Syllabus
Course Program

PHYSICAL CHEMISTRY (part 2)

Specialty
161 Chemical technologies and engineering

Institute
Institute of Education and Science in Chemical Technologies and Engineering

Educational program
Technology of oil, gas and solid fuel refining

Department
Physical Chemistry (194)

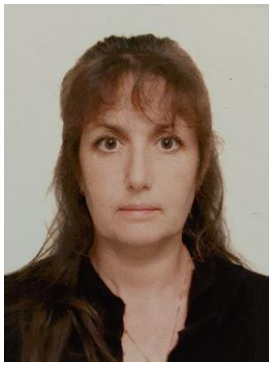
Level of education
Bachelor's level

Course type
Special (professional), Mandatory

Semester
3

Language of instruction
English

Lecturers and course developers



Yuliia Zhelavska

Yuliia.Zhelavska@khpi.edu.ua
Candidate of Technical Sciences (PhD), Associate Professor of the Physical Chemistry Department

Associate Professor of the Physical Chemistry Department, of the Institute of Education and Science in Chemical Technologies and Engineering, completed PhD degree in technical electrochemistry, author of publications in journals indexed in Scopus international science databases, Web of Science and professional editions of Ukraine, patents of Ukraine for invention and utility model, participant in many international scientific conferences, teaching disciplines in English, basic courses: Physical chemistry of dispersed systems, Physical chemistry, Surface phenomena and dispersed systems.

More about the lecturer on the department's website

General information

Summary

The discipline is aimed at forming basic knowledge of physical chemistry for mastering knowledge, abilities and skills in the specialty.

Course objectives and goals

Theoretical bases assimilation by students, principles and laws of physical chemistry, ability formation to understand and analyze processes and phenomena for professional work in the specialty, conducting research methods in physical chemistry is the purpose of the academic discipline teaching.

Format of classes

Lectures, practical classes, consultations, modular control works, calculation tasks; form of control – exam.

Competencies

SC 02 – Ability to apply knowledge in practical situations;
SC 09 – The ability to use the provisions and methods of fundamental sciences to solve professional problems.

Learning outcomes

LR 04 – Carry out qualitative and quantitative analysis of inorganic and organic origin substances, using appropriate methods of general and inorganic, organic, analytical, physical and colloidal chemistry.

Student workload

The total volume of the course is 90 hours (3 ECTS credits): lectures - 16 hours, laboratory classes - 16 hours, self-study - 58 hours.

Course prerequisites

Higher mathematics, physics, general and inorganic, organic and analytical chemistry, physical chemistry (part 1).

Features of the course, teaching and learning methods, and technologies

The course is presented using a systematic approach to form systemic knowledge, integral ideas about the discipline, formation of synthesis skills, comparison and generalization of information.

Program of the course

Topics of the lectures

Topic 1. Basic concepts of chemical kinetics.
The subject and problems of chemical kinetics. Principles of classification of chemical reactions Features of course Simple and complex reactions. Reaction speed. Factors of influence The main postulate of chemical kinetics. Rate constant. Molecularity and reaction order. Half-life.
Topic 2. Formal kinetics of chemical reactions.
Reaction orders. Graphical determination of reaction rate. Methods of determining the reaction order. Differential equations and integration for reactions of the first, second and third orders. Kinetic calculations.
Topic 3. The temperature effect on the course of a chemical reaction.
Temperature coefficient of the rate constant. Van't Hoff's empirical rule. Arrhenius equation. Activation energy. Elementary act of chemical reaction. Model representations of the course of chemical reaction an elementary act.
Topic 4. Kinetics of heterogeneous reactions.
Kinetics of heterogeneous processes. Thermodynamic origin of the kinetic phenomenon of diffusion. Driving force of diffusion. Diffusion and kinetic regions of the heterogeneous reaction.
Topic 5. Catalysis.
Definition and general principles of catalysis. Importance of catalytic processes. Types of catalysis, kinetics and mechanisms of catalysis. Heterogeneous catalysis. Activity and selectivity of catalysts. Catalyst poisoning. Active centers of heterogeneous catalysts. The role of adsorption in the kinetics of heterogeneous catalytic reactions. Activation energy of heterogeneous catalytic reactions. Model representations of the theory of heterogeneous catalysis.
Topic 6. Complex chemical reactions.
Complex reactions: definition and classification. Consecutive reactions. Parallel reactions. Conjugate reactions. Photochemical reactions. Laws of photochemistry. Photochemical reaction rate constants. Quantum output. Chain reactions. Stages of a chain reaction. Peculiarities of the kinetics of reactions with branched and unbranched chains. Oscillatory reactions.
Topic 7. Theoretical foundations of experimental physical methods of chemical substances and processes research.

