**SYLLABUS**

**Fall semester 2023-2024 academic year**

**Educational program "7M05301-Chemistry"**

 **1 course**

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| **ID** **and name** **of course** | **Independent work** **of the student****(IWS)** | **Number of credits** | **General****number** **of credits** | **Independent work** **of the student****under the guidance** **of a teacher (IWST)** |
| **Lectures (L)** | **Practical classes (PC)** | **Lab. classes (LC)** |
| 60317 Theory and Problems of Physical Chemistry | 4 | 1.7 | 3.3 | 0 | 5 | 6 |
| **ACADEMIC INFORMATION ABOUT THE COURSE** |
| **Learning Format** | **Cycle,****component** | **Lecture** **types** | **Types** **of practical classes** | **Form and platform final control** |
| *Offline* | PD, UK | Practical | Problem solving | Standard Written OfflineLMS "Univer" |
| **Lecturer - (s)** | Supiyeva Zhazira, PhD, senior lecturer |
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| **Phone:** | +7-701-391-91-56 |
| **ACADEMIC COURSE PRESENTATION** |
| **Purpose****of the course** | **Expected Learning Outcomes (LO)** As a result of studying the discipline the student will be able to | **Indicators of LO achievement (ID)** |
| To develop knowledge about the basic principles of modern theories and problems of physical chemistry and the use of its theoretical and applied aspects for research purposes to explain and substantiate their results. | * 1. Show knowledge of theoretical and applied aspects of the basic principles of theories and problems of physical chemistry.
 | 1.1. Can explain intermolecular interactions in complex systems. |
| 1.2. Knows the modern concept of the mechanism of formation of solutions of strong and weak electrolytes. |
| 1.3. Knows the main problems when studying interaction in complex systems. |
| 2. Use physical chemistry approaches to explain intermolecular interactions in complex systems and the possibility of solving problems arising in these systems. | 2.1. Able to analyze and compare the physical and chemical nature of solutions, determine the basic thermodynamic and kinetic parameters of molecules and ions in solution. |
| 2.2. Can use methods of physical chemistry theories to determine the crystal lattice energy, solvation energy and thermodynamic parameters of ions. |
| 2.3. Able to explain intermolecular interactions from the point of view of modern concepts of thermodynamic and electrostatic theory of strong electrolytes and statistical thermodynamics. |
| 3. Use modern concepts of the theory of chemical kinetics to determine and analyze the kinetic parameters of complex chemical reactions. | 3.1. Knows methods for calculating the rate and rate constant of complex homogeneous reactions from the point of view of the theory of active collisions. |
| 3.2. Knows methods for calculating the rate and rate constant of complex homogeneous and heterogeneous reactions from the point of view of the activated complex theory. |
| 3.3. Able to analyze the kinetics of complex reactions and determine the kinetic characteristics of such processes. |
| 4. Analyze the thermodynamic and kinetic processes of intermolecular interactions and propose methods for solving certain problems in complex chemical systems.  | 4.1. Justify the use of the Lindemann hypothesis to solve problems of monomolecular reactions in the gas phase. |
| 4.2. Analyze statistical and thermodynamic approaches in determining the rate and rate constant of complex chemical reactions. |
| 4.3. Analyze and reveal the physical meaning of the pre-exponential factor in the Arrhenius equation from the point of view of theories of chemical kinetics. |
| 5. Be able to generalize, analyze and classify theoretical and applied problems of modern physical chemistry. | 5.1. Perform an independent literature search on IWS topics, summarize the data obtained and solve problems posed in the IWS from the point of view of the obtained theoretical material. |
