POZNAN UNIVERSITY OF TECHNOLOGY

EUROPEAN CREDIT TRANSFER AND ACCUMULATION SYSTEM (ECTS)

COURSE DESCRIPTION CARD - SYLLABUS

Course name

Physicochemical basics of chemical and biochemical procesess [S1Bioinf1>FIZCHEM]

Course

Field of study

Bioinformatics

Year/Semester

2/4

Area of study (specialization)

–

Profile of study

general academic

Level of study

first-cycle

Course offered in

Polish

Form of study

full-time

Requirements

elective

Number of hours

Lecture

30

Laboratory classes

15

Other

0

Tutorials

15

Projects/seminars

0

Number of credit points

4,00

Coordinators

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Lecturers

Prerequisites

have knowledge in general chemistry (writing chemical reactions, converting concentrations, knowledge of laboratory glassware and basic laboratory equipment) have knowledge in mathematics and physics enabling the introduction of problems in physical chemistry (basic laws of physics, differential calculus). are able to prepare solutions of specific concentrations. are aware of further development of theirv2 ompetences

Course objective

To familiarise students with the physicochemical basics of chemical and biochemical processes at the academic level in the field of thermodynamics and chemical kinetics.

Course-related learning outcomes

Knowledge:

basic biological phenomena and processes, and their mathematical interpretation on empirical grounds, using machine methods, including statistical and machine methods, K_W01

issues in the field of chemistry useful for the formulation and solving of simple bioinformatics tasks, covering the basic concepts and laws of chemistry, organic chemistry and biochemistry, K_W04 theoretical basis for modeling biological processes K_W17

Skills:
obtain information from literature, databases and other properly selected sources, also in English, K_U01
integrate and interpret the information obtained, as well as draw conclusions and formulate and justify one"s opinions K_U02

Social competences:
lifelong learning and improving competences, K_K01

Methods for verifying learning outcomes and assessment criteria

Learning outcomes presented above are verified as follows:

Lecture: The knowledge acquired during the lecture is verified during the written test. The test consists of 2 open questions for the same number of points and 15 test questions. Minimum threshold: 53% points.

Laboratory classes: the course passing is based on points received for the individual exercise description. Passing exercises from: 53%

Exercises: grade on the basis of points obtained for activity during classes, writing test. Passing exercises from 60% .

If the classes will be held remotely, the forms of course assessments will remain unchanged and will be carried out with the use of tools provided by the Poznań University of Technology (the e-courses platform).

Programme content

This course covers the physicochemical aspects of chemical and biochemical processes in the field of thermodynamics and reaction kinetics. It addresses the thermodynamic description of reactions, which involves defining the state function and determining the direction of chemical and biochemical processes, including their energy effects. It analyzes the effects of temperature, pressure, and catalyst on the rate of these reactions, taking into account the mechanism of the processes (elementary and complex reactions).

Course topics

LECTURES
1. Basic in thermodynamics - 1st Law of Thermodynamics.
Internal energy – total energy of a system. The difference of energy of products and substrates exchanged with the environment - the 1st Law of Thermodynamics. Heat and work as ways of energy exchange. The mean value of the thermal energy of particles. Maxwell-Boltzman distribution. Temperature definition and temperature scales. Thermodynamic temperature scale.
2. The second law of thermodynamics.
Definition of Entropy. Reversibility and irreversibility of the chemical processes. Total entropy change as the sum of the entropy changes of the system and the environment. The zero (third) law of thermodynamics
3. Thermodynamic potentials.
Spontaneous and forces processes. The concept of state functions and mathematical description. Isobaric, isochoric and adiabatic processes. Enthalpy, Free Enthalpy, Free Energy. The heat of isobaric and isochoric processes. When to use which function (p = const or v = const)
4. Thermochemistry.
Energetic effects of the chemical reactions. Heat capacity. Heat measurement - calorimetry. Heat value at constant volume Q_p, heat value at constant pressure Q_p. Dependence of the heat of isobaric and isochoric processes on temperature. Temperature dependence of heat capacity. The difference between C_p and C_v and Q_p and Q_v. Thermochemical equations. The heat of the process and chemical compounds.
5. Standardization of thermodynamic functions.
Arbitrary standard conditions (p = 1 atm, T = 298 K). Standard values of heat of reactions - rules for determining. Standard values of Entropy. Calorimetric measurement of the entropy. Determination of Enthalpy and Entropy values of chemical processes.