Methods of analysis of chemical systems: classification. The nature of molecular spectra. Electronic absorption spectra. Electronic transitions in molecules. Absorption bands. Definition and physical meaning of the main characteristics of absorption bands.

Topic 8. Vibrational spectroscopy.

Vibrational spectroscopy. Lambert-Booger-Behr absorption law. Infrared spectra. Characteristic frequencies. The use of molecular spectroscopy in chemistry. Identification of substances, structural analysis. Quantitative studies. Study of intermolecular interaction.

Topics of the workshops

Practical classes within the discipline are not provided

Topics of the laboratory classes

Laboratory work №1. "Determination the rate constant of acetone iodization reaction".
Laboratory work №2. "Determination rate constant of dissolution".
Laboratory work №3. "Definition of rate constant speed of inversion cane sugar".
Laboratory work №4. "Molecular spectroscopy".

Self-study

Independent work in the discipline includes studying lecture material, preparing for laboratory classes, independent study of topics and issues that are not taught in lecture classes, as well as performing an individual calculation task on the topic ""Electrochemistry", "Chemical Kinetics" according to an individual option for each student. The results of calculations are drawn up in a written report.

Course materials and recommended reading

1. Peter Atkins, Julio de Paula. Physical Chemistry, Oxford University Press, 2018
https://www.scribd.com/document/451516801/Peter-Atkins-Julio-de-Paula-James-Keeler-Atkins-Physical-Chemistry-Oxford-University-Press-2018-pdf
2. A.V. Djenyuk, S.I.Rudneva, N.D. Sakhnenko, O.A. Ovcharenko Physical Chemistry. Laboratory works Part I. – Харків: ФОП Бровін О.В., 2019. – 160 с.
http://web.kpi.kharkov.ua/fchem/wp-content/uploads/sites/30/2020/02/Practicum-I.pdf
3. S.I. Rudneva, N.D. Sakhnenko, A.V. Djenyuk. Physical chemistry: Practical course. – Kharkiv: ФЛП Панов A.H, 2018. – 148 p.
http://web.kpi.kharkov.ua/fchem/wp-content/uploads/sites/30/2020/02/Physical-Chemistry.pdf
.

Assessment and grading

Criteria for assessment of student performance, and the final score structure

100% of the final score consists of assessment results in the form of an exam (20%), ongoing assessment (40%) and an individual assignment (40%).
Exam: written assignment (2 questions on theory) and oral presentation.
Current assessment: defense of laboratory work.

Grading scale

Total points	National	ECTS
90–100	Excellent	A
82–89	Good	B
75–81	Good	C
64–74	Satisfactory	D
60–63	Satisfactory	E
35–59	Unsatisfactory (requires additional learning)	FX
1–34	Unsatisfactory (requires repetition of the course)	F

Norms of academic integrity and course policy

The student must adhere to the Code of Ethics of Academic Relations and Integrity of NTU "KhPI": to demonstrate discipline, good manners, kindness, honesty, and responsibility. Conflict situations should be openly discussed in academic groups with a lecturer, and if it is impossible to resolve the conflict, they should be brought to the attention of the Institute's management.
Regulatory and legal documents related to the implementation of the principles of academic integrity at NTU "KhPI" are available on the website: http://blogs.kpi.kharkov.ua/v2/nv/akademichna-dobrochesnist/

Approval

Approved by	Date, signature	Head of the department Mykola SAKHNENKO
	Date, signature	Guarantor of the educational program Irina SENKEVICH