Jagiellonian University

Faculty of Chemistry

LIST OF COURSES

CHEMISTRY

Ist Cycle Bachelor Program

2007/8

Course title: Mathematics

Course code: WCh-CL-O101-07

Type of course: Lecture (L) + classes (tutorial) (T)

Level of course: Basic

Year of study: First

Semester/trimester: Winter and summer semesters

Number of credits allocated (workload based): 16 ECTS

Name of lecturer: Marian Łoboda, PhD.

Objective of the course (expected learning outcomes and competences to be acquired):

Preparing for solving mathematical problems in physics and chemistry.

Prerequisites: None

Course contents:

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.

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.

Recommended reading:

F. Leja, Rachunek różniczkowy i całkowy, PWN, Warszawa, 1973.

W. Krysicki, L. Włodarski, *Analiza matematyczna w zadaniach*, cz. I, II, PWN, Warszawa, 1976 (and next editions).

L. Maurin, M. Mączyński, T. Traczyk, *Matematyka, podręcznik dla studentów wydziałów chemicznych*, t. I, II, PWN, Warszawa, 1973.

Teaching methods:

Each five hours of lectures are accompanied by seven contact hours in problem solving classes (tutorials) where students can discuss in smaller groups.

Assessment methods:

Continuous assessment (tests written during tutorials) and a written examination at the end of the course.

Course title: Physics **Course code:** WCh-CL-O102-07 **Type of course:** Lecture (L) + classes (tutorial) (T) + laboratory (P) **Level of course:** Basic

Year of study: First

Semester/trimester: Winter and summer semesters

Number of credits allocated (workload based): 12 ECTS

Name of lecturer: Aleksandra Wesełucha-Birczyńska, PhD, DSc (+ Grzegorz Mazur, PhD). **Objective of the course (expected learning outcomes and competences to be acquired):**

The aim of this course is to allow student to gain an understanding of physical phenomena and their mathematical description, what finally makes understanding of the internal unity of science. Physics plays basic role in all of the natural sciences. At calculation classes students learn how to apply mathematics to describe physical phenomena. In laboratory students test practical aspects of physical experiments along with discussion of the measurements precision.

Prerequisites: None

Course contents:

The basis of mathematics in physics – compensatory and complementary course with elements of vectors, derivatives and integrals analysis (dr Grzegorz Mazur).

Fundamentals of classical mechanics with elements of quantum mechanics. Kinematics and dynamics of pointlike (particle) and rigid body. Types of motions: straight-line and curve path motion in two and three dimensions (motion with initial horizontal velocity, projectile motion, uniform circular motion), harmonic motion: simple and complex (Lissajous curves). Inertial and non-inertial reference frames. Principles of conservation of: momentum, angular momentum and energy. Work, power, forms of energy. Waves, propagation of mechanical waves in elastic medium. Elements of acoustic. Elements of hydromechanics.

Electricity. Gravitational, electric, magnetic and electromagnetic fields. Electric and magnetic properties of matter. Motion Electromagnetic oscillations. Maxwell's equations. The electromagnetic spectrum. Dual wave-particle nature of matter and of radiation. Elements of geometrical optics and wave optics. Polarization, interference and diffraction of electromagnetic waves. Elements of solid state physics. Elements of nuclear physics. Nuclear

reactions and elementary particles. Elements of cosmology.

In laboratory there are conducted experiments from mechanics, thermodynamics, electricity, optics and wave motion.

Recommended reading:

A. Bałanda, Fizyka dla chemików, skrypt UJ, Kraków, 1994.

D. Halliday, R. Resnick, J. Walker, Podstawy fizyki, PWN, Warszawa, 2005.

Teaching methods:

Lectures are accompanied by the same number of contact hours in problem solving classes (tutorials) where students can discuss in smaller groups.

Assessment methods:

Written test examination, after winter semester, what gives 1/3 of the final grade (in this 1/5 grade for mathematics in physics test) and written test examination, after summer semester, what gives 2/3 of the final grade.

Additionally, students perform 6 experiments and write 6 protocols.

Course title: Introduction to chemistry

Course code: WCh-CL-O103-07

Type of course: Lecture (L) + classes (tutorial) (T) + laboratory (P)

Level of course: Basic

Year of study: First

Semester/trimester: Winter semester

Number of credits allocated (workload based): 12 ECTS

Name of lecturer: Roman Dziembaj, PhD, DSc, Prof.

Objective of the course (expected learning outcomes and competences to be acquired) Introduction into chemical language, models and rules, illustrated with examples of their usage range and limitations. Presentation of fundamental laws and notions in chemistry – how to understand and use them. Preparation of a background for chemistry studies, especially inorganic, organic, analytical and physical chemistry. Leveling the scope of knowledge and abilities between the graduates of various upper secondary schools. Students will gain good manual skills, learn how to observe the course of an experiment, how to make conclusions and present them in the form of written report. Planning of subsequent stages of experiment on the basis of the results of previous ones is also an important ability gained during the course. The course should help students to achieve such a level of knowledge and skills which enable them to study particular chemical specializations.

Prerequisites: None

Course contents:

Lecture:

Classic chemical ideas and rules. Stoichiometry of chemical reactions. Ideal gas model and real gasses. Thermal effects of chemical reactions with elements of thermodynamics. Chemical equilibrium in single and multi phase systems. Acids and bases according to Bronsted. Redox reactions and electrochemical cells. Chemical kinetics as result of the collision theory. Catalysts and inhibitors. Experimental fundamentals of quantum mechanics. Schroedinger equation for hydrogen atoms, quantum numbers, atomic orbitals. Many-electron atoms in one electron simplification, Slater concept of effective nuclear charge, introduction to atomic terms. Molecular orbitals as linear combination of atomic orbitals, homonuclear diatomic molecules. Heteronuclear diatomic molecules, electronegativity of elements, polarization of chemical bonds. Hybridization as the useful tool to describe many-atom molecules. Examples of molecules showing sp^3 , sp^2 , sp, dsp^2 , and d^2sp^3 hybridizations. Lewis acids and basis, simple examples of coordination compounds. Delocalized orbitals, aromatic molecules, band formation, graphite structure. Introduction to symmetry of molecules. Crystal lattice and unit cells for cubic and hexagonal structures. Elements of solid state chemistry: structural and chemical defects, electrical conductivity, chemical reactions in solids. **Tutorials:**

Stoichiometric calculations, chemical reaction yield, calculation based on the ideal gas law, solutions and their concentrations, calculations based on the first and the second law of thermodynamics, exo- and endothermic processes, the Hess's law, chemical equilibrium and its interpretation, equilibrium constants, Le Chatelier's principle, equilibria in homogenic systems: dissociation of salts, bases and acids (including polyprotic acids), autodissociation of water, pH, hydrolysis, buffer solutions, equilibria in heterogenic systems: solutions of sparingly soluble electrolytes, solubility product, electrochemical calculations: completing and balancing redox equations, standard potentials, chemical reaction in the electrochemical cell, electromotive force, relations between the electrochemical and thermodynamic quantities, first and second order kinetic equations, influence of temperature on chemical reaction rate, activation energy.

Laboratory:

Laboratory techniques, separation of mixtures (crystallization, distillation, extraction, sublimation), synthesis of inorganic compounds, chemical equilibria in aqueous solutions, acid-base equilibria, saturated solutions, buffer solutions, complex compounds, redox reactions, electrochemistry, chemical kinetics, elementary quantitative analysis of cations and anions

Recommended reading: A. Bielański, *Podstawy Chemii Nieorganicznej*, Vol. 1, V edition, PWN, Warszawa, 2006.

A. Śliwa (ed.), Obliczenia chemiczne, PWN, Warszawa, 1987.

A. Reizer (ed.), *Ćwiczenia z podstaw chemii i analizy jakościowej*, Jagiellonian University, 1996.

Teaching methods:

Lectures are accompanied by the same number of contact hours in problem-solving classes (tutorials) where students can discuss in smaller groups.

Assessment methods:

Continuous assessment (tests written during tutorials) and written exam at the end of the course.

Course title: IT (laboratory) Course code: WCh-CL-O104-07 Type of course: classes (tutorial) (T) in computer laboratory Level of course: Basic Year of study: First Semester/trimester: Winter semester Number of credits allocated (workload based): 3 ECTS Name of lecturer: A. Eilmes, PhD,DSc Objective of the course (expected learning outcomes and competences to be acquired): Ability to process experimental data and to write and present laboratory reports using computer software for numerical calculations and text editors. Working knowledge of the facilities provided by the computer network of Faculty of Chemistry. Prerequisites: None Course contents: Basic computer concepts. Introduction to MS Windows and Linux. Functionality of MS

Basic computer concepts. Introduction to MS Windows and Linux. Functionality of MS Office (text processing, spreadsheet, presentations, database). Computer networks. Scientific databases. Data analysis and simple scientific calculations.

Recommended reading:

A. Eilmes, *Word dla chemików*, wyd. MIKOM 2001;
M. Pilch, *Excel dla chemików*, wyd. MIKOM 2001;
A. Michalak, *PowerPoint dla chemików*, wyd. MIKOM 2002;

Materiały do ćwiczeń udostępniane w sieci studenckiej Wydziału Chemii

Teaching methods:

Problem solving classes (tutorials) in small groups. Assessment methods:

Continuous assessment (tests written during tutorials).

Title of the course: Analytical Chemistry

Course code: WCh-CL-0105-07

Type of course: Lecture (L), laboratory (P), classes (tutorials) (T)

Prerequisites: Principles of chemistry (WCh-CL-O103-07).

Level of course: Basic

Year of study: First

Semester/trimester: Summer semester

Number of credits allocated (workload based): 9 ECTS (W – 3, L – 5, K – 1)

Name of lecturer: Stanisław Walas, PhD (L+T), Jolanta Kochana, PhD (P), Joanna Kozak, PhD (T).

Objective of the course (expected learning outcomes and competences to be acquired:

- Instruction of the students about the fundamentals of classical quantitative and instrumental analysis
- 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.

Prerequisites: Introduction to chemistry (WCh-CL-O103-07).

Course contents:

Lecture:

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 gravimetry. Classification of gravimetric methods. The solubility and physical properties of analytical precipitates. Organic reagents used in gravimetry. Advantages, disadvantages and applications of gravimetric methods. The principles of titrimetry. 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. Selected separation techniques. Basics of Chromatography. Division of Spectroscopic methods applied in chemical analysis. Errors in chemical analysis and their origin. Statistical interpretation of analytical data. Standard methods of analysis. Standards and reference materials.

Laboratory:

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 and EDTA. Complexometric determination of the total water hardness. 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.

Tutorial:

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.

Recommended reading:

A. Cygański, Chemiczne metody analizy ilościowej, wyd. 5, Warszawa, WNT, 1999.

A. Rokosz, Wprowadzenie do chemii analitycznej, wyd. UJ, Kraków, 1980.

J. Minczewski, Z. Marczenko, Chemia analityczna, t.1 i 2, Warszawa, PWN, 1985.

W. Szczepaniak, Metody instrumentalne w analizie chemicznej, Warszawa, PWN, 1996.

A. Cygański, B. Ptaszyński, J. Krystek, *Obliczenia w chemii analitycznej*, Warszawa, WNT, 2000.

Teaching methods: Lectures are accompanied by problem solving classes (tutorials) where students can discuss in smaller groups. Every member of the teaching staff offers 1 hour per week to consult and solve particular problems individually. Laboratory classes are crucial for introduction to good laboratory practice

Assessment methods: multiple choice test examination after the lecture, evaluation of results of the analytical process during laboratory classes, multiple choice tests in course of the tutorials

Course title: Organic chemistry

Course code: WCh-CL-O106-07

Type of course: Lecture (L) + classes (tutorial) (T)

Level of course: Basic

Year of study: First

Semester/trimester: Summer semester

Number of credits allocated (workload based): 5 ECTS

Name of lecturer: Janusz Jamrozik, PhD, DSc, Prof. of Jagiellonian University.

Objective of the course (expected learning outcomes and competences to be acquired): 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.

Numerous problems discussed during tutorials should contribute to deeper understanding of a broad area of organic chemistry. 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 take part actively in discussions.

Prerequisites: Introduction to chemistry (WCh-CL-O103-07).

