**SYLLABUS**

**Fall semester 2023-2024 academic year**

**Educational program "6B05301-Chemistry (NIS)"**

**3 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)** |
| 91725  Quantum-chemical methods in thermochemistry | 4 | | 1.7 | 1.7 | 1.6 | 6 | 6 |
| **ACADEMIC INFORMATION ABOUT THE COURSE** | | | | | | | |
| **Learning Format** | **Cycle,**  **component** | **Lecture**  **types** | | **Types**  **of practical classes** | | **Form and platform final control** | |
| *Offline* | Profiling Disciplines, Elective component | Practical | | Problem solving | | Standard Written Offline  LMS "Univer" | |
| **Lecturer - (s)** | Supiyeva Zhazira, PhD, senior lecturer | | | | |
| **e-mail:** | [Zhazira.Supiyeva@kaznu.edu.kz](mailto:Zhazira.Supiyeva@kaznu.edu.kz) | | | | |
| **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)** | |
| Master the skills of using quantum chemical methods in calculating the thermochemical parameters of chemical reactions. | * 1. Explain the content of the basic rules and laws of quantum chemistry | | | | | 1.1. Explain the role of quantum chemistry as the theoretical foundation of modern chemistry | |
| 1.2. Description of basic postulates and methods of quantum-chemical calculations | |
| 1.3. Explain the requirements for calculation methods | |
| 1.4. Explain the methods of solving the Schrödinger equation | |
| 2. Calculation of thermodynamic parameters using methods of quantum chemistry | | | | | 2.1. Selection of properties of the electronic structure of atoms and molecules | |
| 2.2. Perform calculations to obtain information about the limits of application of the laws and theories of quantum mechanics and quantum chemistry | |
| 2.3. Сalculation of thermochemical parameters | |
| 3. Explanation of the reasons for the possibility, optimization, direction, depth of the physico-chemical process based on the calculated parameters | | | | | 3.1. Draw conclusions about the direction of chemical reactions using thermodynamic parameters | |
| 3.2. Analysis of the influence of various factors on the balance in the system | |
| 3.3. Identify similarities and differences between empirical and non-empirical methods | |
| 4. Processing during the comparison of results with software methods based on theoretical and semi-empirical methods using the laws of thermochemistry | | | | | 4.1. By geometrical optimization of the chemical compound  formulation of the heat of chemical reactions using energy parameters | |
| 4.2. Use of quantum mechanical representations and models to analyze chemical problems | |
| 4.3. Use of computer programs | |
| 5. Analysis and conclusion of results obtained by quantum chemical methods | | | | | 5.1. Mastering scientific and reference literature on quantum chemistry | |
| 5.2. Predicting the possibilities of a chemical reaction by working with standard calculation methods of quantum chemistry | |
| 5.3. Draw conclusions by understanding the difference between thermodynamic parameters and results obtained by quantum chemical methods | |
| **Prerequisites** | Physical chemistry, Structure of Matter | | | | | | |
| **Postrequisites** | Writing and defending a thesis (project) | | | | | | |
| **Learning Resources** | **Literature:**  Main:  1. Henry F. Schaefer III (Author) Quantum Chemistry: The Development of Ab Initio Methods in Molecular Electronic Structure Theory (Dover Books on Chemistry) / Publisher: ‎ Dover Publications (February 20, 2004).  2. Rabah Ali Khalil (Editor) A Simple Approach to Quantum Chemistry / 2020, Chemistry, Chemistry Research and Applications, Novinka, Online Books, Special Topics.  3. Fateev A.V., Tuguldurova V.P. Computational Methods in Chemistry (laboratory work) / Tomsk 2021.  4. Tsyshevsky R.V., Garifzyanova G.G., Khrapkovsky G.M. Quantum chemical calculations of chemical reaction mechanisms / Kazan KNRTU Publishing House 2012.  Additional:  1. Mitchell, Erica, "Quantum Chemical Methods: Its history and future" (2019). Chemistry. 19.  https://pillars.taylor.edu/chemistry-student/19.  2. 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/ru  2. <http://sciencedirect.com/> | | | | | | |

