Syllabus
Course Program

PHYSICAL CHEMISTRY (part 1)

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)

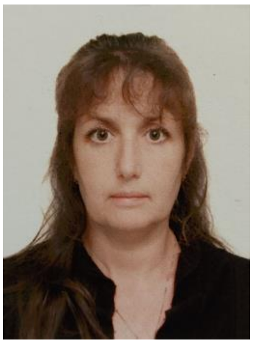
Level of education
Bachelor's level

Course type
Special (professional), Mandatory

Semester
3

Language of instruction
English

Lecturers and course developers



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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 180 hours (6 ECTS credits): lectures - 32 hours, laboratory classes - 48 hours, self-study - 100 hours.

Course prerequisites

Higher mathematics, physics, general and inorganic, organic and analytical chemistry

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. Introduction.
The subject and problems of physical chemistry. Basic sections and methods of physical chemistry. Basic concepts and definitions of thermodynamics – thermodynamic system, state, state parameters, state functions, processes. Work and process heat. Reversible and irreversible processes.
Topic 2. The first law of thermodynamics. Hess's law.
Mathematical formulation of the first law of thermodynamics. Internal energy. Warmth. Enthalpy. Work and change of internal energy in various processes.
Consequences of the first law of thermodynamics. Properties of heat under conditions of constant volume or pressure. The relationship between them. Thermal effect of the reaction (process).Thermochemistry. Hess's law. Consequences of Hess's law. Heat of formation. Heat of combustion. Calculations of thermal effects with the help of binding energies.
Topic 3. Kirchhoff's laws.
Average and true heat capacity, heat capacity of gases and condensed systems, dependence of heat capacity on temperature. Kirchhoff's equation in differential and integral forms. Analysis. Use of the Ulich approximation in calculations of the effect of temperature on the thermal effect of the reaction.
Topic 4. The second law of thermodynamics.
Justification of the second law of thermodynamics. Nernst's thermal theorem. Arbitrary and non-arbitrary processes. Entropy change in various processes. Entropy change of an isolated system and the direction of the process. Entropy change due to the course of chemical reactions. Clausius inequality.
Topic 5. The third law of thermodynamics.
The statistical nature of the second law of thermodynamics. Thermodynamic probability. Entropy and probability. The third law of thermodynamics. Boltzmann's formula. Planck's postulate. Properties of bodies near absolute zero. Absolute values of entropy. Entropy calculations in various processes.
Topic 6. Mathematical apparatus of thermodynamics.
Combined equation of the first and second laws of thermodynamics. Gibbs-Duhem equation. The fundamental Gibbs equation. Definition of the state functions F, G, H, V. Writing the fundamental equations for them. Maxwell's ratio. Characteristic functions, their definitions and properties. Helmholtz and Gibbs energy as criteria for process orientation and equilibrium state. The Gibbs–Helmholtz equation and its various expressions. Temperature dependence of Δ G.
Topic 7. Chemical potential. Law of active masses.

Determination of chemical potential through derivatives of various thermodynamic functions for ideal and real gases. Fugacity, activity, application for calculating the chemical potential of a component in ideal and real solutions. Basic signs and properties of chemical equilibrium. Chemical affinity. Chemical equilibria of reactions at constant temperature. The law of active masses and its various forms. The relationship between different equilibrium constants. Peculiarities of the equilibrium constant of a heterogeneous reaction. Methods of calculating the composition of the equilibrium mixture.

Topic 8. Chemical reaction isotherm.

Van't Hoff isotherm equation. Equilibrium constant. Analysis of the influence of the initial ratio of components on the probable orientation and equilibrium yield of reaction products. The equation of the chemical reaction isotherm for standard conditions. Standard Gibbs energy.

Topic 9. Influence of external factors on chemical equilibria.

Le Chatelier's principle. Its application to chemical reactions. Planck's equation. Analysis. Dependence of the equilibrium constant on the total pressure. The equation of isobars and isochores of a chemical reaction. Calculations of equilibrium constants for different temperatures. Calculations of chemical equilibrium constants with the involvement of tables of standard thermodynamic functions. Determination of thermal effects of reactions from the temperature dependence of the equilibrium constant.

Topic 10. Basic concepts of phase equilibria. Thermodynamics of heterogeneous systems and physico-chemistry of solutions.