Course contents:

Lecture: Isomerism in organic chemistry: constitutional, streoisomerism. Alkanes, cycloalkanes, alkenes, alkynes: preparation and reactivity. Radical substitution, addition to multiple bonds. Radical and carbonium ion structure and stability, carbonium ion rearrangements. Conjugated dienes, resonance. Alkyne electrophilic addition. Stereochemistry: sterogenic centers. Enantiomers, diastereoisomers, meso compounds, racemic mixtures and their separation. Conformational analysis of cyclohexane. Aromatic compounds. Aromaticity, resonance. Electrophilic substitutions. Isomerism of the polysubstituted aromatic compounds. Nucleophilic aromatic substitution. Benzyne. Halogenation of alkylbenzene side chains, benzyl cation, anion radical. Polycyclic aromatic hydrocarbons. Spectroscopy in structure determination of organic compounds. Alyl halides. Nucleophilic substitutions $S_N 1$, $S_N 2$. Elimination reactions E1, E2 – mechanism and stereochemistry. Alcohols, phenols, ethers and epoxides: synthesis and reactivity. 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.

Classes: Tutorial is complementary to the lecture and it emphasises problems that need student co-operation in small groups. The convincing example are here stereochemistry taught with the help of molecular models or reaction mechanisms.

Introduction: The structure of organic molecules resulting from sp^3 , sp^2 and sp hybridisation. Homolytic and heterolytic bond cleavage, acidity and basicity of organic compounds, nucleophilicity and electorphylicity of reagents, inductive and resonance effects. IUPAC rules of nomenclature including *E/Z* and *R/S* configuration. Types of organic reactions. Carbocations, carboanions and radicals.

Stereochemistry: Kinds of stereoisomerism. Configuration of stereogenic centers. Presentation of configuration on the plane. Molecular models. Conformation analysis alkanes: ethane, butane cyclohexane and its mono- and disubstituted derivatives. Stereochemistry of halogen addition to double bond, of S_N1 and S_N2 reactions.

Reaction mechanisms: Substitution (radical, electrophilic, nucleophilic). Addition to multiple bonds. Elimination. Factors having influence on reaction mechanism, mechanism

competition, e.g. S_N/E . Substituent effects in aromatic electrophilic substitution. Aldol condensation.

Recommended reading: J. McMurry, *Chemia organiczna*, PWN, Warszawa, 2000. R.T. Morrison, R.N. Boyd, *Chemia organiczna*, PWN, Warszawa, 1998.

H. Hart, L.E. Craine, D.J. Hart, Chemia organiczna. Krótki kurs, PZWL, Warszawa, 1999.

E. Białecka-Florjańczyk, J. Włostowska, *Chemia organiczna*, WNT, Warszawa, 2003. **Teaching methods:**

Lectures are accompanied by the same number of contact hours in problem-solving classes (tutorials) where students can discuss in smaller groups.

Assessment methods

Continuous assessment (tests written during tutorials) Language of instruction: Polish Course title: Introduction to statistical evaluation of measurement data

Course code: WCh-CL-O107-07

Type of course: Lecture (L)

Level of course: Basic

Year of study: First

Semester/trimester: Summer semester

Number of credits allocated (workload based): 1 ECTS

Tutor: Andrzej Parczewski, PhD, DSc, Prof.

Objective of the course (expected learning outcomes and competences to be acquires: The aim of the lecture is to acquaint the students of the very beginning level of their study with the idea of chemical measurements (chemical metrology) and statistical handling of experimental data. After passing the final test the students should be able to use standard procedures of statistical evaluation of measurement data. Also the lecture is thought to be helpful for students in understanding and practical application of more sophisticated tools of statistics and chemometrics the students will be taught later during the course of their study. **Prerequsites:** None

Course contents:

Measurements in chemistry; chemical metrology. Passive and active experiments. Variables; types of variables; random variables. General population and sample. Selected distributions of random variable, e.g. rectangular, triangular, normal. Estimation of parameters of random variable distribution: sample mean and sample variance; other measures of central tendency and variation within measurement data. Functions of random variables. Distribution of Student's-t variable. Confidence intervals for parameters of random variable distribution. Testing statistical hypotheses. Direct and indirect measurements. Errors and uncertainties of measurements. Error propagation in indirect measurements and in measuring process. Relations between random variables: covariance, correlation coefficient and determination coefficient. Regression analysis; the least squares principle. Calibration graph; statistics of straight line. The most important characteristics of measurement methods: examples concerning analytical methods; validation of analytical procedures.

Presentation of the above ideas is supplemented by numerical examples.

Recommended reading:

J. Czermiński, A. Iwasiewicz, Z. Paszek, A. Sikorski, *Statistical Methods in Applied Chemistry*, PWN, Warszawa; ELSEVIER, Amsterdam-Oxford-New York-Tokio, 1990. Praca zbiorowa, *Ocena i kontrola jakości wyników pomiarów analitycznych*, Wydawnictwa Naukowo-Techniczne, Warszawa, 2007.

J.N. Miller, J.C. Miller, *Statistics and Chemometrics for Analytical Chemistry*, Pearson Education Limited, London, 2005.

Teaching methods:

Lectures

Assessment methods: Final test (written) Language of instruction: Polish **Course title**: Physical education **Course code: Type of course:** Training Level of course: Basic Year of study: First **Semester/trimester:** Winter and summer semesters Number of credits allocated (workload based): 2 ECTS Name of lecturer: **Objective of the course (expected learning outcomes and competences to be acquired):** Prerequisites: None Course contents: Various forms of training (gymnastics, swimming, volleyball, basketball etc.) **Recommended reading: Teaching methods:** Assessment methods: results, scores Language of instruction: Polish

Course title: Inorganic chemistry

Course code: WCh-CL-O201-08

Type of course: Lecture (L) + classes (tutorial) (T) + laboratory (P)

Level of course: Basic

Year of study: Second

Semester/trimester: Winter and summer semesters

Number of credits allocated (workload based): 14 ECTS

Name of lecturer: Janusz Szklarzewicz, PhD, DSc.; Barbara Sieklucka, PhD, DSc, Prof. **Objective of the course (expected learning outcomes and competences to be acquired):**

The main purpose of teaching inorganic chemistry is providing students with a key to understanding periodic table, origin of the elements, electron configuration, bond formation and chemistry of s, p, d and f elements to understand the principles of chemistry. At the end of the course student should be able to solve problems, to think in an abstract way, to apply knowledge in a new situations, to compare and interpret data, to take part actively in discussions. Student should know the limitation of theoretical approach to the structure and reactivity and the perspectives in chemistry of elements.

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 **Prerequisites:** Introduction to chemistry (WCh-CL-O103-07)

Course contents:

Origin of the elements, periodic table, periodicity of physicochemical properties, electronegativity, ionization energy, electron affinity, atom and ionic radii. Electron configuration of atoms and ions, magnetic properties, Slater rules of electron shielding. Lewis structures: resonance, formal charge, exceptions. Molecular Orbital Theory: electronic structure of diatomic molecules and ions. Hybridization: structure of polyatomic molecules. Hybridization and geometry of molecules, examples of coordination polyhedra across periodic table. VSEPR theory, molecule geometry and: number of lone electron pairs, atomic radii, electronegativity, bond multiplicity, shape and size of ligand. The exceptions from VSEPR theory. Hydrogen: properties, hydrides and their classification, hydrogen bonds. Current and perspective utilization of hydrogen. Alkaline metals, occurrence and production, reactivity, coordination numbers across the group. The alkali earth metal, occurrence, production, reactivity, coordination numbers, current trends. The boron family - occurrence, synthesis and reactivity, superconductivity. Boranes, borohydrides, carbaboranes, classification, oxygen acids of boron. p-orbitals energy across the group, s - electron shielding. The carbon family, allotropy of carbon, synthesis of diamond, fullerenes. Compounds, carbides and their classification, hydrogen compounds of silicon - detailed study. Silicon acids, aluminosilicates, properties and structures. The nitrogen family, allotropy, occurrence, preparation, ammonia and nitrogen oxides synthesis, nitric acids. Hydrides, oxides and acids of P, As, Sb, Bi. Polyphosphates. The oxygen family: allotropes, ozone and the environment, hydrides of oxygen family, water allotropy. Ozonides, oxides and peroxides, oxygen acids, polycations. The halogens; compounds with hydrogen, oxygen, acids, interhalogens, pseudohalogens. The noble gases, clathrates, chemical compounds from He to Xe, metal complexes of noble gases.

Coordination compounds. Constitution. Representative ligands and nomenclature. Symmetry of molecules. Application of symmetry (polarity, chirality, symmetry of orbitals). Isomerism. Bonding and electronic structure. Crystal-field theory. Ligand-field splitting parameters.

Spectrochemical series of ligands 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 ion 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. Motonuclear oxo-complexes. Polyoxometalates. Metal-metal bonded compounds and clusters. Metal sulfides and sulfide complexes. Noble metals. Group 12 metals. d-metal organometallic chemistry. Electron counting and oxidation states. d-block carbonyls. Analogs of carbonyls compounds – complexes with other π -acceptor ligands (dinitrogen and nitrogen monoxide). Other organometallic compounds. Metallocenes. The f-block metals.

Recommended reading:

A. Bielański, Podstawy chemii nieorganicznej, Wyd. 5, PWN, 2003.

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

P. A. Cox, Krótkie wykłady: chemia nieorganiczna, PWN 2003.

T. Senkowski, Z. Stasicka, Zarys struktury elektronowej atomów i cząsteczek, skrypt UJ, Kraków 1982.

A. F. Williams, Chemia nieorganiczna, podstawy teoretyczne, PWN, Warszawa, 1986.

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

N. N. Greenwood, A. Earnshaw, Chemistry of the elements, Pergamon Press, 1986.

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

S. Siekierski, Chemia pierwiastków, Szkoła Nauk Ścisłych, 1998.

R. Sołoniewicz, Pierwiastki chemiczne grup głównych, WNT, 1989.

L. Kolditz, Chemia nieorganiczna, PWN, Warszawa, 1994.

L. Jones, P. Atkins, Chemistry, molecules, matter and change, W.H. Freeman & Co., 2002.

B. Staliński, J. Terpiłowski, Wodór i wodorki, WNT, Warszawa, 1987.

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

Teaching methods:

Lectures are accompanied by problem-solving classes (tutorials) where students can discuss in smaller groups. Practical laboratory classes play an essential role.

Assessment methods:

Continuous assessment (written tests during tutorials, assessment of knowledge of theoretical background, written tests and written reports for laboratory work), mid-term written exam and written exam at the end of the course.

Course title: Organic chemistry

Course code: WCh-CL-O206-08

Type of course: Lecture (L) + classes (tutorial) (T) + laboratory (P)

Level of course: Basic

Year of study: Second

Semester/trimester: Winter semester

Number of credits allocated (workload based): 5 ECTS (L+T) + 8 ECTS (L) **Name of lecturer:** Janusz Jamrozik, PhD, DSc, Prof. of Jagiellonian University **Objective of the course (expected learning outcomes and competences to be acquired):**

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.

Numerous problems discussed during tutorials should contribute to deeper understanding of a broad area of organic chemistry. 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 take part actively in discussions.

For laboratory practice the main goals are: knowledge of basic techniques used in a preparative organic chemistry as well as some elements of organic analysis including spectroscopic techniques. During a laboratory practice, partly supervised and partly co-operative, students should learn: how to plan and carry out syntheses, multi-step processes and functional group protection strategies; how to complete experiments safely (especially when flammable or toxic substances are used) and how to protect the environment. Additionally students gain a wide variety of manual skills, learn to observe experiments and to draw conclusions from them, and report experimental results in a written form (often with the help of word processor). Exercises teach how to tackle and solve problems and how to organise own time (students choose the sequence of exercises by themselves).