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| **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](mailto: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 | Unsatisfactory |
| 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 Theoretical methods of quantum chemical research** | | | |
| **1** | **L 1.** Description of modern quantum chemistry. | 1 |  |
| **PC 1.** Discuss the relationship between thermochemistry and quantum chemical methods. Survey on thermodynamic parameters. | 1 | 3 |
| **LC 1.** #1. Work in program GaussView 5.0.Learn the program, all its aspects and tools for modeling the structure of a molecule | 2 |  |
| **2** | **L 2.** The atom in computational methods. One electron atom. A multi-electron atom. | 1 |  |
| **PC 2.** Atoms. Issue reports. | 1 | 3 |
| **LC 2.** #1. Determination of geometric parameters of molecules | 2 | 5 |
| **IWST 1.** Advising on the implementation of the IWS 1. Advising on the implementation of the SOP 1. Geometric calculation of amino acids in aqueous solution by quantum chemical methods. | 1 |  |
| **3** | **L 3.** Semi-empirical methods of electronic structure calculation | 1 |  |
| **PC 3.** Simple molecules. Making reports. | 1 | 3 |
| **LC 3.** #1 Вuilt structures corresponding to transition states of the reaction  nitro-nitrite rearrangement in nitrobenzene and the formation of the aci form of methylnitramine. | 2 | 5 |
| **Module 2. Solving the Schrödinger equation for the helium atom and other multi-electron atoms** | | | |
| **4** | **L 4.** Basic functions of Slater and Gaussian types. | 1 |  |
| **PC 4.** Thermochemistry. Heat effect, heat capacity. Making reports. | 1 | 3 |
| **LC 4.** #2 Carrying out calculations using the Gaussian 09 program | 2 | 5 |
| **5** | **L 5.** Approximate methods for solving the Schrödinger equation for multi-electron systems | 1 |  |
| **PC 5.** Thermochemistry. Heat effect of chemical reactions, heat capacity. Kirchhoff equation. Making reports. | 1 | 3 |
| **LC 5.** #2 Calculate the optimization of geometric parameters and vibration frequencies for molecules | 2 | 10 |
|  | **IWST 2.** IWS 1. Calculation of amino acids in an aqueous solution by quantum chemical methods, preparation of a report in the project structure, presentation of the calculation progress in the Hyperchem program, presentation, oral defense. | 1 | 10 |
| **6** | **L 6.** A molecule in computational methods. Born-Oppenheimer approximation | 1 |  |
| **PC 6.** Calculation of heat effect for a given chemical reaction in two cases Ср=f(Т), Ср≠f(Т). | 1 | 15 |
| **LC 6.** #3 Study of chemical reactions of radical decomposition using the Gaussian 09 program | 2 | 8 |
| **7** | **L 7.** Approximation of the linear combination of MO atomic orbitals. Rutan equations. | 1 |  |
| **PC 7.** Working with errors based on the results of calculation of heat effect, entropy, Gibbs energy for a given chemical reaction in two cases Ср=f(Т), Ср≠f(Т). | 1 | 7 |
| **LC 7**. #3 Study of chemical reactions of radical decomposition using the Gaussian 09 program | 2 | 10 |
| **IWST 3.** Colloquium (project) Comparison of the results of calculating the nitrobenzene molecule using the laws of thermochemistry and the data calculated by quantum-chemical methods. | 1 | 10 |
| **Midterm control 1** | | | **100** |
| **Module 3. Non-empirical, semi-empirical and empirical methods of studying the electronic structure of atoms and molecules** | | | |
| **8** | **L 8.** Hartree-Fock method. | 1 |  |
| **PC 8.** Calculations related to the passage of particles through potential obstacles | 1 | 2 |
| **LC 8.** # 4 Optimization of geometric parameters, calculation of electronic energy. Master the operations of constructing and optimizing molecular models. | 2 | 6 |
| **IWS 2.** Topic: each student takes the structure of 20 amino acids according to the option and chooses the most effective one using semi-empirical methods. Advice on implementation. | 1 |  |
| **9** | **L 9.** Basis sets and pseudopotentials | 1 |  |
| **PC 9.** Atomic orbitals and their properties | 1 | 2 |