| 5.2. Submit a report and presentation on IWS topics, be competent in the field of the material received, be able to summarize, analyze and classify the data received. |
| **Prerequisites** | Selected chapters of organic chemistry, modern problems of inorganic chemistry, analytical chemistry |
| **Postrequisites** | Fundamentals of modern experimental thermodynamics, nonequilibrium thermodynamics |
| **Learning Resources** | **Literature:** Main: 1. C.R. Metz Theory and Problems of Physical Chemistry / McGraw-Hill, 1974.2. Clyde R. Metz Theory and Problems of Physical Chemistry / McGraw-Hill; First edition (January 1, 1976). 3. Dr. RK Gupta Problems in Physical Chemistry / JEE Main and Advanced - 518 р.4. Kenneth Schmitz Рhysical Chemistry Concepts and Theory /1st Edition - November 11, 2016.5. Оспанова А.К., Шабикова Г.Х., Сыздыкова Л.И. Физикалық химиянын теориялары мен мәселерi. Алматы. 2021. с 191.6. Г.Х. Шабикова, Л.И. Сыздыкова Современное состояние теории сольватации и растворения. Алматы.2010.Additional:1.Geerlings, P.; De Proft, F. Chemical Reactivity as Described by Quantum Chemical Methods. Int. J. Mol. Sci. 2002, 3, 276-309. https://doi.org/10.3390/i3040276**Internet resources:**1. http://elibrary.kaznu.kz/ru2. <http://sciencedirect.com/> |
| **Academic****course policy** | The academic policy of the course is determined by [the Academic Policy](https://univer.kaznu.kz/Content/instructions/%D0%90%D0%BA%D0%B0%D0%B4%D0%B5%D0%BC%D0%B8%D1%87%D0%B5%D1%81%D0%BA%D0%B0%D1%8F%20%D0%BF%D0%BE%D0%BB%D0%B8%D1%82%D0%B8%D0%BA%D0%B0.pdf) and [the Policy of Academic Integrity of Al-Farabi Kazakh National University .](https://univer.kaznu.kz/Content/instructions/%D0%9F%D0%BE%D0%BB%D0%B8%D1%82%D0%B8%D0%BA%D0%B0%20%D0%B0%D0%BA%D0%B0%D0%B4%D0%B5%D0%BC%D0%B8%D1%87%D0%B5%D1%81%D0%BA%D0%BE%D0%B9%20%D1%87%D0%B5%D1%81%D1%82%D0%BD%D0%BE%D1%81%D1%82%D0%B8.pdf) Documents are available on the main page of IS Univer.**Integration of science and education.** The research work of students, undergraduates and doctoral students is a deepening of the educational process. It is organized directly at the departments, laboratories, scientific and design departments of the university, in student scientific and technical associations. Independent work of students at all levels of education is aimed at developing research skills and competencies based on obtaining new knowledge using modern research and information technologies. A research university teacher integrates the results of scientific activities into the topics of lectures and seminars (practical) classes, laboratory classes and into the tasks of the IWST, IWS, which are reflected in the syllabus and are responsible for the relevance of the topics of training sessions andassignments.**Attendance.** The deadline for each task is indicated in the calendar (schedule) for the implementation of the content of the course. Failure to meet deadlines results in loss of points.**Аcademic honesty.** Practical/laboratory classes, IWS develop the student's independence, critical thinking, and creativity. Plagiarism, forgery, the use of cheat sheets, cheating at all stages of completing tasks are unacceptable.Compliance with academic honesty during the period of theoretical training and at exams, in addition to the main policies, is regulated by [the "Rules for the final control"](https://univer.kaznu.kz/Content/instructions/%D0%9F%D1%80%D0%B0%D0%B2%D0%B8%D0%BB%D0%B0%20%D0%BF%D1%80%D0%BE%D0%B2%D0%B5%D0%B4%D0%B5%D0%BD%D0%B8%D1%8F%20%D0%B8%D1%82%D0%BE%D0%B3%D0%BE%D0%B2%D0%BE%D0%B3%D0%BE%20%D0%BA%D0%BE%D0%BD%D1%82%D1%80%D0%BE%D0%BB%D1%8F%20%D0%9B%D0%AD%D0%A1%202022-2023%20%D1%83%D1%87%D0%B3%D0%BE%D0%B4%20%D1%80%D1%83%D1%81%D1%8F%D0%B7%D1%8B%D0%BA%D0%B5.pdf) , ["Instructions for the final control of the autumn / spring semester of the current academic year"](https://univer.kaznu.kz/Content/instructions/%D0%98%D0%BD%D1%81%D1%82%D1%80%D1%83%D0%BA%D1%86%D0%B8%D1%8F%20%D0%B4%D0%BB%D1%8F%20%D0%B8%D1%82%D0%BE%D0%B3%D0%BE%D0%B2%D0%BE%D0%B3%D0%BE%20%D0%BA%D0%BE%D0%BD%D1%82%D1%80%D0%BE%D0%BB%D1%8F%20%D0%B2%D0%B5%D1%81%D0%B5%D0%BD%D0%BD%D0%B5%D0%B3%D0%BE%20%D1%81%D0%B5%D0%BC%D0%B5%D1%81%D1%82%D1%80%D0%B0%202022-2023.pdf) , "Regulations on checking students' text documents for borrowings".Documents are available on the main page of IS Univer.