thermal analysis. Separation methods: electrophoresis, gas and liquid chromatography, thin layer chromatography. Other selected problems and methods, e.g. : local and distribution analysis, immunometric methods, genetic fingerprint (DNA) method. Analytical process: problem formulation, sampling, sample preparation for instrumental measurement, calibration and data handling, formulation of conclusions concerning the problem stated. Introduction to automated analysis and process analysis. Selected applications of instrumental methods of analysis: examples and problems.

Method of evaluation: examination

**ECTS:** 4.5

Semester: winter

**Bibiography:** 

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Course code: Ca04 Title of the course: Chemometric and biometric methods Tutor: prof. dr hab. Andrzej Parczewski Teaching objectives:

## Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

Lecture Course code: Ca04 w Type of course: lecture Tutor: prof. dr hab. Andrzej Parczewski Number of hours: 30

## **Description of the course:**

Statistical treatment of experimental data. Introduction to mathematical modeling of processes. Empirical modeling. Linear models: determination of the model parameters and the corresponding variance-covariance matrix, model adequacy testing. Nonlinear models. Design of experiments. Optimization methods: single factor, gradient, simplex, Monte Carlo, Genetic Algorithm. Statistical treatment of multidimensional data. Introduction to the Principal Component Analysis (PCA) and Factor Analysis (FA), Cluster Analysis (CA), Pattern Recognition methods, Artificial Neural Networks (ANN), and other chemometric methods. **Method of evaluation:** credit

ECTS: 3.0 Semester: winter Bibiography:

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Course code: Ca06 Title of the course: CHEMICAL INVESTIGATION IN CRIMINALISTICS AND TOXICOLOGY Tutor: Staff of the Institute of Forensic Research and of FCJU Teaching objectives:

#### Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

Laboratory

Course code: Ca06

**Type of course:** laboratory (l)

Tutor: Staff of the Institute of Forensic Research and of FCJU

Number of hours: 90hrs

**Description of the course:** Ethyl alcohol – selected toxicological and analytical aspects; Intoxicated and psychotropic drugs in toxicological analysis; Application of the GC/MS method to analysis of drugs in biological material; Determination of inorganic poisons in biological material; Examination of car paints; Examination of fibers; Examination of gun shot residues; Examination of inks; Chemical analysis of inks by capillary electrophoresis; Analysis of biological material – simultaneous determination of selenium and arsenic by atomic fluorescence spectrometry; Profiling of narcotics by thin-layer chromatography – part I: LLC extraction; Profiling of narcotics by thin-layer chromatography – part I: SPE extraction.

Method of evaluation: ECTS: 10.5 Semester: summer Bibiography:

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**Course code: Ca08** 

Title of the course: Ecotoxicology and environmental toxicology

Tutor: Prof. dr hab. Wojciech Piekoszewski

**Teaching objectives:** 

#### **Description of the unit included in the course:**

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

## Lecture

Course code: Ca08w

Type of course: lecture

Tutor: Prof. dr hab. Wojciech Piekoszewski

Number of hours: 30

**Description of the course:** Ecotoxicology as a scientific discipline. Contamination of natural environment. Fate of xenobiotics in the environment – atmosphere, water and soil. Bioaccumulation. Evaluation of the influence on the natural environment. Methods used in study the evaluation of the influence on the natural environment. Characteristic of selected contaminations of the natural environment.

Evaluation of the effect of environmental contaminations on human organism. Methods of the evaluation of the exposure to the air pollutions. Threshold Limit Values. Evaluation of carcinogenic risk in humane. Evaluation of the exposure to the mixture of xenobiotics. Biomarkers of exposure, effect and sensitivity. Risk assessment.

Method of evaluation: test exam

**ECTS:** 2

Semester: summer

**Bibliography:** C.H.Walker, S.P.Hopkin, R.M.Sibly: Podstawy ekotoksykologii Curtis D. Klassen: Casatett & Doull's Toxicology. The Basic Science of Poisons. 6<sup>th</sup> edition. McGrow Professional, 2001.

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## **Course code: Cb01**

Title of the course: Modern methods of electroanalysis applied in chemistry and environmental protection Tutor: dr Tadeusz Bieszczad Teaching objectives: does not concern

# Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

## Lecture

Course code: Cb01w

Type of course: lecture

**Tutor:** : dr Tadeusz Bieszczad

## Number of hours: 30 hours

**Description of the course:** Classification of electroanalytical methods, electrolytic conductivity, molar and equivalent conductivity, ionic mobility, conductometric techniques – classic, conductometry of the small and high frequency, conductometric titration, application of conductometric methods, solution equilibrium, activity, activity coefficient, solvation and association of ions, solid state-solution equilibrium, electrochemical potential, Nernst eqation, mixed potential, ion selective electrode potential, Nikolski equation, the measurement of e.m.f., ion selective electrodes – division, application and overpotential, electrogravimetric analysis – classic and potential-controlled electrogravimetry, inner electrogravimetry, coulometry at controlled potential and controlled current, coulometric titration, direct (DCP) and alternating (ACP) current polarography, squere wave polarography (SWP), normal (NPP) and differential (DPP) pulse polarography, lineat sweep voltammetry (LSV), cyclic voltammetry, stripping voltametry (SV), potentiometry stripping analysis (PSA), monitoring systems in environment protection.

Method of evaluation: credits or examination

ECTS: 3.0 Semester: summer Bibiography:

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## **Course code: Cb02**

Title of the course: Statistical methods applied to analysis chemical experiment data Tutor dr Marek Boczar Teaching objectives:

## Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

#### Lecture

Course code: Cb02w

Type of course: lecture

Tutor: : dr Marek Boczar

#### Number of hours: 15 hours

**Description of the course:** Random variable. Distributions of discrete random variables: twopoint distribution, binomial distribution, Pascal's distribution, Poisson distribution. Continuous random variable distributions: uniform distribution, normal distribution, truncated normal distribution, exponential distribution. Estimation of parameters of random variable distribution. Point estimation. Estimation of expected value: sample arithmetic mean, order statistic. Estimation of variance and standard deviation from sample. Confidence interval estimation: general principles of determination of confidence intervals, confidence interval for the expected value, confidence interval for variance and standard deviation, confidence interval for madian. Testing statistical hypotheses. Verification of the significance of the difference between the expected values of two random variables. Verification of the difference between the variance of the random variable and the determined value. Analysis of variance. Correlation and regression. Correlation: model and its verification, measures of dependence, correlation coefficient assessment, study of significance of correlation. Regression: variable, function, regression. The least squares method, the minimum of the multivariable function. Linear regression models by the least square method: defining approximation error, regression of y with regard to x, orthogonal regression, regression of x with regard to y, weighted regression. Residual and its distribution. Testing significance of regression coefficient (slope) and intercept. Confidence intervals determination in regression analysis. Tolerance region for values off the regression line.

#### Method of evaluation: examination

#### **ECTS:** 1.5

#### Semester: winter

#### **Bibiography:**

- J.B.Czermiński, A.Iwasiewicz, Z.Paszek, A.Sikorski, Metody statystyczne dla chemików, PWN Warszawa 1992
- 2. S.Brandt, Analiza danych, PWN Warszawa 1998

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# Course code: Cb03

Title of the course: Physical Chemistry of Nanostructured Surfaces

Tutor: dr Beata Korchowiec

Teaching objectives: does not concern

#### **Description of the unit included in the course:**

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture and classes(i)

Lecture

Course code: Cb03w

Type of course: lecture

Tutor: dr Beata Korchowiec

Number of hours: 30 hours

**Description of the course:** Thermodynamics of surfaces. Contact angle and surface tension: their relation to wetting and spreading phenomena. The Laplace and Young equations. Cohesion, adhesion and spreading. Methods of surface tension and contact angle measurement. Formation and stability of insoluble monolayers; surface pressure. Microstructural phases in monolayers; gaseous, liquid and condensed films. Surface equation of state. Some properties of mixed Langmuir monolayers; ideal mixtures. The Gibbs energy of mixing. Experimental measurement of film pressure. Langmuir film balance. Applications of monolayers and monolayer concepts. Surfactant nanolayers: Langmuir-Blodgett films. Adsorption from solution. The Gibbs equation: two-component systems. Interactions in mixed adsorption monolayers. Thermodynamics of adsorption process. Electrical properties of the free surface of aqueous solutions. Critical micelle concentration and the thermodynamics of micelization.

Method of evaluation: exam ECTS: 3.0 Semester: summer Bibiography:

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# Course code: Cb07

Title of the course: Applied Electrochemistry Tutor: apl. prof. dr hab. Marian Jaskuła Teaching objectives: does not concern

# Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture and classes(i)

Lecture Course code: Cb07w Type of course: lecture Tutor: : apl. prof. dr hab. Marian Jaskuła Number of hours: 15 hours Description of the course:

- electrochemical power sources: barreries, accumulators, fuel cells. Possibilities and limitations of their use,
- electrochemical corrosion and methods of protection,
- some aspects of production of new materials,
- the electrokinetic effects and their application in environment protection (waste water purification, removing heavy metals from soil),
- electrosynthesis of organic compounds,
- conducting polymers and electropolymerization,
- electrochemistry in chemical analysis and in scientific research

Method of evaluation: credit ECTS: 1.5 Semester: winter Bibiography:

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## Course code: Cb08

Title of the course: Electrochemistry of Electrolyte Solutions Tutor: apl. prof. dr hab. Marian Jaskuła Teaching objectives: does not concern

## Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)
Lecture
Course code: Cb08w
Type of course: lecture
Tutor: : apl. prof. dr hab. Marian Jaskuła
Number of hours: 30 hours
Description of the course: Molecular interactions, structure of fluid, ion-solvent interactions,
association and incomplete dissociation of strong electrolytes, theories of ionic interations,
theory of galvanic cells, electrochemistry in non-aqueous solutions

Method of evaluation: examination ECTS: 3.0 Semester: winter Bibiography:

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Course code: Cb09

Title of the course: Advanced Electrochemistry Tutor: apl. prof. dr hab. Marian Jaskuła Teaching objectives: does not concern

## Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

## Lecture

Course code: Cb09w

Type of course: lecture

Tutor: apl. prof. dr hab. Marian Jaskuła

## **Number of hours: 15 hours**

# **Description of the course:**

- The thermodynamics of concentrated electrolyte solutions
- The transport processes in electrolyte solutions
- The double electrical layer
- The physicochemical processes at the phase interface: adsorption,
- charge transfer
- The electrochemistry of non aqueous solutions and fused salts

Method of evaluation: credit ECTS: 1.5 Semester: winter Bibiography:

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# Course code: Cb10

Title of the course: Introduction to polymer spectroscopy and photochemistry Tutor dr Joanna Kowal Teaching objectives:

# Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

## Lecture

Course code: Cb10w

# Type of course: lectur Tutor: : dr Joanna Kowal Number of hours: 15 hours

**Description of the course:** Light absorption, radiative and non-radiative transitions in organic molecules. Kinetics of the deactivation of excited states. Formation of excimers and exciplexes. Energy transfer. Absorption and emission characteristics of polymers. Excimers in polymer systems, energy transfer and migration in polymers, antenna effect. Photodegradation and photooxidation of polymers. Photosensitized degradation. Photostabilization of polymers.

Method of evaluation: written exam ECTS: 1.5 Semester: Bibiography:

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## Course code: Cb11

**Title of the course:** Physicochemistry of polymeric systems **Tutor**: dr Szczepan Zapotoczny, prof. dr hab. Maria Nowakowska

Teaching objectives: does not concern

## Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture and classes(i)

Lecture

Course code: Cb11w

Type of course: lecture

Tutor: : dr Szczepan Zapotoczny, prof. dr hab. Maria Nowakowska

Number of hours: 15 hours

**Description of the course:** Polymer structure, conformation, configuration. Physicochemical methods for polymer studies: end-group analysis, osmometry, light scattering, viscometry, sedimentation, spectroscopies. Phase transitions in polymeric systems, polymer crystals. Correlation between structures of polymers and their physicochemical properties.

Method of evaluation: examination

# ECTS: 1.5 Semester: summer Bibiography:

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# Course code: Cb12

Title of the course: Electron and proton transfer processes Tutor dr hab. Marek Mac Teaching objectives: does not concern Description of the unit included in the course: lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture and classes(i) Lecture

Course code: Cb12w

Type of course: lecture

Tutor: : dr hab. Marek Mac

Number of hours: 15 hours

**Description of the course:** Aim of the lecture is to describe the fundamental photophysical processes such as electron and proton transfer in monomolecular and polymolecular systems. The following topics will be addressed: Marcus theory for electron transfer and its extensions and applications for the description of the photophysical and photochemical behaviours in model systems and in the systems having potential practical applications. Monomolecular and bimolecular electron transfer processes: exciplexes, TICT states, excited singlet and triplet quenching, CT fluorescence band-shape analysis. Photochemical reactions, induced by the electron transfer processes: photosensibilized isomerisation processes, photodechlorination of 9,10-dichloranthracene. Solvent and salt effects on electron transfer processes. Influence of temperature on the electron transfer rate constant.

Method of evaluation: examination

ECTS: 1.5 Semester: summer

**Bibiography:** 

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## Course code: Cb13

Title of the course: Molecular photochemistry and photophysics Tutor prof. dr hab. Jan Najbar Teaching objectives:. Does not concern

#### Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture and classes(i)

Lecture

**Course code:** Cb13w

Type of course: lecture

Tutor: : prof. dr hab. Jan Najbar

Number of hours: 15 hours

**Description of the course** Experimental methods in photochemistry: lifetimes of excited states and quantum yields of photophysical and photochemical processes. Potential energy functions for the ground and electronic excited states of organic molecules. Fluorescence, phosforescence and radiationless transitions in aromatic hydrocarbons, carbonyl and azaaromatic molecules. Properties of the electronically excited molecules: charge distributions, proton affinities, reduction and oxidation potentials. Heavy atom effects on photophysical processes. The role of the conical intersections in the relaxation of the excited states. Monomolecular and bimolecular photochemical processes in solutions. Kinetics and dynamics of the fast multistep photochemical and photophysical processes. Proton and electron transfer, exciplex formation. Photoisomerization processes.

Method of evaluation: examination or credit

ECTS: 1.5 Semester: winter Bibiography:

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# Course code: Cb16

Title of the course: Photochemistry in microheterogenic systems Tutor: prof. dr hab. Maria Nowakowska, dr Krzysztof Szczubiałka Teaching objectives: does not concern

# Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture and classes(i)

Lecture

Course code: Cb16w

Type of course: lecture

Tutor: prof. dr hab. Maria Nowakowska, dr Krzysztof Szczubiałka

## Number of hours: 15 hours

## **Description of the course:**

- 1. Types of microheterogeneous systems.
- 2. Basic photophysical and photochemical terms
- 3. Photophysics and photochemistry in:
  - micelles
  - reversed micelles
  - microemulsions
  - biological microphases
  - monolayers
  - liquid crystalline solvents
  - polymers and polyelectrolytes
  - ion exchange resins
- 4. Photoprocesses in molecular inclusion complexes (cyclodextrins, zeolites, crown ethers, cryptands)
- 5. Photochemistry of molecules adsorbed on the surfaces of inorganic oxides and colloids.

# Method of evaluation: examination

**ECTS:** 1.5

**Semester:** winter

## **Bibiography:**

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Seminar: Physicochemical bases of nanotechnology

**Course code: Cb17** 

Type of course: seminar

Tutor: Professor Maria Nowakowska

Number of hours: 60

**Description of the course: Synthesis and properties of nanostructural objects**. Selfassembly and controlled synthesis/modification. Supramolecular systems. Surface modification and chemical pattering. Experimental methods for studies of nanostructurs.

**Nanomaterials**. Materials for nanotechnology and environmental protection. Polymers, semiconductors and hybrids. Biomaterials and their applications in medicine, pharmacy and biology. Bioinspiration.

Method of evaluation: completion based on the presentation and participation in discussion.

**ECTS:** 6

Semester: winter/summer

Literature : 1. Regis ED, Nanotechnologia, Prószyński i S-ka, Warszawa, 2001

- Ozin G., Arsenault, A., "nanochemistry. Approach to Nanomaterials", RSC Publishing, Cambridge, 2006
- 3. Selected papers from scientific journals

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Course code: Cb18

Title of the course: Physical chemistry of disperse systems

**Tutor:** : prof. dr hab. Maria Paluch

Teaching objectives: does not concern

Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

Lecture

Course code: Cb18w

Type of course: lecture

Tutor: : prof. dr hab. Maria Paluch

Number of hours: 30 hours

**Description of the course:** Classification of colloid systems and their occurrence and preparation. General properties of colloid systems (Brownian motions, diffusion, osmotic pressure, sedimentation), optical properties, electrochemistry of interfaces, structure of the electrical double layer, interfacial potentials, electrocapillary curve, electrokinatic phenomena (electrophoresis, electroosmosis, streaming, potential, Dorn-effect), rheology properties (viscosity, plasticity, thixotropy and dilatancy), foams, emulsions, suspensions, water properties in thin films.

Method of evaluation: written test ECTS: 3.0 Semester: winter Bibiography:

Course code: Cb19

Title of the course: Interactions in disperse systems Tutor: : prof. dr hab. Maria Paluch Teaching objectives: does not concern Description of the unit included in the course: lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture and classes(i) Lecture Course code: Cb19w Type of course: lecture Tutor: : prof. dr hab. Maria Paluch (head) Number of hours: 15 hours **Description of the course:** Electrostatic interactions, charge and potential distribution between two piano-parallel and spherical identical electric double layers. Free energy and repulsion potential at charging diffusion double layers. Dispersion interactions between plano-parallel plates and spherical particles micro- and macroscopic theory, experimental determination of Hameker constant.

The total interaction between colloidal particles, flocculation criterion. Electrostatic and dispersion interactions in heterosystems, potential and charge distribution and free energy in electric double layers, attracting and repulsing dispersion actions, the total interactions and criteria of heterocoagulation.

Method of evaluation: test ECTS: 1.5 Semester: winter Bibiography:

**Course code: Cb20** 

Title of the course: Factor Analysis in Chemistry

Tutor: dr Andrzej Turek

Teaching objectives: does not concern

#### Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture and classes(i)

#### Lecture

Course code: Cb20w

Type of course: lecture

Tutor: dr Andrzej Turek

Number of hours: 15 hours

**Description of the course:** Diverse aspects of the factor analysis methods applied in chemistry are addressed, in particular the techniques allowing to identify and resolve the pure component spectra of the complex reaction products formed in the course of photochemical transformations. The covered theoretical topics and practical applications include Target Factor Analysis (TFA), Evolutionary Rank Analysis (ERA), non-factor algorithms of spectral analysis, conventional and generalized Rank Annihilation Factor Analyses (RAFA and

GRAFA), a comparison between physically constrained and unconstrained methods of factor analysis, the regression models for two-way two-block data analysis (Muliple Linear Regression (MLR), Principal Component Regression (PCR), and Partial Least Squares (PLS) regression), Non-quantitative and Quantitative Structure-Activity Relationships (SAR and QSAR), Multimode Factor Analysis (3DRAFA, Alternating Least Squares Multiple Component Regression (ALS-MCR), the Tucker models and Parallel Factor Analysis (PARAFAC)). All the discussed techniques are illustrated with many practical examples.

Method of evaluation: test ECTS: 1.5 Semester: summer Bibiography:

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#### **Course code: Cb21**

Title of the course: Selected problems of molecular spectroscopy

Tutor: Prof. dr hab. Marek Wójcik

Teaching objectives: does not concern

#### Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture and classes(i)

Lecture

Course code: Cb21w,s

**Type of course:** lecture + seminar

Tutor: : Prof. dr hab. Marek Wójcik

Number of hours: 30 hours

**Description of the course:** Lecture and analysis of selected original spectroscopic publications presented by participants of the course.

Foundations of spectroscopy: characteristics of electromagnetic radiation, division of absorption spectroscopy, intensity of bands, band shape and its description, problems related to presence of background. Experimental methods in absorption spectroscopy: scheme of absorption spectrophotometer, sources of radiation, monochromators - resolving power, detectors and recorders, preparation of samples. Electronic spectroscopy: molecular terms,

correlation diagrams, classification and characteristic of absorption transitions in electronic spectra, chromophores and auxochromes, batho- and hypsochromic shifts, hyper- and hypochrome effects, spectra of saturated compounds, effect of conjugation on electronic spectra, theory of crystal field - spectra of complexes of transition metals, effect of intramolecular and intermolecular perturbations on electronic spectra, applications of electronic spectroscopy - purity control, identification and determination of structure, cis-trans isomerization, tautomerization, determination of molecular mass, spectroscopic titration, chemical kinetics. Vibrational spectroscopy: harmonic and anharmonic oscillator, normal vibrations of molecules, Wilson method of normal modes, characteristic frequencies of vibrations, practical interpretation of infrared spectra, effects of intramolecular and intermolecular perturbations on infrared spectra, adiabatic approximation - Franck-Condon rule, linear crystal, polymers, phonons. Rotational spectroscopy: rotational energy levels, determination of molecular conformation from rotational spectra, interaction of rotations and vibrations. Electronic spectroscopy of selected systems. Vibrational spectroscopy of selected systems.

Method of evaluation: colloquium or examination

ECTS: 3.0 Semester: winter Bibiography:

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**Course code: Cb22** 

Title of the course: : Spectroscopy of hydrogen-bonded systems

Tutor: Prof. dr hab. Marek Wójcik

Teaching objectives: does not concern

#### Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

Lecture

Course code: Cb22w

Type of course: lecture

Tutor: : Prof. dr hab. Marek Wójcik

#### Number of hours: 30 hours

**Description of the course:** Historic outline. Occurrence and importance of hydrogen bonds. Definition of hydrogen bond. Geometric and energetic criteria. Intra and intermolecular hydrogen bonds. Properties of hydrogen-bonded systems. Infrared spectra of hydrogen bonds. Theories of infrared spectra of isolated hydrogen bonds and of systems of interacting hydrogen bonds. Fermi resonance and its occurrence in spectra of strong hydrogen bonds. Model potentials for hydrogen bonds and their application for explanation of spectral and structural correlations in hydrogen-bonded systems. Proton tunneling in systems with hydrogen bonds. Theories of multidimensional proton tunneling. Intra and intermolecular potentials for water. Spectra of hydrogen bonds in ices and aqueous ionic solutions. Theoretical simulation of spectra of ices and aqueous solutions with application of molecular dynamics method.

Method of evaluation: colloquium or examination

ECTS: 3.0 Semester: winter Bibiography:

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## Course code: Cb24

Title of the course: Laser spectroscopy and ultrafast processes in chemistry

Tutor: dr Przemysław Kolek, dr Sebastian Leśniewski

**Teaching objectives:** 

## Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)
Lecture
Course code: Cb24W
Type of course: lecture
Tutor: dr Przemysław Kolek, dr Sebastian Leśniewski
Number of hours: 30
Description of the course:

The lecture is an introduction to laser spectroscopy.

<u>1.Introduction</u>. Absorption and emission of electromagnetic radiation. Width and shape of spectral profiles, spectral broadening..

<u>2. Basics of lasers.</u> Population inversion in active medium, pumping methods. Resonator types, longitudinal and transverse modes of emitted laser radiation. Methods of selecting spectral bands and modes. Methods of producing narrow spectral bands. Spectral and spacial hole burning, mode switching, causes of unstable laser action.

<u>3. Overview of lasers</u> working in the range from microwaves to vacuum UV. Fixed wavelength lasers and tunable lasers.

<u>5. High-sensitivity methods of laser spectroscopy.</u> Fluorescence excitation spectroscopy. Photoacoustic spectroscopy. Intracavity absorption and cavity ring-down spectroscopy. Ionization and optogalvanic spectroscopy. Multiphoton spectroscopy.

<u>6. Doppler-free high-resolution spectroscopy.</u> Spectroscopy in molecular beams, spectroscopy in fast ion beams. Ion trapping. Saturation spectroscopy. Polarization spectroscopy. Nonlinear phenomena. Optical trapping of atoms and optical cooling.

7. <u>Time-resolved laser spectroscopy.</u> Investigation of transient species in photochemical reactions. Spectroscopic methods used for determining the kinetics of photochemical and photophysical processes.

<u>8. Ultrafast processes in chemistry.</u> Generation of ultrashort laser pulses. Mode locking. The titanium-sapphire laser as an example of vibronic lasers. Solvation dynamics, electron solvation, photoisomerization, ultrafast electron and proton processes. Rotational and vibrational relaxation. Photon echo.

## Method of evaluation: exam

**ECTS:** 30

Semester: summer

## **Bibiography:**

1. H. Abramczyk, Wstęp do spektroskopii laserowej, Wydawnictwo Naukowe PWN,

Warszawa, 2000.