6. Mathematical relations of thermodynamic functions.
The dependence of free energy on temperature and volume. The dependence of the free enthalpy on temperature and pressure. The dependence of enthalpy on pressure. The dependence of pressure on volume and temperature. The dependence of internal energy on the volume.
7. Equilibrium of a chemical reaction.
Definition of chemical equilibrium. Equilibrium constant. Relation of the equilibrium constant with Fre energy and free enthalpy: the van"t Hoff isotherm. Dependence of equilibrium constant on temperature, van"t Hoff isobar and isochore. Pressure influence of equilibrium state. Examples. Calculation of equilibrium constant and efficiencies of the reaction based on thermodynamic data.
8. Kinetics - Elementary reactions.
Description of the rate of chemical reactions, the mechanisms and the influence of various factors on the rate of reaction. Molecularity. Order of reaction. Kinetic equations. The half-life of a chemical reaction.
9. Temperature dependencies.
Influence of temperature on the speed of reaction - Energy of activation. Collision theory - Arrhenius equation. Steady-state theory - Eyring equation.
10. Kinetics - complex reactions.
Reversible reactions. Parallel reactions. Chain reactions. Explosion, explosive reaction mechanisms. Steady-state approximation. Oscillating reactions. Catalysis. Catalyst definition. Mechanism of catalytic reactions. Types of catalysis. Heterogeneous catalysis. Homogeneous catalysis. Enzymatic reactions. Examples.
CALCULATION EXCERSICE
students will calculate physicochemical parameters in the field of energetic effects of chemical reactions. equilibrium states, mathematical equations of chemical kinetics, calculations of concentrations values, determination of temperature influence of chemical and biochemical reactions.
LABORATORY CLASSES
Students will conduct four physicochemical experiments focused on the energetic aspects of chemical reactions as well as on the kinetic parameters of chemical reactions. Students will plan, conduct the experiment, analyses the results and draw conclusions.
Topics:
Heat reaction and measurement. General principles of thermodynamics. Heat values at constant pressure and constant volume conditions. Molar enthalpy of formation, combustion, dissolution dilution. Calorimetry. Construction and types of calorimeters.
Speed of the reaction, rate constant. Order and molecularity of reaction, Theory of collisions, steady-state theory. Temperature dependence of the speed of reaction. Eyring equation, Arrhenius equation. The energy of activation. Kinetic equations of 0th, 1st, 2nd and 3rd order.

Teaching methods

Lecture - multimedial presentation.
Laboratory - practical method - laboratory exercises. Planning, execution and analysis of the results of physicochemical experiment
Exercises with discussion. Deductive method. The exercises involve solving partial tasks and solving detailed problems.

Bibliography

Basic
1. K. Pigoń, Z. Ruziewicz, Chemia Fizyczna, PWN Warszawa 2013
2. P. Atkins, Chemia Fizyczna, PWN Warszawa 2019
Additional
1. P. Atkins, Podstawy Chemii Fizycznej, PWN, Warszawa 1999
2. L. Sobczyk, A. Kisza, Chemia fizyczna dla przyrodników PWN Warszawa 1977
3. H. Buchnowski, W. Ufnalski Wykłady z chemii fizycznej WNT Warszawa 1998
4. P.W. Atkins, C.A Trapp, M.P.Cady, C.Giunta Chemia fizyczna. Zbiór zadań z rozwiązaniami.
5. J. Demichowicz-Pigoniowa Obliczenia fizykochemiczne, Wydawnictwo Politechniki Wrocławskiej Wrocław 1997.
6. W.Ufnalski. Obliczenia fizykochemiczne. Wydawnictwo Politechniki Warszawskiej 1998

Breakdown of average student's workload

	Hours	ECTS
Total workload	100	4,00
Classes requiring direct contact with the teacher	60	2,50
Student's own work (literature studies, preparation for laboratory classes/ tutorials, preparation for tests/exam, project preparation)	40	1,50