Heterogeneous system. Component. Number of independent components. Phase. The number of degrees of freedom. Gibbs phase rule. One-component systems. Water state diagram. Clapeyron–Clausius equation and phase transitions of the first kind. Its application to processes of melting, evaporation and sublimation in single-component systems. Ways of expressing concentrations. State diagrams. The principle of construction and interpretation of status diagrams. The Kurnakov principle. Physico-chemical analysis. state The rule of leverage. The main types of diagrams of two-component systems. General definition of ideal solutions. Colligative properties of solutions. Solubility of gases. Henry's Law.

Topic 11. Liquid-vapor equilibrium in a two-component system. Volatile mixtures.

Vapor pressure above the solution. Raoult's laws regarding vapor pressure, cryoscopic and ebulioscopic effects. Their thermodynamic justification Determination of the molecular weight of the dissolved substance. Calculation of pressure and vapor composition above the solution. Konovalov's first law. The rule of leverage. State diagrams "total pressure - composition", "boiling temperature - composition". Distillation (rectification). Azeotropic mixtures. Konovalov's second law Limited liquids solubility. Types of diagrams of limited liquid solubility. Critical solubility temperature. Alekseev's rule

Topic 12. Heterogeneous equilibria: liquid – solid.

Solubility of solids. Dependence of ideal solubility on temperature. Schroeder's equation in differential and integral forms. Analysis. Application for determining heat and melting points. Cooling curve. Types of melting point diagrams (diagrams with eutectic, diagram with the formation of a chemical compound, with unlimited solubility in the solid state, with limited solubility in the solid state).

Topic 13. The Nernst-Shylov distribution law.

Manifestations of law in ideal and real systems.

Extraction. Application in the industry. Zone melting. Application for deep purification of substances. Three-component systems. Determination of the composition. Gibbs triangle. State diagrams of metal alloys. Intermetallics as a reinforcing phase of alloys. Duralumins.

Topic 14. Electrolyte solutions.

Electrochemical systems and processes. Components of electrochemical systems: electrodes, condensed ion conductors. Electrolyte solutions: definition, stages of dissolution, quantitative characteristics. Electrolytic dissociation: definition, quantitative characteristics, Ostwald dilution law. Ion-dipole interaction in electrolyte solutions. Energies of the crystal lattice and solvation of ions. Ion-ion interaction in electrolyte solutions. Ionic strength of the solution

Topic 15. Theory of interionic interaction.

Debye-Hückel theory: the concept of an ionic atmosphere, derivation of the formula for the potential of the ionic atmosphere in a solution of a 1,1-valent electrolyte, the first and second approximations and limitations of the Debye-Hückel theory. The relationship between the average activity coefficient and the activity coefficients of individual ions. Modern concepts of the theory of solutions of strong electrolytes

Topic 16. Electrical conductivity of electrolyte solutions.

Electrical conductivity of electrolyte solutions: specific and molar electrical conductivity, determination of the mobility of individual ions, Kohlrausch's law and equation. Transfer numbers, their dependence on the solution concentration. Methods of determining transfer numbers.
Conductometric method and its application: measurement of electrical conductivity of electrolyte solutions; determination of the dissociation constant and the solubility product. De Baye-Onsager theory of electrical conductivity. Anomalies of electrical conductivity.

Topics of the workshops

Practical classes within the discipline are not provided.

Topics of the laboratory classes

Laboratory work №1. "Determination of thermal effects processes and chemical reactions by calorimetric method".
Laboratory work №2. "Determination of thermodynamic characteristics of chemical reaction by EMF method".
Laboratory work №3. "Determination of the heterogeneous reaction equilibrium constant".
Laboratory work №4. "Construction of the solubility diagram of two solutions with limited solubility".
Laboratory work №5. "Construction of the melting diagram of a two-component system with eutectics".
Laboratory work №6. "Construction of a diagram of a volatile mixture distillation".
Laboratory work №7." Cryoscopic method of determining the dissolved substance molecular weight".
Laboratory work №8. "Determination of a weak electrolyte dissociation constant".

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 "Thermodynamics of chemical reactions" 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 А.Н, 2018. – 148 p.
http://web.kpi.kharkov.ua/fchem/wp-content/uploads/sites/30/2020/02/Physical-Chemistry.pdf
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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 (20%) and an individual assignment (60%).
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