2. W. Demtroeder, Spektroskopia laserowa, Wydawnictwo Naukowe PWN, Warszawa, 1993.

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## Course code: Cb27

Title of the course: Photopolymerization and photocrosslinking

Tutor: dr Mariusz Kępczyński

**Teaching objectives:** 

## **Description of the unit included in the course:**

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)
#### Lecture

Course code: Cb27w

Type of course: w

Tutor: dr Mariusz Kępczyński

Number of hours: 15 hours

**Description of the course:** Introduction to the kinetics of photochemical processes. Difference between polymerization and photopolymerization. Types of photoinitiators. Kinetics of photopolymerization. PLP- pulse laser polymerization. Application of photopolymerization. Photocrosslinking. Types of photoresists. Photolithography. Application of photolithography in microelectronics. Photochromic processes and its applications. Photochromism in the polymer systems. Photochemical reactors.

Method of evaluation: essay ECTS: 1.5 Semester: Bibiography:

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Lecture: Surface active compounds in nanotechnology

Course code: Cb28

Type of course: lecture

Tutor: dr Paweł Wydro

Number of hours: 15

**Description of the course:** Structure and properties of solutions containing surfactants: periodic surfaces (phase structure: hexagonal - H<sub>1</sub>, H<sub>2</sub>; lamellar – L<sub> $\alpha$ </sub>, cubic- I<sub>1</sub>, I<sub>2</sub>, V<sub>1</sub>, V<sub>2</sub>, micellar L<sub>1</sub>, L<sub>2</sub>).Molecular sieves. Nanoemulsions – properties and applications. Modeling of biological systems with monolayer and bilayer technique. Correlation between monolayers and bilayers. Liposomes and nanocapsules as a novel method of drug delivery. Biosensors.

Method of evaluation: exam or credit

**ECTS:** 1.5

Semester: summer

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# Course code: Cb30

Title of the course: Spectroscopic methods of surface analysis

Tutor: dr Dorota Jamróz

#### **Teaching objectives:**

### Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

Lecture

Course code: Cb30W

Type of course: lecture

**Tutor:** dr Dorota Jamróz

Number of hours: 15

**Description of the course:** The following non-invasive methods of surface analysis shall be discussed: Reflection-Absorption IR Spectroscopy (RAIRS), Attenuation Total Reflection (ATR), Surface-Enhanced Raman Spectroscopy (SERS), X-ray Photoelectron Spectroscopy (XPS/ESCA), UV Photoelectron Spectroscopy (UPS), Auger Electron Spectroscopy (AES), Electron Energy Loss Spectroscopy (EELS).

Each of the methods shall be presented in the following way: it's theoretical background, construction of the equipment and the measuring procedure, analysis of typical spectra, the advantages and limitations of the method.

Method of evaluation: ECTS: Semester: Bibiography:

# **Cb31**

#### INTRODUCTION TO NANOMATERIALS ENGINEERING AND NANOTECHNOLOGY

- general characterization of nanotechnology and nanostructured materials, various approaches for synthesis of nanostructured materials, properties of nanostructured materials: thermal stability, mechanical, electrical, optical and magnetic properties, advantages and disadvantages of size reduction to nanoscale, nanotechnology limits and undesirable phenomena, typical methods of nanostructured materials fabrication, properties and technological applications of nanomaterials, magnetic, electronic, optical, and biological nanodevices (metallic, semiconductor and oxides nanodots, nanoparticles, nanowires, nantubes, CMOS and MOSFET transistors, Micro, and Nano Electro Mechanical systems (MEMS & NEMS), nanomaterials for modern batteries and fuel cells, nonoreactors, photonic crystals, biomaterials), pH and humidity nanosensors, nanosensor for determination of single virus, DNA and its reactivity, nanoelectrodes and others, perspectives on the future of nanotechnology and its development.

# **Cb32**

#### FABRICATION OF NANOSTRUCTURED MATERIALS

nanotechnology and nanostructured materials, nanomaterials fabricated by lithographic techniques: classical lithography, electron beam lithography (EBL), ion beam lithography (IBL), X-ray lithography, interference and holographic lithography, soft lithography techniques including microcontact printing and nanotransfer patterning (µCP and nTP), nanoimprint lithography (NIL), fabrication of nanoscale structures using STM, AFM and NSOM microscopy, deep-pen lithography (DPL), molecular beam epitaxy (MBE), vapour-phase synthesis of nanomaterials: physical and chemical vapour deposition (PVD and CVD), vapour-liquid-solid (VLS) growth method, metal-organic chemical vapour deposition (MOCVD), liquid phase epitaxy (LPE), other physical methods including self-organised nanosphere lithography, chemical methods for synthesis of nanomaterials using reverse micelles, self-assembled close-packed monolayers or bilayers, sol-gel and electrochemical techniques used for fabrication of nanostuctured materials, template methods of nanofabrication employing block copolymers, porous silicon, porous polymeric and alumina membranes together with electroless deposition and atomic layer deposition (ALD)

# **Cb34**

#### SYNTHESIS OF NANOSTRUCTURED MATERIALS BY ANODISING

various semiconductors and metals anodization, aluminium anodising as a method of synthesis of ordered nanostructures, type of formed anodic film, electrolytes used for Al anodization, structural features of anodic porous alumina (AAO), effect of operating conditions on structural features of nanostructures (nanopore diameter, interpore distance, thickness of the barrier layer, aspect ration and porosity), incorporation of anions during anodization, cell-wall structure, density of anodic porous alumina, charge of anodic porous film, anodising techniques, theories of pore initiation and porous alumina growth, volume expansion during anodization, kinetics of self-organised nanopore growth, self-organised and pre-patterned anodising of aluminium, type of materials used for anodization, pre-treatment of aluminium, anodising procedures, characterization of nanostructures formed by anodization of aluminium in various electrolytes, ordering degree and defects in nanostructures, direct and template AAO assisted methods used for fabrication of various modern nanomaterials and their applications in microelectronics and microoptics, nanosensor and biomaterials.

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### Course code: Cb33

Title of the course: Polymeric materials for applications in nanotechnology

Tutor: dr Krzysztof Szczubiałka i dr Mariusz Kępczyński

**Teaching objectives:** 

# Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture and classes(i)

Lecture

Course code: Cb33

**Type of course:** w

Tutor: dr Krzysztof Szczubiałka i dr Mariusz Kępczyński

Number of hours: 30 hours

**Description of the course:** Introduction to nanotechnology. Reactions of polymerization in homogenous systems: radical, living and controlled polymerization. Reactions of polymerization in dispersed systems: suspension, emulsions, miniemulsions and microemulsions. Reactions of polymerization in self-organizing systems. Nanoencapsulation. Photopolymerization and photocross-linking. Photolithography. Polymeric nanolayers. Self-organizing processes of amphiphilic polymers. Techniques: SLS/DLS, TEM/SEM, AFM. Controlled release of drugs. Conductive polymers. Electronics. Biosensors. Photonics.

Method of evaluation: exam

**ECTS:** 3.0

Semester:

**Bibiography:** 

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#### Course code: Cc01

Title of the course: Phase transitions in solid state Tutor: dr hab. Anna Migdał-Mikuli, dr hab. Edward Mikuli Description of the unit included in the course: Lecture Course code: Cc01 Type of course: lecture and classes Tutor: dr hab. Anna Migdał-Mikuli, dr hab. Edward Mikuli

#### Number of hours: 60

**Description of the course:** The framework of the course includes discussing various methods of determining phase transitions such as: adiabatic calorimetry, differential scanning calorimetry, Raman and infrared band shape spectroscopy, inelastic and quasi-elastic neutron scattering, nuclear magnetic resonance, electron paramagnetic resonance, dielectric relaxation and magnetic susceptibility measurement. Issues concerning interpretation of the results obtained through these methods, particularly the problem of molecular reorientation (formalism correlation functions, correlation and relaxation times, activation energy, molecular reorientation models) will also be discussed. The lab sessions include introduction to the construction and activity of calorimeters as well as measuring phase transitions /specific heat/ by applying the method of differential scanning calorimetry (DSC) for the crystal hexaammine and hexaaqua complexes of divalent metals. The participants will also learn how to determine the correlation time and activation barriers for reorientation movement based on temperature-related shape of the chosen spectroscopic bands of the compounds. The seminars also include discussions on ways of presenting the results of other methods of measuring phase transitions and molecular reorientation.

\* the course consists of 30 hours of lectures and 30 hours of lab sessions

#### Method of evaluation: written exam

### **ECTS: 6.5**

#### **Semester:** summer

**Bibliography:** "Komplementarne metody badania przemian fazowych", praca zbiorowa pod red. E. Mikulego i A. Migdał-Mikuli, Wydawnictwo UJ, Kraków 2005. "Przemiany fazowe", praca zbiorowa pod red. A. Graji i A. R. Ferschmina, Ośrodek Wydawnictw Naukowych, Poznań 2003.

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# Course code: Cc02

Title of the course: Spectroscopic instrumentation Tutor: prof. dr hab. Leonard M. Proniewicz

# Description of the unit included in the course:

Lecture Course code: Cc02w Type of course: lecture Tutor: prof. dr hab. Leonard M. Proniewicz Number of hours: 15

**Description of the course:** The lecture provides an introduction to instrumental tools and methods of spectroscopic studies useful in wavelength (frequency) and/or spectral line shape measurements. Applications of selected apparatuses using their technical parameter, e.g. sensitivity, spectral resolution, optimal signal to noise ratio, constitute the major emphasis of the course. The fundamental features and working principles of some tools (prismatic and mesh monochromators, interferometers) and detection methods (thermal and photoemission detectors, photocells, photomultiplier, photon counting, photoresistors, photodiodes, CCD and others) will be discussed. The light sources of the various spectroscopic techniques also will be presented, especially the applied lasers.

Method of evaluation: exam ECTS: 1.5 Semester: summer

Course code: Cc03

Title of the course: Raman spectroscopy in catalysis and new materials. Tutor: prof. dr hab. Leonard M. Proniewicz, dr Aleksandra Wesełucha-Birczyńska Description of the unit included in the course: Lecture Course code: Cc03w

#### Type of course: lecture

**Tutor:** prof. dr hab. Leonard M. Proniewicz, dr Aleksandra Wesełucha-Birczyńska **Number of hours:** 15

**Description of the course:** Theoretical introduction: interaction of radiation with matter, Raman efect, selection rules, advantages and disadvantages of the Raman method in application of structure determination of catalysts and new materials. Modern instrumentation and techniques applied in the Raman measurements. Examples of application: catalytic processes of petroleum and carbon desulfunation (MoO<sub>3</sub> and WO<sub>3</sub> catalysts), of SO<sub>2</sub>, CO<sub>2</sub>, NO and hydrocarbons oxidations of (catalysts consisting of vanadium, manganese, iron, molybdenum and bismuth oxides), of olefins' hydrogenation and dehydrogenation, and also of synthetic gases formation (CO/H<sub>2</sub>) and others. Structure determination of zeolites, ceramics, polymers (especially, their orientation on various surfaces), semi- and superconductors is discussed in details.

Method of evaluation: exam

**ECTS**: 1.5

Semester: summer

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#### **Course code: Cc04**

**Title of the course:** Rotational and Vibrational Spectroscopy in Environmental Protection **Tutor**: dr Małgorzata Barańska, prof. dr hab. Leonard M. Proniewicz

Description of the unit included in the course:

Lecture

Course code: Cc04w

Type of course: lecture

Tutor: dr Małgorzata Barańska, prof. dr hab. Leonard M. Proniewicz

Number of hours: 15

**Description of the course:** Introduction to theoretical fundamentals of radiation-matter interaction, rigid rotor, harmonic and anharmonic oscillators, selection rules. Students acquaint with apparatus for measurements of rotational and vibrational spectra (IR, RS and RR), and selected measurement techniques applied in solution of environmental protection problems. Examples of qualitative and quantitative analysis of substances polluting of

atmosphere (CO, SO<sub>2</sub>, nitrogen oxides,  $CH_4$  and other hydrogencarbons), water and soil are discussed. Spectroscopic quality and quantity analysis of selected bioactive compounds occurring in plants.

Method of evaluation: paper ECTS: 1.5 Semester: summer

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**Course code: Cc05** 

Title of the course: Oscillation reactions (order and chaos)

Tutor: dr Małgorzata Rachwalska

#### Description of the unit included in the course:

Lecture

Course code: Cc05w

Type of course: lecture

Tutor: dr Małgorzata Rachwalska

Number of hours: 15

**Description of the course:** During the lecture the following items will be considered: oscillation reactions in light of nature laws, some unstabilities: physical and physico-chemical, some models of chemical oscillation reactions, some sequential oscillators, subcritical and supercritical Hopf's bifurcation, some elements of deterministic chaos.

Method of evaluation: Problems

**ECTS:** 1.5

Semester: summer

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Course code: Cd01

Title of the course: Phase analysis. Multidisciplinary applications

Tutor: Barbara Borzęcka-Prokop

**Teaching objectives:** not given (nonobligatory course)

#### Seminar

**Course code:** Cd01 + s

Type of course: seminar

Tutor: Barbara Borzęcka-Prokop

Number of hours: 30 hrs

**Description of the course:** (seminar 10 hrs + classes 20 hrs). Introduction to X-ray phase analysis. Instrumentation and accuracy (use of external and internal standards). Creation of experimental databases: diffraction line analysis in relation to Hanawalt and Fink methods. Reference structure databases and their application in qualitative analysis. Specific approaches to phase analysis of: i) polymorphic modifications, ii) catalysts, iii) minerals, iv) biomaterials and v) nanostructural compounds.

Method of evaluation: written reports

**ECTS:** 3,5

Semester: winter/summer terms

Bibliography: seminar notes and materials

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#### **Course code: Cd02**

Title of the course: Biomimetics in chemistry of novel materials

Tutor: Barbara Borzęcka-Prokop

Teaching objectives: not given (nonobligatory course)

#### Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

Lecture

Course code:Cd02

**Type of course:** lecture (w)

Tutor: Barbara Borzęcka-Prokop

Number of hours: 15 hrs

**Description of the course:** Biomimetics: general terms, principles and multidisciplinary applications. Biomineralisation and strategies in syntheses of biomimetic systems. Types and functions of main biominerals. Bacterial biomineralisation. Biocorrosion. Molecular tectonics

in biomineralisation. Biomimetic approach to nanostructural synthesis. Template-directed nucleation and growth of novel materials. SAMs. Biogenic semiconductors. Structure and characteristics of inorganic biomimetic compounds.

Method of evaluation: written work ECTS: 1,5 Semester: winter term Bibliography: lecture notes and materials

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# Course code: Cd03

Title of the course: POWDER DIFFRACTOMETRY IN THE INVESTIGATION OF

MATERIALS

Tutor: prof. dr hab. Stanisław Hodorowicz

**Teaching objectives:** 

#### Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

Lecture

Course code: Cd03w

**Type of course:** lecture(w)

Tutor: prof. dr hab. Stanisław Hodorowicz

Number of hours: 15

**Description of the course:** 

Degree, range and the kind of ordering in the crystalline and pseudo-crystalline phases; real structures, crystallinity, size of crystallites; examination of defects and strains in crystals; investigation of polycrystalline phases in the chemical reaction conditions and structural phase transitions; modern diffraction techniques in the study of composite polycrystalline materials.

Method of evaluation: test ECTS: 1.5 Semester: winter or summer Bibliography:

- Fundamentals of Powder Diffraction and Structural Characterization of Materials.
   V. Pecharsky, P. Zavalij. Cluwer Academic Publishers, 2003;
- The Rietveld method (IUCr Monograph on Crystallography, No. 5.) Ed. R. A. Young, Oxford University Press, 1995.

# Formularz aktualizacyjny

Opis ogólny kursu:

Course code: Cd04

Title of the course : Protein structure and function

Tutor : dr hab. Krzysztof Lewiński

Teaching objectives : Introduction to relationship between 3-dimensional structure of

proteins and their role in biological processes.

# Opis jednostki wchodzącej w skład kursu.

np. wykład (w), ćwiczenia(n), laboratorium (l), konwersatorium (k), seminarium (s),

ćwiczenia rachunkowe (c), wykład + ćwiczenia (i)

Course code : Cd04w

**Type of course :** 

**Tutor :** 

Number of hours :

**Description of the course :** Elements of protein structure, aminoacids, peptide bond, conformation of polypeptide chain. Side-chain conformations. Secondary structure. Motifs of protein structure. Structural hierarchy of protein structures: examples of alpha, alpha/beta and beta structures. Interactions stabilizing proteins. Proteins folding and molecular diseases, amyloids. Structure and mechanism of activity of selected groups of proteins: enzymes, immunoglobuline, spherical viruses, membrane proteins, DNA-binding proteins. The structure of DNA and RNA.

Method of evaluation : test

# **ECTS:** 3

Semester: (zimowy, letni, zimowy/letni) winter

Bibliography: Berg J.M., Tymoczko J.L., Stryer L., Biochemia, PWN, 2005

Branden C., Tooze J., Introduction to Protein Structure, Garland Publishing, 1999

# Course code: Cd05

Course:	POLYCRYSTAL STRUCTURE INVESTIGATION
Tutor:	Wiesław Łasocha PhD, DSc
Type of course:	Lecture + tutorials
Number of hours:	30  hrs lec + 15  hrs tut
ECTS:	5

Short description of the course:

Powder diffraction techniques including: measurement conditions, lattice parameters and space group determination. Limitation factors of intensities determination of individual reflections, sources of errors (texture or reflections overlapping), Methods enabling preparation of 'texture free' specimens, special methods for retrieving intensities of overlapping peaks. Classic and new methods for structure solution in powder diffractometry. Rietveld refinement, available packages their limits and applicability.

In practica part: structure solution and refinement using powder diffraction data. Software for powder diffractometry: EXPO, DBWS, XRS-82, GSAS.

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#### **Course code: Cd07**

Title of the course: Methods of Crystal Preparation

Tutor: Dr. Andrzej Olech

**Teaching objectives:** 

#### Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture

and classes(i)

Lecture and classes

Course code: Cd07 i

Type of course: lecture and classes

Lecturer and Tutor: Dr. Andrzej Olech

**Number of hours:** 30 (15 w + 15 n)

#### **Description of the course:**

Processes of nucleation and growth; laboratory growing: ways of temperature control, inorganic and organic preparation ABC, microcrystallization, crystal microanalysis; methods of industrial production: mass and bulk crystallization, influence of nucleation processes on crystallite properties, crystallization of metals and metal monocrystals, casts, dendrites and wiskers, zone melting, epitaxy, defects; flux growth and growth in microgravity conditions.

**Method of evaluation:** Preparation of a took on a selected topic; test miniproject on a crystallization method.

**ECTS:** 3,5 (2,0 w + 1,5 n)

Semester: summer

# **Bibliography:**

- 1. "Wzrost kryształów" (in polish), Ed. Keshra Sangwal, wyd. WSP w Częstochowie, 1990.
- "Modeling Crystal Growth Rates from Solution" M.Ohara, R.C.Reid, Prentice-Hall, New Jersey (1973).
- "Vyrashtshivanije kristallov iz rastvorov" (in rus.), T.G.Pietrov, E.B.Treivus, Ju.O.Punin, A.P.Kasatkin; Niedra, Leningrad, 1983.
- 4. "Krystalizacja i krystalizatory" (in polish), Z.Rojkowski, J. Synowiec, WNT, Warszawa 1991.

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# Course code: Cd08

Title of the course: Structure and activity of small bioactive molecules

Tutor: prof. dr hab. Barbara Oleksyn

**Teaching objectives:** 

# Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture and classes(i) Lecture and classes Course code: Cd08i Type of course: lecture and classes Tutor: prof. dr hab. BarbaraOleksyn Number of hours: 30

**Description of the course:** 

Role of small molecules in living organisms, endo- and exogenic molecules, drugs. Small molecule and biological membranes: structure and interaction of small molecules with proteins: enzyme substrates and inhibitors, protein receptor stimulants and blockers. Interactions of small molecules with DNA. Physico-chemical properties of drugs and their fate in organism, Quantitative Structure-Activity Relationship (QSAR) and three dimensional structure of drug molecules. Determination of biological activity of drugs. Employment of X-ray structure analysis and theoretical calculations for studies of

macromolecule – small molecule interactions. Selected models of drug interactions with macromolecule active sites. Drug design.

The course comprises 15 hours of lecture and 15 hours of laboratory which are included in specialization laboratory for 4<sup>th</sup> year Chemistry students.

Method of evaluation: writing test + classroom report ECTS: 3.5

Semester: winter

**Bibliography:** selected publications

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# Course code: Cd09

Title of the course: Crystal structure of selected organic compounds

Tutor: prof. dr hab. Barbara Oleksyn

**Teaching objectives:** 

# Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture and classes(i)

Lecture and classes

Course code: Cd09i

Type of course: lecture and classes

Tutor: prof. dr hab. Barbara Oleksyn

Number of hours: 45

# **Description of the course:**

Review of molecular and crystal structures of selected groups of compounds together with discussion of the following problems: chemical properties an *versus* molecular geometry, chirality of molecules and absolute structure, mutual recognition of molecules, effect of the environment in the crystal on molecular conformation, packing of molecules in the crystal and intermolecular interactions, polymorphism, the role of intra- and intermolecular hydrogen bonds, thermal motion and disorder in crystal structures. Crystallographic databases as the source of information on molecular structure and intermolecular interactions in crystals. Search in database and data analysis. Studies of variation of molecular geometry and of

coordination polyhedra in different crystalline environment. Search for structure correlations

and for information about possible reaction paths.

The course comprises 30 hours of lecture and 15 hours of laboratory concerning usage of Cambridge Structural Database which are included in specialization laboratory of the profile Chemistry of New Materials and Catalysis.

Method of evaluation: writing test + classroom report

**ECTS:** 5.0

Semester: summer

Bibliography: selected articles from monographies and journals

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Course code: Cd10 Title of the course: CRYSTAL STRUCTURE AND PHYSICAL PROPERTIES Tutor: dr hab. Katarzyna Stadnicka Teaching objectives:

# Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)
Lecture

Course code: Cd10w Type of course: lecture(w)

Tutor: dr hab. Katarzyna Stadnicka

Number of hours: 30

**Description of the course:** 

Symmetry of physical properties and symmetry of crystals; tensorial description of physical properties – basic tensor algebra; of the absolute structure: structure polarity, structure chirality; structural characteristics of the selected crystalline materials from the viewpoint of their physical properties: ferroic, magnetic, mechanical, optical – linear and non-linear, thermal, transport properties etc.

*Remark:* Cd10w is one of the obligatory lectures in the Profile Chemistry of New Materials and Catalysis.

**Method of evaluation:** an essay and 15 min. presentation for the given problem concerning the subject of the lecture.

# **ECTS:** 3.0

Semester: winter

# **Bibliography:**

- 1. J. Chojnacki, Elementy krystalografii chemicznej i fizycznej, PWN, 1971;
- 2. R.E. Newnham, Structure Property Relations, Springer-Verlag, 1975;

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# Course code: Cd11

**Title of the course:** ORGANIZATION OF CRYSTAL STRUCTURE – SPACE GROUPS **Tutor**: dr hab. Katarzyna Stadnicka

# **Teaching objectives:**

# Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes (c), lecture and classes (i)

#### Lecture and classes

Course code: Cd11i

Type of course: lecture and classes (i)

Tutor: dr hab. Katarzyna Stadnicka

**Number of hours:** 30 + 15

# **Description of the course:**

Isometric transformations in crystallography: passive – transformations of the coordinate system (unit-cell), active – transformations of symmetry operations (motions), invariants; one-dimensional (2), two-dimensional (17 plane groups) and three-dimensional (230) space groups – examples of space-group description, matrix representations, Wyckoff positions, Bragg reflection conditions; experimental determination of space-group symmetry from diffraction patterns – diffraction symbol, investigation of the normalized structure-factors distribution; maximal subgroups and minimal supergroups; practical usage of the International Tables for Crystallography Vol. A: Space-group symmetry; isometric

transformations and the description of the structural mechanism of phase transitions; color space-groups and their applications; multidimensional space groups and their applications.

Remark: the lecture of Cd11 course is included in the Profile Chemistry of New Materials and Catalysis whereas the classes are obligatory only for the students choosing the Panel on Designing Crystalline Phases and Structure Determination.

**Method of evaluation:** written solution of three selected problem concerning the subject of the course

#### **ECTS:** 3.0 + 2.0

# Semester: winter

# **Bibliography:**

- 1. International Tables for Crystallography, Vol. A: Space-group Symmetry,
- 2. T. Hahn (ed), D. Reidel Publishing Company, 1983;

Fundamentals of Crystallography, C. Giacovazzo (ed.), Oxford University Press, 1992

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# Course code: Ce01

Title of the course: Numerical analysis Tutor: Dr. Habil. Janusz Mrozek Teaching objectives: Teaching students basic operations in numerical analysis

# **Description of the unit included in the course:**

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture and classes(i)

Lecture

**Course code:** 

**Type of course:** 

Tutor: Dr hab. Janusz Mrozek

Number of hours: 20

# **Description of the course:**

Mathematical foundations of basic operations in numerical analysis: interpolation, polynomial approximation, numerical differentiation and integration, solving sets of linear equations,

matrix diagonalization, solving differential equations, optimization of functions. Use of computer libraries and numerical packages.