| **LC 9.** # 4 Compare the relative stability of three isomers - acetaldehyde and two conformers of vinyl alcohol with a C-C-O-H dihedral angle of 180° and 0° | 2 | 6 |
| **10** | **L 10.** Electronic characteristics | 1 |  |
| **PC 10.** Analysis of the energy spectrum of a hydrogen-like atom | 1 | 2 |
| **LC 10.** # 5 Calculation of vibrational spectra | 2 | 6 |
| **IWST 4.** Topic: choosing an effective method by taking the structure of 20 amino acids by each student and calculating with the help of semi-empirical methods. Interpretation of calculation results. Presentation, report preparation and oral defense | 1 | 10 |
| **Module 4. Theory of chemical bonding** | | | |
| **11** | **L 11.** Methods of accounting for electronic correlation. Methods of function theory | 1 |  |
| **PC 11.** Slater orbital. Analysis of parameters necessary for the calculation of quantum chemical methods | 1 | 2 |
| **LC 11.** # 5 Calculate vibrational spectra of organic compounds and visualize types of vibrations to decipher experimental data. | 2 | 6 |
| **12** | **L12.** Geitler-London, Pauling-Slater method of valence bonds, concepts of hybridization and resonance from the perspective of quantum mechanics | 1 |  |
| **PC 12.** Diatomic molecules. Analysis of parameters necessary for the calculation of quantum chemical methods | 1 | 2 |
| **LC 12.** # 6 Calculation of thermochemical parameters of substances | 2 | 5 |
| **IWST 5**. **IWS** 3. To study the stability of different states of amino acids in the gas phase and to draw conclusions on the thermochemistry of amino acids in an aqueous medium by analyzing the results of quantum chemical methods. | 1 | 10 |
| **13** | **L 13.** Geitler-London, Pauling-Slater method of valence bonds, concepts of hybridization and resonance from the perspective of quantum mechanics. Homonuclear diatomic molecules, calculation of their MO energy using the variational principle. | 1 |  |
| **PC 13.** Calculation of vibrational and rotational frequencies of molecules by quantum-chemical methods and interpretation of the results showing the connection with thermochemistry. | 1 | 2 |
| **LC 13.** # 6 Master the operations of calculating the enthalpy, entropy and Gibbs energy of substances and, with their help, evaluate the stability of isomers. | 2 | 5 |
| **IWS 3.** Studying the stability of different states of amino acids in the gas phase and drawing conclusions on the thermochemistry of amino acids in aqueous media by analyzing the results of quantum chemical methods (Project). Presentation, reporting and oral defense. | 1 | 10 |
| **14** | **L 14.** Designing a task for calculating simple molecules. The problem of choosing the basis of AO. Geometric optimization. Analysis of AO complementation and communication order according to Mulliken | 1 |  |
| **PC 14.** States and reactivity of molecules. | 1 | 2 |
| **LC 14.** # 7 Calculation of thermochemical parameters of reactions. learn to calculate enthalpy changes, entropy and Gibbs energy of the reaction. | 2 | 5 |
| **IWST 6.** Colloquium. Making analyzes on the topics of the IWS and the data of the laboratory work. Protection of the report in the form of a project. | 1 | 10 |
| **15** | **L 15.** Molecular quantum numbers. MO method-basic rules and tasks. One electron approximation, concept of molecular orbital. Linear combination approximation of MO atomic orbital in the Hartree-Fock method, Rutan equations and their solution methodology. | 1 |  |
| **PC 15.** Analyzing a molecule by multi-configurational methods. | 1 | 2 |
| **LC 15.** # 7 Calculate ΔrH and ΔrG for the reaction of ethylene hydrogenation using  using the Hartree-Fock method and the 6-31G(d,p) basis set. | 2 | 5 |
| **IWST 7.** Advice on exam preparation. Rules for creating a project. | 1 |  |
| **Midterm control 2** | | | **100** |
| **Final control (exam)** | | | **100** |
| **TOTAL for course** | | | **100** |

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

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