Prerequisites: Organic chemistry (WCh-CL-O106-07)

Course contents:

Lecture:

Carboxylic acids and their derivatives. Synthesis of carboxylic acids and their reactivity. Formation of esters, acid chlorides, amides and acid anhydrides. Acyl substitution reactions. Carbonyl α -substitution reactions: keto-enol tautomerism, α -halogenation, alkylation and acylation of enolate ions. The application of acetoacetic and malonic esters in organic synthesis. Carbonyl condensation reactions: Claisen condensation, Michael addition and similar reactions. Enamines and their application in synthesis. Amines, their basicity and nucleophilicity. Synthesis and reactions of amines: alkylation, acylation. Diazonium salts and their application in organic synthesis. Heterocyclic compounds. Their structure, nomenclature and reactions with electrophilic and nucleophilic reagents, oxidation and reduction, basic and acidic properties. Examples of biologically active heterocyclic compounds: alkaloids, vitamins, medicines, pyrimidine and purine bases, nucleotides. Structure, synthesis and importance of nucleic acids. Carbohydrates: classification, structure and reactivity. Configuration of monosaccharides, Fischer projections, cyclic structure, formation of hemiacetals; epimers, anomers, mutarotation. Disaccharides, polysaccharides and their properties. Aminoacids: dipolar structure, isoelectric point, synthesis and stereochemistry. Peptide bond, Important methods of peptide synthesis, determination of peptide sequence, Edman degradation. Lipids: fats, waxes, oils, terpenes, steroids. Saponification of fats, soaps and detergents. Synthetic polymers, structure and properties of polymers. Radical and ionic polymerization of alkenes, polycondensation reactions, polyesters, polyamides.

Classes:

Tutorial is complementary to the lecture and it emphasises problems that need student cooperation in small groups. The convincing example are here stereochemistry taught with the help of molecular models, structure elucidation by spectroscopic methods or reaction mechanisms.

Stereochemistry: Stereoisomerism of monosaccharides and amino acids. *D* and *L* configurations. Stereochemistry of polymers and biopolymers.

Reaction mechanisms: Interconversions of acid derivatices. Reactions of amines. Cleisen condensation, Michael addition, reactions of enolates and enamines. Rearrangements. Synthesis and reactivity of heterocyclic compounds.

The outlines of organic synthesis planning. Protecting groups, inter-conversion of functional groups, formation of carbon skeleton, sequence of reactions in the synthesis of polysubstituted aromatic compounds, 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; simple fragmentation pathways of basic classes of organic compounds. Infrared spectroscopy: absorption bands characteristic for typical structural elements and functional groups. ¹H and ¹³C nuclear magnetic resonance: chemical shifts, intensity of signals, spin-spin couplings; determination of simple structural elements and their sequence in organic molecules. Complementary usage of all the mentioned methods for structure elucidation of simple organic compounds.

Laboratory:

Students get acquainted with the application of the following unit operations (some of them known from the Introduction to chemistry course) for the separation, purification and identification of reaction products: crystallization from organic solvent (the choice of a proper solvent included), distillations (simple, fractionated, and steam distillation), the usage of a rotary evaporator, chromatographic techniques (thin layer and column chromatography), extraction with organic solvents, heating of reaction mixtures under reflux condenser, filtration under reduced pressure, drying of solutions and solids, determination of physical properties (melting and boiling points, refraction).

Organic synthesis experiments are ordered into seven classes 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: seven syntheses of various classes, among them an example of a multi-step synthesis; one special exercise (e.g. separation of a natural product from a plant material) or one experiment prescribed by a tutor, fitting in level of difficulty student's ability and very often related to research done in the Department of Organic Chemistry. The products obtained are characterized by spectroscopic methods (MS, IR, ¹H and ¹³C NMR).

Analytical part of laboratory includes structure elucidation of two unknown samples by spectroscopic methods proved additionally by classical methods.

Recommended reading:

Lecture and classes:

J. McMurry, Chemia organiczna, PWN, Warszawa, 2000.

R.T. Morrison, R.N. Boyd, Chemia organiczna, PWN, Warszawa, 1998.

H. Hart, L.E. Craine, D.J. Hart, Chemia organiczna. Krótki kurs, PZWL, Warszawa, 1999.

E. Białecka-Florjańczyk, J. Włostowska, *Chemia organiczna*, WNT, Warszawa, 2003. *Laboratory:*

A. Czarny, B. Kawałek, A. Kolasa, P. Milart, B. Rys, J. Wilamowski *Ćwiczenia laboratoryjne z chemii organicznej*, Adamantan, Warszawa 2008 (*on-line electronic version*: www.skryptoszafa.pl).

A. Vogel, Preparatyka organiczna, WNT, Warszawa, 2007.

Praca zbiorowa, ed. J. T. Wróbel, *Preparatyka i elementy syntezy organicznej*, PWN, Warszawa, 1983.

Praca zbiorowa, tłum. z jęz. niemieckiego, *Preparatyka organiczna*, PWN, Warszawa, 1983. R. Walczyna, J. Sokołowski, G. Kupryszewki, *Analiza związków organicznych*,

Wydawnictwo Uniwersytetu Gdańskiego, Gdańsk, 2001.

Z. Jerzmanowska, *Analiza jakościowa związków organicznych*, PZWL, Warszawa, 1951. **Teaching methods:**

Lectures are accompanied by the same number of contact hours in problem-solving classes (tutorials) where students can discuss in smaller groups. Practical laboratory classes play an essential role.

Assessment methods:

Continuous assessment (tests written during tutorials, assessment of knowledge of theoretical background, results of experiments and written reports for laboratory work), written examination at the end of the course

Course title: Physical chemistry

Course code: WCh-CL-0202-08

Type of course: Lecture (L) + laboratory (P)+ calculation classes (T) + tutorials (solving problem classes) (T).

Level of course: Preliminary

Year of study: Second

Semester/trimester: Winter and summer semesters

Number if credits allocated: 18 ECTS (6 for lab.)

Name of lecturer: Marek Wójcik, PhD, DSc, Prof.; Maria Nowakowska, PhD, DSc, Prof. **Objective of the course:**

The main objective of this course is to provide students with basic knowledge and its applications in the area of physical chemistry, to highlight the basic laws and the advances of physical chemistry, to demonstrate the importance of that discipline for the development of modern science. Major aspects of chemistry such as characteristics of different states of matter, principle of thermodynamics, kinetics, catalysis, electrochemistry, relations between bulk properties and properties of individual molecules will be considered. Theories describing these phenomena and their experimental verification will be discussed. The course will develop the skill to analyze the material and to obtain the general concept. The information-management competences will be also developed. The main objective of the laboratory exercises is experimental verification of the fundamental laws and relationships between different quantities which describe the physicochemical properties of the chemical systems. To help in understanding the main concepts of physical chemistry calculation classes and tutorials are delivered.

Prerequisites:

Basic courses of mathematics (WCh-CL-0101-07) and physics (WCh-CL-0102-07).

Course content:

First law of thermodynamics, thermochemistry. Second law of thermodynamics, Helmholtz and Gibbs functions, chemical potential. Planck's theorem and its consequences. Phase transitions of pure substances, phase diagrams, Clausius-Clapeyron equation. Phase transitions of simple mixtures. Real solutions: activity and activity constant, fugacity. Phase transitions in multi-component systems. Equilibrium in chemical reactions. Molecular spectroscopy: polarization, rotational and vibrational spectra of molecules, characteristics of electronic transitions, elements of photochemistry, nuclear magnetic resonance, electron spin resonance, mass spectrometry. 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. Collision theory, active complex, transition state, entropy and enthalpy of activation. Catalysis. Equilibrium in electrochemical systems: thermodynamical properties of ions, 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.

Recommended reading:

K. Pigoń, Z. Ruziewicz, Chemia fizyczna, PWN, Warszawa, 1980, 2005.

G.M. Barrow, Chemia fizyczna, PWN, Warszawa, 1978.

Praca zbiorowa, Chemia fizyczna, PWN, Warszawa, 1980.

Z. Kęcki, Podstawy spektroskopii molekularnej, PWN, Warszawa, 1992.

P.W. Atkins, Chemia fizyczna, PWN, Warszawa, 2001.

K. Gumiński, Termodynamika, PWN, Warszawa, 1972.

J. O. Bockris, Modern Aspects of Electrochemistry, Plenum Press, London, 1979.

T. Bieszczad, M. Boczar, D. Góralczyk, W. Jarzęba, A.M. Turek, *Ćwiczenia laboratoryjne z chemii fizyczne*, Wyd. UJ, Kraków 2000.

Teaching methods: multimedia techniques, performing experiments, applying equipment, dealing with experimental data, solving numerical problems.

Assessment methods: evaluation of the report and of the oral presentation of results at laboratory classes, tests and oral presentations at tutorials, written examination.

Course title: Crystallography **Course code:** WCh-CL-O203-08

Turne of course Lecture (L) is chosen (

Type of course: Lecture (L) + classes (tutorial) (T)

Level of course: Basic

Year of study: Second

Semester/trimester: Winter semester

Number of credits allocated (workload based): 2 ECTS

Name of lecturer: Stanisław Hodorowicz, PhD, DSc, Prof.

Objective of the course (expected learning outcomes and competences to be acquired):

The main purpose of teaching crystallography is providing students with a key to understanding the nature and symmetry of the ordered phases, showing that the knowledge is necessary to understand spatial structure of chemical compounds, their mutual packing and interactions in crystalline phases, underlying the influence of crystallographic achievements on material sciences, 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 take actively part in discussions.

Prerequisites: Mathematics (WCh-CL-O101-07), Physics (WCh-CL-O102-07) and Introduction to chemistry (WCh-CL-O103-07).

Course contents:

Crystals as the ordered phases: the order range in various states of matter, mesomorphous phases. Geometric crystallography: point symmetry, lattice symmetry and Bravais lattices, space groups. Structural crystallography: diffraction methods in structure determination (X-ray, neutron and electron diffraction) – Laue, Bragg and Ewald approach, outline of X-ray structure analysis and application in chemistry. Crystal chemistry: outline of crystal structures classification according atomic interactions: metallic, ionic, covalent, coordination, van der Waals and hydrogen bonding.

Recommended reading:

Z. Bojarski, M. Gigla, K. Stróż, M. Surowiec, *Krystalografia, podręcznik wspomagany komputerowo*, PWN, Warszawa, 1996 (and next editions).

J. Chojnacki, *Elementy krystalografii chemicznej i fizycznej*, PWN, Warszawa, 1971 (and next editions).

Teaching methods:

Lectures are accompanied by the same number of contact hours in problem solving classes (tutorials) where students can discuss in smaller groups.

Assessment methods:

Continuous assessment (tests written during tutorials) and a written examination (multi-choice test) at the end of the course.

Course title: Introduction to quantum chemistry

Course code: WCh-CL-O204-08

Type of course: Lecture (L) + classes (tutorial) (T) + computer laboratory (P)

Level of course: Basic

Year of study: Second

Semester/trimester: Summer semester

Number of credits allocated (workload based): 8 ECTS

Name of lecturer: A. Michalak, PhD, DSc; J. Korchowiec, PhD, DSc.

Objective of the course (expected learning outcomes and competences to be acquired):

To acquire knowledge and basic concepts and ideas of quantum mechanics and quantum chemistry, and a specificity of description on the quantum level, a relationship between a description of molecular systems on the microscopic and macroscopic levels. To develop the competence and confidence of the students in performing quantum-chemical calculations and interpreting their results..

Prerequisites: Mathematics (WCh-CL-O101-07), Physics (WCh-CL-O102-07), Introduction to chemistry (WCh-CL-O103-07).

Course contents:

Postulatem of quantum mechanics; model systems: particle in a box, harmonic oscillator, Brigid rotor, hydrogen atom and H_2^+ ; approximate methods, variational metod, Born-Oppenheimer approximation, LCAO MO method, elements of the group theory, one-electron approximation, Hartree-Fock method, errors of the SCF calculations, electronic structure of many-electron atoms and diatomic molecules, atomic orbitals, molecular orbitals, localized orbitals, natural orbitals, hybridization, ionization potential, Koopmans theorem, basis sets in ab initio calculations, semiempirical methods, correlation energy, post-HF methods and DFT – basic ideas, accuracy of quantum cemical calculations, geometry optimization, stationary points on the potential energy surface, chemical reactions, thermodynamics and kinetics, reactivitycriteria and indices, molecular electrostatic potential, population analysis, bondorders, frontier orbitals, electronegativity, harness, Fukui function, Woodward-Hoffmann rules, canonical ensamble and determination of thermodynamical functions.