Method of evaluation:

**ECTS:** 4.5

Semester: summer

Bibiography: Bjork and Dahlquist, Metody numeryczne, PWN

Laboratory

**Course code:** 

**Type of course:** 

Tutor: Dr. Habil. Janusz Mrozek

Number of hours: 25

#### **Description of the course:**

Learning basic operations in numerical analysis: interpolation, polynomial approximation, numerical differentiation and integration, solving sets of linear equations, matrix diagonalization, solving differential equations, optimization of functions. Use of computer libraries and numerical packages (Scilab, Octave).

Method of evaluation: 1 project work during the semester

ECTS:

Semester:

**Bibiography:** Introduction to Scilab

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Course code: Ce02

Title of the course: Operating systems and network services

Tutor: Dr hab. Janusz Mrozek

#### **Teaching objectives:**

Teaching basic commands of Linux and MS Windows and using network services (ssh, ftp,

ntp)

nauczenie podstawowych poleceń systemów operacyjnych Linux i Windows oraz korzystania z podstawowych usług sieciowych

# Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture and classes(i)

Lecture Course code: Type of course: Tutor: Dr.Habil. Janusz Mrozek Number of hours: 15 Description of the course: Students are given an overview of basic commands of both Linux and MS Windows and description of network services such as ssh, ftp and ntp Method of evaluation: 1 test after the lectures ECTS: 2.5 Semester: summer Bibiography:

Course code: Ce03

Title of the course: Design and applications of molecular modeling software

Tutor: Dr. Habil Janusz Mrozek and Dr. Habil. Marek Frankowicz

**Teaching objectives:** 

#### Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture and classes(i)

Lecture

Course code: Ce03w

Type of course: lecture and classes

Tutor: Dr. Habil. Janusz Mrozek and Dr. Habil. Marek Frankowicz

Number of hours: 60

#### **Description of the course:**

The scope of discussed subjects includes i.a.:

Students are learning the principles of work and software design of typical quantum-chemical programs used in molecular modeling. The GAMESS package is used as an example of organization of typical ab initio program, while MOPAC and MOLDEN are used as exemplary cases of semiempirical calculations and molecular structure editing and visualization, respectively.

Within the practical part of the course students are doing modifications of program codes, learning, i.a., the ways of extending the functionality of particular packages by including extra modules and/or writing codes allowing for retrieving data from workfiles

generated by GAMESS and MOPAC. Part of the course is also devoted to ways of implementing quantum chemical codes on computing clusters. About one third of course material is related to characterization of simulation methods: molecular dynamics, Monte Carlo, cellular automata. Examples of application: modellning of chemical reactions, simulations of surface processes. Software for molecular modeling (PHASER, Dynamics).

Method of evaluation: several software miniprojects

ECTS: 7 Semester: winter Bibiography:

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Course code: Ce04 Title of the course: Statistical methods and data analysis Tutor: Dr Mariusz Pilch Teaching objectives:

## Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture and classes(i)

Lecture

**Course code:** Ce04w

**Type of course:** w

Tutor: dr Mariusz Pilch

Number of hours: 30

#### **Description of the course:**

Introductory information on calculus of probability and random variables (probability, random variable, cumulative distribution function). Theory of errors (rounding errors, significant digits, propagation of errors). Random variable distributions (Poly's distribution, Poisson's distribution, Gauss's distribution, geometric distribution). Least square methods.

Matching functions to experimental data (linear function, Gaussian function, exponential function, logarithmic function). Testing statistical hypotheses. Introduction to function minimisation.

Method of evaluation: ECTS: 3.0 Semester: Bibiography:

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# Course code: Ce05

Title of the course: Mathematical Methods in Chemistry I Tutor: Dr. Grzegorz Mazur ...... Teaching objectives: The course supplements the basic course in mathematics and extends it by the issues directly related to theoretical chemistry. The emphasis is put on the material connected with quantum chemistry. The purpose of the course is to present basic mathematic apparatus used in quantum mechanics, and to develop proficiency in using it.

# Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)
Lecture
Course code:Ce05
Type of course:lecture
Tutor:Dr. Grzegorz Mazur
Number of hours:
Description of the course:Elements of combinatorics, complex numbers, functions of
complex numbers, elements of the group theory, linear space over real and complex fields,
Hilbert space.
Method of evaluation:exam
ECTS:.5
Semester: winter
Bibiography:

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Course code: Ce06 Title of the course: Mathematical Methods for Chemists II Tutor: dr Grzegorz Mazur

**Teaching objectives:** 

# Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

Lecture

Course code: Ce06w

Type of course: w

Tutor: dr Grzegorz Mazur

Number of hours: 30

**Description of the course:** Victor analysis with element sof tensor caculus (gradient, divergence, curl, Gauss's theorem, Stokes's theorem; curved coordinates and tensor analysis). Introduction to the group theory (discreate and continuous groups). Elements of complex function theory and partial differential equations. , . Special functions (gamma function and Stirling's series, Legendre functions, Bassel Functions, Hermite functions) as well as orthogonal polynomials. Fourier transformation and Dirac delta function.

Method of evaluation: exam

ECTS: 4.5 Semester: summer Bibiography:

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**Course code: Ce07** 

Title of the course: Advanced programming in Fortran

# Tutor: Dr hab. Janusz Mrozek

# **Teaching objectives:**

Teaching students with advanced techniques of Fortran programming exceeding those taught in standard courses of FTN 77. Extra stress is put on various extensions to the language including some historical solutions. This should help the students understand the work of Fortran codes, especially those still commonly used in quantum chemical packages. Some introduction is given to software solutions used in writing parallel codes for the multiprocessor machines and computer clusters. owych jak i klastrach obliczeniowych.

# Description of the unit included in the course:

lecture(w), classes(n), laboratory(l), tutorials(k), seminar(s), calculation classes(c), lecture

and classes(i)

Lecture

**Course code:** 

**Type of course:** 

Tutor: Dr hab. Janusz Mrozek

Number of hours: 30

# **Description of the course:**

The scope of discussed subjects includes i.a.:

i. the detail description of I/O operations in formatted, unformatted and binary modes, OPEN and ENQUIRE instructions, I/O operations for sequential and direct access files, operations involving "internal" files, description of fields and modifiers of FORMAT statement.

- a. Description of library subroutines and functions of modern FORTRAN compilers (based on Intel and OPEN WATCOM compiler libraries, with specialstress on routines used in communicating the operating system
- b. Constructions like COMON, EQUIVALENCE, IMPLICIT, PARAMETER, INCLUDE, their internal relations and potential problems resulting from their misuse
- c. Relations between program modules, ENTRY statement, nonstandard solutions like e.g. RETURN statement to the label in calling module
- d. Compilation, optimization and linker options
- e. Creating and using software libraries, connecting modules in other languages
- f. Parallel codes using MPICH and OpenMP
- g. Code optymization

Method of evaluation: several software miniprojects

**ECTS:** 4.5

Semester: winter

**Bibiography:** 

### Course code: Ce08

Title of the course: Techniques of programming scientific calculations in C++

Tutor:dr Grzegorz Mazur

**Teaching objectives:**The main objective of the course is that students learn how to effectively and efficiently create/modify software for scientific calculations. To achieve that, the course covers most important methods and techniques of modern software design and implementation. The emphasis is put on hands-on approach.

#### **Prerequisites:**

Theoretical Chemistry (A514)

Computer Science (A512)

Molecular Modelling (???)

Recommended but not obligatory: Mathematical Methods in Chemistry (Ce05/Ce06)

Description of the unit included in the course.

Lecture and classes

Course code:Ce08

Type of course:lecture and classes

Tutor:dr Grzegorz Mazur

Number of hours:45 (15 lecture + 30 classes)

**Description of the course:**Introduction to object programming with emphasis on the C++ object model. Introduction to generic programming in C++. Modern techniques of C++ libraries construction, mainly based on the C++ Standard Library and Boost Library (<u>http://www.boost.org/</u>). Basics of computational applications design and implementation. Introduction to optimization techniques. Introduction to parallel programming with the Message Passing Interface. Advanced methods of implementing quantum-chemical calculations, based on the niedoida project (<u>http://www.chemia.uj.edu.pl/~niedoida/en</u>).

Method of evaluation:semester project

**ECTS:**5

Semester: winter

**Bibliography:** 

B. Stroustrup, The C++ Programming Language

Tao Pang, An Introduction to Computational Physics

T. Helgaker, P. Jorgensen, J. Olsen, Molecular Electronic-Structure Theory

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# **Course code: Cf01**

Title of the course: Methodics od Chemistry Teaching

Tutor: Dr. Michał M. Poźniczek

**Teaching objectives:** 

# Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture

and classes(i)

Lecture

Course code: Cf01W

**Type of course:** lecture

Tutor: Dr. Zofia Kluz

Number of hours: 30

**Description of the course:** "Principles of Chemistry Didactics". The lecture includes problems of general didactics illustrated by the examples necessary for the chemistry teacher in the lower and higher secondary schools (methods, principles, didactic tools etc.). Moreover, within the framework of the lecture the issues of principles of pupils' knowledge testing and estimation are discussed (preparing the tools of didactic measurement, principles of criterial estimation).

The second part of the lecture consists of methodology of curricula formation, detailed analysis of chosen curricula and the way of chosen issues introduction.

Method of evaluation: written examination

**ECTS:** 13.0 W

Semester: winter semester

**Bibiography:** 

Classes

Course code: Cf01

Type of course: classes

Tutor: The staff of the Department of Chemistry Education

#### Number of hours: 90

**Description of the course:** The classes has been divided into 2 blocks – 45 hours each. The first one contains the problems of chemistry teaching in lower secondary schools and the second one – in higher secondary schools. During the classes, basing on the lecture, students elaborate summaries of the lessons, acquaint with the technics of school chemical experiment, use of technical tools in teaching (computers, contemporary technics of presentations etc.). The second part of each block are the classes in schools, where students elaborate summaries and carry on lessons by themselves.

Method of evaluation: written test (lesson summary)

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#### **Course code: Cf05**

Title of the course: Basic of chemistry for teachers

Tutor: dr M.M.Poźniczek

**Teaching objectives:** Aim of the curse is introduction to students essential problems of teaching chemistry in classes with natural science profile.

#### Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture

and classes(i)

# Lecture

Course code: Cf051

Type of course: lecture

Tutor: dr M.M.Poźniczek

Number of hours: 30

Description of the course: 1. Modern way of teaching chosen issues of chemistry

- 2. Rule of erudition
- 3. Various treatment of the same topic
- 4. Teaching in problem context

Method of evaluation: revision exam

**ECTS:** 3.0

Semester:

**Bibiography:** 

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Course code: Cf06

Title of the course: Methodics of Nature Study Teaching Tutor: Dr. Michał M. Poźniczek

**Teaching objectives:** 

# Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture

and classes(i)

Lecture

Course code: Cf06 W

Type of course: lecture

Tutor: Dr. Michał M. Poźniczek

Number of hours: 30

**Description of the course:** "Principles of Biology for Nature Historians". Within the framework of the lecture, the basic issues relating to the organisation of vivacious matter (from a cell to the whole organism) are discussed. The issues resulting from the Curriculum Base of Science are especially emphasised.

Method of evaluation: written credit ECTS: 3,0 Semester: winter semester Bibiography:

**Course code: Cf06 W** 

Type of course: lecture

Tutor: Dr. hab. Krystyna German

Number of hours: 30

**Description of the course:** "Principles of Geography". The contents of the lecture – just as in the case of the Principles of Biology for Nature Historians – is based on the Curriculum Base

of Science and contains three main issues: 1) structure and organisation of the natural environment, 2) environment as a dynamic system, 3) landscapes of Poland. **Method of evaluation:** written test

**ECTS:** 3

Semester: summer semester

**Bibiography:** 

Classes

Course code: Cf06n

Type of course: classes

Tutor: Dr. Ewa Odrowąż, Dr. Małgorzata Krzeczkowska

Number of hours: 45

**Description of the course:** "Didactics of Nature Study Classes". Within the framework of the classes the students get acquainted with different curricula for teaching nature study – *science* (the subject in primary schools) and didactic tools and obtain knowledge of teacher's work. A separate part of classes is to prepare didactic tools useful for teaching the subject and different summaries of lessons.

Method of evaluation: written test ECTS: 4,5 Semester: winter semester Bibiography:

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**Course code: Cf09** 

Title of the course: Problem Based Learning

Tutor: dr Iwona Maciejowska

**Teaching objectives:** 

Acquaintance students with PBL and various techniques of teaching/learning at different levels of education

### Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

Lecture and classes

Course code: Cf09i

Type of course: Lecture and classes

Tutor: dr Iwona Maciejowska

Number of hours: 15

# **Description of the course:**

Problem solving methods of teaching/learning – structure and principles (Problem and Context Based Learning).

Method of evaluation: scenario of a class using a problem solving method, active

participation in the course (individual and group work: preparation of metaplan, project,

mental map)

**ECTS:** 1,5

Semester: summer

# **Bibiography:**

- 1. E. Brudnik, A. Moszyńska, B. Owczarska, Ja i mój uczeń pracujemy aktywnie. Przewodnik po metodach aktywizujących, Zakład Wydawniczy SFS, Kielce 2000.
- 2. E. Brudnik, Ja i mój uczeń pracujemy aktywnie 2, Oficyna Wydawnicza Nauczycieli, Kielce 2003.
- 3. B. Borowska, V. Panfil, Metody aktywizujące w edukacji biologicznej, chemicznej i ekologicznej, Wydawnictwo TEKST, Bydgoszcz 2001.
- 4. Aktywne metody nauczania w szkole wyższej, red. M. Jaroszewska, D. Ekiert-Oldroyd, Wyd. Nakom, Poznań 2002.
- 5. K.Chałas, Metoda projektów i jej egzemplifikacja w praktyce, wydawnictwo nowa era, Warszawa 2000
- 6. Problem Solving In Analytical Chemistry, The Education Division, The Royal Society of Chemistry, London, 1998

ASE Guide to Secondary Science Education

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# Course code: Cf11

Title of the course: Basics of creating interactive multimedia applications using Macromedia

software.

Tutor: dr Michał M. Poźniczek

# **Teaching objectives:**

# Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture and classes(i)

# Lecture and classes

**Course code:** 

Type of course: i

Tutor: mgr Paweł Bernard, mgr Paweł Broś

# Number of hours: 15

# **Description of the course:**

- 1. Evolution of Information Technology in teaching.
- 2. Elements of eLearning and blended learning.
- 3. Basics of creating static graphics.
- 4. Creating interactive applications using Authorware software.
- 5. Creating animations using Flash software.
- 6. Director as a tool similar to Authorware and Flash.

Method of evaluation: presence on classes, miniproject

**ECTS:** 1,5

Semester: second

# **Bibiography:**

'Biblia Flash 2004' MX, Robert Reinhardt, Snow Dowd, Helion 2004

'Using Authorware' 7, Macromedia 2003

'Director MX. Szybki start', Andre Persidsky, Mark Schaeffer, Helion 2004

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# Course code: Cg01

Title of the course: Heterogeneous catalysis Tutor: Prof. Dr Jerzy Datka Teaching objectives

# Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

Lecture

Course code: Cg01 Type of course: lecture Tutor: Prof. Dr Jerzy Datka Number of hours: 30

**Description of the course:** 1. The elements of chemical kinetics and thermodynamics. 2. Definition of catalyst. 3. Various aspects of catalyst selectivity (selectivity in consecutive reactions, shape selectivity, selectivity in enzyme reactions). 4. Methods of comparing of catalytic activity and selectivity. 5. Homogeneous and heterogeneous catalysis. 6. Basic steps of catalytic reactions (diffusion, adsorption, and surface reactions). 7. Description of adsorption process on catalysts. 8. Physisorption and chemisorption. 9. Adsorption isotherms. 10. Kinetics of catalytic reactions with adsorption

Method of evaluation: examination or acceptance

**ECTS:** 3.0

Semester: winter

**Bibiography:** 

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# Course code: Cg02

Title of the course: Application of IR spectroscopy to the problems of catalysis

Tutor: Prof. Dr Jerzy Datka, Dr Barbara Gil, Dr Paweł Kozyra

**Teaching objectives** 

#### Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture and classes(i)

Lecture and classes

Course code: Cg02

Type of course: lecture and classes

Tutor: Prof. Dr Jerzy Datka, Dr Barbara Gil, Dr Paweł Kozyra

Number of hours: 30

**Description of the course:** 1. The IR spectrometer. 2. The software used to treatment of IR spectra. 3. IR studies of acidity of surface of solids. 4. IR studies of Lewis acid sites with CO as probe molecule. 5. CO as probe molecule for the studies of electronic properties of

transition metal cations. 6. IR studies of the interaction of reactant molecules with active sites in zeolites. 7. The IR spectra of catalysts recorded at liquid helium temperature.
Method of evaluation: acceptance
ECTS: 3.0
Semester: summer
Bibiography:

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Course code: Cg03 Title of the course: Chemistry of zeolites Tutor: Prof. Dr Jerzy Datka Teaching objectives

#### Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture and classes(i)

Lecture

Course code: Cg03

Type of course: lecture

Tutor: Prof. Dr Jerzy Datka

Number of hours: 30

**Description of the course:** 1. Systematic of silicates. 2. Definition and the most important properties of zeolites. 3. Description and structures of the most important zeolites. 4. Mesoporous materials. 5. Application of zeolites in refinery industry. 6. Izomorphous substitutions in zeolite framework. 7. Stability of zeolite structures. 8. Modifications of zeolites (ionic exchange, dealumination, "grafting"). 9. NMR studies of zeolites. 10. Acidity of zeolites. 11. Perspectives of development of chemistry of zeolites in the future.

Method of evaluation: examination or acceptance

**ECTS:** 3.0

Semester: winter and summer

**Bibiography:** 

# Course code: Cg06

Course:	INTRODUCTION TO SURFACE CHEMISTRY
Tutor:	Dr. Andrzej Kotarba
Type of course:	Lecture + tutorials
Number of hours:	30 hrs
ECTS:	3

Short description of the course:

The course is focused on the following problems of Surface Chemistry:

Surfaces – an Introduction: classification, properties (surface concentration, clusters, thin films, clean surfaces, adsorption, techniques of surface science); Structure of Surfaces: surface diffraction, reconstruction, defects, epitaxial growth; Thermodynamics of Surfaces; Dynamics of Surfaces: elementary processes of gas-surface interaction, sticking probability, surface diffusion, desorption; Electrical Properties of Surfaces: work function, DOS, electron excitation, charge transfer, field and surface ionisation, electron emission, XPS, STM; Surface Chemical Bond: chemisorption, thermal activation of bond breaking, coadsorption.

The lectures are illustrated with laboratory classes organised in the research groups of Inorganic Chemistry Department (TPD of probe molecules, BET isotherm, Kelvin Probe CPD measurements, XPS.

# Course code: Cg07

Course:	HIGH VACUUM TECHNOLOGY
Tutor:	Dr. Andrzej Kotarba
Type of course:	Lecture + tutorials
Number of hours:	30 hrs
ECTS:	3

Short description of the course:

The course addresses the following problems of high vacuum technology: basic tasks and problems of high vacuum, gasses in vacuum systems, pumping process, vacuum hardware (materials and fittings), construction of chambers and systems, measurements in vacuum conditions.

The lectures are illustrated with laboratory classes organised in the research groups of Inorganic Chemistry Department. Students perform typical experiments using vacuum apparatus, interpret the results and prepare short reports.

#### Course code: Cg09

Title of the course: New materials in heterogeneous catalysis

Tutor: dr Piotr Kuśtrowski

#### **Teaching objectives:**

#### Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

## Lecture

Course code: Cg09w

Type of course: Lecture

Tutor: dr Piotr Kuśtrowski, dr Lucjan Chmielarz

Number of hours: 15

**Description of the course:** Review of the most important types of new materials, which are used in catalysis (modified zeolites and silicalites, superacids, superbases, bifunctional catalysts, synthetic and natural mesoporous catalysts, polimetallic catalysts, sulphides, nitrides and carbides, homogeneous immobilized catalysts). Influence of chemical composition, structure and texture of a catalyst on its physicochemical and catalytic properties. The main methods of catalysts preparation, the most important technological applications and the perspectives in scientific research of new types of catalysts.

Method of evaluation: final examination or final report

**ECTS:** 1.5

Semester: winter

**Bibiography:** 

Laboratory

Course code: Cg091

Type of course: laboratory

Tutor: dr Piotr Kuśtrowski, dr Lucjan Chmielarz, mgr Janusz Surman

Number of hours: 30

**Description of the course:** Four complex laboratory practices concerning on the new types of catalytic materials (modified zeolites and silicalites, superacids, superbases, bifunctional catalysts, synthetic and natural mesoporous catalysts, polimetallic catalysts, sulphides, nitrides and carbides, homogeneous immobilized catalysts). The preparation of catalysts and the

studies on relation between chemical composition, structure and texture of a catalyst on its physicochemical and catalytic properties
Method of evaluation: Final report
ECTS: 3.0
Semester: winter
Bibiography:

# Seminar Course code: Cg09s Type of course: seminar Tutor: dr Piotr Kuśtrowski, dr Lucjan Chmielarz Number of hours: 15 Description of the course: Theoretical preparation of student for performing of laboratory classes by analysis of state of art obtained from scientific literature Method of evaluation: Preparation of procedure for the preparation of new type of catalyst ECTS: 1.5 Semester: winter Bibiography:

Course code: Cg13 Title of the course: ENVIRONMENTAL CATALYSIS Tutor: prof. dr hab. Mieczysława Najbar Teaching objectives: Lecture: Course code: Cg13W Type of course: lecture(w) Tutor: prof. dr hab. Mieczysława Najbar Number of hours: 30 Description of the course: Basic catalytic processes leading to the low temperature purification of exhaust gases produced by engines and industrial sources of emission,

DENOX – Selective Catalytic Reduction of nitrogen oxides, DESONOX – Selective Catalytic

Reduction of nitrogen oxides connected with oxidation of sulphure dioxide, VOC – oxidation of volatile organic compounds, VXOC – oxidation of volatile organic compounds containing halogens (X). Monolithic oxidic and metallic catalysts for particular purification processes – synthesis, efficiency and durability. Methods of analysis of gases containing 10-10 000 ppm pollutant particles.

Method of evaluation: examination

ECTS: 3.0 Semester: winter Bibiography:

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# Course code: Cg14

Title of the course: Physico-chemical bases of the Contact Catalysts' Synthesis

Tutor: Mieczyslawa Najbar

**Teaching objectives:** The scientific bases of the planning the structure of the catalyst surface being active in the HC oxidation, SCR of NO decomposition.

# **Description of the unit included in the course:**

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

Lecture

**Course code:** Cg14(w)

Type of course: lecture

Tutor: M. Najbar

#### Number of hours: 60

**Description of the course:** The scientific bases of the planning the catalyst surface structure to achieve maximal activity and selectivity in determined processes.

The following method of the catalyst synthesis will be discussed: i) the exchange of the anions and cations of the substrates with basic OH groups or protons of the acidic OH groups, respectively, ii)"grafting" with the use of the volatile substrates containing component of the active phase, iii) hydrothermal formation of the high-surface- area one- and multi-component active phases, iv) formation of the high-surface-area multi-component active phases by sol-gel method, v) wet impregnation and impregnation. The physico-chemical
processes occurring during: i) substrates' deposition at the catalyst surface (anionic and cationc exchange, hydrolysis, condensation, adsorption), ii) calcinations of the catalyst precursors (ion diffusion, oxidation-induced cations' segregation), iii) catalysts' pretreatment in atmospheres of different redox potentials ( surface segregation of the active forms, dissolution of the active species in supports or intermediate phases.

The influence of the crystallographic matching the active species and the support on the species structure.

The structure investigation of the catalyst precursors and the catalysts, with a powder X-ray diffraction (XRD), electron diffraction in Transmission Electron Microscope (TEM) and structure imaging in the High Resolution Transmission Electron Microscope (HRTEM), will be presented.

The following methods for the investigation of the surface species will be discussed: i) X- ray photoelectron spectroscopy (XPS), ii) Fourier Transform Raman spectroscopy iii) Fourier Transform IR spectroscopy (FTIR).and iv) Difussion Reflectance Infrared Fourier Transform Spectroscopy (DRIFTS)

The methods of the determining the catalyst activity and selectivity, the thermoprogramed surface reaction (TPSR) and stationary state reaction (SSR), will be presented. The examples of relations between the catalytic activity and the surface structure will be discussed.

