KAPITAŁ LUDZKI
NARODOWA STRATEGIA SPÓJNOŚCI

Projekt współfinansowany przez Unię Europejską w ramach Europejskiego Funduszu Społecznego

UNIA EUROPEJSKA
EUROPEJSKI
FUNDUSZ SPOŁECZNY

Course title	ECTS code
Physico-chemical analytical methods	13.3.0860

Name of unit administrating study

Faculty of Chemistry

Studies

faculty	field of study		
Wydział Chemii	Chemia	type	pierwszego stopnia
		form	stacjonarne
		specialty	analityka i diagnostyka chemiczna
		specialization	wszystkie

Teaching staff

dr hab. Karol Krzymiński, profesor uczelni; dr inż. Beata Zadykowicz

Forms of classes, the realization and number of hours

Forms of classes

Auditorium classes, Laboratory classes, Lecture

The realization of activities

classroom instruction

Number of hours

Lecture: 30 hours, Laboratory classes: 30 hours, Auditorium classes: 15 hours

ECTS credits

5
classes - 75 h
tutorial classes – 25 h
student's own work – 25 h

Total: 125 h - 5 ECTS

The academic cycle

2024/2025 winter semester

Type of course

obligatory

Language of instruction

polish

Teaching methods

- - calculation exercises activating students' self-activity
- - laboratory experiments in small groups;
- individual processing and evaluation of experimental results;
- multimedia-based lecture

Form and method of assessment and basic criteria for eveluation or examination requirements

Final evaluation

- Graded credit
- Examination

Assessment methods

- written exam (test)
- - written test exam, requiring performance of basic physicochemical calculations
- oral correction exam
- step in (entrance) colloquia (laboratory exercises)
- reports on laboratory experimental exercises
- final tests (auditorium calculation exercises)
- oral exam

The basic criteria for evaluation

Course attendant possesses basic knowledge on physicochemical issues, allowing him to understand more complex problems in this field. He can read and understand source texts in the area of the course and acquire, analyse, evaluate and process information from various sources. He is able to gain a new knowledge in a „research way" – by observing, verifying, drawing conclusions and generalizing by himself

Method of verifying required learning outcomes

Required courses and introductory requirements

A. Formal requirements

Completion of courses at the bachelor level: mathematics, physics, general chemistry, physical chemistry

B. Prerequisites

Aims of education

Familiarize students with theoretical (general knowledge, calculations) and practical aspects (experimental skills) contained in the contents of the course; Deepening and enriching physicochemical knowledge with experimental aspects related to the application of instrumental measurements in modern analysis (both qualitative and quantitative); Understanding physicochemical processes with the emphasis on natural environment and everyday life; Development of practical skills related to the implementation of physicochemical measurements with the participation of apparatus and calculations, processing and evaluation of results associated with them. Acquainting with the methodologies of physicochemical measurements based on modern techniques,. Inspiring students to select and evaluate the acquired information by themselves in order to develop skills of self-education by acquiring and analysing information derived from various sources.