**Basic principles of inclusive education.** The educational environment of the university is conceived as a safe place where there is always support and equal attitude from the teacher to all students and students to each other, regardless of gender, race / ethnicity, religious beliefs, socio-economic status, physical health of the student, etc. All people need the support and friendship of peers and fellow students. For all students, progress is more about what they can do than what they can't. Diversity enhances all aspects of life.All students, especially those with disabilities, can receive counseling assistance by phone / e- mail Zhazira.Supiyeva@kaznu.edu.kz or via video link in ZOOM <https://us04web.zoom.us/j/73331417104?pwd=6a0l5WzWKT2aT3IgEBNmaaWr8JgQ5I.1>. **Integration MOOC (massive open online course).** In the case of integrating MOOC into the course, all students need to register for MOOC. The deadlines for passing MOOC modules must be strictly observed in accordance with the course study schedule. **ATTENTION!** The deadline for each task is indicated in the calendar (schedule) for the implementation of the content of the course, as well as in the MOOC. Failure to meet deadlines results in loss of points. |
| **INFORMATION ABOUT TEACHING, LEARNING AND ASSESSMENT** |
| **Score-rating letter system of assessment of accounting for educational achievements** | **Assessment Methods** |
| **Grade** | **Digital****equivalent****points** | **points,****% content** | **Assessment according to the traditional system** | **Criteria-based assessment** is the process of correlating actual learning outcomes with expected learning outcomes based on clearly defined criteria. Based on formative and summative assessment.**Formative assessment is** a type of assessment that is carried out in the course of daily learning activities. It is the current measure of progress. Provides an operational relationship between the student and the teacher. It allows you to determine the capabilities of the student, identify difficulties, help achieve the best results, timely correct the educational process for the teacher. The performance of tasks, the activity of work in the classroom during lectures, seminars, practical exercises (discussions, quizzes, debates, round tables, laboratory work, etc.) are evaluated. Acquired knowledge and competencies are assessed.**Summative assessment** -type of assessment, which is carried out upon completion of the study of the section in accordance with the program of the course.Conducted 3-4 times per semester when performing IWS. This is the assessment of mastering the expected learning outcomes in relation to the descriptors. Allows you to determine and fix the level of mastering the course for a certain period. Learning outcomes are evaluated. |
| A | 4.0 \_ | 95-100 | Great |
| A- | 3.67 | 90-94 |
| B+ | 3.33 | 85-89 | Fine |
| B | 3.0 | 80-84 | **Formative and summative assessment** | **Points % content** |
| B- | 2.67 | 75-79 | Activity at lectures | 0 |
| C+ | 2.33 | 70-74 | Work in practical classes | 20 |
| C | 2.0 | 65-69 | Satisfactorily | Independent work | 30 |
| C- | 1.67 | 60-64 | Design and creative activity | 10 |
| D+ | 1.33 | 55-59 | Final control (exam) | 40 |
| D | 1.0 | 50-54 | TOTAL | 100 |
| FX | 0,5 | 25-49 | Unsatisfactorily |
| F | 0 | 0-24 |
| **Calendar (schedule) for the implementation of the content of the course. Methods of teaching and learning.** |