Recommended reading:

R. F. Nalewajski, Podstawy i metody chemii kwantowej: wykłady, PWN, Warszawa, 2001.

A. Gołębiewski, Elementy mechaniki i chemii kwantowej, PWN, Warszawa, 1982.

K. Gumiński, P. Petelenz, Elementy chemii teoretycznej, PWN, Warszawa 1989.

L. Piela, Idee chemii kwantowej, PWN, Warszawa, 2003.

A. Cotton, Teoria grup - zastosowania w chemii, PWN, Warszawa 1973.

F. Jensen, Introduction to Computational Chemistry, Wiley, 1999.

A.R. Leach, Molecular Modeling. Principles and Applications, Pearson Education, 2001.

Teaching methods:

Lectures are accompanied by the same number of contact hours in problem solving classes (tutorials) where students can discuss in smaller groups and the computer laboratory where the opractical quantum chemical calculations are performed to illustrate the concepts introduced and to solve qualitative and quantitative practical problems.

Assessment methods:

Test

Language of instruction: Polish or English

Course title: English **Course code: Type of course:** Foreign language course Level of course: Advanced, intermediate or basic (depending on the language) Year of study: Second **Semester/trimester:** Winter and summer semesters Number of credits allocated (workload based): 5 ECTS Name of lecturer: **Objective of the course (expected learning outcomes and competences to be acquired): -Prerequisites:** None Course contents: Students (vast majority of) choose English, usually at the advanced level, but there is a possibility to choose any other language **Recommended reading:** Teaching methods: Foreign language course supported by multimedia Assessment methods: Tests Language of instruction: English or any other chosen language

Course title: Biochemistry and biology **Course code:** (WCh-CL-O301-09)

Type of course: Lecture

Level of course: Basic

Year of study: Third

Semester/trimester: Winter semester

Number of credits allocated (workload based): 4 ECTS

Name of lecturer: Jerzy Silberring PhD, DSc, Prof.

Objective of the course (expected learning outcomes and competences to be acquired):

Competences concerning the description and interpretation of phenomena and processes present in nature. Knowledge of important biopolymers, their properties and structure-activity relationship, basic biochemical techniques and applications of biological processes in chemistry and technology.

Prerequisites: Organic chemistry (WCh-CL-O106-07, WCh-CL-O206-08)

Course contents: Molecular basis of life. Theories describing the origin of life on the Earth. Life organization levels – acellular forms, cells, tissues, organs. Unicellar and complex organisms. Biological concept of species, processes of species creation and dying off. Structure and physiology of procariotic and eucariotic organisms. Structure and functions of physiological membranes. Structure and biological functions of proteins, nucleic acids, lipids and carbohydrates. Structure activity relationship of biologically active compounds. Basic metabolic pathways. Photosynthesis and other anabolic pathways. Introduction to classic, population and molecular genetics. Principles of biotechnology.

Recommended reading: J. M. Berg, J. L. Tymoczko, L. Stryer, *Biochemia*, PWN, 2005. **Teaching methods:** Lecture supported by multimedia.

Assessment methods: Written examination

Course title: Chemical technology

Course code: WCh-CL-O302-09

Type of course: Lecture (L) + classes (problem-solving and laboratory) (T+P)

Level of course: Basic

Year of study: Third

Semester/trimester: Winter semester

Number of credits allocated (workload based): 5 ECTS

Name of lecturer: Roman Dziembaj PhD, DSc, Prof.

Objective of the course (expected learning outcomes and competences to be acquired):

Fundamentals of chemical technology addressed to students with basics chemistry knowledge (inorganic chemistry, organic chemistry, analytical and physical chemistry, thermodynamical and kinetic aspects) as well as in mathematic and physics. The course provides for students a basic knowledge and practice training in industrial and applied chemistry of the most popular technological reactions and processes. Students should be able to solve qualitative and quantitative problems of a familiar nature and recognize and implement good measurements science and practice connected to chemical technology. They should demonstrate competences in evaluation, interpretation and synthesis of chemical information and data as well as in presenting scientific material and arguments in writing and orally. Skills in processing data by computer software, monitoring of chemical properties by observation and measurements with systematic documentation, conducting standard laboratory procedures should be acquired. Students should be able to apply safely chemicals used during laboratory classes, interpret data derived from laboratory observations and measurements, conduct risk assessment concerning use of chemical substances and laboratory procedures. This course should moreover develop skills in calculation of technological parameters with error analysis, correct use of units, team-working, planning and time management. Students should be ready to analyze material resulting in a fast decision making.

Prerequisites:

Introduction to chemistry (WCh-CL-O103-07), Physical chemistry (WCh-CL-O202-08). Course contents:

Course contents:

Fundamentals in physicochemistry of technological processes (mass and heat transport, unit operations, similarity theory). Technological rules and charts. Specifics of industrial chemistry – scale up of processes. Raw materials in industrial chemistry. A review of main chemical technologies. Biotechnology – enzymatic reactions. Quality control of raw materials and products – selected analytical techniques in industrial processes. Green chemistry. Government regulations (law regulations) in chemical industry – REACH regulation. The exercises and laboratory practice in unit operations, technical analysis of raw materials and products in chemical industry, methods of preparation of industrial catalysts and polymers, and selected biotechnological processes.

Recommended reading:

E. Bortel, H. Koneczny, Zarys technologii chemicznej, PWN, Warszawa, 1992.

R. Gayer, Z. Matysikowa, *Zbiór zadań z technologii chemiczne*", Wydawnictwa Szkolne i Pedagogiczne, Warszawa, 1978.

M. Serwiński, *Zasady inżynierii chemicznej i procesowej*, WNT, Warszawa, 1982. **Teaching methods:**

Lectures, seminars, exercises and laboratory practice.

Assessment methods:

Written examination (lecture) and evaluation of reports and tests (classes). Language of instruction: Polish/English

Course title: Chemistry of materials

Course code: WCh-CL-A303-09

Type of course: Lecture (L)

Level of course: Basic Year of study: Third

Semester/trimester: Winter semester

Number of credits allocated (workload based): 2 ECTS

Name of lecturer: Marcin Molenda, PhD; Ewa Witek, PhD.

Objective of the course (expected learning outcomes and competences to be acquired):

Applying of chemical methodology in describing the relationships between structure and properties of solid state materials and polymers. Students should be able to demonstrate knowledge on basic chemical materials, evaluate the application of materials and their process properties as well as utilization (recycling) of used materials. They should gain competences in evaluation, interpretation and synthesis of chemical information and data, presenting scientific materials. Ability to recognize and implement good measurement science and skills required for use of instrumentation in synthetic and analytic work in characterization of materials should be acquired. Students should demonstrate skills in processing and interpretation of chemical information and data, safe handling of chemical materials, monitoring of characteristic properties of solid materials. They should be able to analyze material, synthesize concepts, apply information technology for collecting and acquisition of data. They should enlarge competences in written communication in Polish and English languages.

Prerequisites: Introduction to chemistry (WCh-CL-O103-07), Organic chemistry (WCh-CL-O106-07), Inorganic chemistry (WCh-CL-O201-08).

Course contents:

Introduction to materials science, supra-molecular chemistry and nanotechnology. Solid state materials: metals, alloys, ceramics and glasses – the basics of preparation methods, characteristic properties, application, terminology. Introduction into polymers chemistry, preparation methods, structure, properties and applications of polymers. Basic polymers classification: polyolefins, phenol resins, polyesters, epoxides and polymer blends. Biodegradable polymers. Basics of composites and advanced functional materials.

Recommended reading:

M. Hetmańczyk, *Podstawy nauki o materiałach*, Oficyna Wydawnictwa Politechniki Śląskiej, Gliwice, 1999.

M. Blicharski, *Wstęp do inżynierii materiałowej*, WNT, Warszawa, 1998. **Teaching methods:**

Lecture accompanied by short experimental presentations.

Assessment methods:

Evaluation of a written report based on literature survey. Language of instruction: Polish/English

Course title: Applied chemistry and chemicals management **Course code:** WCh-CL-O304-09

Type of course: Classes (problem-solving) (T)

Level of course: Basic

Year of study: Third

Semester/trimester: Winter semester

Number of credits allocated (workload based): 2 ECTS

Name of lecturer: Ewa Witek, PhD; Marcin Molenda, PhD.

Objective of the course (expected learning outcomes and competences to be acquired):

The main goal of this course is to provide the rules of sustainable growth in daily life as well as the safe handling of chemical materials including specific hazards associated with their use. Students should know terminology associated with applied chemistry and be ready to propagate the sustainable use of natural and synthetic materials. They should conduct risk assessment concerning the use of chemical substances. Knowledge of law on chemicals management should be acquired. Students should gain competences in presenting scientific materials and arguments during oral presentations of material retrieved through on-line computer searches and library studies. They should be able to use subject-related Internet databases and to prepare presentations supported by multimedia techniques.

Prerequisites: Introduction to chemistry (WCh-CL-O103-07).

Course contents:

Concept of sustainable growth – environmentally friendly chemistry ("green chemistry"). Pollution and protection of air. Cleaning and using of water for commercial and industrial applications. Sewage purification. Soil pollution, fertilizers, recultivation. Additives used in food production. Household wastes – segregation, recycling, utilization, reuse. Washing and cleaning agents – use, environment impact, waste utilization. Chemical plant protection – use, toxicity. Building materials, paint cover, fuels, oils, solvents – protection during use, waste utilization. Renewable resources of raw materials and energy.

Recommended reading: -

Teaching methods:

Short lectures with oral presentations given by students followed by a problem discussion. Assessment methods:

Literature survey and evaluation.

Language of instruction: Polish/English

Course title: Chemical analysis

Course code: WCh-CL-A301-09

Type of course: Lecture (L), laboratory (P), classes (T).

Level of course: Intermediate

Year of study: Third

Semester/trimester: Winter semester

Number of credits allocated (workload based): 7 ECTS (L – 3, P – 2, T – 2)

Tutor: Paweł Kościelniak, PhD, DSc, Prof. (L); Stanisław Walas, PhD (L); Małgorzata Herman, PhD (P); Teaching staff of the Department of Analytical Chemistry (T).

Objectives of the course(expected learning out comes and competences to be acquired:

- Introduction to main problems and methods of chemical analysis.
- Instruction in techniques of atomic spectrometry and of chromatography.
- Training in lab work related to fundamental steps of an analytical process.
- Validation of analytical methods and appropriate data handling.
- Achieving of practical skills in realization of particular steps of analytical procedure as well as in operation of analytical instruments in order to prepare the students to be employed in analytical laboratories.

Prerequisites: Analytical chemistry (WCh-CL-O105-07)

Course contents:

Lecture:

Analytical procedure. Methods of sample digestion. Optimization of analytical parameters. Advanced methods of analyte separation and preconcentration. Analytical calibration. Matrix effects and interferences. Analytical signal and data handling. Interpretation of analytical results. Multicomponent analysis and speciation. Reference materials. Interlaboratory trials. Techniques of atomic spectrometry and inorganic mass spectrometry – analytical performance and applications. Techniques of chromatography – analytical performance and applications Laboratory:

Introduction to the most important practical issues of analytical procedure. Acquaintance with construction, work and operation of atomic spectrometers and chromatographs. Sample preparation and analysis using selected techniques of atomic absorption spectrometry and chromatography.

Classes:

Introduction to the most important practical issues of analytical procedure. Acquaintance with construction, work and operation of atomic spectrometers and chromatographs. Sample preparation and analysis using selected techniques of atomic absorption spectrometry and chromatography.

Recommended reading:

Praca zbiorowa, *Ocena i kontrola jakości wyników pomiarów analitycznych*, WNT, Warszawa, 2007.

W.W. Kubiak, J. Gołaś (editors), *Instrumentalne metody analizy chemicznej*, WN AKAPIT, Kraków, 2005.

E. Bulska, K. Pyrzyńska (editors), *Spektrometria atomowa, Możliwości analityczne, Ocena i kontrola jakości wyników pomiarów* analitycznych, (praca zbiorowa), Wydawnictwa Naukowo-Techniczne, Warszawa, 2007.

Z. Witkiewicz, *Podstawy chromatografii*, WNT, Warszawa 2005; MALAMUT, Warszawa, 2007.

P. Kościelniak, M. Trojanowicz, red., *Analiza przepływowa, Metody i zastosowania*, T.1, Wydawnictwo Uniwersytetu Jagiellońskiego, Kraków, 2005.

P. Kościelniak, M. Trojanowicz, red., *Analiza przepływowa, Metody i zastosowania*, T.2, Wydawnictwo Uniwersytetu Jagiellońskiego, Kraków, 2008. (in print).