Course contents

Course contents
Lectures
Part 1: General physicochemistry with reference to the surrounding world and practical aspects. Features of matter and methods of its research; Energy values of fuels and food; Standard enthalpy of processes of practical importance and examples of its determination; Calculation of and trends among energies of chemical bonds; Dependence of enthalpy of bonds depending on the length and chemical environment; Using enthalpy of bonds to estimate energy effects of reactions; Crystal lattice energies vs. solubility and melting of substances; Application of Born-Haber cycle for thermochemical calculations; Spontaneity of processes vs. entropy changes; The dependence of entropy on temperature; Determination of the entropy of chemical transformations of practical use; Entropy, enthalpy and the natural surroundings; Analysis of free Gibbs energy in chemical processes of economic importance; The effect of temperature on the Gibbs free energy - practical consequences. Chemical kinetics in natural processes; Reaction profiles and their analysis; Examples of applications of chemical kinetics in technology; Graphical form of the Arrhenius equation and conclusions; The dependence of reaction speed on temperature - examples; Catalysis and inhibition in natural and industrial processes; Components and phases - characteristics; Thermodynamic stimuli, speed and temperature of phase transformations; Phase diagrams - methods of construction, characteristic points, analysis; Boiling temperature vs. pressure - practical aspects and examples; Supercritical state and its use; Gibbs phase rule - analysis on examples; Phase diagrams - analysis including natural transformations; Anomalies of water phase changes and their consequences; Changes of free enthalpy in different phases vs. temperature - analysis of charts for exemplary substances; Elevation / diminution of melting and freezing temperatures - thermodynamic reasons; Analysis of the graphs of dependence of chemical potential on temperature; Analysis of the Gibbs phase rule for mixtures of liquids; Phase diagrams for zeotrope and azeotrope systems – examples and practical problems; Industrial fractional distillation; Refractometry – principles and practical aspects; Application of colligative properties of solutions - cryometric and viscometric determination of molar masses; Consequences of raising / lowering of boiling points - analysis on examples including natural systems; Osmosis, osmotic pressure and osmometric measurements – principles and methods; Osmometric determination of molar mass; Osmosis in practice: iso-, hyper- and hypotonic environment; Reverse osmosis and its use.
Part 2: Modern physicochemical analysis - selected applications. Practical UV-Vis absorption spectroscopy: quantitative assays - calibration charts; pKa determining of organic subst. chromophores and auxochromes, bato-, hipso-, hyper- and hypochromic effects. Practical FT-IR spectroscopy: the effect of deuteration on the IR spectrum, estimation of the binding force constants, investigation of hydrogen bonds. Practical aspects of NMR spectroscopy: construction of NMR spectrometer, generation of NMR spectra (animated films); Applications of dynamic NMR methods in physicochemical analysis, study of equilibria. Emission spectroscopy - fluorimetric techniques: Characteristics of fluorescence, Jabłoński's diagram; Kasha's and Wawiłow's law and consequences thereof; Stokes shift; Concentration quenching FL; Measurements of FL spectra; Determination of theOK dipole moments and equilibrium constants in the excited state; Determination of quantum yield; Quantitative fluorimetric analysis analysis; Properties for FL probes; FL polarizing measurements; FRET processes and their utility. Emission spectroscopy: chemiluminescence (CL) techniques: Advantages of luminometric methods; Requirements for CL occurrence; Quantum yield of CL; Methods of CL measurements; General properties of light probes; CL labels and indicators; Luminometric immunochemical tests; Characteristics and analytical applications of bioluminescence (BL). Chromatography - selected aspects: types of chromatography; Determination of parameters characteristic for HPLC/UPLC technique (retention coefficients, number of theoretical plates, selectivity, resolution and others); Efficiency and of the HPLC system; Types and requirements for mobile and stationary phases used in the HPLC / UPLC techniques; Quantitative HPLC analysis - calibration charts; Practical aspects of thin layer (TLC) and column (LC) chromatography. MS spectrometry and mixed techniques: Construction of MS spectrometer; Formation of typical MS spectra; ionization methods and analyzers used in MS techniques; LC-MS other combined techniques; Applications of combined MS methods in trace analysis.

Auditorium classes
Calculations of the cryoscopic, ebuloscopic and other colligative effects; osmosis: determination of osmotic pressure, molar mass and isotonic ratio using the osmotic measurement method; spectroscopy: rotational and vibrational spectra: calculation of the frequency and width of rotational and vibrational signals, calculation of moments of inertia of the molecule, bond length and force constants; calculations of molar absorption coefficients, wave numbers of electron transitions, calculation of the lifetime of a phosphorescent state

Laboratory classes
• Measurement of the heat of dilution and neutralization of inorganic substance.
• Determination of acetic acid partition coefficient between organic and inorganic phase.
• Refractometric determination of glycerine content in cosmetic products and sugar content in fruit juices.

