Topic list for Physical Chemistry II exam

1. **Transport phenomena** (Different states of matter (different phases) and their properties, similarities and differences. Transport processes: diffusion, thermal conductivity, viscosity. Interpretation of transport processes with the kinetic theory of gases. Effusion. Barometric formula. The diffusion equation (Fick's 2nd law).)

2. **Homogeneous dynamic electrochemistry** (Conductivity of electrolytes. Law of the independent migration of ions. Strong electrolytes. Kohlrausch law. Weak electrolytes. Ostwald's dilution law. Mobilities of ions, definition and determination of ion transport number.)

3. **Reaction kinetics** (Concept of reaction rate. Graphical representation of reaction rate. Experimental methods to measure reaction rates. Rate equation. First-order, second-order kinetics, other reaction orders. Multiterm rate equations: consecutive, parallel, reversible reactions. Steady-state and fast pre-equilibrium approximation. Steps for determining the rate equation.)

4. **Reaction mechanisms** (Concept and properties of elementary reactions. Law of kinetic mass action. Unimolecular and termolecular reactions. Interpretation of higher reaction orders. Negative reaction order and its rationalization. Enzyme catalysis. Gas phase formation of hydrogen halides. Branching chain reactions, explosions. Catalysis, autocatalysis, oscillation.

5. **Theories of reaction rates** (Temperature dependence of rate constants. Arrhenius equation. Collision theory in gas and in solution phase. Activated complex theory: thermodynamic, quantum mechanical and statistical mechanical approach.)

6. **Processes at solid surfaces** (Application examples of surface reactions. Surface: concept, nature; formation, growth, size; composition, structure; measuring methods. Physisorption and chemisorption. Langmuir and BET isotherms. Kinetics of adsorption and desorption. Catalytic activity of surfaces, Langmuir–Hinshelwood and Eley–Rideal mechanisms.)

7. **Heterogeneous dynamic electrochemistry** (Current density–overpotential, their connection, exchange current densities, Tafel equations. The structure of the double layer, Nernst diffusion layer. Volta- and Galvani potentials. Kinetics of electrode processes. Butler–Volmer equation. Polarization, limiting current density.)

8. **Non-thermal activation** (Types of radiations. Characteristics of radiations. Electromagnetic radiation ranges. The interaction between matter and radiation: reflection, passing over, absorption. Hot flames. Comparison of photochemistry and radiation chemistry. Ionizing radiations. Magnetochemistry, sonochemistry, mechanochemistry, tribochemistry.)

9. **Basics of photochemistry** (The nature of light. Characterization of electromagnetic radiation. Basic laws of photochemistry: Grotthus–Draper law, Bunsen–Roscoe law, Stark–Einstein law, Lambert–Beer law. Quantum yield and quantum efficiency. Jablonski diagrams. Kinetics of photochemical processes. Sensitization.)

10. **Chemistry of the atmosphere** (The structure of the atmosphere. The most important gases in the atmosphere. CO_2 emission and global warming. The CO_2 cycle. Ozone generation, ozone decay, the role of ozone in the atmosphere. Atmospheric pollutants. Halogenated hydrocarbons.)

11. **Quantum theory: definitions, apparatus** (Limitations of classical physics: black body radiation, photoelectric effect, Compton effect, electron diffraction. Heisenberg's uncertainty principle. Schrödinger equation and its solution: free particle, particle in a box, harmonic oscillator and circular motion in quantum mechanics. Variational principle.)

12. **Atomic structure and atomic spectra** (Elementary particles in atoms. Hydrogen-like atomic particles: convention for designating the wave function, radial and angular wave function, degeneration. Radial density function and average distance from the nucleus. Spectra of hydrogen-like particles. Fermions and bosons. Multielectron particles, SCF method.)

13. **Electron structure of molecules** (Classical bonding theories. Quantum chemical description of the hydrogen molecule ion, bonding and antibonding orbitals. MO method, MO correlation diagrams. Hückel method. VB method. Hybridization.)

14. **Quantum mechanical calculations** (PES: minima, saddle points. Calculation methods: Molecular mechanics, HF method, semiempirical calculations, post-HF, DFT. Calculated properties: energy, structure, vibrations, electron density. Comparison of calculated and measured geometric parameters. Statistical thermodynamics, partition function. Reaction path and reaction coordinate.)