Wybrane normy PN EN-ISO.

Teaching methods:

Lecture supported by multimedia, practical classes, problem solving classes (tutorials). Lecturer offers 1 hour per week to consult and solve particular problems individually.

Assessment methods:

Multiple choice test examination (L), written tests, reports (P), evaluation of particular tasks (T).

Course title: Flow analysis Course code: WCh-CL-A302-09 Type of course: Lecture (L) Lever of course: Intermediate Year of study: Third Semester /trimester: Summer semester Number of credits allocated (workload based): 1 ECTS Name of lecturer: Paweł Kościelniak, PhD, DSc, Prof. Objective of the course (expected learning outcomes and competences to be acquired): • Introduction to main issues of flow analysis, its role and place in analytical chemistry.

- Making the students familiar with different flow techniques and their application in analytical practice.
- Transfer of skills in construction and operation of flow systems as the tolls for realization of particular steps of the analytical procedure.

Prerequisites: Introduction to chemistry (Ch-CL-O103-07), Analytical chemistry (WCh-CL-0105) and Introduction to statistical evaluation of measurement data (WCh-CL-0107). **Course content:**

Review, characteristics and comparison of flow analysis techniques. Flow systems – designing and operation. Instrumental parameters of flow injection analysis. Chemical reactions in flow systems. Methods of dilution. Methods of separation and preconcentration. Calibration procedures. Multicomponent analysis and speciation. Flow analysis based on the International Standards. Trends and prospects of flow analysis.

Recommended reading:

B. Karlberg, G.E. Pacey, *Wstrzykowa analiza przepływowa dla praktyków*, WNT, Warszawa, 1994.

M. Trojanowicz, Automatyzacja w analizie chemicznej, WNT, Warszawa, 1992.

P. Kościelniak, M. Trojanowicz, red., *Analiza przepływowa, Metody i zastosowania*, T.1, Wydawnictwo Uniwersytetu Jagiellońskiego, Kraków, 2005.

P. Kościelniak, M. Trojanowicz, red., *Analiza przepływowa, Metody i zastosowania*, T.2, Wydawnictwo Uniwersytetu Jagiellońskiego, Kraków, 2008 (in print).

Teaching methods: Lecturer offers 1 hour per week to consult and solve particular problems individually.

Assessment methods: Written examination .

Course title: Adsorption and catalytic processes

Course code: WCh-CL-A303-09

Type of course: Lecture (L) + classes (tutorial) (T)

Level of course: Intermediate

Year of study: Third

Semester/trimester: Summer semester

Number of credits allocated (workload based): 2 ECTS

Name of lecturer: Piotr Kuśtrowski, PhD, DSc; Lucjan Chmielarz, PhD, DSc.

Objective of the course (expected learning outcomes and competences to be acquired): The course offers an introduction to adsorption and catalysis. Students should collect basic knowledge on quantitative and qualitative description of adsorption and catalysis phenomena. They should be able to recognize and implement good measurements science and practice using in catalytic and adsorption processes. Skills in the monitoring of changes in chemical properties as well as the processing and interpretation of data derived from laboratory measurements should be acquired. Students should be able to analyze the collected materials and calculate basic parameters related to effectiveness of adsorption and catalytic activity together with error analysis. They should gain competences in information retrieval, communication in English and Polish languages and presenting scientific material with use of information technology to an informed audience.

Prerequisites:

Introduction chemistry (WCh-CL-O103-07), Physical chemistry (WCh-CL-O202-08). Course contents:

Physical and chemical adsorption. Thermodynamics of adsorption processes. Methods used for determination of adsorption isotherms. Kinetics of adsorption and desorption. Models describing kinetics and equilibrium as well as parametric dependences. Adsorbent (structure, texture, micro- and mesoporous solids). Kinetics of catalytic processes. Experimental methods used for study on activity and selectivity of catalysts. Diffusion limitations. Activation, deactivation, reactivation and recycling of catalysts.

Recommended reading : -

Teaching methods:

Lecture, problem-solving classes, literature surveys. Assessment methods: Oral examination Language of instruction: Polish/English

Course title: Introduction of polymer science Course code: WCh-CL-A304-09 **Type of course:** Lecture (L) + classes (problem-solving) (T) Level of course: Intermediate Year of study: Third Semester/trimester: Summer semester Number of credits allocated (workload based): 3 ECTS

Name of lecturer: Ewa Witek, PhD.

Objective of the course (expected learning outcomes and competences to be acquired):

Students should know what the consequences of chain structure encountered in polymers are. They should know major aspects of chemical terminology used in polymer field. A particular emphasis is laid on types of polymerization reactions, relations between chain-topology, tacticity and physicochemical properties of polymers as well as possibilities of steering polymerization and polycondensation reactions toward achieving polymers with preset properties. The main aim of problem-solving classes is to acquire by students experimental techniques which are used for the synthesis of macromolecular substances, Knowledge on methods employed to determine physicochemical properties of polymers should be also acquired. Students should be able to recognize and implement good measurement science, interpret data derived from laboratory observations, conduct risk assessments concerning the use of chemicals needed for polymer synthesis. They should present skills in the safe handling of chemical materials used in polymer synthesis. A part of classes demands literature survey through computer searches in Internet databases, analysis of collected information and presentation of conclusions during discussion in a small group.

Prerequisites:

Introduction to chemistry (WCh-CL-O103-07), Physical chemistry (WCh-CL-O202-08). **Course contents:**

Chain structure of macromolecular compounds. Criteria diversifying macromolecular compounds. Definitions of "mer" and "constitutional unit". Isomers in polymer chemistry, especially concerning tacticity. Concept of average molecular masses and molecular mass distributions. Reactivity of monomers. Kinetics of chain reactions and polycondensations. Thermodynamics and mechanisms of polymerization reactions.

Recommended reading:

E. Bortel, Wprowadzenie do chemii polimerów, Wydawnictwo UJ, 1994.

Z. Florjańczyk, S. Penczek, Chemia polimerów, T. I, II, III, Oficyna Wydawnicza Politechniki Warszawskiej, 1995-98.

Teaching methods:

Lectures supported by multimedia techniques accompanied by problem-solving classes with demonstrated short experiments.

Assessment methods:

Written examination.

Course Title: Advanced Inorganic Chemistry

Course code: WCh-CL-B301-09

Type of course: Lecture (L) + classes (tutorial) (T)

Level of course: Intermediate

Year of study: Third

Semester/trimester: Summer semester

Number of credits allocated (workload based): 5 ECTS

Name of lecturer: Barbara Sieklucka, PhD, DSc, Prof.; Grażyna Stochel, PhD, DSc, Prof.; Zbigniew Sojka, PhD, DSc, Prof.

Objective of the course (expected learning outcomes and competences to be acquired): The main purpose of the course is to get students acquainted with advanced branches of inorganic chemistry such as modern coordination chemistry, bioinorganic chemistry and chemistry of solids, by showing the principal concepts and machinery of those disciplines. The special emphasis is put on explaining the structure-property and function relationships. After passing successfully the tutorial, students should be able to solve problems in various fields of inorganic chemistry, to think in an abstract way, to compare and interpret data, to take part actively in discussions as well.

Prerequisites:

Inorganic Chemistry (WCh-CL-O201-08), Physical Chemistry (WCh-CL-O202-08) **Course contents:**

Electronic spectra and magnetism of d- and f-electron metal complexes (10 h).

Spectroscopic terms. Ligand field electronic transitions: weak field and strong field limits, Tanabe-Sugano diagrams, the nepheloauxetic series. Charge-transfer bands. Selection rules and intensities. Electronic spectra of f-block ions. Magnetism of d- and f-electron metal complexes. Different forms of magnetism. Curie-Weiss law. Ferro-, antiferro- and ferrimagnetic ordering. The magnetism of d-electron metal ions. Spin equilibria. The magnetism of lanthanide ions. Magnetic molecular materials.

Bioinorganic chemistry (10 h)

Problems and research methods in bio-inorganic chemistry, important elements in biology and medicine, co-ordination chemistry vs. bio-inorganic chemistry, properties if bio-ligands, selection, absorption and formation of metal complexes in biology, transport and storage of metal ions, communication functions of metals, functions of metals in metallo-bioparticles. Functions of metallo-enzymes, biochemistry of small particles, metals in the environment, metals and their compounds in medicine, perspectives of bio-inorganic chemistry.

Structure and Properties of Solids (10 h)

Thermodynamics of condense matter. Structural principles and chemical classification of solids based on the ordering and the nature of chemical bonding. Crystalline and amorphous materials - their basic properties and applications. Nanostructural materials - dimension and size related effects. Electronic structure models, band theory, Brillouin zones and density of states, metals and metallic oxides, semiconductors, insulators, Point defects and extended defects, non-stoichiometry, chemical equilibria of defects in daltonides and bertolides, doping and impurity. Diffusion in solid state - phenomenological and atomic level description. Electronic and ionic conductivity. Mechanical, electrical, optical and magnetic properties of solids. Surfaces and interfaces. Reactivity of solids.

Recommended reading:

A. Bielański, Chemia Nieorganiczna, PWN, Warszawa, 2003.

S. F. A. Kettle, Fizyczna Chemia Nieorganiczna, PWN, Warszawa, 1999.

D. F. Shriver, P. W. Atkins, T. L. Overton, J. P. Rourke, M. T. Weller, F. A. Armstrong, *Inorganic Chemistry*, Oxford, 2006.

J. E. Huheey, E. A. Keiter, R. L. Keiter, *Inorganic Chemistry. Principles of Structure and Reactivity*, Harper Collins, 1994.

S. J. Lippard, J. M. Berg, Podstawy Chemii Bionieorganicznej, PWN, Warszawa, 1998.

J. Dereń, J. Haber, R. Pampuch, Chemia Ciała Stałego, PWN, Warszawa, 1977.

A. F. Wells, Strukturalna Chemia Nieorganiczna, WNT, Warszawa, 1993.

R. Zallen, Fizyka Ciał Amorficznych, PWN, Warszawa, 1994.

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

A. R. West, Basic Solid State Chemistry, J. Wiley, Chichester, 1996.

R. Tilley, *Understanding Solids. The Science of Materials*, Wiley, Chichester, 2004. **Teaching methods:**

Lectures are accompanied by seminars where students are working in smaller groups using problem-solving approach.

Assessment methods:

Continuous assessment (written tests during tutorials, written examination at the end of the course.

Course Title: Experimental techniques and measuring instruments

Course code: WCh-CL-B302-09

Type of course: Lecture (L)

Level of course: Basic

Year of study: Third

Semester/trimester: Winter semester

Number of credits allocated (workload based): 1 ECTS

Name of lecturer: Witold Piskorz, PhD.

Objective of the course (expected learning outcomes and competences to be acquired):

The aim of the lecture is to introduce students to the fundamentals of the measuring instruments, experimental data acquisition and processing.

Prerequisites: Physical Chemistry (WCh-CL-O202-08)

Course contents:

The lecture covers various topics of measurements of the physical quantities such as: temperature and heat, pressure, mass, time and frequency, flow, charge, electric measurements (current and voltage, conductivity, resistivity, capacitance) using modern transducing devices in the context of chemical applications. Principles of controlling and programming of experimental parameters and processes. Hardware and software for interface systems data acquisition and processing. Switching and connecting devices. Standards for transmission protocols. Converters ADC, DAC, amplifiers. Pressure and vacuum lines building blocks. Optical devices and fibber optic techniques.

Recommended reading:

Handouts prepared by the lecturer.

Teaching methods

Lecture using multimedia facilities, scientific data mining.

Assessment methods

Final test examination

Language of instruction: Polish/English.

Course Title: Inorganic chemistry open laboratory

Course code: WCh-CL-B303-09

Type of course: Laboratory (P)

Level of course: Intermediate

Year of study: Third

Semester/trimester: Summer semester

Number of credits allocated (workload based): 8 ECTS

Name of lecturer: Andrzej Kotarba, PhD, DSc.

Objective of the course (expected learning outcomes and competences to be acquired): The main aim of the open laboratory is to develop the theoretical knowledge and practical skills in the field of inorganic and structural chemistry. The students learn: methods of inorganic materials synthesis and materials characterization, document, analyze, interpret and

discuss experimental data.

Prerequisites: Introduction to chemistry (WCh-CL-O103-07), Physical Chemistry (WCh-CL-O202-08), Inorganic Chemistry (WCh-CL-O201-08).