- Spectrophotometric determination of caffeine concentration in tea/coffee.
- Fluorimetric determination of vitamin B1 (thiamine).
- Luminometric determination of of antioxidant properties of dietary supplements.

Bibliography of literature

Literature required to pass the course
Monographic works provided by assistants leading classes
Extracurricular readings
P.W. Atkins, Chemia fizyczna, Wydawnictwo naukowe PWN, Warszawa 2003.
L. Sobczyk, A. Kisza, K. Gatner, A. Koll, Eksperymentalna chemia fizyczna, PWN Warszawa 1982.
E. Więckowska-Bryłka, Eksperymentalna chemia fizyczna, Wydawnictwo SGGW, Warszawa 2007.
J. Demichowicz-Pigoniowa, Obliczenia fizykochemicze, PWN Warszawa, 1984.
S. Paszyc, Podstawy fotochemii, PWN, Warszawa 1992.
P. Suppan, Chemia i światło, PWN Warszawa 1998.

The learning outcomes (for the field of study and specialization)

Knowledge

Student:
- knows and understands basic physicochemical methods used in the study of matter and gives examples of their applications;
- provides examples of colligative properties of solutions and knows how to use them to determine basic properties of chemical substances;
- knows theoretical principles of HPLC, TLC and LC chromatography and gives examples of applications of these methods;
- knows what parameters characterize the quality of chromatographic separations;
- provides methods of calculation of chromatographic parameters, characterizing the quality of separation, basing on experimental data;
- knows what a partition coefficient is, its practical importance and how it can be determined;
- knows what are the adsorption isotherms are how they can be determined;
- gives examples of relationships between the structure of molecules and their spectroscopic features;
- knows the principles of construction and data acquisition for crucial spectroscopic methods (NMR, MS, UV-Vis, FL);
- knows what are luminescent labels and indicators, their properties and gives examples of their applications;
- knows what solvatochromic measurements are and gives examples of their use;
- distinguishes basic types of luminescence, can characterize them and knows what applications they have;
- knows how to calculate the discussed physicochemical parameters on the basis of electronic absorption spectra and emission spectra;
- describes the physicochemical changes occurring in surroundings in terms of thermodynamics;
- distinguishes the concept of thermodynamic and kinetic control of chemical reactions;
- knows how is described and what depends on speed of chemical transformations;
- knows basic methods of calculating the kinetic and thermodynamic parameters of transformations;
- understands the terms of crystal lattice energy and the energy of chemical bond and knows how these parameters can be assessed.
- can explain the origin of the colour, the emission of fluorescence as well as chemi- of and bioluminescence of organic substances;
- is able to predict the direction of physicochemical changes basing on thermodynamic data.

Skills

Student:
- is able to calculate the refraction of substances on the basis of optical measurements and use them to calculate the composition of mixtures of chemical substances;
- can assess the molar masses of the macromolecular substance basing on the knowledge of the osmotic pressure;
- can use selected equipment for physicochemical tests: refractometer,

	conductometer calorimetric kit, UV-Vis spectrophotometer, stationary spectrofluorimeter and plate luminometer; - can determine the rate constants of the chemical reaction based on experimental data; - possess basic skills in the interpretation and determination of parameters of electronic spectra (absorption and emission) and HPLC chromatograms; - can calculate the acidity constants of organic compounds based on spectroscopic measurements; - can calculate and evaluate the discussed HPLC parameters basing on experimental data; - can calculate crucial parameters and on this basis predict their thermodynamic stability.
	Social competence
	Student: - shows interest in physicochemical problems; - understands the physicochemical principles of surrounding world and the principle of sustainable development resulting from them; - shows activity and commitment in experimental work; - demonstrates creativity and activity in independent acquisition of information; - demonstrates curiosity and the ability to acquire chemical knowledge from various sources; - understands the complexity of nature and presents the commitment in deepening of physicochemical knowledge.

Contact

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