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# Course code: Cg17

Title of the course: Inorganic Reaction Mechanisms

Tutor: dr hab Janusz Szklarzewicz

**Teaching objectives:** The knowledge of kinetic measurements and interpretation of kinetic data. Typical approximations used in kinetic measurements and theirs limits. Order of the reaction. Activation parameters - determination, limits and typical problems with their interpretation. Typical reaction mechanism for compounds of different geometry on the basement of literature data. Stereochemical change and the coordination number - inversion, pseudorotation, isomerization. Problem of isolation of isomers for specific coordination polyhedra. Substitution and solvent exchange reaction. Medium effects (solvent effect, salt effect, organized media). Oxidation-reduction reactions - mechanisms and distinguishing between them. Typical oxidants and reductants - typical mechanisms and literature compendium. Two-electron processes - do they exists in typical systems? Multielectron transfers - examples. Activation of small molecules - problems in modern chemistry of metal complexes. Insertion, migration, activation, addition and elimination. Reaction on ligands.

Catalysis, homo- and hetero-genous. Catalysators and organic reaction rules (are they general and what is their origin?). Instrumental methods for kinetic measurements - selected problems.

### **Description of the unit included in the course:**

lecture(w)

Lecture

Course code: Cg17W

Type of course: obligatory for IV year of study

Tutor: dr hab. Janusz Szklarzewicz

Number of hours: 30h

#### **Description of the course:**

Determination of the kinetic equation: order of the reaction, rate constants, reversible reactions, parallel reactions, multistep reactions, approximations: steady state, pseudo firstorder. Activation parameters, modes of activation, type of reaction mechanisms. Reactions in solution, molecularity of the process, Langford-Gray nomenclature. Occurrence and types of coordination polyhera. Substitution reaction at 2-8 coordinate centres - overview of literature data. Stereochemical change, classification, pseudorotation, inversion and the coordination number. Rearrangement with change of coordination number, hydrido complexes. Substitution reaction of carbonyl and related compounds. Solvent exchange and coordination number, special case of complex formation in aqua complexes. Salvation of ground and transient state. Medium effects: solvent and its structure, typical and specific salt effect, organised media. Redox reactions: inner- and outer- sphere mechanisms (details, intermediates, distinguishing between mechanisms, Marcus theory and their limits). Redox reactions of sp- and d- block species, radicals and solvated electron. Activation, addition, insertion and catalysis. Activation of ligands and small molecules (O<sub>2</sub>, N<sub>2</sub>, CO, NO, CO<sub>2</sub>, SO<sub>2</sub>, NO<sub>2</sub>, isonitriles, H<sub>2</sub>, alkenes, alkynes, alkanes), examples. Homogeneous calatysis: isomerization, methathesis, hydroboration, hydrogenation and other important processes. Reactions of explosives - typical mechanisms, difference in comparison with typical kinetic measurements.

Method of evaluation: exam

**ECTS:** 4.5

### **Semester: winter**

### **Bibiography:**

1. Martin L. Tobe, J. Burgess, "Inorganic Reaction Mechanisms", ed. Longman Ltd, England, 1999.

2. J.P. Candlin, K.A. Taylor, D.T. Thompson, "Reactions of Transition-Metal Complexes", ed. Elsevier, Amsterdam, 1968.

3. J. D. Atwood, "Inorganic and Organometallic Reaction Mechanisms", ed. Cole Publish., Comp., California, 1985 4. R.W. Hay, "Comprehensive Coordination Chemistry", vol. 6, eds G. Wilkinson, R.D. Gillard, J.A. McCleverty, Pergamon, Oxford, 1987.

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Course code: Cg20 Title of the course: EPR spectroscopy Tutor: Prof. dr hab. Zbigniew Sojka Teaching objectives:

# Description of the unit included in the course:

Lecture

Course code: CG20W

**Type of course:** lecture (w)

Tutor: Prof. dr hab. Zbigniew Sojka

Number of hours: 15

#### **Description of the course:**

Basic notions and definitions (magnetic electronic and nuclear moments, quantization, spinorbit and spin-spin coupling). Zeeman effect, resonance conditions, relaxation. Experimental techniques, continuous wave and pulse methods, quantitative measurements. Classification of EPR spectra and their parameters, spin Hamiltonian. Isotropic spectra, hyperfine interaction  $S \times A \times I$ , equivalent and nonequivalent nuclei. Anisotropic spectra of oriented systems and systems averaged in time and space. Tensor g and tensor A - determination and molecular interpretation, EPR spectra of organic and inorganic radicals and transition metal ions (monoand polinuclear centers). Calculation of g and A tensors from molecular structure data. Fine structure interactions  $S \times D \times S$ , determination and interpretation of D and E parameters. Computer analysis of complex spectra, relationship between spectral and molecular symmetry Advanced techniques (ENDOR, ESEEM, HF-EPR). Application of EPR spectroscopy in chemistry (case studies).

Method of evaluation: exam

#### **ECTS:** 1,5 (1,5 W)

#### Semester: winter

#### **Bibiography:**

- R. Kirmse, J. Stach, "Spektroskopia EPR. Zastosowania w chemii", Wyd. UJ, Kraków 1994

- S.K. Hoffman, W. Hilczer, "Elektronowy Rezonans Paramagnetyczny. Podstawy

spektroskopii impulsowej", Wyd. Nakom, Poznań 1997.

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Course code: Cg21

**Title of the course: Principles of Catalysis** 

Tutor: Prof. dr hab. Zbigniew Sojka

**Teaching objectives:** 

# **Description of the unit included in the course:**

Lecture

Course code: CG21W

**Type of course:** lecture (w)

Tutor: Prof. dr hab. Zbigniew Sojka

Number of hours: 15

### **Description of the course:**

Basic notions and definitions, description levels of catalytic phenomena, kinetic and molecular picture, time and space scales.

Catalytic cycle - thermodynamic and kinetic analysis. Energetic diagrams and analysis of simple and complex catalytic cycles (description of the cycle, identification of elementary steps, kinetic coupling, thermodynamic and kinetic reaction products).

Survey of typical catalytic systems and experimental techniques used for their characterization: structure-reactivity relationships.

Microscopic picture of heterogeneous catalysis, adsorption, diffusion, surface reaction, Langmuir-Hinshelwood and Eley-Riedl mechanisms, oscillatory processes.

Dynamics of surface reactions, elementary processes, potential energy surfaces, analysis of molecular pathways of surface reactions.

Description of simple and complex catalytic processes, transport limitations, introductory reactor engineering.

# Method of evaluation: exam

**ECTS:** 1,5 (1,5 W)

Semester: winter

# **Bibliography:**

- B. Grzybowska-Świerkosz, "Elementy katalizy heterogenicznej", PWN, Warszawa 1993
- F. Pruchnik, "Kataliza homogeniczna", PWN, Warszawa 1993
- G.C. Bond, "Kataliza heterogeniczna. Podstawy i zastosowania", PWN, Warszawa 1979.

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Course code: Cg22

Title of the course: Experimental techniques of catalysis and surface chemistry Tutor: prof. dr hab. Zbigniew Sojka Teaching objectives:

### Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

Lecture Course code: Cg22W Type of course: lecture (w) Tutor: prof. dr hab. Zbigniew Sojka Number of hours: 15 Description of the course:

Survey of experimental methods, interaction of electromagnetic radiation with the matter-Probst diagram, basic types of measurements, application of molecular probes. Imaging and microscopy: SEM, TEM/AEM and EPMA (examination of sample morphology and point composition), AFM and STM (surface atomic microscopy). Determination of phase and elemental composition- XRD/ED, XRF, XRE (global composition, crystallinity, grain size). Surface analysis: sorption methods (specific surface area, porosity, pore distribution). XPS/UPS, AES, SIMS techniques (examination of surface composition, valence and coordination states), LEED (structure of ordered surfaces and adsorbate layers). Investigation of molecular structure of active sites, adsorbed molecules and reaction intermediates: UV-VIS-NIR (electronic structure, coordination, valence states), IR/RS, DRIFT (identification of surface species, reaction mechanism), EXAFS, SEXAFS, XANES, NEXAFS (coordination and bond lengths in amorphous systems), MAS NMR and EPR spectroscopy (investigation of active centers, adsorbed species, surface reaction mechanisms, radical processes).

Method of evaluation: ECTS: 1,5 Semester: Bibiography:

Course code: Cg23

**Title of the course**: Solid State Chemistry **Tutor**: prof. dr hab. Zbigniew Sojka

### **Teaching objectives:**

### Description of the unit included in the course:

Lecture

Course code: CG23W

**Type of course:** lecture (w)

Tutor: prof. dr hab. Zbigniew Sojka

Number of hours: 15

### **Description of the course:**

Classification of solids: crystalline (molecular, ionic, covalent, metallic), porous, amorphous, hybride, nano- and supramolecular materials., inorganic polymers, highly dispersed substances.

Preparation methods of solid materials, nucleation, particle growth and sintering, hydrothermal methods, sol-gel.

Electric, magnetic and optical properties of solids (metals, insulators and semiconductors, diamagnetic, paramagnetic, antiferro- ferro- and ferrimagnetic materials.

Electronic structure (band theory and chemical bonding, Bloch functions, Fermi level and surfaces, DOS, local and cluster models, Hubbard and Anderson approach.

Point and linear defects (classification and Kroger-Vink notation, thermodynamics of defects, transport properties, diffusion, donor and acceptor levels, electronic and chemical properties, chemical doping, p-n junctions.

Surface (surface energy, work function, electronic states, band curvature, interaction with adsorbate). Interfacial phenomena and chemistry. Heterogeneous solid state reactions in ionic solids, metals, amorphous materials.

18. Method of evaluation: exam

### 19. ECTS: 1,5 (1,5 W)

20. Semester: winter

### 21. Bibliography:

- J. Dereń, J. Haber, R. Pampuch, "Chemia ciała stałego", PWN, Warszawa 1977

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# Course code: Cg25

Title of the course: Photocatalysis in homogeneous systems

Tutor: Prof. dr hab. Zofia Stasicka

**Teaching objectives:** To present photocatalytic processes from the mechanistic point of view and to show their importance

# Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

# Lecture

Course code: Cg25w Type of course: lecture Tutor: Prof. dr hab. Zofia Stasicka Number of hours: 15

# **Description of the course:**

- Introduction (origin, definitions, general meaning);
- Types of photocatalytic processes (true photocatalysis and photoenhancement: calalysed photoreactions, assisted photoreactions, sensitized photoreactions);
- Transition metal complexes in photocatalysis (effect of coordination on ligand properties and reactivity, photochemical behaviour of coordination compounds, influence of ligand, central atom and medium nature on the photoreaction type and photosensitivity spectral range);
- Applications (photocatalysis in organic synthesis, photocatalysis in environment, photocatalysis in energy production: conversion of solar energy).

# Method of evaluation:

ECTS: Semester: Bibiography:

# Course code: Cg28

Course:	BIOINORGANIC CHEMISTRY
Tutor:	Prof. Grażyna Stochel PhD, DSc
Type of course:	Lecture + seminar
Number of hours:	30  hrs lec + 15  hrs sem
ECTS:	4.5
Short description of the course:	

Important elements in biology and medicine, physical methods in bioinorganic chemistry, choice, uptake and assembly of metal containing units in biology, bioligands, communication roles for metals in biology, metal functions in metalloproteins, metalloenzymes, metal ion transport and storage, biochemistry of small molecules (O2, N2, CO, CO2, NO, etc), biomineralization, metals in environment and medicine, perspectives of bioinorganic chemistry.

Course:	PHOTOCHEMISTRY IN BIOLOGY AND MEDICINE		
Tutor:	Prof. Grażyna Stochel PhD, DSc		
Type of course:	Lecture		
Number of hours:	15 hrs		
ECTS:	1.5		
Short description of the course:			
Light and life; photochemical and photophysical principles; excited states, transient species,			
radicals; direct and sensitize	d photoprocesses; photochemical reactions and kinetics;		
photochemistry in nature:	photosynthesis, vision, bioluminescence; phototoxicity,		
photocancerogenesis, photoalergy, photoaging; elements of photomedicine: direct phototherapy,			
photodynamic therapy and diagnosis, phototargeting, photostability of drugs, photoprotection;			

modern experimental technics in photochemistry, photophysics and photobiology.

# Course code: Cg30

Course:	INORGANIC AND BIOINORGANIC REACTIONS - KINETICS AND MECHANISMS	
Tutor:	Prof. Grażyna Stochel PhD, DSc	
Type of course:	Lecture	
Number of hours:	15 hrs	
ECTS:	1.5	
Short description of the cour	se:	
Reaction rate and rate law; deduction of mechanism, experimental determination of the rate of		

Reaction rate and rate law; deduction of mechanism, experimental determination of the rate of reaction, substitution reactions, oxidation-reduction reactions, modification of ligand reactivity by complex formation, isomerism and stereochemical change, photochemical reactions.

# Course code: Cg31

Course:	MEDICAL INORGANIC CHEMISTRY			
Tutor:	Prof. Grażyna Stochel PhD, DSc			
Type of course:	Lecture			
Number of hours:	15 hrs			
ECTS:	1.5			
Short description of the course:				
Introduction; inorganic compounds in prophylaxis, therapy and diagnosis, Bertrand diagrams,				
radiometal-labeled agents for diagnostic imaging, contrast agents for X-ray, magnetic resonance				
imaging (MRI), therapeutic	radiopharmaceuticals, metal complexes as photo- and			
radiosensitizers, cis-platin and other antitumor metallopharmaceuticals, vanadium compounds as				

insulin mimics, treatment of Wilson and Menkens diseases, gold-based therapeutic agents, bismuth compounds, inorganic pharmacology of lithium, metal complexes as enzyme inhibitors, chelation treatment of metal intoxication, recognition and reactions of metallointercalators with DNA, transport of metal ions.

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# Course code: Cg32

Title of the course: Chemistry under Extreme Conditions & Cryogenics

Tutor: Dr. Wojciech Macyk, Dr. Konrad Szaciłowski

**Teaching objectives:** 

# Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture

and classes(i)

### Lecture

Course code: Chemistry under Extreme Conditions & Cryogenics

**Type of course:** i

Tutor: Dr. Wojciech Macyk, Dr. Konrad Szaciłowski

### Number of hours: 30

### **Description of the course:**

The subject of the course covers physical and chemical processes under extreme and nonclassical conditions. The following aspects will be discussed in detail:

- Cryogenics properties of cryogenic liquids, methods of various gases condensation, physical and chemical processes at low temperatures, applications of cryogenics. Polish scientists as pioneers of cryogenics (Karol Olszewski, Zygmunt Wróblewski).
- High pressures influence of high pressure on selected physical and chemical processes, thermodynamic parameters, etc. Application of high pressures in synthesis of chemicals and in mechanistic studies of chemical processes.
- Supercritical fluids properties of supercritical fluids, physical and chemical processes in supercritical solutions, application of supercritical fluids.
- Physical and chemical processes under other non-classical conditions ionic liquids, ultrasounds (sonochemistry), microwaves, plasma.

### Method of evaluation: exam

### **ECTS:** 3.0

#### Semester: summer

#### **Bibliography:**

- van Eldik, R.; Hubbard, C. D. (Eds.) Chemistry under Extreme or non-Classical Conditions, Wiley, 1996.
- Jha, A. R. Cryogenic Technology and Applications, Butterworth-Heinemann, 2005.
- Szczepaniec-Cięciak, E. Karol Olszewski (1846-1915). Chemik, światowej sławy kriogenik. in Złota Księga Wydziału Chemii UJ, E. Szczepaniec-Cięciak (Ed.), Wydawnictwo UJ, Kraków 2000, pp. 143-168.
- Selected review papers.

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### Course code: Cg35

Title of the course: Modern methods of inorganic synthesis Tutor: J. Szklarzewicz

# **Teaching objectives:**

Practical knowledge of the methods used in inorganic synthesis. Stability of coordination compounds and the isolation problems (including isomerisation, reaction on coordinated ligands etc.). Methods of inorganic synthesis including use of: ultrasonic, plasma and microwave activation. Synthesis under anaerobic, low and high pressure. Solvents, cations and anions and crystal quality.

lecture (W)

**Course code:** Cg35W **Type of course:** lecture **Tutor:** J. Szklarzewicz 22. Number of hours: 30 **Description of the course:** 

General description of coordination numbers in periodic table. The structure stability and the problem of product isolation. Isomerisation and methods of isomers synthesis and purification. Solvents, influence on reactivity and on product. Methods of reaction activation and its impact on products. Some techniques in synthesis: ultrasonic and microwave radiation, low and high pressure. Synthetic procedures in phases: gas; gas-liquid, liquid-solid sate, solid-solid. Anaerobic procedures, synthesis in supercritical liquids, hydrothermal methods, gels, use of current flow in synthesis (including synthesis by reduction, oxidation, electrodeposition and synthesis of compounds with metal on extreme oxidation states). Synthesis of heterometallic compounds and polymers. Substitution and redox and thermal dissociation reactions in synthesis. Activation of ligands- short review. Evaluation of cations, anions and solvent in crystal growth. Practical examples. Methods of crystal growth (including change in solubility, crystallization of non soluble compounds, electrocrystallization). Composite materials and molecular wires and their synthesis.

Method of evaluation: presence ECTS: 4.5 Semester: winter Bibiography: literature Laboratory Course code: Cg351 Type of course: ? Tutor: J. Szklarzewicz Number of hours: 15 Description of the course:

Method of evaluation: exam and report ECTS: Semester: winter Bibiography:

### Course code: Cg38

Title of the course: Coordination Chemistry of Inorganic Molecular Materials

Tutor: prof.dr hab.Barbara Sieklucka

**Teaching objectives:** 

#### **Description of the unit included in the course:**

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture and classes(i)

Lecture

**Course code:** Cg38 (w)

**Type of course:** 

Tutor: prof.dr hab.Barbara Sieklucka

Number of hours: 30

#### **Description of the course:**

From molecular coordination chemistry to coordination chemistry of inorganic materials. Chelate Metal-ligand bonding. and macrocyclic effects. Pre-organization and complementarity. Coordination of inorganic cations and anions. Design and characteristics of polynuclear coordination compounds. Synthetic strategy - from molecule to inorganic molecular material. Building blocks and self-assembly. Types of metal moieties (connectors) and linkers. Nature of interactions (coordination bonds, electrostatic interactions, hydrogen bonding,  $\pi$ - $\pi$  stacking, dispersion forces, solvatophobic effects, steric effects). Structural topology. Clusters and aggregates - zero-dimensional assemblies. Inorganic-organic hybrid materials one-, two- and three-dimensional. Coordination polymers. Functionality of polynuclear coordination compounds. Porous materials. Magnetic molecular materials. Spin

cross-over materials. Chromism. Non-linear potical properties. Redox properties. Conductivity.Multifunctionality.

Method of evaluation: credit or exam

**ECTS:** 3.0

Semester: winter

### **Bibiography:**

1. P.D.Beer, P.A.Gale, D.K.Smith, Supramolecular Chemistry, OUP Oxford 1999.

2. J.W.Steed, J.L.Atwood, Supramolecular Chemistry, Wiley 2000.

3. M.T.Weller, Inorganic Materials Chemistry, OUP Oxford 1999.

4. B.J.Holliday, Ch.A.Mirkin, Supramolecular Coordination Chemistry, Angew.Chem.Int.Ed., 2001, 40, 2022-2043.

5. S.Leiniger, B.Olenyuk, P.J.Stang, Self-assembly of discrete cyclic nanostructures mediated by transition metals, Chem.Rev.,2000, 100, 853-908.

6. B.Moulton, M.J.Zaworotko, From molecules to crystal engineering: supramolecular isomerism and polymorphism in network solids, Chem.Rev., 2001, 101, 1629-1658.

7. Ch.Janiak, Engineering coordination polymers towards applications, Dalton Trans., 2003, 2781-2804.

8. A.F.Orchard, Magnetochemistry, OUP Oxford 2003.

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# Course code: Cg39

Title of the course: Molecular devices and molecular logic gates

Tutor: dr Konrad Szaciłowski

**Teaching objectives:** Course is devoted to different aspects of molecular devices and especially to chemical logic gates and other chemical systems for information storage and processing.

# Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

Lecture

Course code: Cg39w

### **Type of course:** w

Tutor: dr Konrad Szaciłowski

### Number of hours: 15

**Description of the course:** The course encompasses basic notions related to molecular machines with special emphasis on information processing at molecular level.Introductory topics: introduction to Boolean algebra and digital information processing, Moore's law and principles of oparation of logic gates.Control of motion in supramolecular systems, application of supramolecular systems as information carriers. Application of electrochemical and photochemical techniques in control and monitoring of supermolecules.Molecular information processing as an alternative to conventional electronics. Chemical systems in information processing: chemomechanical systems: "molecular mecano", rotaxanes, catenanes, rotacatenanes, photochromic materials, fluorescent sensors as logic gates. Chemical algebraic systems. Molecular logic systems based on simple coordination compounds.

Method of evaluation: essay or written exam

### **ECTS:** 1.5

Semester: winter

### **Bibiography:**

F. Crick "The Astonishing Hypothesis", Scribner Book Company, 1995

R. Penrose "The Large, the Small and the Human Mind", Cambridge University Press, 1997

S. Greenfield "The Human Brain: A Guided Tour", Basic Books, 1998.

E. Regis "Nano : The Emerging Science of Nanotechnology", Back Bay Books , 1996.

G.J. Milburn "Quantum technology", Allen & Unwin, 1996.

W.D. Hills "Pattern on the Stone", Perseus Books Group, 1999.

G.J. Milburn "The Feynman Processor: Quantum Entanglement and the Computing Revolution", Perseus Publishing, 1999.

# Seminar

**Course code:** Cg39S

**Type of course:** s

Tutor: dr Konrad Szaciłowski

Number of hours: 15

**Description of the course:** This course is devited to extension of the material presented during lectures, desing and analysis of various logic circuits (both electronic and chemical) and theorwetical analysis of logic systems. A part of the course is devited to numerical modelling of electronic circuits.

### Method of evaluation: oral presentation

**ECTS:** 1.5

Semester: winter

Bibiography: 1. P. Bonhôte, E. Gogniat, F. Campus, L. Walder, and M. Grätzel, Displays,

1999, 20, 137. 2. G. J. Brown, A. P. de Silva, and S. Pagliari, J. Chem. Soc. Chem. Commun.,

2002, 2461. 3. Y. Chen, G.-Y. Jung, D. A. A. Ohleberg, X. Li, D. R. Stewart, J. O. Jeppesen,
K. A. Nielsen, J. F. Stoddart, and R. S. Williams, Nanotechnology, 2003, 14, 462. 4. A. P. de
Silva, D. A. Fox, A. J. M. Huxley, and T. S. Moody, Coord. Chem. Rev., 2000, 205, 41. 5. A.
P. de Silva, H. Q. N. Gunaratne, T. Gunnlaugsson, A. J. M. Huxley, C. P. McCoy, J. T.
Rademacher, and T. E. Rice, Chem. Rev., 1997, 97, 1515. 6. V. Balzani, M. Venturi, and A.
Credi, 'Molecular Devices and Machines - A Journey into Nanoworld', WILEY-VCH, 2003.

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### **Course code: Cg40**

Title of the course: Introduction to environmental chemistry Tutor: dr Magdalena Kurdziel Lecture Course code: Cg 40w Type of course: lecture Tutor: dr Magdalena Kurdziel Number of hours: 15

**Description of the course:** Basic concepts and definitions. The role of environmental chemistry in realization of the idea of sustainable development. Composition of the atmosphere. Chemical and photochemical reactions in the atmosphere. Air pollutants and their sources. Chemistry of hydrosphere. Water pollution. Water quality – classification of waters. Water and sewage treatment. Soil pollution and degradation. Protecting the environment against pollution.

### Method of evaluation: examination

### **ECTS:** 1,5

#### Semester: summer

#### **Bibiography:**

- S. E. Manahan, Environmental chemistry, 8th edition, CRC Press, Boca Raton-London-New York-Washington 2005.
- 2. P. O'Neill, Chemia środowiska, Wydawnictwo Naukowe PWN, Warszawa-Wrocław 1997.
- 3. L. Falkowska, K. Korzeniowski, Chemia atmosfery, Wydawnictwo Uniwersytetu Gdańskiego, Gdańsk 1995.
- 4. B. J. Alloway, D. C. Ayres, Chemiczne podstawy zanieczyszczania środowiska,

Wydawnictwo Naukowe PWN, Warszawa 1999.