Course contents:

The laboratory covers various topics of coordination chemistry, photochemistry, solid state chemistry and chemistry of materials. The emphasis is put on structural problems and correlation between the structure and materials' properties. Students consult the tutors and after the literature studies they propose the sample preparation method, prepare samples for their own research: structural (spectroscopic and diffraction), photochemical, reactivity, kinetic measurements etc. The laboratory is carried out within a cooperative model - students perform most of the activities by themselves under the supervision of the tutor using the apparatus and equipment of the research groups. Each exercise has a mini-project character and is accomplished by the project report prepared using the data processing and presentation software (statistical and graphic programs as well as a text editor).

Recommended reading:

S. Paszyc, Podstawy Fotochemii, PWN, 1992

A. Fujishima, K. Hashimoto, T. Watanabe, *TiO*₂ *Photocatalysis*. *Fundamentals and Applications*, BKC Inc. 1999.

J. Dereń, J. Haber, R. Pampuch, Chemia Ciała Stałego, PWN, 1975.

Z. Bojarski, E. Łągiewka, Rentgenowska analiza strukturalna, PWN, 1988.

D. F. Shriver, P. W. Atkins, Inorganic Chemistry, OUP, 1999.

Teaching methods:

Scientific data mining (reading of scientific papers). Problem-solving classes (tutorials) where students can discuss their activity with the tutor or in smaller groups. Practical laboratory classes play an essential role. Report writing.

Assessment methods:

Continuous assessment (assessment of knowledge of theoretical background, results of experiments and written reports for laboratory work).

Course Title: Properties of crystalline phases

Course code: WCh-CL-B304-09

Type of course: Lecture (L) + classes (tutorial) (T)

Level of course: Intermediate

Year of study: Third

Semester/trimester: Summer semester

Number of credits allocated (workload based): 2 ECTS

Name of lecturer: Katarzyna Stadnicka, PhD, DSc, Prof.

Objective of the course (expected learning outcomes and competences to be acquired):

Presentation of contemporary knowledge in the field of materials properties in the aspect of anisotropy, symmetry and structure of crystalline phases. Developing the skills of solving problems related to structure-property relationships

Prerequisites: Crystallography (WCh-CL-O203-08).

Course contents:

Symmetry of physical properties and symmetry of crystals – the Neumann's principle; tensorial description of physical properties – basic tensor algebra; the properties of polar and axial tensors, the meaning of extended term of absolute structure: structure polarity / structure chirality; structural characteristics of the selected crystalline materials from the viewpoint of their physical properties: thermodynamic, pyroelectric, dielectric, piezoelectric, elastic, magnetic, ferroic, mechanical, optical – linear and non-linear, thermal, transport properties etc.

Recommended reading:

J. Chojnacki, Elementy krystalografii chemicznej i fizycznej, PWN, 1971.

R. E. Newnham, Properties of materials, OUP, 2005.

J. F. Nye, *Physical Properties of Crystals*, Clarendon Press - Oxford, 1979.

C. Giacovazzo (ed.), Fundamentals of Crystallography, OUP, 1992.

Teaching methods:

Lectures are accompanied by the same number of contact hours in problem-solving classes (tutorials).

Assessment methods:

An essay and an oral presentation (15 min) comprising a given problem concerning the subject of the lecture.

Course Title: Introduction to chemistry of new materials

Course code: WCh-CL-B305-09

Type of course: Lecture (L) + classes (tutorial) (T)

Level of course: Intermediate

Year of study: Third

Semester/trimester: Summer semester

Number of credits allocated (workload based): 2 ECTS

Name of lecturer: Wiesław Łasocha, PhD, DSc, Prof.

Objective of the course (expected learning outcomes and competences to be acquired):

Presentation of the contemporary methods of synthesis and investigations of new materials. Developing the skills of selection and proper modification of new materials required by modern science and technology.

Prerequisites: Crystallography (WCh-CL-O203-08).

Course contents:

Contemporary methods of synthesis of new materials, solvothermal methods, gas phase deposition, self-propagating reactions, synthesis with the use of microwaves.

Obtaining materials with high purity, crystallization techniques, structural characterization of new materials.

Synthesis and properties of selected groups of materials;

- high temperature superconductors, fullerenes, inorganic-organic hybrid electronic materials.

- porous materials, inorganic polymers, nanotubes, MOF materials and their applications.

- DNA and biological materials as components and inspiration in material science.

Recommended reading:

A. Bielański, Podstawy chemii nieorganicznej, wyd. 5, PWN, Warszawa, 2003.

U. Schubert, N. Husing, Synthesis of Inorganic materials, Wiley-VCH, 2000.

L. E. Smart, E. A. Moore, *Solid State Chemistry*, 3rd Ed., Taylor and Francis, 2003. **Teaching methods:**

Lectures are accompanied by the same number of contact hours in problem-solving classes (tutorials) where students can discuss case studies described in the literature, design synthesis and computer experiments.

Assessment methods:

Continuous assessment (tests written during tutorials), written exam at the end of the course. Language of instruction: Polish

Course title: Advanced organic chemistry – laboratory

Course code: WCh-CL-C301-09

Type of course: Laboratory (P)

Level of course: Intermediate

Year of study: Third

Semester/trimester: Winter semester

Number of credits allocated (workload based): 4 ECTS

Name of responsible person: Jarosław Wilamowski, PhD.

Objective of the course (expected learning outcomes and competences to be acquired):

Extension of student's knowledge concerning new laboratory techniques and other aspects of organic chemistry e.g. "green chemistry", getting familiar with the unique analytical equipment and keeping alive basic laboratory techniques. Students should also learn how to present their results to the informed audience, how to adapt general methods to certain experiments and how to use scientific literature and data bases.

Prerequisites: Organic chemistry (WCh-CL-O106-07 and WCh-CL-O206-08) **Course contents:**

Students learn new techniques (column chromatography connected with the choice of its conditions, vacuum distillation, sublimation, syntheses on a semi-micro scale, reactions carried out in a complex glass equipment, manipulation of water sensitive compounds), get familiar with the unique analytical equipment, and keep alive basic laboratory techniques. Students perform experiments including multi-step syntheses, tandem reactions or processes with modern catalysis. Results of some experiments (e.g. chemoluminescence, solvatochromic effects) are presented to other members of a student group. Some exercises are enriched by usage of spectroscopic methods for the structure elucidation of a product. The others require the adaptation of a general method for a certain experiment done by a student as well as taking advantage of data bases and scientific literature.

Recommended reading:

A. Czarny, B. Kawałek, A. Kolasa, P. Milart, B. Rys, J. Wilanowski, *Ćwiczenia laboratoryjne z chemii organicznej*, Adamantan, Warszawa, 2008; (*on-line electronic version*: www.skryptoszafa.pl).

A. Vogel, Preparatyka organiczna, WNT, Warszawa, 2007.

Praca zbiorowa, red. J. T. Wróbel, *Preparatyka i elementy syntezy organicznej*, PWN, Warszawa, 1983.

Praca zbiorowa, tłum. z jęz. niemieckiego, *Preparatyka organiczna*, PWN, Warszawa, 1983. J. Gawroński, K. Gawrońska, K. Kacprzak, M. Kwit, *Współczesna synteza organiczna. Wybór eksperymentów*, Wydawnictwo Naukowe, PWN, Warszawa, 2004.

Teaching methods:

Practical courses in laboratory

Assessment methods:

Continuous assessment of theoretical background for experiments, experimental results, and written laboratory reports.

Course Title: Application of spectroscopy to organic chemistry

Course code: WCh-CL-C302-09

Type of course: Problem solving classes (T)

Level of course: Basic

Year of study: Third

Semester/trimester: Winter semester

Number of credits allocated (workload based): 1 ECTS

Name of lecturer: Anna Kolasa, PhD.

Objective of the course (expected learning outcomes and competences to be acquired):

Skills in application of spectroscopic methods for structure elucidation of organic molecules. Ability to solve problems, to think in an abstract way, to apply known methods to new situations. Preparation for taking part in discussions and for team work.

Prerequisites: Organic chemistry (WCh-CL-O106-07 and WCh-CL-O206-08) **Course contents:**

Ultraviolet and visible spectroscopy: spectra of dienes, enones and aromatic compounds. Infrared spectroscopy: bands typical for functional groups and structural units, interpretation of spectra.

Mass spectrometry: ionisation methods and their influence on spectra; fragmentation pathways for main classes of organic compounds.

Nuclear magnetic resonance: interpretation of spectra with complicated spin patterns, coupling constants and their application to structure elucidation, application of NMR in stereochemistry, NMR of various nuclei (¹H, ¹³C, ¹⁹F, ³¹P), heteronuclear couplings. A range and limitations of methods under consideration. Complementary usage of all the methods for structure elucidation of complex organic compounds.

Recommended reading:

Praca zbiorowa, red. W. Zieliński, A. Rajca, *Metody spektroskopowe i ich zastosowanie do identyfikacji związków organicznych*, WNT, Warszawa, 2000.

R. M. Silverstein, F. X. Webster, D. J. Kremle, *Spektroskopowe metody identyfikacji związków organicznych*, PWN, Warszawa, 2007.

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

Teaching methods:

Problem solving classes in small groups

Assessment methods:

Written test at the end of the course.

Course Title: Principles of bioorganic chemistry

Course code: WCh-CL-C303-09

Type of course: Lecture (L)

Level of course: Basic

Year of study: Third

Semester/trimester: Summer semester

Number of credits allocated (workload based): 1 ECTS

Name of lecturer: Maciej Góra, PhD.

Objective of the course (expected learning outcomes and competences to be acquired):

The main purpose of teaching bioorganic chemistry is providing students with a key to understanding the structure and reactivity of biomolecules including kinetics and biocatalysis as well as some aspects of molecular biology and biotechnology. **Prerequisites:** Organic chemistry (WCh-CL-O106-07 and WCh-CL-O206-08), Biochemistry and biology (WCh-CL-O301-09).

Course contents:

- 1. Enzymes. a. Characteristic of enzymatic reactions. b. Course of enzymatic reactions. c. Influence of kinetic parameters on enzyme catalysed reactions. d. Selectivity of enzymatic reactions.
- 2. Chemical enzyme models. a. Micellar catalysis. b. Cyclodextrines and macrocyclic compounds as enzyme models.
- 3. Biogenetic and biomimetic processes. a. Biomimetic models of enzymatic reactions. c. Models of oxygen bounding proteins. d. Biological membrane mimics.
- 4. Designing of biologically active compounds. a. Natural products as leading substances.b. Structure bioactivity relationship of chemical compounds.
- 5. Enzymes and artifical enzymes as tools for molecular biology and biotechnology.

Recommended Reading:

P.Kafarski, B. Lejczak, Chemia Bioorganiczna, PWN, Warszawa, 1994.

Teaching methods: Lectures

Assessment methods:

Written examination at the end of the course.

Course Title: Principles of biological chemistry Course code: WCh-CL-C304-09 **Type of course:** Lecture (L) + Tutorial (T) Level of course: Intermediate Year of study: Third Semester/trimester: Summer semester Number of credits allocated (workload based): 4 ECTS Name of lecturer: Grażyna Stochel, PhD, DSc, Prof. (Lecture, part I)

Barbara Oleksyn, PhD, DSc, Prof. (Lecture, part II)

Krzysztof Lewinski, PhD, DSc (Lecture, part III)

Katarzyna Kurpiewska, PhD (Tutorial)

Małgorzata Brindel, PhD (Tutorial)

Objective of the course (expected learning outcomes and competences to be acquired):

The main purpose of teaching biological chemistry is providing students with a knowledge on chemical understanding of molecules and processes in biological systems.

Prerequisites: Organic chemistry (WCh-CL-O106-07 and WCh-CL-O206-08), Analytical chemistry (WCh-CL-O105-07), Inorganic chemistry (WCh-CL-O201-08), Biochemistry and biology (WCh-CL-O301-09).