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| **A week** | **Topic name** | **Number of hours** | **Max.****ball** |
| **Module 1 Modern concept of the theory of electrolyte solutions** |
| **1** | **L 1.** Concepts of physical and chemical (hydrate) theory of solutions. | 1 |  |
| **PC 1.** Introductory lesson. Familiarization with the requirements for seminar classes and receiving an assignment for IWS No. 1. | 2 |  |
| **2** | **L 2.** Energy of the crystal lattice. The Born, Kapustinsky model and the Born-Haber cycle for calculating the energy of a crystal lattice. | 1 |  |
| **PC 2.** Critical analysis of the physical and chemical theory of solutions. Solving problems to determine the energy of a crystal lattice using various methods. | 2 | 10 |
| **IWST 1.** Consultations on implementation of IWS 1. | 1 |  |
| **3** | **L 3.** Solvation energy. Born model and Born-Haber cycle for calculating solvation energy. Ionophores and ionogens. | 1 |  |
| **PC 3.** Application of various methods for calculating solvation energy for chemical compounds. Analysis of the results obtained, generalizations and conclusion. | 2 | 10 |
| **IWS 1.** Study of the influence of the radius and charge of ions on the energy of the crystal lattice in the groups and periods of the Mendeleev | 1 | 20 |
| **4** | **L 4.** Modern concepts about the mechanism of formation of solutions of strong and weak electrolytes. Chemical and real energy of solvation. | 1 |  |
| **PC 4.** Theoretical survey on the Born model for calculating the crystal lattice energy and solvation energy, analysis, problems and generalization. | 2 | 5 |
| **5** | **L 5.** The modern concept of thermodynamics of ionic solvation in solutions, determination of enthalpy, Gibbs energy and entropy of formation of ions in solution. | 1 |  |
| **PC 5.** Calculations of enthalpy, Gibbs energy and entropy of ions of various metals, analysis and generalization. | 2 | 10 |
| **6** | **L 6.** Intermolecular interaction in solutions of strong electrolytes. Lewis thermodynamic theory, activity, activity coefficient. | 1 |  |
| **PC 6.** The influence of various parameters on the activity coefficient, problem solving, analysis and generalization. | 2 | 10 |
| **IWST 2.** Report of individual research work on IWS 1, presentation, analysis. Receiving assignments and advice on completing IWS 2 | 1 | 20 |
| **7** | **L 7.** Debye and Hückel's ideas about the nature of the average ion activity coefficient. Modern concept of the theory of strong electrolytes. | 1 |  |
| **PC 7.** Theoretical survey on all the material covered. | 2 | 15 |
| **IWST 3.** Consultations on implementation of IWS 2. | 1 |  |
| **Midterm control 1** | **100** |
| **Module 2 Fundamentals of statistical thermodynamics and kinetic analysis of complex chemical reactions** |
| **8** | **L 8.** The influence of the ionic strength of a solution on the rate of ionic reactions. Application of the Debye-Hückel theory to solutions of weak electrolytes. | 1 |  |
| **PC 8.** Solving problems on the topic of the lecture, presentation on the scientific research of Arrhenius, Debye, Hückel and modern scientists in the field of solution theory. | 2 | 5 |
| **IWS 2.** The influence of concentration, temperature and nature of the solvent on the average ionic activity coefficient of strong electrolytes. IWS assignment No. 3. | 1 | 20 |
| **9** | **L 9.** Fundamentals of statistical thermodynamics. Boltzmann's law on the distribution of particles in macrosystems. | 1 |  |
| **PC 9.** Properties of micro- and macrosystems. Liouville theory and ergoid hypothesis. Theoretical survey, analysis and synthesis. | 2 | 5 |
| **10** | **L 10.** Gibbs statistical ensembles. Total particle energy. Energy distribution of molecules, Boltzmann's law. | 1 |  |
| **PC 10.** Solving problems on the energy distribution of molecules, Boltzmann's law. | 2 | 5 |
| **11** | **L 11.** Statistical sum on the state of the system and molecule. Relationship between the molecular sum by state and thermodynamic functions. | 1 |  |
| **PC 11.** Solving partition function problems for individual molecules. Quiz survey.  | 2 | 5 |
| **IWST 4.** Consultation on implementation of IWS 3. Presentation on the work of Maxwell, Boltzmann and Gibbs. | 1 | 10 |
| **12** | **L12.** Theoretical foundations of the theory of active collisions. Methods for determining rate, rate constants for various types of reactions. | 1 |  |
| **PC 12.** Application of the theory of active collisions to monomolecular reactions, Lindemann's hypothesis. Theoretical survey.  | 2 | 5 |
| **IWST 5**. Consultation on implementation of IWS 3. Problem solving | 1 | 5 |
| **13** | **L 13.** Theoretical foundations of the theory of the activated complex, the Eyring model, the basic equation of the theory of the transition state. Potential energy surface. | 1 |  |
| **PC 13.** Solving problems on the theory of active collisions and activated complex | 2 | 5 |
| **IWS 3.** Consultation on implementation of IWS 3. | 1 |  |
| **14** | **L 14.** Statistical and thermodynamic aspects of the transition state theory. Methods for determining the rate, rate constants of complex reactions. | 1 |  |
| **PC 14.** Justification of the physical meaning of the pre-exponential factor in the Arrhenius equation from the point of view of the theory of active collisions and the theory of the activated complex. | 2 | 5 |
| **IWST 6.** Report and presentation of IWS No. 3. Determination of the amount based on the state of some molecules. | 1 | 15 |
| **15** | **L 15.** Comparative analysis of active collision theories and transition state theory. Distinctive features and applications of these theories for the kinetic analysis of complex reaction reactions. | 1 |  |
| **PC 15.** Theoretical survey on the basics of statistical thermodynamics and theories of chemical kinetics. | 2 | 15 |
| **IWST 7.** Consulting on exam questions | 1 |  |
| **Midterm control 2** | **100** |
| **Final control (exam)** | **100** |
| **TOTAL for course** | **100** |

**Dean \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_** A.K. Galeyeva

**Head of Department \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_**Ye.A. Aubakirov

**Lecturer \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_** Zh.A. Supiyeva