Classes Course code: Cg40n Type of course: classes Tutor: dr Magdalena Kurdziel Number of hours: 15 Description of the course: Calculations in environmental chemistry. Problem solving tasks Method of evaluation: graded credits ECTS: 1,5 Semester: summer Bibiography:

Seminar

Course code: Cg40s

Type of course: seminar

Tutor: dr Magdalena Kurdziel

Number of hours: 30

**Description of the course:** Green chemistry. Global environmental problems: greenhouse effect, ozone layer destruction, acid rains. Persistent organic pollutants and heavy metals in the environment. Wastes management. Food contamination. The state of the environment in chosen regions of Poland. Problems of local communities caused by environment degradation. Human pression.

Method of evaluation: graded credits

**ECTS:** 3

Semester: summer

Bibiography: 1. Chemia środowiska. Ćwiczenia i seminaria. Cz. 1 i 2., pod red. E.

Szczepaniec-Cięciak

i P.Kościelniaka, Wydawnictwo Uniwersytetu Jagiellońskiego, Kraków 1999.

- Web sites: Inspectorate of Environmental Protection (www.pios.gov.pl), Ministry of Environment (www.mos.gov.pl), local administration (municipalities, communes, counties, etc.)
- 3. Teaching materials supplied by tutor.

Title of the course: Actual problems in chemistry of new materials and catalysis
Tutor: Prof. Dr Jerzy Datka, Prof. Dr Barbara Sieklucka, Prof. Dr Zbigniew Sojka, Dr hab.
Katarzyna Stadnicka, Dr hab. Wiesław Łasocha

**Teaching objectives** 

### Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

Lecture

Course code: Cg41

Type of course: lecture

**Tutor:** Prof. Dr Jerzy Datka, Prof. Dr Barbara Sieklucka, Prof. Dr Zbigniew Sojka, Dr hab. Katarzyna Stadnicka, Dr hab. Wiesław Łasocha

Number of hours: 30

**Description of the course:** 1. basing information concerning zeolites 2. industrial application of zeolites. 3. Thermodynamic, kinetic and molecular description of surface processes and catalytic reactions. 4. Introduction to chemistry of nanostructural materials. 5. what is supramolecular coordination chemistry. 6. Examples of inorganic functional molecular materials, topology, structure and properties. 7. Introduction to crystal structure designing. 8. Intermolecular interactions useful in crystal engineering. 9. Crystallographic and powder diffraction methods in material science. 10. Application of new materials as solid hydrogen storage materials.11. Preparation of literature miniproject concerning chemistry of new materials and catalysis.

Method of evaluation: acceptance and evaluation of literature miniproject

**ECTS:** 7.0

Semester: summer

**Bibiography:** 

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Title of the course: Photomaterials

Tutor: dr Wojciech Macyk, dr Konrad Szaciłowski

Teaching objectives: Course is devoted to practical applications of photoactive materials

### Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

#### Lecture

**Course code:** Cgw

**Type of course:** w

Tutor: dr Wojciech Macyk, dr Konrad Szaciłowski

Number of hours: 15

**Description of the course:** Introduction: interactions of light with matter (reflection, dispersion, scattering, interference, diffraction), basic photophysical and photochemical processes. Definition of photomaterials. Photomaterials in biology and medicine: fluorescent labelling (fluorophores and quantum dots), fluorescent chemisensors, photoactive materials in therapy, cosmetic photoprotective filters, plant and animal pigments. Photomaterials and information: photography (B&W and colour), photocopying, optical discs (CD, CD-R, CD-RW, DVD, DVD-R, DVD-RW), displays (LCD, LED, OLED, CRT, plasma displays), thermal and self-copying paper. Photomaterials in environmental protection: photocatalysts for air and water purification, self-cleaning and self-sterilizing surfaces, superhydrophobicity and superhydrophylicity. Other photomaterials: photovoltaic cells, photo-, thermo- and elecgtrochromic materials for various applications, light-hardened resins, photopolymers in electronics and medicine, photolitography.

**Method of evaluation:** essay or written exam **ECTS:** 1.5

#### Semester: summer

### **Bibiography:**

(1) Fujishima, A.; Hashimoto, K.; Watanabe, T. *TiO*<sub>2</sub> *photocatalysis. Fundamentals and Applications*; BKC, Inc.: Tokyo, 1999.

- (2) Bonhôte, P.; Gogniat, E.; Campus, F.; Walder, L.; Grätzel, M. Displays 1999, 20, 137.
- (3) Carp, O.; Huisman, C.L.; Reller, A. *Progr. Solid State Chem.* **2004**, *32*, 33.
- (4) de\_Saja, J.A.; Rodríguez-Méndez, M.L. Adv. Colloid Interface Sci. 2005, 116, 1.

(5) de\_Silva, A.P.; Gunaratne, H.Q.N.; Gunnlaugsson, T.; Huxley, A.J.M.; McCoy, C.P.; Rademacher, J.T.; Rice, T.E. *Chem. Rev.* **1997**, *97*, 1515.

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Title of the course: Nanoelectronics and molecular electronics

Tutor: dr Konrad Szaciłowski

**Teaching objectives:** principles of nanoelectronics and molecular electronics, chemistry of components used in molecular electronics, techniques for fabrication and research on nanostructures

### Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture and classes(i)

Lecture

**Course code:** Cg43w

**Type of course:** w

Tutor: dr Konrad Szaciłowski

Number of hours: 15

**Description of the course:** The course consists of three parts. The first part deals with basic principles of classical electronics: construction and operational properties of basic active components (diodes, bipolar transistors, FET transistors), structure and fabrication technology of monolithic integrated circuits. Technological and physical limits of classical electronic semiconducting devices are also included in this part.

The second part is mostly devoted to synthesis, properties and electronic structure of molecular precursors used in molecular electronics (fullerenes, porphyrins, phthalocyanines, policenes, tetrathiafulvalenes and carbon nanotubes). Properties critical for applications of these materials in electronics are especially emphasized.

The third part of the course discusses techniques used for fabrication and investigation of nqnoelectronic structures using single molecules and thin layers. Organic field effect transistors (OFET), organic photovoltaic systems and molecular optoelectronic switches are described in detail.

Method of evaluation: essay or test exam

**ECTS:** 1.5

Semester: summer

#### **Bibiography:**

A. W Gosh, P.S. Damle, S. Datta, A. Nitzan "Molecular electronics: theory and device prospects", *MRS Bulletine*, **2004**, 391-395.

R. McCreery "Carbon-based molecular electronic junctions", *Electrochem. Soc. Interface*, **2004**, 46-51.

J.A. Hutchby, G.I. Bourianodd, V.V. Zhirnov, J.E. Brewer "Extending the road beyond CMOS", *IEEE Circ. Dev. Mag.* 2002, (03), 28-40.

K.S. Kwok "Materials for future electronics", NANO Today 2003, (12), 20-27.

S.M. Lindsay "Single molecule electronics", *Electrochem. Soc. Interface* **2004**, 26-30.

R.L. Carroll, C.B. Gorman "The genesis of molecular electronics", Angew. Chem. Int. Ed. 2002, 41, 4378-4400.

K.P. Zauner "Molecular information technology", Crit. Rev. Solid State Mat. Sci. 2005, 30, 33-69.

"Springer Handbook of Nanotechnology", ed. B. Bhushan, Springer Verlag, Berlin 2004 "Handbook of Nanoscience, Engineering and Technology", ed. W.A. Goggard III, CRC Press, New York, 2003.

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# Course code: Cg45

Title of the course: Mechanisms of photochemical reactions

#### Tutor:

**Teaching objectives:** 

### Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture

and classes(i)

Lecture

**Course code:** Cg45w

Type of course: w

Tutor: Dr. Wojciech Macyk

Number of hours: 15

#### **Description of the course:**

- Fundamental photochemical laws: Jabłoński diagram, radiative and nonradiative processes, fluorescence, phosphorescence, selection rules, excited states quenching, kinetics of photochemical processes
- Tools used in studies on mechanisms of photochemical reactions and photophysical processes continuous and flash photolysis, quantum yield measurements, photoelectrochemistry, spectroelectrochemistry
- Chemical actinometry
- Photochemical reactions of organic compounds pericyclic reactions, symmetry in photochemistry, various types of photochemical reactions (substitution, addition, polymerisation, redox, etc.)
- Chemiluminescence
- Photochemical reactions of coordination compounds
- Mechanisms of selected photochemical processes in biology, medicine, environmental protection, industry

### Method of evaluation: essay or exam

# **ECTS:** 1.5

# Semester: summer

# **Bibliography:**

- S. Paszyc *Podstawy fotochemii*, PWN, Warszawa 1992
- J. A. Baltrop, J. D. Coyle Fotochemia. Podstawy, PWN, Warszawa 1987
- Selected review papers

# Course code: Cg46

Title of the course: Heterogeneous photocatalysis

**Tutor**: Dr Wojciech Macyk

**Teaching objectives:** 

# Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture

and classes(i)

### Lecture

**Course code:** Cg46w

### Type of course: w

Tutor: Dr. Wojciech Macyk

### Number of hours: 15

# **Description of the course:**

- Basic processes at illuminated semiconductors (excitation, recombination, interfacial electron transfer)
- Photocatalytic degradation and mineralization of water and air pollutants mechanistic aspects
- Modification of heterogeneous photocatalysts photosensitisation, tuning of redox properties and basic physicochemical parameters
- Spectroscopy of broad bandgap semiconductors
- Photoelectrochemistry of broad bandgap semiconductors flatband measurements, efficiency of photocurrent generation (incident photon to current efficiency; *IPCE*), current doubling effect, spectroelectrochemistry, semiconductor-based photochemical switches
- Selected photocatalytic processes photocatalysed organic synthesis, nitrogen photofixation, CO<sub>2</sub> photoreduction, photosensitised singlet oxygen generation
- Practical applications of heterogeneous photocatalysis, especially in the presence of TiO<sub>2</sub> – photocatalytic water and air purification, self-cleaning and self-sterilising surfaces, superhydrophilic surfaces, photovoltaic cells (Graetzel cell)

# Method of evaluation: essay or exam

# **ECTS:** 1.5

### Semester: summer

### **Bibliography:**

- Fujishima, A.; Hashimoto, K.; Watanabe, T. *TiO*<sub>2</sub> *Photocatalysis. Fundamentals and Applications*; BKC, Inc.: Tokyo, 1999.
- Selected review papers

# Course code: Cg47

Title of the course: Photoelectrochemistry and photovoltaics

Tutor: Dr. Konrad Szaciłowski, Dr. Wojciech Macyk

**Teaching objectives:** The main objective of the course is to present the basic aspects of spectroscopy and electrochemistry of semiconductors and practical applications of these materials for construction of solar cells. Furthermore, much attention will be paid to various practical aspects of solar energy conversion: from thermodynamic efficiency of the devices to the economical and environmental factors.

# **Description of the unit included in the course:**

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture

and classes(i)

Lecture and classes

Course code: Cg47i

Type of course: i

Tutor: Dr. Konrad Szaciłowski, Dr. Wojciech Macyk

Number of hours: 30

**Description of the course:** The course is divided into two parts. The first part encompasses the basics of electronic structure of semiconductors, synthesis of semiconductor powders and thin layers of precisely designed structure as well as various photoelectrochemical phenomena. Detailed problems: determination of band gap energy and band edge potentials, polarity of semiconductor surfaces, bulk doping and surface modification, generation and recombination of charge carriers, photocurrent doubling effect, thermodynamic and kinetic aspects of photocurrent generation, photocurrent switching effects and its application in optioelectronics, semiconductor-based sensors.

The second part is devoted to various types of photovoltaic cells: monocrystalline, polycrystalline, thin layer cells, polymer PV cells, photosensitized solar cells. Detailed topics: thermodynamic efficiency of various solar cells, electronic phenomena in single- and multilayer semiconducting cells, semiconductor matching and parasitic processes associated therewith, photonic phenomena in thin layer cells, photonic and fluorescent energy concentrators, economical and environmental issues of solar energy conversion.

Method of evaluation: test exam

# **ECTS:** 3.0.

### Semester: winter

# **Bibiography:**

V. Lehman "Electrochemistry of Silicon. Instrumentation, Science, Materials and Applications", Wiley-VCH 2002.

K. Iizuka *Elements of Photonics, Volume I: In Free Space and Special Media.* John Wiley & Sons, Inc. 2002

K. Iizuka *Elements of Photonics, Volume II: For Fiber and Integrated Optics*. John Wiley & Sons, Inc., 2002.

J.G. Vos, R.J. Forster, T.E. Keyes "Interfacial Supramolecular Assemblies" John Wiley & Sons, Ltd., 2003

G. Decher, J.B. Schlenoff "Multilayer Thin Films", Wiley-VCH 2002

T. Markvart, L. Castanier "*Practical Handbook of Photovoltaics: Fundamentals and Applications*", Elsevier 2003

C.J. Brabec, V. Dyakonov, J. Parisi, N.S. Sariciftci "Organic photovoltaics. Concepts and realization", Springer Verlag: Berlin, 2003.

J. Gellings, H.J.M. Bouwmeester "*The CRC Handbook of Solid State Electrochemistry*", CRC Press 1996

N. Tsuda, K. Nasu, A. Fujimori, K. Siratori "*Electronic Conduction in Oxides*", Springer, 2000.

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# Course code: Ci01

Title of the course: Metals in organic synthesis

Tutor: Dariusz Cież Ph.D.

**Teaching objectives:** 

# Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture and classes(i)

Lecture

Course code: Ci01

Type of course: lecture

Tutor: Dariusz Cież Ph.D.

Number of hours: 30

**Description of the course:** Topics include the Wurtz coupling, "soft" enolization techniques, syntheses of enolates and their application in aldol reactions, alkylation and arylation processes and couplings. Addition reactions of metalorganic compounds to  $\alpha$ , $\beta$ -unsaturated systems, carbonyl groups and imines. Applications of palladium, cobalt, chromium and molybdenum compounds in carbon-carbon bond formations. Olefin metathesis using the Schrock's and Grubb's catalysts. Metal mediated functionalization of olefins. Lewis acid-catalyzed enantioselective cycloadditions. Radical and carbene reactions – formation of free radical species using metal salts. Oxidation and reduction of organic compounds. Homogeneous and heterogenous hydrogenations of unsaturated compounds using palladium, platinum and Wilkinson's catalysts. Application of aluminum trihydride, LAH and cerium trichloride in reduction of functional groups.

Method of evaluation: exam

**ECTS:** 3.0

Semester: winter semester

Bibiography: 1) R. P. Houghton "Kompleksy metali w chemii organicznej"

2) F. Pruchnik "Chemia metaloorganiczna – pierwiastki przejściowe"

3) W. Carruthers, I. Coldham "Modern methods of organic synthesis"

4) J. Gawroński, K. Gawrońska, K. Kacprzak, M. Kwit "Współczesna synteza organiczna"

5) J. Skarżewski "Wprowadzenie do syntezy organicznej"

6) F. Pruchnik "Kataliza homogeniczna"

**Supramolecular Chemistry** 

**Course code: Ci03** 

**Type of course: lecture** 

Tutor: dr hab. Julita Eilmes

Number of hours: 30

#### **Description of the course:**

Nature of supramolecular interactions: Terminology of supramolecular chemistry, definitions and their historical development (host, guest, receptor, molecular inclusion, clathrates, cavitates, complementarity, preorganisation). Classification of supramolecular interactions (ion-ion, ion-dipole, dipole-dipole, cation- $\pi$ , hydrogen bonding,  $\pi$ - $\pi$  stacking, hydrophobic effects, close packing in the solid state). Supramolecular aspects of biological processes – metalloproteins, enzymes, nucleic acids Molecular recognition: Cation binding hosts - crown ethers, lariat ethers, podands, cryptands, spherands. Natural receptors of cations. Complexation and transport of ions. Ionophores. Activation of anions - Phase Transfer Catalysis. Calixarenes, cyclophanes, carcerands. Receptors for anionic guests. Neutral guest binding. Chiral recognition. Cyclodextrins - inclusion properties and applications. Self-assembly: Self-assembly in natural and synthetic systems. Molecular template effect.  $\pi$ -Electron donor-acceptor systems. Transition metal ions in self-assembly and in template effects. Hydrogen bond directed assemblies. Synthesis of catenanes, rotaxanes and knots. Molecular boxes, racks and ladders. Helicates. Molecular rosettes and ribbons. Cucurbituril and peptide nanotube. Materials, devices and supramolecular technology: Dendrimers. Liquid crystals. Molecular sensors, switches and logic gates. Supramolecular catalysis.

Method of evaluation: colloquium or examination

ECTS: 3 Semester: summer Bibliography: Chemistry of Macrocyclic Complexes Course code: Ci04 Type of course: lecture Tutor: dr hab. Julita Eilmes Number of hours: 15

### **Description of the course:**

Nomenclature rules for macrocyclic systems. Thermodynamic and kinetic aspects of macrocyclic systems formation - coordination template effect, macrocyclic and cryptate effects. Synthetic approach to macrocyclic systems: Non-template procedures - high dilution techniques. Metal - ion templated synthesis, Crown ethers, aza-oxa, thia-crowns, cryptands. Macrocyclic Schiff bases. Metal complexes of phtalocyanine, Tetraaza[14]annulenes. Synthesis of porphyrins (TPP, OEP, meso-substituted derivatives). Reactivity of macrocyclic complexes: Metal centered reactions. Reactivity of the ligand oxidative dehydrogenation, hydrogenation, addition-insertion, electrophilic substitution alkilation, acylation. Natural macrocyclic systems: Macrocycyclic antibiotics and related systems. Natural porphyrins and corrins - Vit. B<sub>12</sub>, chlorophyll, hemoglobin, myoglobin and cytochromes. Oxygen transport and storage. Design and synthesis of biomimetic macrocycles: Functionalisation of porphyrins - capped, fenced, bridged and dimeric porphyrins as models of natural oxygen transporting systems. Synthetic models of metaloenzymes (monooxygenase-cytochrom P-450, B<sub>12</sub> coenzyme). Oxygen binding and activation. Synthetic biomimetic catalysts.

### Method of evaluation: colloquium or examination

ECTS: 1.5 Semester: winter Bibliography:

### **Recent Advances in Synthetic Organic Chemistry**

**Course code: Ci05** 

**Type of course: lecture** 

**Tutor:** dr hab. Julita Eilmes

Number of hours: 30

#### **Description of the course:**

**Organic chemistry of fullerenes:** Methods of fullerenes separation and purification. Chemical reactivity of C<sub>60</sub>. Reactions with nucleophiles and electrophiles. Oxidation, reduction and halogenation. Cycloaddition as method of fullerene functionalisation. Methanofullerenes. Heterofullerenes. Diels-Alder cycloadducts. Preparation of bioconjugates. Fullerene modified polymers. Endohedral metal complexes. Supramolecular chemistry of fullerenes – complexes with calixarenes, cyclodextrins and cyclotriveratrylenes. Buckybowls – synthesis of semibuckminsterfullerenes. Perspectives and applications. **Organic chemistry on solid supports:** Resins, linkers and reagents for solid phase organic synthesis (SPOS). Cleavage strategies. Solid phase organic reactions – representative examples. Solid phase peptide synthesis. Combinatorial chemistry. Synthetic strategies in combinatorial and parallel synthesis of peptides, oligonucleotides, oligosaccharides and small- molecular-weight compound libraries. **Expanded, contracted and isomeric porphyrins:** Synthetic aspects of porphyrins chemistry. Procedures leading to expanded, contracted and isomeric porphyrins. Biomimetic approach to porphyrinoid systems. Medical applications of expanded porphyrins – Magnetic Resonance Imaging (MRI), Photodynamic Therapy (PDT), Antisense applications – RNA hydrolysis and DNA photolysis. **Unconventional methods in organic synthesis:** Use of microwaves, ionic liquids and enzymes. Solvent-free organic synthesis. High pressure methods. Transition metals in organic synthesis – selected examples.

Method of evaluation: colloquium	
ECTS: 3.0	
Semester: winter	
Bibiography:	

### Course code: Ci07

### Title of the course: Application of spectroscopy in the organic chemistry

Tutor: Dr. Anna Kolasa

**Teaching objectives:** Except the subject related competences students should learn some generic competences like problem solving, abstract thinking, applying known solutions in new situations, critical evaluation of data as well as taking part in discussions and team-work

# Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

**Tutorials** 

**Course code:** Ci07k

Type of course: tutorials

Tutor: Dr. Anna Kolasa

Number of hours: 30

**Description of the course:** The course is a continuation of basic principles of spectroscopic methods gained by students in the course of organic chemistry. The following methods are discussed:

*Ultraviolet and visible spectroscopy*: spectra of dienes, enones and aromatic compounds; steric effects and UV-VIS spectra; influence of solvents on absorption bands; application of UV-VIS spectra for structure elucidation, monitoring of reactions, determination of dissociation constants, investigation of equilibria (tautomerism, complex formation), analysis of mixture composition.

*Mass spectrometry*: HRMS and molecular formula; ionisation methods and their influence on spectra; fragmentation pathways for main classes of organic compounds and the methods to prove them; rearrangements; combination of MS with chromatography (GC/MS).

*Infrared spectroscopy*: Bands typical for functional groups and structural units; interpretation of spectra; application of IR in stereochemistry and quantitative analysis.

*Nuclear magnetic resonance*: interpretation of spectra with complicated spin patterns; NMR of various nuclei (<sup>1</sup>H, <sup>13</sup>C, <sup>19</sup>F, <sup>31</sup>P, <sup>15</sup>N), heteronuclear couplings; coupling constants and their application for structure elucidation; decoupling technique; chemical shift reagents; application of NMR in: stereochemistry, investigation of dynamic processes, biology and medicine.

A range and limitations of methods under consideration. Complementary usage of all the methods for structure elucidation of complex organic compounds.

Method of evaluation: written examination

**ECTS:** 3.0

Semester: summer (VI)

### **Bibiography:**

R. M. Silverstein, F. X. Webster; "Spectrometric identification of organic compounds"; John Wiley & Sons 1989

M. Hesse, H. Meier, B. Zeeh; "Spektroskopische Methoden in der organischen Chemie"; Georg Thieme Verlag 1995

#### Course code: Ci08

**Title of the course:** Retrosynthetic analysis

Tutor: Dr. Anna Kolasa

#### **Teaching objectives:**

Except the subject related competences students should learn some generic competences like problem solving, applying known solutions in new situations, as well as an active participation in discussions and team-work

Lecture and classes Course code: Ci08i Type of course: lecture and classes

### Tutor: Dr. Anna Kolasa

### Number of hours: 30

**Description of the course:** This course should provide students with the ability to design the pathways of synthesis for complex organic molecules, including natural compounds and synthetic biologically active compounds. Topics: multistep syntheses and their yields; synthons, disconnections and thinking backwords: from final product to educts; selection of proper functional groups in starting materials and proper reactions to achieve the product wanted; formation of certain bonds as a crucial point of retrosynthetic analysis; chemo-, regio-, and stereoselective strategies; application of software and biomimetic pathways in retrosynthetic analysis; retrosynthetic analysis of some complex molecules taken from literature.

Method of evaluation: written examination

**ECTS:** 3.0

**Semester:** winter (VI)

### **Bibiography:**

Ch. Willis, M. Wills "Organic synthesis" Oxford University Press 1997M. B. Smith "Organic Synthesis" McGraw-Hill International Editions 1994E. J. Corey, Xue-Min Cheng "The logic of chemical synthesis" John Wiley & Sons 1989

# Course code: Ci10

# **Title of the course: TWO-DIMENSIONAL NMR SPECTROSCOPY**

Type of course: lecture and classes

Tutor: Barbara Rys PhD, DSc

Number of hours: 15

**ECTS:** 1,5

# **Description of the course:**

Prerequisite: Application of spectroscopic methods in organic chemistry. Application of COSY, TOCSY, HTCOR, HMQC, HMBC, NOESY, ROESY and INADEQUATE methods to structure elucidation.

### **Course code: Ci13**

# **Title of the course: MECHANISMS OF ORGANIC REACTIONS**

Type of course: lecture and classes

Tutor: Janusz Sepioł PhD, DSc

#### Number of hours: 45

#### **ECTS:** 4,5

#### **Description of the course:**

The main types of organic reactions have been presented during fundamental lecture on organic chemistry. The present lecture will deal with the discussion of some other important organic reactions and rearrangements, which are essential for those students who will specialise in organic chemistry. The reactions of Jacobsen, Curtius, Hofmann, Losen, Schmidt, Konoevenagel, Wittig, Wagner-Meerwein and also Phase-Transfer catalysis (PTC) and Vicarious Nucleophilic Substitution (VNS) reactions will be presented. The Claisen, Beckmann and benzidine rearrangements will also be included in the lecture.

Mechanisms of organic reaction – a seminar:

The variety and complexity of organic reactions is especially plentiful. It is of substantial importance that students learn the methods how to formulate hypotheses concerning the mechanisms of the reactions and ways of proving these hypotheses. During the seminar the participants will study the analysis of several reactions in connection with the structure of products obtained in these reactions. Methods useful for predicting the structure of final products on the basis of their relation to the structure of substrates and conditions of the reactions will also be included in the seminar. Recent publications dealing with the above areas will be used in the seminar.