Course contents:

Lecture, Part I. Biological chemistry of the elements:

Elements of life; metalome vs genome and proteome; chemical and physical factors controlling bioelements; abundance and speciation; chemical networks in biology, thermodynamic and kinetic aspects of biological processes; energy in biological systems and hydrogen biochemistry; functional properties of elements in biological systems (Na, K, Mg, Ca, Mn, Fe, Co, Ni, Cu, Zn, Mo, Cl, C, N, O, P, S, Si, Se)

Lecture, Part II. Structure and function of small bioactive molecules:

The role of small molecules in living organisms, endo- and exogenic molecules and drugs. Small molecules and biological membranes: structure and function of selected ionophores. Structure and interactions of small molecules with proteins: substrates and inhibitors of enzymes, stimulators and blockers of protein receptors. Role of small molecule chirality. Interactions of small molecules with DNA. Fate of drugs in organisms vs. their physicochemical properties. QSAR (Quantitative Structure-Activity Relationship) with regard to the three-dimensional molecular structure. Basic knowledge of biological activity measurements. Principles of drug design, selected models of drug interactions with active sites of macromolecules.

Lecture, Part III. Structure of biomacromolecules:

Structure of amino acids. Peptide bond. Conformational restrictions of polypeptide chain. Side-chain conformations. Elements of secondary structure: helices and beta-sheets. Motifs of protein structure. Structural hierarchy of protein structures. Structure of DNA and RNA. Structure of oligosaccharides

Tutorial:

Theoretical introduction to analytical methods in biochemistry.

Recommended reading: J. M. Berg, J. L. Tymoczko, L. Stryer, Biochemia, PWN, Warszawa, 2005.

Teaching methods: Lectures and tutorials

Assessment methods: Test

Course Title: Laboratory of biological chemistry

Course code: WCh-CL-C305-09

Type of course: laboratory (P)

Level of course: Intermediate

Year of study: Third

Semester/trimester: Summer semester

Number of credits allocated (workload based): 2 ECTS

Name of lecturer: Katarzyna Kurpiewska, PhD; Małgorzata Brindel, PhD.

Objective of the course (expected learning outcomes and competences to be acquired): During a laboratory practice, partly supervised and partly co-operative, students should learn: the basic techniques and methods used in qualitative analysis of biomolecules. Students also learn to interpret the results of experiments, to draw conclusions and to report them in a written form.

Prerequisites: Laboratory courses in organic chemistry (WCh-CL-O206-08).and analytical chemistry (WCh-CL-O105-07).

Course contents:

Laboratory classes "Introduction to analytical methods in biochemistry".

Chemical properties and qualitative analysis of main classes of biological compounds: amino acids proteins, saccharides, nucleic acids. Biological activity of proteins, protein-ligand interactions. Methods of isolation and molecular characterization of selected biologically active compounds.

Recommended Reading: A.Dubin, B.Turyna (red.), *Praktikum z biochemii dla studentów biologii i biotechnologii*, IBM UJ, 1999.

Teaching methods: Laboratory experiments and discussions on problem solving methods. **Assessment methods:** Continuous assessment during laboratory work and written reports. **Language of instruction:** Polish Title of the course: Advanced methods in physical chemistry Course code: WCh-CL-D301-09 Type of course: Lecture (L) + laboratory (P) Level of course: intermediate Year of study: third Semester/trimester: Winter semester Number if credits allocated: 4 ECTS Name of lecturer: Jan Najbar, PhD, DSc, Prof. Objective of the course:

The course will develop the skill to analyze the material and to be familiar with basic physicochemical 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 will be discussed. The main objective of the laboratory classes is to familiarize students with techniques and problems in advanced physical chemistry and to show the importance of the physical chemistry methods as tools in other chemical branches. The problems discussed and solved during the course allow to understand wide scope of modern physical chemistry, i.e. surface physical chemistry, electrochemistry, chemical kinetics and spectroscopy. Solution of all occurring scientific problems requires use of modern computer programs, which additionally enhances the attractivity of the course.

Prerequisites: Physical chemistry (WCh-CL-O202-08).

Course contents:

Lecture:

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.

Laboratory:

Application of the factor analysis for simultaneous determination of the contents of the organic mixtures. Spectrometric measurements and application of the computer programs for distribution of the absorption spectra to the spectra of individual components.

Determination of the critical micelle concentration (CMC) of the ionic surfactants in the presence of electrolytes. Electrochemical measurements (conductivity) of the solutions of the ionic micelle and the determination of the CMS and the number of aggregation of the micelle. Nanocrystallic solar battery. Construction of the simple solar photovoltaic battery based on semiconductor (TiO₂) sensibilized by organic dyes. Discussion of the photoinduced electron transfer processes occurring in the photovoltaic cell. Investigations of the vapour-liquid equilibrium in bicomponent mixtures. Construction of the phase diagram on the basis of the analysis of the temperature of boiling of the mixtures of organic liquids. Determination of the content of the liquid mixture by refractometric measurements.

Concentration cells. Determination of the transport numbers. First and second kind electrodes. Potentiometric titration. Determination of the solubility product of AgCl (AgI) from titration

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curves. Discussion of the stability of the complexes of silver with ammonia and tiosulphate anions on the basis of potentiometric measurements.

Broensted salt effect. Absorptiometric investigations of the bimolecular reaction of the phenolphthalein dianion with hydroxide anion. Theory of electrolytes (Debye-Hueckel equation). Kinetics of first and second order. Lambert-Beer law.

Recommended reading:

P.W. Atkins, Chemia fizyczna, PWN, Warszawa, 2006.

K.Pigoń, Z. Ruziewicz, Chemia Fizyczna, PWN, Warszawa, 2005.

Praca zbiorowa, Chemia Fizyczna, wyd. IV, PWN, Warszawa, 1980.

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

Teaching methods: Multimedia teaching techniques, the use of experimental techniques with the use of such equipment as e. g.: UV-Vis spectrometry, conductometry, refractometry, potentiometry to investigate physicochemical phenomena.

Assessment methods: evaluation of the report and of the oral presentation of results, written examination.

Course title: Mathematical Methods in Chemistry I Course code: WCh-CL-E306-09 Type of course: Lecture (L) + classes (tutorial) (T) Level of course: Basic Year of study: Third Semester/trimester: Winter semester Number of credits allocated (workload based): 1 ECTS Name of lecturer: Grzegorz Mazur, PhD Objective of the course (expected learning outcomes and competences to be acquired):

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.

Prerequisites:

Course contents:

Elements of combinatorics, complex numbers, functions of complex numbers, elements of the group theory, linear space over real and complex fields, Hilbert space. **Recommended reading:**

Teaching methods:

Lectures are accompanied by the same number of contact hours in problem solving classes (tutorials) where students can discuss in smaller groups.

Assessment methods: exam

Title of the course: Physical chemistry of surface and electrochemistry **Course code**: WCh-CL-D303-09

Type of course: Lecture (L)

Level of course: intermediate

Year of study: third

Semester/trimester: Summer semester

Number if credits allocated: 2 ECTS

Name of lecturer: Paweł Wydro, PhD, Tadeusz Bieszczad, PhD.

Objective of the course: The objective of that lecture is to present the physicochemical and electrochemical processes occurring at the interfaces. The course brings the understanding of theoretical backgrounds of the problems discussed as well as to familiarizes them with basic and modern experimental techniques used to study interfacial phenomena. The main objective of that lecture is to demonstrate the importance of interfaces in nature and its role in functioning of the living organisms. Moreover, the application of interfacial science to industry and technology is thoroughly presented. Thus, the lecture is aimed at showing the surfaces and interfaces as a place of variety, crucial for physiological and industrial processes. The second objective of that lecture is to acquaint students with principles of modern electrochemistry. The reversible and irreversible electrochemical processes and their fundamental role in electrolysis, corrosion, electrocatalysis and electroanalytical methods will be demonstrated.

Prerequisites: Physical chemistry (WCh-CL-0202-08).

Course contents: Interfaces and its role in nature, physicochemical phenomena at the interfaces, modern experimental method in studying of the interfacial processes (Brewster angle microscopy, fluorescence microscopy, UV-Vis, elipsometry, surface potential), the structure and properties of the surfactants aqueous solutions (association colloids, liquid crystalline phases, bilayers, liposomes), physical and chemical processes in micellar solutions: luminescence, microviscosity, energy transductions, kinetics of reactions Application of surfactants in industry: detergents, molecular sieves, catalyst, battery, nanoreactors, solubilisation and wetting. Application of amphiphiles in medicine and pharmacy. Modeling of biological membranes, the study of the mechanism of action of drugs. Drug carriers. Reversible electrode processes, the electromotive force of reversible cells, electrode potentials, reversible electrodes, application of e.m.f. measurements to a determination of the thermodynamic properties of reactions, irreversible electrode processes, overpotential, electrolysis, electrode kinetics, electrochemical corrosion, electrocatalysis, bioelectrochemistry.

Recommended reading: F. MacRitchie, *Chemistry at interfaces*, Academic Press, Inc. New York, 1990. P. A. Kralchevsky, K. Danov, N. D. Denkov, *Chemical Physics of Colloid Systems and Interface, Handbook of Surface and Colloid Chemistry*, CRC Press, New York, 2002. J. N. Israelachvili, *Intermolecular and surfaces forces – with applications to colloidal and biological systems*, Academic Press, Inc. New York, 1987. P. C. Hiemenz, *Principles of colloid and surface chemistry*, Marcel Dekker Inc., New York, Bazylea, 1986. A. Kozubek, A. F. Sikorski, J. Szopa, *Molekularna organizacja komórki*, Wydawnictwo Uniwersytetu Wrocławskiego, Wrocław 1996. R. H. Tredgold, *Order in thin organic films*, Cambridge University Press, Cambridge, 1994. G. T. Barnes, I. R. Gentle, *Interfacial Science*, Oxford University Press, New York, 2005. J. Eastoe, *Surfactant Chemistry*, Bristol UK, 2003. Selected articles published in scientific journals.

Teaching methods: Multimedia teaching techniques.

Assessment methods: written examination or credit.

Title of the course: Physicochemistry of macromolecular systems

Course code: WCh-CL-D304-09

Type of course: Lecture (L)

Level of course: intermediate

Year of study: third

Semester/trimester: Summer semester

Number if credits allocated: 1 ECTS

Name of lecturer: Szczepan Zapotoczny, PhD, Maria Nowakowska, PhD, DSc, Prof. Objective of the course:

The course aims in understanding correlations between structures of polymers and their physicochemical properties. The objective of the lecture is also to introduce modern methods of polymer characterizations. Major aspects of chemical terminology in relation to macromolecular chemistry will be addressed. The principal techniques of structural analysis of macromolecules in bulk solution and at the interfaces will be discussed. The relation between macroscopic properties of polymeric material and the properties of individual macromolecules will be presented. The study competences needed for continuing professional development will be developed.

Prerequisites: Physical chemistry (WCh-CL-0202-08).

Course contents:

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.

Recommended reading:

H. Galina, *Fizykochemia polimerów*, Oficyna Wydawnicza Politechniki Rzeszowskiej, 1998. Z. Florjańczyk, S. Penczek, (editors), *Chemia polimerów*, volumes II, III, Oficyna Wydawnicza Politechniki Warszawskiej, 1995-98.

Teaching methods:

multimedia teaching techniques Assessment methods: written examination or credit Language of instruction: Polish Title of the course: Photochemistry Course code: WCh-CL-D305-09 Type of course: Lecture (L) Level of course: preliminary Year of study: third Semester/trimester: Winter semester Number if credits allocated: 1 ECTS Name of lecturer: Joanna Kowal, PhD, Marek Mac, PhD, DSc. Objective of the course:

The objective of this course is to give students a basic knowledge and understanding of the photophysical and photochemical processes in organic molecules and polymer systems. The major aspects of chemical terminology and nomenclature used in photochemistry will be considered and the principal procedures of photochemical experimental techniques will be discussed. The practical aspects of photochemistry will be demonstrated. The ability to demonstrate knowledge and understanding the basic concepts and principles of molecular photochemistry will be developed.

Prerequisites: Physical chemistry (WCh-CL-0202-08).

Course contents:

Light absorption, electronic excited states of molecules and molecular aggregates, radiative and non-radiative transitions in excited molecules. Kinetics of the deactivation of excited states. Formation of excimers and exciplexes. Energy transfer. Quenching of excited states. Photochemical reactions – photoinduced electron transfer, photolysis, photoisomerization, photoaddition, hydrogen abstraction. Absorption and emission characteristics of polymers. Excimers in polymer systems, energy transfer and migration in polymers, antenna effect. Photodegradation and photoaxidation of polymers. Photosensitized degradation. Photostabilization of polymers. Photochemical modification of polymers.

