POZNAN UNIVERSITY OF TECHNOLOGY

EUROPEAN CREDIT TRANSFER AND ACCUMULATION SYSTEM (ECTS)

COURSE DESCRIPTION CARD - SYLLABUS

Course name

Thermodynamics and kinetics basics of chemical and biochemical processess [S1Bioinf1>TERDYN]

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

dr hab. Maciej Galiński prof. PP
maciej.galinski@put.poznan.pl

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 basic problems in thermodynamics and kinetics at the academic level in the field of the first and second laws of thermodynamics, thermodynamics potentials, thermochemistry, energetic effects of chemical reactions, mathematical relations of thermodynamic functions. To familiarise students with basic kinetics description of chemical and biochemical reactions, basic equations of elementary and complex reactions, determination of mechanisms of chemical and biochemical reactions, the influence of the external factors on the rate of the reactions. Chemical catalysis, homo- and heterogeneous and enzymatic catalysis.

Course-related learning outcomes

Knowledge:
podstawowe zjawiska i procesy biologiczne, a ich interpretacja matematyczne na podstawach empirycznych, wykorzystując metody maszynowego, w tym statystyczne oraz metody maszynowego, 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_K0

Methods for verifying learning outcomes and assessment criteria

Learning outcomes presented above are verified as follows:

Learning outcomes presented above are verified as follows:
Lecture - multimedial presentation - exam
Laboratory classes: The course passing is based on points received for the individual exercise description. Passing exercises from 56% .
Execises: grade on the basis of points obtained for activity during classes, writing tests. Passing exercises from 75%

Programme content

It will be discussed the basics of the physicochemical description of chemical processes: energetic effects, chemical equilibrium and kinetics of chemical and biochemical reactions, including catalyzed. Basic equations of thermodynamics. Thermodynamic functions. Heat capacity. Chemical equilibrium. Energetics of reaction. Influence of temperature and pressure on the equilibrium state of the reaction as well as on the heat of reaction. Chemical kinetic equations. Elementary reactions. Complex reactions. Catalytic reactions. Enzymatic reactions. Molecular interpretation of chemical reactions, order and molecularity of the chemical reaction. Temperature dependencies. The energy of activation. Arrhenius empirical equation. The theory of collisions. Steady-state theory.
LECTURE
1. First law of thermodynamics - the energy of preservation rule.
Internal energy – total energy of a system. Energy balance of the reaction (process) - internal energy balance. The difference of energy of products and substrates exchanged with the environment. The Energy of preservation rule - mathematical description. Thermodynamic definition of work. Work: electrical, surface expansion, volume work. How internal energy is stored. Thermal energy. 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 - The concept of entropy.
Total entropy can increase but not decrease. Reversible reactions in thermodynamics. Total entropy change as the sum of the entropy changes of the system and the environment. The zero (third) law of thermodynamics.
3. Driving force of processes - thermodynamic potentials.
Work and heat depending on the path of the process. Why we don"t use the quantities we are used to in thermodynamics (heat, work). The concept of a state function, its mathematical expression. Isobaric, isochoric and adiabatic processes. The concept of enthalpy. The heat of isobaric and isochoric processes. Free energy concept. Free enthalpy. When to use which function (p = const or v = const).
4. Thermochemistry.
Heat capacity. Heat measurement - calorimeter. Heat value at constant volume Qp, heat value at constant pressure Qp. Dependence of the heat of isobaric and isochoric processes on temperature. Temperature dependence of heat capacity. The difference between Cp and Cv and Qp and Qv. Thermochemical equations. The heat of the process and chemical compounds.
5. Standardization of thermodynamic functions.

Standard heat values - rules for determining. Arbitrary standard conditions (p = 1 atm, T = 298 K). We standardize the energy values of substances, not processes - this reduces the amount of the data. Standard Entropy values - determination. Calorimetric measurement of the entropy.
6. Mathematical thermodynamic relations.
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.
Equilibrium constant. Relation of equilibrium constant exchange with internal energy and enthalpy: the van"t Hoff isotherm. Dependence of equilibrium constant on temperature, van"t Hoff isobar and isochore. Pressure dependence 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 dependence of reaction rate - activation energy. 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.
11. 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 several 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 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.

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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