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Course code: Ci14 Title of the course: Heterocyclic Chemistry Tutor: Prof.Barbara Zaleska Teaching objectives:

### Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)
Lecture
Course code: Ci14
Type of course: lecture (w)

#### Tutor: Prof.Barbara Zaleska

#### Number of hours: 15

**Description of the course:** Systematic nomenctature for heterocyclic systems, mono- and policyclic. I. Non-aromatic heterocycles. Three- and four-membered ring compounds. Interaction in the rings and influences on reactivity. II.Aromatic heterocycles. Some criteria of aromaticity in heterocycles. Five-membered systems  $\pi$ -excessive . Six-embered systems  $\pi$ -deficiency (pyridine). Synthesis of various heterocyclic systems. III. Fused heterocyclic rings. Quinolines, isoquinolines, acridines, phenantridines, indol, indolizines. Other fused systems cyclization reactions, characteristic reactivity.

Method of evaluation: examination

**ECTS:** 1.5

#### Semester: summer

**Bibiography:** Thomas Gilchrist "Heterocyclic Chemistry"; Jacek Młochowski "Chemia zwiazków heterocyklicznych" G.R.Newkone, W.V.Paudler Contemporary Heterocyclic Chemistry.

#### Seminar

**Course code: Ci14** 

Type of course: seminar

Tutor: Prof.Barbara Zaleska

Number of hours: 15

**Description of the course:** The general methods, available for the construction of heterocyclic compounds from open-chain precursors and their mechanism. Characteristic reactions of  $\pi$ -excessive as well as  $\pi$ -deficiency heterocyclic systems.

Method of evaluation: examination

### **ECTS:** 1.5

#### Semester: summer

**Bibiography:** Thomas Gilchrist "Heterocyclic Chemistry"; Jacek Młochowski "Chemia zwiazków heterocyklicznych" G.R.Newkone, W.V.Paudler Contemporary Heterocyclic Chemistry.

### Course code: Ci15

Title of the course: Chemistry of bioactive natural products. Tutor: Prof.Barbara Zaleska Teaching objectives:

### Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)
Lecture

**Course code: Ci15** 

**Type of course:** lecture (w)

Tutor: Prof.Barbara Zaleska

Number of hours: 30

**Description of the course:** This lecture included a groundwork in natural product chemistry, by considering biosynthesis leading to various selected classis of natural product present in nature (plants) . Biological activity. Fatty acids, prostaglandins, terpenes, steroids. Flavones. Natural-dyes . Alkaloids. Feromone. Atibiotics.

Method of evaluation: examination

**ECTS:** 3.0

### Semester: summer

**Bibiography:** Paul M Dewick "Medicinal Natural Products" Graham L.Patrick Medicinal Chemistry. A.Kołodziejczyk "Naturalne Związki Organiczne" S. Kohmutzer "Farmakognozja".

Course code: Ci17

# **Title of the course: CHEMISTRY AND TECHNOLOGY OF MATERIALS**

Type of course: lecture

Tutor: Dr Ewa Witek

Number of hours: 15

**ECTS:** 1,5

**Description of the course:** Organic and inorganic raw materials in chemical industry; products of chemical industry: synthetic fertilisers; preparations for plants protection; dyes; preparation for food preservation; detergents; plastics; polymer aid preparations.

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Title of the course: HYDROPHILIC POLYMERS

Tutor: Prof. Edgar Bortel, PhD, DSc

**Teaching objectives:** 

#### Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

Lecture

**Course code:** Cj01 (w)

Type of course: lecture

Tutor: Prof. Edgar Bortel, PhD, DSc

Number of hours: 30

**Description of the course:** In the lectures newest achievements in the field of synthesis and applications of water-soluble resins and hydrogels are presented. The focus is particularly directed on the processes carried out in inverse micro emulsions (w/o) and on nanolatexes thus obtained

Method of evaluation: based on participation in lectures

ECTS: 3 Semester: summer Bibiography: Seminar Course code: Cj01 (s) Type of course: seminar Tutor: Dr Ewa Witek Number of hours: 30 Description of the course: Zgodna z tematyką wykładu Method of evaluation: obecność i test końcowy ECTS: 3 Semester: summer

Title of the course: FUNDAMENTALS OF POLYMER CHEMISTRY

Tutor: Prof. Edgar Bortel, PhD, DSc

**Teaching objectives:** 

#### Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture and classes(i)

Lecture

**Course code:** Cj02 (w)

Type of course: lecture

Tutor: Prof. Edgar Bortel, PhD, DSc

Number of hours: 30

**Description of the course:** Discovery of chain structure in high molecular substance and the origin of polymer science. Topology and isomers possible in the chain structures. Differences between low- and high-molecular weight substances. Tactic and atactic polymers Conditions enabling a monomer to participate in polyreactions. Mechanisms of polymerization (radical, ionic, stereospecific, polymerization). Possibilities to control polyreactions. Determination of average molecular masses. Chemical reactions on polymers. Theory of copolymerization. Linear polycondensation

**Method of evaluation:** Examination for profile of Application Chemistry for the rest of the students on participating in lectures

**ECTS:** 3

Semester: summer Bibiography:

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Course code: Cj03

Title of the course: FUNDAMENTALS OF POLYMER CHEMISTRY II

**Tutor**: Prof. Edgar Bortel, PhD, DSc, Dr Andrzej Kochanowski, Dr Marian Piasecki, Dr Ewa Witek

### **Teaching objectives:**

#### Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

Lecture

**Course code:** Cj03 (w)

Type of course: lecture

Tutor: Prof. dr hab. Edgar Bortel,

Number of hours: 30

**Description of the course:** The course comprises of lectures, seminars and laboratory. Different techniques of polymerizations are discussed and classification of polymers based on the Hooke's law is reviewed. Physicochemical fundamentals of behaviour of macromolecules in solutions are elucidated. Molecular weight determination by means of such methods like cryometry, membrane– and vapour osmometry, light-scattering, analytical centrifugation and viscosimetry is subject of theoretical consideration and practical excercizes.

**Method of evaluation:** Examination for students belonging to the panel "Chemistry and Technology of Polymers" for others on participation in lectures

ECTS: 3 Semester: winter Bibiography:

#### Laboratory

Course code: Cj031

Type of course: laboratory

Tutor: , Dr Andrzej Kochanowski, Dr Marian Piasecki, Dr Ewa Witek

Number of hours: 90

**Description of the course:** Purification of vinyl monomers. Techniques of radical polymerization and copolymerization: bulk polymerization, solution polymerization, precipitation polymerization, emulsion and microemulsion polymerization, pearl polymerization. Chemical methods of determination of degree of polymerization. Prepare of hydrogels. Purification of polymers

Method of evaluation: presents and raports

#### **ECTS:** 9

Semester: summer Bibiography:

Seminar Course code: Cj03 (s) Type of course: seminer Tutor Dr Andrzej Kochanowski, Dr Marian Piasecki, Dr Ewa Witek Number of hours: 30/15 Description of the course: according with lecture Method of evaluation: presents on seminar ECTS: 4,5 Semester: winter/summer Bibiography:

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# Course code: Cj04

Title of the course: INDUSTIAL SYNTHESIS OF POLYMERS AND NATURAL

POLYMERS

Tutor: Prof. Edgar Bortel, PhD, DSc, Prof. Andrzej Barański, PhD, DSc, Dr Ewa Witek Teaching objectives:

### Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

Lecture

**Course code:** Cj04 (w)

Type of course: lecture

Tutor: Prof. Edgar Bortel, PhD, DSc, Prof. Andrzej Barański, PhD, DSc

Number of hours: 30

**Description of the course:** The course deals with syntheses and applications, as well as with physicochemical properties of commercial polymers like polyolefins, polyamides, polyesters, polyurethanes etc. .Natural polymers are also taken into consideration, i.e. cellulose, starch,

chitine – with the focus on paper production, restoration of acid paper in order to save documents and valuable writings.

Method of evaluation: based on participation in lectured

ECTS: 3 Semester:summer Bibiography: Seminar Course code: Cj04 (s) Type of course: seminar Tutor: Dr Ewa Witek Number of hours: 1,5 Description of the course: compatible with lecturer content Method of evaluation: credit for mark ECTS: 1,5 Semester: summer Bibiography:

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Course code: Cj05 Title of the course: Chemical reactors Tutor: dr Lucjan Chmielarz Teaching objectives:

# Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)
Lecture
Course code: Cj05w
Type of course: Lecture
Tutor: dr Lucjan Chmielarz
Number of hours: 15
**Description of the course:** Types of chemical reactors, rules of mass and energy balance calculations for chemical reactors. Project equations for the model reactors (tank reactor, plug-flow reactor, cascade reactor etc), kinetic equations, examples of industrial catalytic reactors (fix-bed, fluidized etc). Effects of mass and heat diffusion.

Method of evaluation: Solving of the problem related to reactor engineering

ECTS: 1.5 Semester: summer Bibiography: Laboratory Course code: Cj051 Type of course: Laboratory Tutor: dr Lucjan Chmielarz Number of hours: 15 Description of the course: Solving the problems related to reactor engineering with using professional computer software. Method of evaluation: Solving the problem related to reactor engineering ECTS: 1.5 Semester: summer Bibiography:

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Course code: Cj07 Title of the course: Industrial catalysis Tutor: dr Lucjan Chmielarz, dr Piotr Kuśtrowski Teaching objectives:

# Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

Lecture

Course code: Cj07w

Type of course: Lecture Tutor: dr Lucjan Chmielarz, dr Piotr Kuśtrowski Number of hours: 30 Description of the course: The main parameters which characterize industrial catalysts; conditions of performance of catalytic industrial processes; rules of selection of optimal composition of industrial catalyst; examples of using of catalytic processes in large-scale inorganic technologies (e.g. synthesis of ammonia, oxidation of ammonia, synthesis of

removal of industrial pollution

Method of evaluation: final examination

ECTS: 30 Semester: summer Bibiography:

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sulphuric acid); application of catalysis in refinery and petrochemistry; catalytic methods of

Course code: Cj08

Title of the course: Modeling of technological processes Tutor: dr Piotr Kuśtrowski Teaching objectives:

### Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)
Lecture
Course code: Cj08w
Type of course: Lecture

Tutor: dr Piotr Kuśtrowski

Number of hours: 30

**Description of the course:** Presentation of computer software package for modeling of technological processes; design of main unit operations (dynamical, diffusion and heating operations); simulation of chosen unit processes; modeling of complex technological units. In

the frame of the course students could develop skill of computer usage, especially for the simulation of complex industrial processes

Method of evaluation: Solving of problem related to modeling of technological processes

**ECTS:** 3.0

Semester: summer

**Bibiography:** 

Classes

Course code: Cj08c

Type of course: classes

**Tutor:** dr Piotr Kuśtrowski

Number of hours: 15

**Description of the course:** Solving of complex problems related to modeling of technological processes presented in the frame of lecture, including application of computer software for the simulation of chosen operation and process units.

Method of evaluation: Solving of problem related to modeling of technological processes ECTS: 1.5 Semester: summer Bibiography:

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Course code: Cj09 Title of the course: WASTELESS TECHNOLOGIES Tutor: dr Marian Piasecki Teaching objectives:

# Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)
Lecture
Course code: Cj09w
Type of course: lecture

### Tutor: dr Marian Piasecki

### Number of hours: 15

**Description of the course:** Main technological focus directed on savings of Raw materials and energy :rules concerning usage of raw materials under environmental point of view (wastes) and synthesis of products liable to recycling after being wasted, or liable to biodegradation. Presentation of some selected wasteless technologies (i.e. winning of gypsum from wastes released from desulfuration of gases)

Method of evaluation: attendance during the lectures ECTS: 1,5 Semester: summer

**Bibiography:** 

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# Course code: Cj12

Title of the course: Formal kinetics

Tutor: Dr Wacław Makowski

**Teaching objectives:** 

## Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

Lecture

**Course code:** Cj12

Type of course: w

Tutor: Dr Wacław Makowski

Number of hours: 15

## **Description of the course:**

Basic concepts of chemical kinetics: reaction rate, reaction order, molecularity, differential and integrated rate equations. Temperature dependence of rate constants - the Arrhenius equation. Collision theory and transition state theory. Kinetics of complex reactions - reversible, parallel and consecutive. Steady state approximation, rate determining step, most abundant reaction intermediate. Autocatalytic and oscillating reactions. Kinetic measurements - fitting the experimental data with empirical rate laws. Relationship between

rate equation and reaction mechanisms. Mechanisms of gas phase reactions. Kinetics of catalytic reactions. Chemisorption, Langmuir isotherms. Langmuir-Hinshelwood, Eley-Rideal and Mars-van Krevelen mechanisms. Kinetics of temperature programmed desorption. Kinetics and mechanisms of solid state reactions. Parabolic law, shrinking core model, Jander equation.

Method of evaluation: attendance and final test

**ECTS:** 1.5

Semester: summer

## **Bibiography:**

P. W. Atkins, Chemia fizyczna, PWN, 2001, chapters 25-28

A. Barański, Kinetyka chemiczna, in: Chemia fizyczna, PWN, 1980, pp. 776-890

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Course code: Cj13

Title of the course: Industrial catalytic methods Tutor: Prof. dr hab. Roman Dziembaj, dr Piotr Kuśtrowski, dr Lucjan Chmielarz Teaching objectives:

## Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture and classes(i)
Lecture
Course code: Cj13w
Type of course: Lecture
Tutor: of. dr hab. Roman Dziembaj
Number of hours: 30
Description of the course: Presentation of the most up-to-date chemical technologies based
on catalytic processes and perspectives of their application
Method of evaluation: evaluation of report
ECTS: 3.0
Semester: winter
Bibiography: Seminar Course code: Cj11s Type of course: seminar Tutor: dr Piotr Kuśtrowski, dr Lucjan Chmielarz Number of hours: 60 Description of the course: Presentation of results of the studies obtained by diploma students including different problems related to catalysis and chemical technology Method of evaluation: Evaluation of oral presentation ECTS: 6.0 Semester: winter and summer Bibiography:

# Course code: Ck02

Title of the course: Self-organization in chemical and biological systems

Tutor: dr hab Marek Frankowicz

Description of the unit included in the course:

Lecture

Course code: Ck02w

Type of course: lecture

Tutor: dr hab Marek Frankowicz

Number of hours: 30

### **Description of the course:**

Elements of theory of dynamical systems: phase space, phase trajectories, attractors. Bifurcations, elements of catastrophe theory.. Deterministic chaos. Strange attractors. Fractal geometry. Examples: Brusselator, van der Pol oscillator, enzymatic systems, Lorenz model, logistic map. Reaction-diffusion systems. Turing struktures. Waves and impulses. Elements of theory of stochastic processes. Markov processes. Master equation. Stochastic simulation techniques. Noise induced phase transitions.

Method of evaluation: students prepare essays on chosen topics

**ECTS:** 3

Semester: summer

### **Bibliography:**

A.L. Kawczyński: Reakcje chemiczne od równowagi poprzez struktury dyssypatywne do chaosu, WNT, 1990

M. Orlik: Reakcje oscylacyjne porządek i chaos, WNT, 1996

S.K. Scott: Oscillations, Waves, and Chaos in Chemical Kinetics, OUP, 1994

A. Harrison: Fractals in Chemistry, OUP, 1995

M. Tempczyk: Teoria chaosu dla odważnych, PWN, 2002

D. Kaplan and L. Glas: Understanding Nonlinear Dynamics, Springer 1995.

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# Course code: Ck03

Title of the course: Density Functional Theory

Tutor: Professor Roman F. Nalewajski

**Teaching objectives:** This course introduces to the audience (IVth-year undergraduates and graduate students) the elements of the modern Density Functional Theory (DFT), which dominates both the current *ab initio* calculations of the electronic structure of large molecular and solid-state systems and contemporary conceptual developments in the theory of chemical reactivity

### Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

Lecture

Course code: Ck03w

Type of course: lecture

Tutor: Professor Roman F. Nalewajski

Number of hours: 30

**Description of the course:** Mathematical and physical supplement: functional derivative and statistical ensembles in quantum mechanics. Hohenberg-Kohn Theorems and their implications, Levy's constrained-search principle. Equilibrium (thermodynamic) states of

molecular systems in the Grand-Canonical ensemble. The discontinuity of the chemical potential at T = 0 K, as function of the system average number of electrons, and its physical implications. The Kohn-Sham (KS) method: variational derivation of the effective Schrödinger equation for orbitals, physical interpretation of KS orbitals, Janak's Theorem. The Kohn-Sham-Mermin theory for ensembles. The density functional for the exchangecorrelation energy: uniform-scaling properties, local and non-local (gradient) approximations, relation to the classical Thomas-Fermi-Dirac-Weizsäcker and Slater theories. Adiabatic connection between the hypothetical (non-interacting) KS system and the real (interacting) system of the same electron density, and expressing the exchange-correlation energy as functional of the exchange-correlation hole. The Hartree and Hartree-Fock theories as references in definitions of the exchange and correlation holes. Examples of the functionals used in molecular DFT calculations: LDA, GGA, and hybrid functionals. Survey of the accuracy level of KS calculations in typical ground-state applications. Orbital-dependent density functionals: the Optimized Potential Model and Optimized Effective Potential theory, the Krieger-Li-Yafrate approximation. Selected generalizations of Hohenberg-Kohn theorems. Elements of the Time-Dependent theory and the excited states in DFT. Importance of DFT for conceptual chemistry: electronegativity and hardness descriptors of the electron gas in molecules, reactivity criteria of open molecular systems - the Fukui Function and charge sensitivities of reactants.

Method of evaluation: essay, after completion of lectures.

## **ECTS:** 3.0

### Semester: Summer

**Bibiography:** (1) R. F. Nalewajski, *Podstawy i metody chemii kwantowej*. PWN, Warsaw 2001 (In Polish); (2) R. G. Parr, W. Yang, *Density Functional Theory of Atoms and Molecules*. Oxford University Press, New York 1989; (3) R. M. Dreizler, E. K. U. Gross, *Density Functional Theory: An Approach to the Quantum Many-Body Problem*. Springer-Verlag, Heidelberg 1990; (4) R. F. Nalewajski (red.), *Density Functional Theory I-IV*, Topics in Current Chemistry, Vols. 180-183. Springer-Verlag, Heidelberg 1996; (5) R. F. Nalewajski and J. Korchowiec, *Charge Sensitivity Approach to Electronic structure and Chemical Reactivity*. World-Scientific, Singapore 1997.

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## Course code: Ck04

Title of the course: Theoretical spectroscopy Tutor: Professor Marek Pawlikowski Teaching objectives:

### Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

Lecture

Course code: Ck04W

**Type of course:** lecture(w)

Tutor: Professor Marek Pawlikowski

Number of hours: 30

**Description of the course:** The interactions between electronic and nuclear degrees of freedom (adiabatic and non-adiabatic BO approaches, vibronic couplings, Jahn-Teller and Franck-Condon effects); The probability of optical transitions in molecules (one- and two-photon processes: absorption, emission and Raman scattering); The optical phenomena in a presence of external fields (Stark and Zeeman effects); The magnetic circular dichroism (MCD) spectroscopy and the relative phenomena such as NMR and EPR; The natural circular dichroism in the dipole-allowed and dipole forbidden electronic states. The Cotton effect in molecules consisting of identical units (dimers, tetramers); The theoretical background of the resonance Raman spectroscopy (RRS) (scattering tensors in the resonance limit, interferences in the Raman cross-section, excitation profiles and depolarization dispersions); The fate of the energy upon molecular excitations (radiative and non-radiative transitions, energy transfer between molecules and environment, quantum yield and the lifetimes of the excited states, Jablonski diagram); The computational methods in the electronic spectroscopy; The spectral characteristics evaluations in terms of quantum chemical approaches based on CASSCF and (TD) DFT methodologies.

Method of evaluation: examination in writing or oral questions ECTS: 3 Semester: summer Bibliography: D.C. Harris, M.D.Bertolucci, Symmetry and spectroscopy, New York, Oxford University
Press, 1978 (in English)
A.Gołębiewski, Elementy mechaniki i chemii kwantowej, PWN, 1982 (in Polish)
P.W.Atkins, Molekularna mechanika kwantowa, PWN, 1974 (in Polish)
R.M Golding, Applied wave mechanics, van Nostrand Comp. Ltd., London 1969 (in English)

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## Course code: Ck06

Title of the course: Elements of theoretical solid state physics Tutor: Professor Piotr Petelenz hTeaching objectives:

### Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture and classes(i)

Lecture

Course code: Ck06W

Type of course: lecture

Tutor: Professor Piotr Petelenz

Number of hours: 30

**Description of the course:** Translational symmetry and its consequences: reciprocal lattice, quasimomentum, Brillouin zone, Bloch Theorem. Crystal lattice dynamics; phonons. Electrons in a crystal: band theory, pseudo-one-particle picture; metals: free and quasi-free electrons, effective-mass approximation; other crystals: tight-binding approximation, electrons vs holes. Electron-phonon interaction: scattering, band narrowing, polarons; "band" and "hopping" transport. Electron-hole interaction and basic semiconductor physics; Wannier, Frenkel and intermediate excitons. Excitons in molecular crystals; Davydov splitting. Electron-electron interaction and basic metal physics: screening, interaction mediated by phonons, introduction to the theory of superconductivity (BCS).

Method of evaluation: oral examination

**ECTS:** 3.0

Semester: winter term Bibiography:

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# Course code: Ck07

Title of the course: Information theory of molecular systems Tutor: Professor Roman F. Nalewajski Teaching objectives:

Introduction to the audience (4<sup>th</sup>-year undergraduates and graduate students) of the main concepts and techniques of the information theory: Shannon entropy, Fisher information, information distance (entropy deficiency, missing information) of Kullback and Leibler, information variational principles, as well and with their applications in a chemical and thermodynamic-like interpretation of the electronic structure of molecular systems.

# Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

Lecture Course code: Ck07w Type of course: lecture(w) Tutor: Professor Roman F. Nalewajski

Number of hours: 30

**Description of the course:** Entropy/information and communication channels: a survey od basic concepts, theorems and principles of the information theory: complementary uncertainty/information measures of Shannon and Fisher, cross-entropy (information distance) of Kullback and Leibler. Principles of the maximum entropy, minimum entropy-deficiency, and the extreme physical information. Combination rules for the entropy-information descriptors of subsystems. Electronic kinetic energy as measure of the Fisher information in molecular electron distributions. Schrödinger equation as information principle. Information-theoretic analysis of molecular electron densities, relative to the promolecular distribution due to non-bonded atoms: relations between the local missing-information densities and the density difference function, diagrams of the density difference

and entropy-deficiency densities relative to the promolecular reference. Shannon entropy densities and the electron-localization function. Atoms-in-Molecules from the information theory: partition of the molecular electron density into atomic fragments, properties of the so called "stockholder" atoms from the partition of the one- and two-electron densities, and their in information theory. Molecule as justification information system and the entropy/information interpretation of the global bond-multiplicity of molecular systems and their covalent/ionic composition. Entropy/ information descriptors of bond multiplicities involving molecular subsystems. A comparison between the bond indices from the communication theory and predictions from the Valence-Bond and Molecular-Orbital theories for simple orbital models. Illustrative applications of the information theory to reactive systems. Elements of the local "thermodynamics" of molecular systems and their fragments in the combined description within the Density Functional and information theories.

## Method of evaluation: esay

**ECTS:** 3.0

### Semester: Summer

### **Bibiography:**

N. Abramson, *Teoria informacji i kodowania*, PWN, Warszawa, 1969.
B. R. Frieden, *Physics from Fisher Information – A Unification*, Cambridge University Press, Cambridge, 2000.
R. F. Nalewajski, *Information Theory of Molecular Systems*, Elsevier, Amsterdam, 2005 (w druku).
L. Brillouin, *Nauka a teoria informacji*, PWN, Warszawa 1969.
A, M. Jagłom, I. M. Jagłom, *Prawdopodobieństwo i informacja*, Książka i Wiedza , Warszawa 1963.
A. Dąbrowski, *O teorii Informacji*, Wydawnictwo Szkolne i Pedagogiczne, Warszawa, 1974.
J. R. Pierce, *Symbole, sygnały i szumy – wprowadzenie do teorii informacji*, PWN, Warszawa, 1967.

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## Course code: Ck08

Title of the course: Quantum-chemical molecular modeling

Tutor: Dr. Artur Michalak

**Teaching objectives:** The main goal of the course is a <u>practical</u> introduction to the computational methods of quantum chemistry. After completing the course student should be familiar with practical aspects of computational chemistry, and be able to apply quantum

chemical programs in the description of electronic structure of organic, inorganic, and organometallic systems, as well as in the theoretical analysis of chemical reactivity.

