

Physical Chemistry Final Exam Rules and questions

Each candidate will receive three questions:

- one from block I
- one from the themes of block II chosen by the candidate
- one from the remaining three themes of block II

Students are advised to choose the topics from block II, which is related either to the physical chemistry subjects taken by the candidate during the MSc or to the topic of the dissertation.

Block I: Electronic structure of molecules

- **Principles of quantum mechanics:** Interpretation of the most important concepts based on postulates (state, measurement, stationary state), presenting them on the example of the “particle in the box” model. Quantum mechanical interpretation of angular momentum.

- **Electronic structure of atoms:** Solutions of the Schrödinger equation of hydrogen atom, interpretation of the results (energy, orbits, density); Quantum mechanical discussion of the electronic structure of many-electron atoms in the framework of the Independent Electron Model, characterization of the states and interpretation of their notation; Atoms in magnetic field.

- **Symmetry of molecules, basics of group theory:** spatial symmetry of molecules, basic concepts of group theory, character table, notion of representations, the role of symmetry in quantum mechanics.

- **Electronic structure of molecules:** Schrödinger equation, Born-Oppenheimer approximation, introduction of molecular orbitals. Diatomic molecules, water molecule. Simple MO descriptions: Hückel theory, electronic structure of transition metal complexes.

- **Basic methods of computational chemistry:** Hartree-Fock method, DFT methods, theoretical foundations of electron correlation methods. One-electron basis sets.

- **Applications of quantum chemical methods:** geometry optimization, calculation of vibrational spectra, and obtaining thermochemical data.

Block II

Thermodynamics

The three laws of classical thermodynamics: The criteria of thermodynamic equilibrium in various thermodynamics systems. S, U (or E), H, A (or F) and G thermodynamic potential function.

Equilibrium in single and multi-component systems: Ideal and real mixtures. Phase equilibria and phase diagrams. Chemical equilibria. Equilibrium constant of homogeneous and heterogeneous reactions.

Changes in thermodynamic systems

-Molecular theories of chemical reactions: Collision theory and transient state theory. Rate equations and mechanism of complex reactions.

-Transport processes: Thermal conductivity, diffusion, viscosity, electrical conductivity.

Electrochemistry

-Electrodes and electrochemical cells. Cell diagrams. Measurement of the electromotive force. Potentials of cell and electrode reactions, standard electrode potentials. Nernst's equation. Pourbaix diagrams. Batteries, electrochemical power sources. The definition and measurement of pH.

-The kinetics of electrode reactions. Electrolysis. The most important steps of electrode processes. The rate of electrode reactions (charge transfer) and its dependence on the electrode potential and the concentrations of reactants according to the Erdey-Grúz–Volmer equation. The conductance of electrolyte solutions, its experimental determination. Kohlrausch's law.

Colloids and interfaces

-Basics of interfacial thermodynamics: Surface excess energy, surface tension, pressure difference between phases separated by a curved surface. The Gibbs adsorption equation and its applications

- Colloidal systems: Association colloids, micelle formation. Macromolecular colloids. Polymer solutions. Dispersion colloids. Classical (DLVO) theory of colloidal stability.