Recommended reading:

Z. Kęcki, Podstawy spektroskopii molekularnej, PWN, Warszawa, 1998.

Praca zbiorowa, J. Pączkowski (ed.), Fotochemia polimerów. Teoria i zastosowanie,

Wydawnictwo Uniwersytetu Mikołaja Kopernika, Toruń, 2003.

W. Schnabel, Polimer degradation, Akademie-Verlag, Berlin, 1981.

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

S.Paszyc, Podstawy fotochemii, PWN

Teaching methods: Multimedia teaching techniques

Assessment methods: written examination

Course title: Mathematical Methods for Chemists II Course code: WCh-CL-E312-09 Type of course: Lecture (L) + classes (tutorial) (T) Level of course: Basic Year of study: Third Semester/trimester: Summer semester Number of credits allocated (workload based): 1 ECTS Name of lecturer: G. Mazur, PhD Objective of the course (expected learning outcomes and competences to be acquired):

Prerequisites:

Course contents:

Vector analysis with elements of tensor calculus (gradient, divergence, curl, Gauss's theorem, Stokes's theorem; curved coordinates and tensor analysis). Introduction to the group theory (discrete 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). Orthogonal polynomials. Fourier transformation and Dirac delta function.

Recommended reading:

Teaching methods:

Lectures are accompanied by the same number of contact hours in problem solving classes (tutorials) where students can discuss in smaller groups.

Assessment methods: exam

Course title: Quantum-chemical molecular modeling Course code: WCh-CL-D306-09 Type of course: Classes (tutorial) (T) Level of course: Basic Year of study: Third Semester/trimester: Summer semester Number of credits allocated (workload based): 2 ECTS Name of lecturer Artur Michalak, PhD, DSc Objective of the course (expected learning outcomes and competences to be acquired): 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

Prerequisites: Introduction to quantum chemistry (WCh-CL-O204-08)

Course contents:

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.

Recommended reading:

practical aspects of computational chemistry:

as in the theoretical analysis of chemical reactivity.

- 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

Teaching methods:

Practical problem solving excercises

Assessment methods:

course evaluation: written test (50%), lab reports (50%)

Course title: Introduction to computer programming

Course code: WCh-CL-E301-09 Type of course: Lecture (L) Level of course: Basic Year of study: Third Semester/trimester: Winter semester Number of credits allocated (workload based): 1 ECTS Name of lecturer: Objective of the course (expected learning outcomes and competences to be acquired): Understanding of basic concepts of computer architecture and function.

Prerequisites:

Course contents:

Concept of algorithm. Recurrence. Data representation and arithmetic operations implementation. Low-level architecture (memory system, CPU, I/O devices). Introduction to operating systems. File systems. Multitasking. Parallel computing.

Recommended reading:

Teaching methods:

Assessment methods: test

Course title: The C programming language Course code: WCh-CL-E302-09 Type of course: Lecture (L) + classes (tutorial) (T) Level of course: Basic Year of study: Third Semester/trimester: Winter semester Number of credits allocated (workload based): 2 ECTS Name of lecturer: M. Makowski, PhD Objective of the course (expected learning outcomes and competences to be acquired): The course presents modern low-level general application programming language. The aim

of the course is to develop basic programming skills, with emphasis on correctnes of the

program structure, dynamic memory allocation, recurrence and numerical methods.

Prerequisites: IT laboratory

Course contents:

Physical form of a program. Preprocessor, compilation phases. Type system. Functions.
Assignment instruction. Conditional instructions. Iteration. Pointers. Standard library.
Dynamic memory allocation. Input/output operations. Creating and using libraries.
Implementing numerical algorithms using the GSL library
Recommended reading: Kernighan B.W., Ritchie D.M., "The C Programming Language",
2nd Edition, Prentice Hall, 1988;
Tondo C.L., Gimpel S.E., "C Answer Book", Prentice Hall, 1990.

Teaching methods:

Lectures are accompanied by the same number of contact hours in problem solving classes (tutorials) where students can discuss in smaller groups.

Assessment methods: Semester project Language of instruction: Polish.

Course title: Computer networks.

Course code: WCh-CL-E303-09 Type of course: Lecture (L) Level of course: Basic Year of study: Third Semester/trimester: Winter semester Number of credits allocated (workload based): 5 ECTS Name of lecturer: Janusz Mrozek, PhD, DSc Objective of the course (expected learning outcomes and competences to be acquired): Basic understanding of typical network architectures. Ability to manage simple networks. Prerequisites: Course contents: Introduction to computer networks. OSI/ISO model. Physical layer. Network devices.

Addressing and routing in IP networks. Transport layer protocols: UDP and TCP. Application layer. HTTP protocol. Security in computer networks and data encryption. Firewalls. Network management.

Recommended reading:

: D.E. Comer: "Sieci komputerowe TCP/IP. Zasady, protokoły i architektura", WNT, 1997; K.S. Siyan, T. Parker: "TCP/IP. Księga eksperta", Helion, 2002

Teaching methods:

Assessment methods: One test after the lectures.

Course title: Statistical methods and data analysis Course code: WCh-CL-E304-09 Type of course: Lecture (L) + classes (tutorial) (T) Level of course: Basic Year of study: Third Semester/trimester: Winter semester Number of credits allocated (workload based): 2 ECTS Name of lecturer: A. Eilmes, PhD, DSc Objective of the course (expected learning outcomes and competences to be acquired):

Application of statistical methods to data analysis in chemistry.

Prerequisites: Mathematics (WCh-CL-O101-07).

Course contents:

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.

Recommended reading:

W.Feller, Wstęp do rachunku prawdopodobieństwa, PWN, Warszawa 1987; S.Brandt, Analiza danych, PWN, Warszawa 1999. **Teaching methods:**

Lectures are accompanied by the same number of contact hours in problem solving classes (tutorials) where students can discuss in smaller groups.

Assessment methods:

Continuous assessment (tests written during tutorials).

Course title: Software packages for symbolic and numerical calculations.

Course code: WCh-CL-E305-09 Type of course: Classes (tutorial) (T) Level of course: Basic Year of study: Third Semester/trimester: Winter semester Number of credits allocated (workload based): 2 ECTS Name of lecturer: A. Eilmes, PhD, DSc Objective of the course (expected learning outcomes and competences to be acquired): Application of software packages to solving simple model problems.

Prerequisites:

Course contents:

Problems specific to symbolic and numerical calculations. Application of Computer Algebra Systems to model problems. Performing typical scientific computations in numerical packages. Data visualisation.

Recommended reading:

Podręczniki użytkownika pakietów Octave i Mathematica;

D.A.McQuarrie, "Matematyka dla przyrodników i inżynierów", PWN

Teaching methods:

Problem solving classes (tutorials) where students can discuss in smaller groups.

Assessment methods:

Student project.

Course title: Algorithms and Data Structures Course code: WCh-CL-E307-09 Type of course: Lecture (L) + classes (tutorial) (T) Level of course: Basic Year of study: Third Semester/trimester: Summer semester Number of credits allocated (workload based): 3 ECTS Name of lecturer: Grzegorz Mazur, PhD

Objective of the course (expected learning outcomes and competences to be acquired):

The course presents basic data structures, the notion of algorithm, selected typical algorithms and elements of software engineering. The aim of the course is to develop ability to select and implement the right data structure and algorithm to solve problem at hand.

Prerequisites: The C Programming Language

Course contents:

Basic types and data structures. Representation of data. Pointers. Dynamic data structures. Algorithm complexity analysis. Recurrential algorithms. Sorting. Hash tables. Introduction to software engineering (software design, requirements specification, testing).

Recommended reading:

N. Wirth, "Algorithms and Data Structures", Prentice Hall, 1988

Teaching methods:

Lectures are accompanied by the same number of contact hours in problem solving classes (tutorials) where students can discuss in smaller groups.

Assessment methods:

Exam.

Course title: Numerical methods

Course code: WCh-CL-E308-09 Type of course: Lecture (L) + classes (tutorial) (T) Level of course: Basic Year of study: Third Semester/trimester: Summer semester Number of credits allocated (workload based): 3 ECTS Name of lecturer: Andrzej Eilmes, PhD, DSc Objective of the course (expected learning outcomes and competences to be acquired):

The aim of the course is to introduce students to basic algorithms used in scientific calculations and their implementation in available numerical packages. After completing the course students should be able to choose the numerical method appropriate to the problem.

Prerequisites:

Course contents:

Floating-point arithmetic. Estimation of the condition number. Estimation of the computational complexity. Basic problems of the numerical analysis: linear algebra, interpolation and approximation, numerical integration and differentiation, differential equations and equation systems, optimization.

Recommended reading:

Bjork and Dahlquist, Metody numeryczne, PWN; D. Kincaid, W. Cheney, "Numerical analysis", 3rd ed. Brooks/Cole Publishing **Teaching methods:**

Lectures are accompanied by the same number of contact hours in problem solving classes (tutorials) where students can use the numerical packages to perform typical scientific calculations

Assessment methods:

One project work during the semester. Language of instruction: Polish.

Course title: Databases

Course code: WCh-CL-E309-09 Type of course: Lecture (L) + classes (tutorial) (T) Level of course: Basic Year of study: Third Semester/trimester: Summer semester Number of credits allocated (workload based): 2 ECTS Name of lecturer: Objective of the course (expected learning outcomes and competences to be acquired): Understanding of the relational model of the database. Ability to construct simple database.

Prerequisites:

Course contents:

Database systems. Data modelling. Normal forms. Relational algebra. Relational databases. Query languages. Design of relational databases. Transaction processing. Hypertext and hypermedia.

Recommended reading:

Teaching methods:

Lectures are accompanied by the same number of contact hours in problem solving classes (tutorials) where students can discuss in smaller groups.

Assessment methods:

Continuous assessment (tests written during tutorials).

Course title: Scripting languages

Course code: WCh-CL-E310-09 Type of course: Lecture (L) + classes (tutorial) (T) Level of course: Basic Year of study: Third Semester/trimester: Summer semester Number of credits allocated (workload based): 2 ECTS Name of lecturer: Objective of the course (expected learning outcomes and competences to be acquired): Ability to solve simple problems using available libraries.

Prerequisites: C Programming Language

Course contents: Programming paradigms. Virtual machines. Concepts specific to scripting languages. The Python Language. Extending and embedding mechanisms. Applications of scripting languages in scientific computing, data presentation and data management.

Recommended reading: M. Lutz, D. Ascher, "Python. Wprowadzenie", Wyd. Helion

Teaching methods:

Lectures are accompanied by the same number of contact hours in problem solving classes (tutorials) where students can discuss in smaller groups.

Assessment methods:

Continuous assessment (tests written during tutorials).

Course title: Proteins and their complexes with ligands: computer modeling. Course code: WCh-CL-E311-09 Type of course: Lecture (L) + classes (tutorial) (T) Level of course: Basic Year of study: Third Semester/trimester: Summer semester Number of credits allocated (workload based): 2 ECTS Name of lecturer: Ewa Brocławik, PhD, DSc, Prof. (Institute of Catalysis, PAS),

Prof. Dr. Habil. Irena Rotterman-Konieczna (Collegium Medicum UJ)

Objective of the course (expected learning outcomes and competences to be acquired):

Prerequisites: Course contents:

The course is focused on modern computer-aided techniques for simulating conformational changes in proteins and protein-ligand complexes. Such information is indispensable in modern drug design. The course is composed of the following modules: Ligand structure I and II; Protein structure; Structure of protein-ligand complex; Structure of receptor protein in membranes.

Recommended reading:

Teaching methods:

Lectures are accompanied by the same number of contact hours in problem solving classes (tutorials) where students can discuss in smaller groups.

Assessment methods: Semester work

Course title: Humanities **Course code:** Type of course: Any course at the University. Level of course: Advanced, intermediate or basic (depending on the subject). Year of study: Third Semester/trimester: Winter and/or summer semester Number of credits allocated (workload based): 4 ECTS Name of lecturer: **Objective of the course (expected learning outcomes and competences to be acquired): Prerequisites:** None Course contents: Students can choose any course at the University but majority of them chooses either philosophy or economics. **Recommended reading**: depending on the course **Teaching methods**: depending on the course Assessment methods: depending on the course Language of instruction: Polish