### Description of the unit included in the course:

lecture(w), computer laboratory (l),

Lecture Course code: Ck08w Type of course: lecture Tutor: Dr. Artur Michalak Number of hours: 30

**Description of the course:** Using quantum chemical software – general rules; input data for quantum chemical calculations; available software. Born-Oppenheimer approximation; potential energy surface (PES), stationary points on PES. Practical aspects of geometry optimization of molecular systems; optimization of minima (reactants, products) and saddle points (transition states); reaction paths on PES. Commonly used computational methods; variational and perturbational methods; Hartree-Fock method (HF); restricted and unrestricted HF (RHF and UHF); ab initio and semiempirical methods. Basis sets in ab initio calculations. Molecular orbitals, electron density, populational and bond-order analysis. Visualisation methods. Chemical bond; differential density (deformatyion density); delocalized and localized orbitals; localization methods. Vibrational analysis; normal modes. Electron correlation; Configuration interaction methos (CI), Moller-Plesset perturbational method (MP). Density functional theory (DFT) and Kohn-Sham (KS) method. Practical aspects of DFT calculations; exchange-correlation functional choice. Modeling of large systems; hybrid methods (QMMM). Solvent effects; continuum models. Chemical reactivity; single- and two reactant reactivity indices; interaction energy partitioning methods. Modeling of elementary reactions of complex processes. Thermodynamic properties; free-energy of chemical reactions; ab initio molecular dynamics approaches.

Method of evaluation: project/essay or exam (arranged with lecturer)

ECTS: 3 or 5 (exam)

Semester: summer (on Tuesdays)

## **Bibiography:**

### practical aspects of computational chemistry:

- web page
- F. Jensen, Introduction to Computational Chemistry, Wiley, 1999

- W. Koch, M.C. Holthausen, A Chemist's Guide to Density Functional Theory, Wiley, 2001.
- A.R. Leach, Molecular Modeling. Principles and Applications. Pearson Education 2001.
- Encyclopedia of Computational Chemistry. Wiley, 1998. (wybrane artykuły)
- selected articles from scientific journals

theoretical basis of the quantum-chemica methods:

- R.F. Nalewajski Podstawy i metody chemii kwantowej. PWN 2001.
- L.Piela, Idee chemi kwantowej. PWN 2001
- A. Szabo, N.L. Ostlund, Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory, Dover, 1989

# Laboratory

Course code: Ck081

Type of course: computer laboratory

Tutor: Dr. Artur Michalak

Number of hours: 60

**Description of the course:** Computer exercises - quantum-chemical calculations performed by students will illustrate applications of various quantum-chemical methods in the description of the electronic structure of simple organic, inorganic and organometallic molecules and in the problems of chemical reactivity.

Method of evaluation: lab reports

**ECTS:** 6

Semester: summer (on Tuesdays)

**Bibiography**:

- web page
- selected articles from scientific journals

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Course code: Ck09 Title of the course: Biospectroscopy Tutor: Professor Marek Pawlikowski Teaching objectives:

## Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

Lecture Course code: Ck09W Type of course: lecture Tutor: Professor Marek Pawlikowski Number of hours: 30

**Description of the course:** The nuclear motions in large molecules (local and normal mode representations); The infrared and Raman spectroscopy in applications to large biologically important molecules (e.g., peptide, protein, metalo-organic complexes, etc.); A role played by symmetry; The spectroscopy of vis-UV transitions and their description based on the molecular orbital theory and the configuration interaction scheme; The vibrational structure of absorption and emission bands due to vibronic interactions and FC principle in the excited electronic states. The carotenoids and porphyrins discussed as illustrative examples; The natural circular dichroism (CD-Cotton effect) and its significance for a structural analysis of large molecules; The energy transfer processes in the excited states of peridinin-chlorofil-propein (PCP) (light harvesting) complexes. The resonance Raman spectroscopy (RRS) as a tool to study large molecules containing biologically active chromophores. The excitation profiles and depolarization dispersions of totally and nontotally symmetric RR fundamentals for selected molecules such as chlorofil-a, vitamin B12 and cytochrome-c.

Method of evaluation: examination in writing or oral questions

**ECTS:** 3.0

**Semester:** 2<sup>nd</sup> semester (summer)

## **Bibliography:**

- a. D.C. Harris, M.D.Bertolucci, *Symmetry and spectroscopy*, New York, Oxford University Press, 1978 (po angielsku)
- b. A.Gołębiewski, Elementy mechaniki i chemii kwantowej, PWN, 1982

### Course code: Ck10

Title of the course: Theory of excitons

Tutor: Prof. Piotr Petelenz

**Teaching objectives:** Formation of intuitive understanding of the main concepts of exciton theory, viewed in the context of semiconductor physics, physics of molecular crystals and optoelectronics

Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture and classes(i)

Lecture

**Course code:** 

Type of course: lecture

Tutor: Prof. Piotr Petelenz

Number of hours: 30

**Description of the course:** Second-quantization formalism, commutation rules for bozon, fermion and paulion operators. Electrons and holes in semiconductors. Consequences of translational symmetry: band structure, quasimomentum, Brillouin zone, Bloch theorem. Low-energy electronic excitations in periodic structures. Delocalization in orbital and excitonic sense; classification of excitons and their limiting cases: Wannier-Mott, Frenkel, CT excitons, intermediate excitons.  $\Delta \mathbf{k}=0$  selection rule. Wannier excitons: hydrogenic model and its shortcomings. Screening of Coulombic interaction in semiconductors; electron-hole interaction via phonon field. Wannier exciton complexes exemplified by the complex with ionized donor; biexcitons. Excitons in molecular crystals and aggregates: molecular exciton, mechanisms of Frenkel exciton propagation, singlet and triplet excitons, Davydov splitting. Coupling to vibrational degrees of freedom; limiting cases of vibronic coupling. Lattice sums. macroscopic polarization, role of boundary conditions., non-analytic energy contributions. Interaction with electromagnetic radiation: polaritons, stopping bands, metallic reflection. Experimental methods: absorption, reflection, emission spectroscopy, photocurrent spectra, electro-absorption. Energetics of molecular crystals; electric and optical band gap.

Chcarge-transfer excitons: consequences of charge delocalization, mixing of different CT configurations and couling to Frenkel excitons. Interpretation of electro-absorption spectra.

Transport properties of excitons: band model and hopping model. Method of evaluation: oral examination ECTS: 4 Semester: summer or winter Bibliography:

# Course code: Cl04

# **Title of the course:** ISOLATION AND IDENTIFICATION OF ENDOGENOUS COMPOUNDS

**Tutor**: Dr. Piotr Suder, MSc, Dr. Marek Smoluch, Prof. Jerzy Silberring PhD, DSc, Prof. Adam Dubin PhD, DSc (IMB JU)

Number of hours: 30

# **ECTS: 3,5**

**Description of the course:** Practical aspects of the isolation of proteins, peptides and other endogenous molecules. Bioinformatics. Applications of modern analytical techniques: mass spectrometry, HPLC, LC/MS, nanospray, capillary zone electrophoresis, peptide map, aminoacid analysis, protein/peptide sequencing.

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## Course code: Cl06

Title of the course: The art of presentation

Tutor: Prof. dr hab. Jerzy Silberring, dr Agnieszka Kraj

## **Teaching objectives:**

To acquire the practical knowledge on scientific data presentation, including talks and posters for the conferences.

## Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

Classes

Course code: C106

**Type of course:** classes (n)

Tutor: prof. dr hab. Jerzy Silberring, dr Agnieszka Kraj

### Number of hours: 30

### **Description of the course:**

The course is organized in a form of workshop with actors (pronounciation, intonation), psychologist (coping with stress), psychiatrist (gaining atypical situations). Topics include, among others, methods for lecture and poster preparation and advanced options of the PowerPoint software. Presentations will be recorded with a video camera for further discussion of eventual drawbacks and improvements.

**Method of evaluation:** presentation of a 5-min. talk on a selected topics. Preparation of the 15-min.presentation on a selected topics. Obligatory presence on at least 80% classes.

**ECTS:** 3

Semester: summer

Bibiography: none

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Course code: Cv01

Title of the course: METHODS AND TECHNIQUES OF DATA PRESENTATION Tutor: Dr. Grzegorz Stopa Teaching objectives:

## Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture and classes(i)

Lecture

Course code: Cv01

**Type of course:** lecture (w)

Tutor: Dr. Grzegorz Stopa

Number of hours: 15

## **Description of the course:**

Description of methods and techniques how to present effectively different kind of data. These knowledge is used to: writing of diploma thesis, preparing and delivering short conference speeches or lectures, preparing conference posters. There are also given examples how to introduce and present oneself to employer during process of application for a job. Method of evaluation: preparation of the final project ECTS: 1,5 Semester: summer Bibiography:

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Course code: Cv02

# Title of the course: Alumnus on the Labour Market

Tutor: dr Iwona Maciejowska

Teaching objectives: Preparation of graduates to enter job market

# Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture

and classes(i)

Lecture and classes

Course code: Cv02i

Type of course: lecture and classes

Tutor: dr Iwona Maciejowska

Number of hours: 15

**Description of the course:** 

cv, application letter, interview, tests, assessment centre, negotiations

Method of evaluation: cv and application letter; enterprise description; written test

**ECTS:** 1,5

## Semester: winter/summer

# **Bibiography:**

- 1. Bronisław Szydłowski, *Praktyczny Poradnik Poszukiwania Pracy. Listy motywacyjne i curriculum vitae*, Kraków 2000
- 2. Eric Tyson, Jim Schell, Własna Firma, IDG Books, Warszawa 1999
- 3. Gavin Kennedy, Negocjacje doskonałe, Rebis, Poznań 2000
- 4. Biuletyny i poradniki Urzędu Pracy: Jak znaleźć odpowiednią pracę, Indywidualny Plan Działania. Poradnik dla Absolwenta, Wejście i powrót na rynek pracy

- 5. Katalogi: Praktyki przewodnik dla studentów poszukujących praktyk, Pracodawcy, Absolwent, Pracuj.pl, Hobsons Kariera w Polsce, Profile:Polska International Casebook
- Absolwent na rynku pracy. Skrypt do ćwiczeń, wyd. Wydział Chemii UJ, Kraków 2003

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# Opis ogólny kursu:

(Cele dydaktyczne wypełnia się w stosunku do kursów obowiązkowych oznaczonych A i B)

# Course code: Cw02

Title of the course : Biological chemistry laboratory

Tutor : dr hab. Krzysztof Lewiński (kierownik)

**Teaching objectives:** To develop competence of student applying modern experimental and computational methods in research

# Opis jednostki wchodzącej w skład kursu.

np. wykład (w), ćwiczenia(n), laboratorium (l), konwersatorium (k), seminarium (s),

ćwiczenia rachunkowe (c), wykład + ćwiczenia (i)

# Laboratorium

Course code: Cw021

**Type of course** 

Tutor: dr hab. Krzysztof Lewiński (kierownik)

Number of hours : 90

## **Description of the course:**

Laboratory exercises cover: kinetics of enzymatic processes, proteomics, X-ray structural analysis of proteins and utilization of data bases (Protein Data Bank, Cambridge Structural Data Base, SwissProt,Medline, Science Citation Index. Students are using modern spectroscopic and analytical methods as mass spectroscopy, HPLC, Raman and IR spectroscopy, UV-VIS, spectrofluorimetry, X-ray diffractometry.

Method of evaluation : raport

**ECTS:** 9

**Semester:** (zimowy, letni, zimowy/letni)

## **Bibiography:**

### Course code: Cw03

### **Title of the course: CHEMISTRY OF NEW MATERIALS - LABORATORY**

Tutor: Wiesław Łasocha PhD, DSc (head)

Number of hours: 75

### **ECTS:** 9

### **Description of the course:**

Synthesis of selected materials (e.g. superconducting, layred, fibrillar compounds etc.). Investigations of phase composition as a function of temperature and atmosphere. Measurements of selected properties of crystalline samples.

Sample preparation, X-Ray measurements and structure solution. Study of relations between crystal structure and chemical, physical or biological properties and applications.

### Course code: Cw04

# **Title of the course:** CATALYSIS AND CHEMISTRY OF SOLID STATE SURFACE - LABORATORY

Tutor: Dr Andrzej Kotarba (head)

Number of hours : 120

### **ECTS:** 14

**Description of the course:** The course serves as a complementary unit to the lecture on Catalysis and Chemistry of Solid State Surfaces. The laboratory classes are organized in the research groups of Inorganic Chemistry Department and Regional Laboratory of Physicochemical Analyses and Structural Research and are focused on the following problems:

surface morphology: scanning electron microscopy, BET-surface area, porosity, X-ray microanalysis, spectroscopy and surface science: IR of adsorbed molecules, UHV hardware, X-ray photoelectron spectroscopy, electrical properties of surfaces: work function, surface ionization, thermal electron emission, surface chemical bond: TPD of probe molecules, temperature programmed surface reaction on catalytic surfaces.

Students perform instructed experiments, interpret the results and prepare short reports.

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Course code: Cw05

## Title of the course: CRYSTAL STRUCTURE ANALYSIS

Tutor: dr hab. Katarzyna Stadnicka

### **Teaching objectives:**

### Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

## Laboratory

Course code: Cw051 Type of course: laboratory (l)

Tutor: dr hab. Katarzyna Stadnicka

Number of hours: 30

## **Description of the course:**

Selection of crystals for X-ray experiment - crystal optical homogeneity (polarizing microscope), absorption coefficient from chemical composition for given wavelengths, estimation of optimal crystal size; measuring with the Nonius KappaCCD diffractometer: diffraction power of investigated crystal, preliminary determination of the unit cell parameters and Laue class, strategy choice for the diffracted beams intensities measurements; data processing, determination of Bravais lattice type, character of normalized structure factor distribution and the space group; choice of the structure solution method (programs SIR and/or SHELXS); refinement of the structural parameters using non-linear least-squares method (program SHELXL) - strategy of refinement, selection of weighting scheme, reliability indices, problem of twinning; structure analysis: configuration of the molecules, atomic bond lengths, the values of valence angles and torsion angles - conformation of the molecules, best planes of aromatic moieties, puckering parameters for saturated rings, mutual packing of the chemical units in the structure - coordination polyhedra, detection of strong, moderate and weak hydrogen bonds, intermolecular distances typical for Van-der Waals interactions; Visualization of chemical units in anisotropic description of atomic displacements (program ORTEP) and unit-cell contents (program MERCURY) with the hydrogen bonds marked; CIF file preparation and structure validation (program PLATON); comparison of the obtained results with the similar structures found in databases (Cambridge Structural Database, Inorganic Structure Database, Powder Database etc.).

**Method of evaluation:** Written report from the experiments / calculations performed and discussion of the results obtained.

## **ECTS:** 4.0

## Semester: summer

## **Bibiography:**

- 1. J.P. Glusker, K.N. Trueblood, Zarys rentgenografii kryształów, PWN, 1977;
- J.P. Glusker, M. Lewis, M. Rossi, Crystal Structure Analysis for Chemists and Biologists, VCH 1994;
- M.M. Woolfson, An Introduction to X-ray Crystallography, Cambridge University Press, 1997.

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# Course code: Cw06

Title of the course: DESIGNING CRYSTALS WITH REQUIRED PROPERTIES Tutor: dr hab. Katarzyna Stadnicka (course supervisor), prof.. dr hab. Barbara Oleksyn, Teaching objectives:

### Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

Lecture

Course code: Cw06w

**Type of course:** lecture(w)

Tutor: dr hab. Katarzyna Stadnicka, prof.. dr hab. Barbara Oleksyn

Number of hours: 30

## **Description of the course:**

Goals in designing crystalline material from the viewpoint of chemical, physical and biological properties; choice of the building blocks, *i.e.* basic chemical units to be used for construction of crystalline phases (synthons or tectons), intermolecular interactions as criteria for selection of spacers or connectors, which ascertain three-dimensional architecture of the crystals under design; choice of crystal growth method and optimization of crystallization conditions; polymorphism phenomena; crystal structure determination methods using X-ray diffraction techniques (for single crystals and powdered samples); verification methods of

expected properties of the materials engineered; case studies of the most spectacular crystal engineering achievements.

*Remark: Cw06w is one of the obligatory lectures in the Profile Chemistry of New Materials and Catalysis.* 

Method of evaluation: multi-choice test

**ECTS:** 3.0

Semester: summer

# **Bibiography:**

- 1. J.W. Steed, J.L. Atwood, Supramolecular Chemistry, John Wiley & Sons, Ltd, 2000;
- Crystal Design Structure and Function, G.R. Desiraju (ed), John Wiley & Sons Ltd, 2003;
- 3. J. Bernstein, Polymorphism in Molecular Crystals, Oxford University Press, 2002;
- 4. collection of original papers from international scientific journals.

# Laboratory

Course code: Cw061

**Type of course:** laboratory(l)

Tutor: dr hab. Katarzyna Stadnicka, prof.. dr hab. Barbara Oleksyn

Number of hours: 45

# **Description of the course:**

The workshop consists of four-stage individual work of students: designing crystal structure with specified polar, chiral or other type of chemical, physical or biological properties; search through the literature data and choice of a procedure leading to formation of single crystals; crystal growing experiments, X-ray structure determination, verification of the potential properties of the obtained crystalline phases. Writing a report on the project performed and conclusion drawn.

Remark: Cw06l is the part of specialization laboratory of the Panel on Designing Crystalline Phases and Structure Determination in the Profile Chemistry of New Materials and Catalysis. Method of evaluation: written report and 20 min. presentation of the achieved results

# **ECTS:** 6.0

# Semester: summer

# **Bibiography:**

- 1. W. Steed, J.L. Atwood, Supramolecular Chemistry, John Wiley & Sons, Ltd, 2000;
- Crystal Design Structure and Function, G.R. Desiraju (ed), John Wiley & Sons Ltd, 2003;

- 3. J. Bernstein, Polymorphism in Molecular Crystals, Oxford University Press, 2002;
- 4. collection of original papers from international scientific journals.

## Course code: Cw07

# **Title of the course: CO-ORDINATION CHEMISTRY - LABORATORY**

Tutor: Dr Ewa Wasielewska (head)

Number of hours : 120

# **ECTS:** 14

**Description of the course:** Synthesis and characterisation of coordination compounds: X-ray structural analysis, elemental analysis, thermogravimetry.

Spectroscopic properties of coord. compds.: UV-Vis, EPR, IR, NMR. Redox properties of coord. compds.- different electrochemical techniques: CV, DPV, CC; spectroelectrochemistry.

Kinetic and mechanistic investigation of reactivity of coord. compds.: stopped-flow, conventional kinetics, high pressure kinetics,  $\mu$ s - flash kinetics, ns - laser photolysis.

Photochemistry of coord. compds.: continuous photolysis,  $\mu$ s - flash photolysis, ns flash photolysis, quantum yield measurements, photoelectrochemistry, photochemistry of coord.

compds. deposited on semiconductor surfaces.

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# Course code: Cw08

Title of the course: Methods of catalyst characterization Tutor: dr Piotr Kuśtrowski, dr Lucjan Chmielarz Teaching objectives:

# Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

Lecture Course code: Cw08w Type of course: Lecture Tutor: dr Piotr Kuśtrowski, dr Lucjan Chmielarz

# Number of hours: 15

**Description of the course:** Physicochemical methods for characterization of heterogeneous catalysts: temperature-programmed techniques (TPR, TPOx, TPD, TPSR); thermal analysis (TG, DSC), texture studies, structural analysis (XRD). Studies of the reactions with the gas reagents and vapor of organic compounds in differential and integral reactors, stability of catalysts (influence of poisons), study on reaction mechanisms

Method of evaluation: final examination or oral presentation

**ECTS:** 1.5

Semester: winnter

**Bibiography:** 

Laboratory

Course code: Cw081

Type of course: Laboratory

Tutor: dr Piotr Kuśtrowski, dr Lucjan Chmielarz, mgr Janusz Surman

**Number of hours:** 75

**Description of the course:** Scientific mini-project related to application of different experimental methods in catalytic studies..

Method of evaluation: Evaluation of report describing results of scientific mini-project.

**ECTS:** 7.5

Semester: summer

**Bibiography:** 

Seminar

**Course code:** Cw08s

Type of course: Seminar

Tutor: dr Piotr Kuśtrowski, dr Lucjan Chmielarz

Number of hours: 30

Description of the course: Theoretical preparation of student tfor performing of scientific

mini-project

Method of evaluation: Presentation of the plan of scientific mini-project

**ECTS:** 3.0

Semester: summer

**Bibiography:** 

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# Course code: Cw10

Title of the course: Physicochemical methods of polymer characterization Tutor: dr Andrzej Kochanowski Teaching objectives:

### Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture and classes(i)

Lecture

Course code: Cw10w

**Type of course:** w + 1

Tutor: dr Andrzej Kochanowski

**Number of hours:** 15 + 60

Description of the course: Qualitative analysis of polymers. Determination of

macromolecule structure. Methods of determination of average molecular mass of polymers..

Method of evaluation: graded credits for "Chemistry and Technology of Polymers" panel;

credits for the lectures within "Industrial Catalysis" panel

**ECTS:** 7,5 (1,5 + 6,0)

Semester:

**Bibiography:** 

Laboratory

Course code: Cw101

**Type of course:** 

Tutor: dr A. Kochanowski, dr E. Witek, dr M. Piasecki,

dr S. Zapotoczny

Number of hours: 60

**Description of the course:** Analysis of H<sup>1</sup> NMR i C<sup>13</sup> NMR spectra, gel chromatography, determination of average molecular mass with various methods (viscosimetry, cryoscopy, light scattering, analytical ultracentrifugation), analysis of size of the disperged particles in various types of emulsions

## Method of evaluation:

ECTS: 6,0 Semester: Bibiography:

## **Course code:** Cw13

Title of the course: Laboratory in Photochemistry and Spectroscopy

**Tutor:** dr Andrzej Turek (head)

Teaching objectives: does nor concern

### Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

### Laboratory

Course code: Cw131

Type of course: laboratory

**Tutor:** dr Andrzej Turek

Number of hours: 180 hours

Description of the course: Laboratory provides an opportunity of practical acquaintance with modern methods of molecular spectroscopy and photochemistry applied to study the structure and transformations of various chemical species. The methods of electronic spectroscopy include actinometry, determination of quantum yields of photochemical and photophysical processes, spectrofluorimetry, fluorescing probes, polarization effects, measurements of transient absorption, laser spectroscopy used in laboratory are: FT Raman and infrared spectroscopy, resonance Raman spectroscopy and surface enhanced Raman spectroscopy. The studied problems refer to various aspects of photochemistry and photophysics such as photochromism, hydrogen bonding, solvation dynamics in binary solvents, charge transfer, proton transfer, photoisomerisation, determination of structure of biologically active molecules, investigation of photoelectrochemical properties of semiconductors and many others. Laboratory activities give students a chance to learn many experimental techniques and give them also a practical knowledge how to interpret the obtained experimental results.

### Method of evaluation: raports

ECTS: 21.0 Semester: winter/summer Bibiography:

Laboratory: Experimental physicochemical methods in nanotechnology Course code: Cw14

Type of course: laboratory

Head of the panel: prof. dr hab. Maria Nowakowska

Tutor: dr Paweł Wydro

Number of hours: 150

**Description of the course: The properties of nanostructures formed in the surface layer at the liquid – gas interface.** Properties and structure of Langmuir monolayers ( $\pi$ -*A* isotherms, Brewster Angle Microscopy –*BAM*). Molecular interactions between components in mixed monolayers. Surface potential. Chemical reactions in monomolecular films. Equilibrium constants at the air/water interface. **Polymeric and hybrid nanostructures – synthesis and properties.** Nano- and microcapsules for controlled release of drugs. Emulsion polymerization. Osmometry, osmotic pressure, isotonic coefficient. Atomic force microscopy (*AFM*). Electrochemical methods of the controlled modification of metals surfaces and. **their applications in nanotechnology.** Electrochemical corrosin, Pourbaix diagrams, passivation of metals, Tafel plots. Rotating disc electrode (*RDE*), diffusion coefficient, mass transport, Levich equation. Plarografy. Elecktrode kinetics, cyclic voltamperometry. Ion selective electrodes, potentiometric titration, electrode potentials in aqueous-organic environments.

Method of evaluation: completion of lab experiments, reports, graded credits ECTS: 17 Semester: winter/summer

Advanced Organic Chemistry Laboratory Cw15C

Assessment: Written reports.

Advanced Laboratory Techniques:

Techniques for performing experiments in anhydrous condition, in the atmosphere o inert gasses, and at low temperatures. Vacuum techniques. Experiments with gaseous reagents. Synthesis of metallic catalysts and organo-metallic reagents. Modern techniques in chromatography and extraction.

Organic Synthesis:

A set of exercises includes the classical advanced procedures of proven value, as well as experiments, that illustrate recently developed methods of modern organic synthesis. There are also special exercises focused in experimental specificity of current M.Sc. research projects. All synthetic projects have been carefully designed, so as to correlate laboratory experiments with the lecture part of the advanced organic chemistry course, In addition, most products synthesized by students are well suited for the structure elucidation with use of advanced NMR techniques, and for the later physicochemical experiments.

Organic Physicochemistry:

Application of spectroscopic methods to study reaction kinetics and mechanisms and hydrogen bonds, to determine the reaction products stereochemistry and tautomeric equilibrium. Investigation of the steric and electronic effects of substituents.

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**Course code:** Cw17

Title of the course: Instrumental methods in environmental analysis

Tutor: dr Jolanta Kochana

### **Teaching objectives:**

### Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture and classes(i)

### Laboratory

**Course code:** Cw17 (l)

Type of course: laboratory

Tutor: dr Jolanta Kochana

Number of hours: 40

### **Description of the course:**

Potentiometric determination of cations and anions using ion-selective electrodes; Stripping voltammetry in trace analysis; Selective catalytic reduction of NO over a V-O-Mn catalyst; Application of Raman Spectroscopy for identification and determination of organic compounds; FTIR spectroscopy applied to study environmental pollution; Mass spectrometry and hyphenated techniques (LC-MS and GC-MS); Quantitative analysis in gas chromatography. Determination of components in gaseous and liquid mixtures; Diffraction methods in industrial analysis: powder X-ray diffraction (PXRD); Application of structural databases in industrial analysis; SPE in environmental analysis. Determination of trace amounts of phenol in water.

Method of evaluation: test ECTS: 4.5 Semester: summer Bibiography:

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Course code: Cw20 Title of the course: Laboratory of chemical processes Tutor: dr Lucjan Chmielarz, dr Piotr Kuśtrowski Teaching objectives:

# Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture and classes(i)
Laboratory
Course code: Cw201
Type of course: Laboratory
Tutor: dr Lucjan Chmielarz, dr Piotr Kuśtrowski
Number of hours: 30
Description of the course: Solving of the problems related to thermodynamic, kinetics of chemical reactions and chemical engineering with using professional computer software.
Presentation of abilities of computer data bases for solving complex chemical problems and advanced literature studies.
Method of evaluation: Presentation of mini-project
ECTS: 3.0
Semester: summer
Bibiography:

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# Course code: Cz04

Title of the course: Applied quantum chemistry for catalysis Tutor: prof. dr hab. Ewa Brocławik (Institue of Catalysis and Surface Chemistry PAN) Teaching objectives:

# Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)
Lecture
Course code: Cz04W
Type of course: lecture
Tutor: prof. dr hab. Ewa Brocławik (Institue of Catalysis and Surface Chemistry PAN)
Number of hours: 45

**Description of the course:** Quantum chemistry has emerged as a modern tool in chemical research, including traditionally experimental areas such as catalysis. Therefore we offer the course tailored to: a) refresh fundamental knowledge on quantum chemistry; b) interpret basic axioms and approximations from the point of view of physical implications; c) indroduce quantum chemical methods in the context of usefulness in research, in to particular to catalysis: surfaces, adsorption, active sites and reaction mechanisms. The course will have the form merging lectures with worksops. Examples will be selected from personal sciantific activity of students focused on advantages and limitations of advanced quantum chemical methods in the field of catalysis and modern computer modeling.

Method of evaluation: active participation

ECTS: 4.5 Semester: Summer Bibiography:

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### Course code: Cz05

Title of the course: FORENSIC TOXICOLOGY

Tutor: dr Zofia Chłobowska

**Teaching objectives:** 

### Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture and classes(i)

Lecture

Course code: Cz05w

Type of course: Lecture

Tutor: dr Zofia Chłobowska (Institute of Forensic Research)

Number of hours: 30 hrs

### **Description of the course:**

Basic concepts in toxicology (poison, routes of intoxication, cooperating factors in poisoning, mechanisms of poisons action, detoxication processes, and the like); chemistry and toxicology of selected ecological poisons; food contamination; tobacco; intoxicating agents in the problems connected with ecotoxicology; environmental contaminations monitoring.

## Method of evaluation: written examination

# **ECTS:** 3

### Semester: winter

Bibiography: : Alloway B. I., Ayres D.C. Chemiczne podstawy skażenia środowiska Wydawnictwo Naukowe PWN Warszawa 1999; Baran-Furga H., Steinbarth-Chmielewska K. Uzależnienia. Obraz kliniczny, leczenie, Wydawnictwo Lekarskie PZWL Warszawa 1999 r., Brandy J. (red.) Toksykologia-wybrane zagadnienia, Wydawnictwo Uniwersytetu Jagiellońskiego, Kraków 1999 r., Danysz A. (red.) Leki a kierowcy, PZWL, Warszawa 1980r., Dutkiewicz T. Chemia toksykologiczna, PZWL, Warszawa 1968 r., Grochowalski A. Badania nad oznaczaniem polichlorowanych dibenzodioksyn, dibenzofuranów i bifenoli, seria: Inżyniera i Technologia Chemiczna, monografia 272, Politechnika Krakowska, Kraków 2000 r., Gubała W., Toksykologia alkoholu wybrane zagadnienia, Wydawnictwo Instytutu Ekspertyz Sądowych, Kraków 1997 r., Kościelniak P., Piekoszewski W. (red.), Chemia sądowa, Wydawnictwo Instytutu Ekspertyz Sądowych, Kraków 2002 r., Maciejewski H., Ekologiczne i ekonomiczne skutki wynikające z niezadowalającego stanu środowiska atmosferycznego (w:) Postęp w pomiarach emisji substancji zanieczyszczających powietrze atmosferyczne, Wisła s. (1-20). "Markiewicz J., Niektóre problemy toksykologii metali ciężkich w aspekcie skażenia środowiska, Komisja Nauk Medycznych-Oddział PAN w Krakowie, Kraków 1990 s. 117., Mędrzycka K. (red.), Gospodarka odpadami niebezpiecznymi, Wydział Chemiczny Politechniki Gdańskiej, Gdańsk 1998., Namieśnik J., Jaśkowski J. (red. 0, Zarys Ekotoksykologii, EKO Farma, Gdańsk 1995 r., Seńczuk W., Toksykologia PZWL, Warszawa 1999r., Szczepaniec-Cięciak Е., Kościelniak P.,(red.),Chemia środowiska. Ćwiczenia i seminaria, t. I i II Wydawnictwo Uniwersytetu Jagiellońskiego, Kraków 1999 r., Zakrzewski S.F. Podstawy toksykologii środowiska, Wydawnictwo Naukowe PWN, Warszawa 1995r.

Biological chemistry: the principles of biology Course code: Cz08

**Type of course:** Lecture

Tutor: dr Jerzy Galas

Number of hours: 30

**ECTS:** 3

Semester: winter

Principles of biochemistry:Chemical constituents of living organisms, water and it's functions in the organism, metabolism and its pathways, organic compounds present in living organisms, the role of enzymes in the metabolism. Description of more important methods of separation and analysis of selected biological compounds.

Cytology: principles of molecular organization of the cell, the structure of cell membrane and its derivatives, structure and function of plant and animal cells. Cell cytoskeleton and its functioning. Compartmental organization of the eukaryotic cell. Functions of the vacuolar system, cell cycle, intercellular communication.

Histology: elementary information on the structure of tissues: epithelial, nervous, muscle, connective, blood and sensory organs. The rules of taxonomical classification of organisms, selected groups of organisms: occurrence, importance of bacteria, fungi, algae and their role in nature, economy and life of humans, methods of plant reproduction, ecological forms of flowering plants. Physiology: description of the functioning of selected systems of vertebrates and humans: nervous, hormonal, alimentary, circulatory systems and the role of body fluids (blood circulation in the frog, pulse in the human – blood pressure measurement), excretory system, reproductive system including the process of spermatogenesis and oogenesis in the human, sex determination, menstrual cycle, pregnancy tests, discussion of selected hereditary diseases. The subjects discussed during lectures can accommodate wishes expressed by the participants.

Within the scope of the course there will be visits to the Anthropological and Nature Museums of UJ Institute of Zoology, Theatrum Anatomicum CMUJ (Normal and Pathological Anatomy Museum) and to the UJ Botanic Garden.

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Course code: Cz09

Title of the course: LEGAL ASPECTS OF FORENSIC EXPERT'S JOB

Tutor: Aleksander Głazek MSc, Prof. dr hab. Józef Wójcikiewicz PhD, DSc (Institute of

Forensic Research)

**Teaching objectives:** 

## Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture and classes(i)

Lecture

Course code: Cz09w

**Type of course:** lecture(w)

Tutor: mgr Aleksander Głazek, prof. dr hab. Józef Wójcikiewicz (Institute of Forensic

Research)

Number of hours: 15

### **Description of the course:**

Scientific evidence in legal proceeding – introduction. Forensic expert's status and role in legal proceeding. Forensic expert's rights and obligations. Legal basis of forensic expertise.

Scope and subject of forensic expertise. Forms of forensic expertise. Scheme of the physicochemical expertise. Drawing of final conclusions. Appearance before the court. Method of evaluation: ECTS: 2.0 Semester: summer Bibiography:

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Course code: Cz14

Title of the course: RADIOMETRIC ANALYSIS Tutor: PhD Jerzy Ostachowicz (University of Science and Technology-AGH) Teaching objectives:

# Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture and classes(i)

Lecture Course code: Cz14W

**Type of course:** lecture (w)

Tutor: PhD Jerzy Ostachowicz

Number of hours: 30

# **Description of the course:**

Radioactivity. The radioactive decay law; radioactive equilibrum. Nuclear reactions and reaction cross section. Nuclear reactions with charged particle, with neutrons, photonuclear reactions. Interaction of the radiation with matter. Interaction with charged particles: specific ionisation, range, bremstrahlung radiation. Interaction with gamma and X-rays: the photoelectric effect, the Compton effect and pair production, linear and mass absorption coefficients. Interaction with neutrons: elastic and inelastic scattering, absorption. Natural radioactivity. The sources of the radioactive contamination and measurements of its level.

Measurement of nuclear radiation: ionisation chamber, proportional counters, Geiger-Muller counters, scintillation detectors, semiconductor detectors. Single channel spectrometer. Multichannel spectrometer. Dosimetry: limits of dose, methods of dose measurement,
radiation protection. Radiometric methods of the density, thickness and level of liquid online measurements. Radiometric methods of the humidity measurements.

Neutron Activation Analysis (NAA): basics, the neutron sources. NAA with the use of the thermal neutrons: the instrumental method, the method with chemical separation of radionuclides. Energy Dispersive X-Ray Fluorescence Analysis (EDXRF): basics. Sources of the XRF excitation: radiosotope sources, X-ray tubes, synchrotron radiation. Total Reflection XRF (TXRF). Analytical devices with the use of EDXRF method in laboratory and for on-line control in the industrial processes.

Uncertainty and detection and determination levels in the radiometric analysis..

Method of evaluation: exam ECTS: 3.0 W Semester: winter Bibiography:

## Laboratory

Course code: Cz14 L

Type of course: laboratory (l)

**Tutor:** PhD Jerzy Ostachowicz

Number of hours: 45

**Description of the course:** 

#### **RADIOMETRY:**

Statistic errors of the radioactivity measurements (No.1)

Gamma -ray spectrometer with the scintillation counter (No.4)

Dosimetry of the ionization radiation (No.7)

Determination of iron in the iron sands using gamma-absorption method and radioisotope source <sup>241</sup>Am. (No.17)

Gamma-ray spectrometer with the semiconductor detector Ge(Li). Determination of

manganese by NAA method. (No 3+22)

Measurement of the humidity of the industrial material with the use of neutron flux (No.25) EDXRF method in the analytical laboratory.

Total Reflection method (TXRF) applied for the analysis of the biological materials.. RADIOCHEMISTRY:

Introduction - how to work with radioactive materials (open sources) ?

Separation of the Fe-59 and Co-60 using ion exchange resin (No.13)

Thorium separation from uranyl nitrate with the use of the extraction. (No12)

Determination of iodine content with the use of isotope dilution analysis (No.6)

Determination of the PbJ<sub>2</sub> solubility. (No.10)

Method of evaluation: credit

**ECTS:** 4,5L

Semester: summer

# **Bibiography:**

1.B.Dziunikowski, S.Kalita: Ćwiczenia laboratoryjne z jądrowych metod pomiarowych, Wydawnictwa AGH, skrypt nr 1440, 1995, Kraków.

2. Laboratory of Radiochemistry, Instructions - : internet page: <u>www.ftj.agh.edu.pl</u> -

Zakłady,, Zakład Radiometrii ,, dydaktyka ,, ćwiczenia laboratoryjne z radiochemii)

# INSTRUMENTAL BIOCHEMICAL ANALYSIS Course code: Cz18

**Type of course:** Labolatory (l), Seminar (s)

Tutor: Prof. dr hab. Andrzej Kozik

**Number of hours:** 45 (l), 15 (s)

## **ECTS:** 6

Semester: winter

## Seminar

General problems of analytical biochemistry, theoretical principles of specific methods, areas of analytical applications, statistical analysis of results and construction details of the equipment used.

## Laboratory practice

The most important instrumental methods of quantitative and qualitative analysis of biochemical compounds and their composite mixtures. Spectrophotometry in visible and ultraviolet light, fluorometry, nefelometry and turbidymetry. Liquid chromatography, electrophoresis and isoelectrofocusing.

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Course code: Cz23

Title of the course: CLINICAL TOXICOLOGY

Tutor: Prof. dr. Wojciech Piekoszewski (Institute of Forensic Research)

# **Teaching objectives:**

Introduction to clinical toxicology with pointed out the role of analytical toxicologist in clinical toxicology

# Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

## Lecture

Course code: Cz23

**Type of course:** lecture(w),

**Tutor:** Prof. dr. Wojciech Piekoszewski (Institute of Forensic Research), Zakład Toksykologii Analitycznej i Terapii Monitorowanej CM UJ oraz Instytut Ekspertyz Sądowych w Krakowie.

#### Number of hours: 30

**Description of the course:** Introduction to clinical toxicology, therapeutic monitoring of adverse drug reaction, the role of the laboratory in diagnosis and treatment of poisoning, analytical methods in clinical toxicology, introduction to toxicokinetics, poisoning control centers, antidotes, toxicodromes, manegement of poisoned patients, epidemiology of poisoning i Poland, toxicity of therapeutic agents, toxicity of nontherapeutic agents, drug of abuse, plant poisoning.

## Method of evaluation:

ECTS: 3.0 Semester: winter Bibiography:

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# Course code: Cz25 Title of the course: BIOCHEMISTRY Tutor: prof. dr hab. Kazimierz Strzałka (Faculty of Biotechnology UJ) Teaching objectives:

# Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)

#### Lecture

Course code: Cz25w

Type of course: lecture

Tutor: prof. dr hab. Kazimierz Strzałka (Faculty of Biotechnology UJ)

Number of hours: 60

#### **Description of the course:**

Basic life processes occuring in the cells of autotrophic and heterotrophic organisms. Problems: structure and properties of macromolecules, molecular structure of the cell, catalysis of biochemical processes, enzymes, energetics of plant and animal cell, selected anabolic and catabolic processes and their subcellular localization, regulation of biochemical processes, biogeochemical cycle, biochemical aspects of of adaptation of organisms to environment, realization of genetic information (replication, transcription, translation), elements of genetic engineering.

Method of evaluation: Z

ECTS: 9 Semester: summer Bibiography: Classes Course code: Cz25n Type of course: classes Tutor: prof. dr hab. Kazimierz Strzałka (Faculty of Biotechnology UJ) Number of hours: 90 Description of the course:

Program of laboratories contains: (1) qualitive and quantitive analysis of molecules building living organisms: amino acids, proteins, saccharides, nucleic acids and lipids. (2) Selected topics in enzymology: enzymatic activity of certain enzymes, enzyme specificity; influence of substrate concentration on rate of enzymatic reactions; introduction to enzyme kinetics ( $V_{max}$ ,  $K_M$ ); influence of competitive and uncompetitive inhibitors. (3) Protein-ligand interactions. (4) Selected techniques applied in biochemistry: adsorption and TLC chromatography, electrophoresis, histochemical staining; gel filtration, spectrophotometry. (5) Selected topics in plant biochemistry: isolation and spectral characteristic of photosynthetic pigments, measurement of fluorescence induction; measurements of photochemical activity in isolated chloroplasts/ thylakoid membranes via <sup>1)</sup> absorption measurements and <sup>2)</sup> Clark electrode, analysis of  $\Delta pH$  in isolated thylakoids membranes; influence of uncouplers.

ECTS: 6 Semester: summer Bibiography:

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# Course code: Cz27

Title of the course: Management in Practice

Tutor: Dr. Stefan Witkowski

**Teaching objectives:** 

## Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture and classes(i)

Lecture

Course code: Cz27

Type of course: lecture (w) part A

Tutor: Dr. Stefan Witkowski

Number of hours: 16

## **Description of the course:**

Part "A" introduces students to the management. Typical problems that may be encountered in real conditions and methods of solving are presented.

Topics:

Aim, Process, Optimisation.

The Employee in an Enterprize, in Science and Selfemployment.

Ethics in Business.

Building Cooperation.

Intelectual Property .

Six Sigma Optimized Production.

A visit to General Motors Manufacturing Poland Plant in Gliwicach

## Method of evaluation: colloqium

ECTS: 1,5 Semester: summer Bibiography: Lecture Course code: Cz27

**Type of course:** lecture (w) part B

Tutor: Dr inż. Kazimierz Miga, mgr inż. Andrzej Korpak

Number of hours: 16

**Description of the course:** 

Part "A" focuses on chosen detailed topics of practical management:

Safety Management in Contemporary Enterprize

What is Process and Process Control **GM GMS (Global Manufacturing System)** 

**Standarized Communication HR Management under Lean Conditions** Practical Problem Solving Integrated Quality System

Method of evaluation: colloqium

**ECTS:** 1,5

Semester: summer

**Bibiography:** 

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Course code: Cz31 Title of the course: Electronics and automatics Tutor: D. Sc. Roman Płaneta Teaching objectives:

## Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture
and classes(i)
Lecture
Course code: Cz31.w
Type of course: lecture
Tutor: : D. Sc. Roman Planeta
Number of hours: 30
Description of the course:

Electric signals: analogue and digital.Basic electronics units. Thevenin and Norton theorems. RC and Wien circuits.Delay line.Band structure of crystals.Extrinsic semiconductors of type n and p.Junction model. Basic diode types: Zener, tunneling and fotodiode. Rectifiers.

Voltage regulator circuit with Zener diode. Bipolar transistors. Transistor working configurations with common base, emitter and collector . Hybrid parameters for bipolar transistors. Application of "h" parameters for amplifier analysis. Common-Emitter and Common-Collector Amplifier . Feedback theory. Operational amplifier. Operational amplifier in circuits with negative feedback. Bistable multivibrator. Astable multivibrator.

Generator with Wien bridge. Binary, octal and hexadecimal digits representation. Boolean algebra.Basic logic circuits.Functional blocks: combinatorial and sequential.

Flip-Flops circuits: R-S, J-K i D.Shift registers, multiplexers, demultiplexers and decoders. Sum unit . Elementary memory cell and memory circuits. Converters classification. Digitalanalog converters. Sampling circuits. Voltage comparators. Analog-digital converters. Serial (CENTRONICS) and parallel (RS-232C) transmission

Method of evaluation: written exam

**ECTS:** 3.0W

#### **Semester:**winter

## **Bibiography:**

M.Rusek i J.Pasierbiński: "Elementy i układy elektroniczne", Wydawnictwo Naukowo-

Techniczne, Warszawa, 1997;

P.Górecki, "Układy cyfrowe", Wydawnictwo btc, Warszawa, 2004

R.A.Colclaser, "Electronic circuit analysis", John Wiley & Sons, 1984

T.Hayes, P.Horowitz, "Student manual for the art of electronics", Cambridge University Press

## Laboratory

Course code: Cz31.1

Type of course: laboratory

Tutor: D.Sc. Marcin Wójcik

Number of hours: 60

## **Description of the course:**

Obligatory excercises: invesitgation of passive circuits; analoge and digital oscilloscope; delay line, wave reflection, measurement of phase velocity; transistor amplifier with common emitter, transistor as a current source; operational amplifier, diode in a feedback circuits as a temperature detector; logical circuits, NAND gate applications, TTL binary counter. Facultative excercises: analog-to-digital converter, investigation of generating and steering circuits, memory programming, tunneling and capacity diode, simulation of electronic circuits in frame of the MICRO-LOGIC II simulation program. Method of evaluation: get a credit ECTS: 6.0L Semester: winter Bibiography:

# PHYSICAL BASIS OF MOLECULAR DYNAMICS SIMULATION OF BIOMOLECULES Course code: Cz35

Lecturer: Prof. dr. hab. Marta PASENKIEWICZ-GIERULA

Hours and points: 60 h (30 h lecture, 30 h classes) (ECTS 5)

Scheduled time: Fall semester

#### **Contents**:

- 1. Definition and perspectives of molecular modelling.
- 2. 3D structure of molecules and inter-atomic interactions.
- 3. Potential function, interaction parameters computational problem and approximations
- 4. Numerical methods: molecular mechanics (MM, structure optimisation); molecular dynamics (MD, generation of motion) approximations
- 5. Classical approach justification; point charges.
- 6. Control of thermodynamic parameters temperature and pressure.
- 7. Models of water.
- 8. Analyses of MD trajectories: equilibrium structure of biomolecules and equilibrium dynamics of biomolecules.

Laboratory practice is intended to introduce students to the latest commercial and academic programs for molecular modelling and demonstrate their research potential. Practice will be conducted on graphic workstations (2 students per workstation).

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Course code: Cz37

Title of the course: Forensic physico-chemistry

Tutor: doc. dr hab. Janina Zięba-Palus

**Teaching objectives:** 

#### Description of the unit included in the course:

lecture(w), classes(n), laboratory (l), tutorials(k), seminar (s), calculation classes(c), lecture and classes(i)

#### Lecture

Course code: Cz37w

**Type of course:** lecture (w)

Tutor: dr. Janina Zięba-Palus (Institute of Forensic Research)

#### Number of hours: 30

**Description of the course:** Subject of forensic chemistry. Interdisciplinary character of forensic sciences. Historical overview of toxicological and criminalistic examinations. Application of chemical methods in forensic examinations. Evidence and control materials. The types of materials analysed in criminalistics. The purpose of criminalistic expertise. The interpretation of the analytical results for criminalisctic purposes. Criminalistic traces and microtraces - definition, kind, collection and method of examination. Classification of microtraces. Contact and non-contact traces. Preparation of expert reports. Documentation of results obtained. Identification and comparison in trace evidence analysis. Individual and group identification.

Method of evaluation: exam

**ECTS:** 3,5 (3,5 W)

Semester: summer

**Bibiography:** Kościelniak P., Piekoszewski W. (red.), Chemia sądowa, Wydawnictwo Instytutu Ekspertyz Sądowych, Kraków 2002 r.,

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Course code: Cz42

Title of the course: philosophy

Type of course: lecture, classes

Number of hours: 60

Tutor: dr Marek Suwara

**ECTS: 5** 

**Teaching objectives:** familiarizing students with the history of basic philosophical problems with the special attention put on philosophical foundations of science

#### **Description of the course:**

a.history of the main problems in philosophy: ontology, epistemology, basic

elements of methodology os science b.basic problems in contemporary philosophy of science c.elements of philosophical anthropology, ethics and social ethics

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#### Course code: Cz43

Title of the course: Analytical Chemistry of Natural Products Tutor: Dr. Caroline West Number of hours: 15 ECTS: 3 Description of the course: HPLC methods, reverse-phase HPLC, detectors, cation-exchange chromatography, natural products

#### Course code: Cz45

Title of the course: Programming Tools for the Contemporary Teaching

Tutor: dr Stefan Witkowski

**Teaching objectives:** 

Number of hours: 16 (lecture 4h) + (laboratory 12h)

**Description of the course:** Reasons and aims of internet use in teaching practice. Web pages. XHTML and CSS. Teaching materials, their logical structure, SCORM standard for teaching materials. Tools for editing teaching aids and for converting them into web pages. Web based support for teaching. The course, its structure, building tools, managing the course. Open and confidential parts of the teaching course. Adveritizing. Professional web pages creation

# Method of evaluation: exam

**ECTS:** 1.5

#### Semester:summer

**Bibiography:** Zastosowanie Technologii Informatycznych w Akademickiej Dydaktyce Chemii, Wydział Chemii UJ, Kraków 2007, pr. zbiorowa pod red. I. Maciejowska, M.Ruszak, S. Witkowski.

www.exelearning.org

www.moodle.pl

www.plone.org.pl

www.wordpress.org