

I Equilibrium

1. Properties of gases
 - 1.1. Ideal gas: states of gases, the gas laws, kinetic model of gases
 - 1.2. Real gases: intermolecular interactions, van der Waals equation
2. The first law of thermodynamics
 - 2.1. Work and heat: expansion work, heat transactions, enthalpy, adiabatic changes
 - 2.2. Thermochemistry: standard enthalpy changes, standard enthalpy of formation
 - 2.3. The temperature-dependence of reaction enthalpies, temperature dependence of enthalpy, relationship between C_V and C_p
3. The second law of thermodynamics
 - 3.1. Direction of spontaneous changes, energy dissipation, entropy, entropy change accompanying selected processes
 - 3.2. The third law of thermodynamics
 - 3.3. Free energy and enthalpy, standard molar free enthalpy
 - 3.4. Properties of the internal energy
 - 3.5. Properties of the free enthalpy
 - 3.6. Chemical potential of pure substances
 - 3.7. Real gases: fugacity, standard state of real gases, relationship between fugacity and pressure
4. Physical transformations of pure substances
 - 4.1. Phase diagrams, phase stability, phase equilibrium boundaries: phases, components and degrees of freedom, phase rule, two-component systems, vapour pressure diagrams, temperature-composition phase diagrams, liquid-liquid phase diagrams, liquid-solid phase diagrams
 - 4.2. Stability of phases and phase transitions: The thermodynamic criterion of equilibrium, the dependence of stability on the conditions, the location of phase boundaries, the Ehrenfest classification of phase transitions
 - 4.3. Liquid surface: surface tension, curved surfaces, capillary phenomena
 - 4.4. Simple mixtures
 - 4.4.1. Thermodynamic description of mixtures: partial molar quantities, thermodynamics of mixing, chemical potential of a liquid component
 - 4.4.2. Properties of solutions: liquid mixtures, colligative properties
 - 4.4.3. Activity: solvent activity, solute activity
5. Chemical equilibrium
 - 5.1. Spontaneous chemical reactions, minimum free enthalpy
 - 5.2. The influence of external conditions on the state of equilibrium: the influence of pressure and temperature
 - 5.3. Acids and bases
6. Electrochemistry of equilibrium systems
 - 6.1. Thermodynamic properties of ions in solutions: thermodynamic functions of formation, ion activity
 - 6.2. Electrochemical cells: half-reactions and electrodes, varieties of cells, standard potentials

- 6.3. Application of standard potentials: electrochemical series, solubility constants, pH and pK measurements, determination of thermodynamic values from cell potential measurements

II Structure

1. Quantum theory
 - 1.1. Wave-particle duality, dynamics of microscopic systems: Schrödinger equation, Born interpretation of the wavefunction
 - 1.2. Quantum mechanical principles: information in a wavefunction, the uncertainty principle
 - 1.3. Translational motion: particle in the box, motion in two dimensions
 - 1.4. Oscillating motion: energy levels, wavefunctions
 - 1.5. Rotational movement: rotation in two dimensions, rotation in three dimensions, spin
2. Atomic structure and atomic spectra
 - 2.1. Structure and spectra of hydrogenic atoms: structure of hydrogenic atoms, atomic orbitals and their energies, spectral transitions and selection rules
 - 2.2. Structure of multi-electron atoms, orbital approximation
 - 2.3. Spectra of complex atoms: singlet and triplet states, spin-orbit coupling, term symbols and selection rules
3. The structure of molecules
 - 3.1. Born-Oppenheimer approximation: hydrogen molecule, homonuclear diatomic molecules, polyatomic molecules
 - 3.2. Theory of molecular orbitals: structure of diatomic molecules, diatomic heteronuclear molecules
 - 3.3. Molecular orbitals of polyatomic systems: Hückel approximation, band theory of solids
 - 3.4. Symmetry of molecules: operations and elements of symmetry, symmetry classification of molecules, vanishing integrals and overlapping orbitals, vanishing integrals and selection rules
4. Spectroscopy
 - 4.1. Rotational and vibrational spectra
 - 4.1.1. Purely rotational spectra: moments of inertia, rotational energy levels, rotational transitions
 - 4.1.2. Oscillations of diatomic molecules: molecular oscillations, selection rules, anharmonicity
 - 4.1.3. Oscillations of polyatomic molecules: normal vibrations, oscillation spectra of polyatomic molecules, Raman vibrational spectra
 - 4.2. Electronic transitions
 - 4.2.1. Characteristics of electronic transitions: oscillatory structure, types of transitions
 - 4.2.2. The fate of electronically excited states: fluorescence and phosphorescence, general principles of laser action
 - 4.3. Nuclear magnetic resonance: nuclear magnetic moments, energies of nuclei in magnetic fields, chemical shift, fine structure
 - 4.3.1. Pulse techniques in NMR: magnetization vector, line width and rate of processes, the nuclear Overhauser effect, solid state NMR
 - 4.4. Electron paramagnetic resonance: g factor, hyperfine structure

5. Statistical thermodynamics
 - 5.1. Distribution of molecular states: macro states of the system and thermodynamic probability, molecular partition function
 - 5.2. Internal energy and entropy, statistical entropy, canonical ensemble and canonical partition function
 - 5.3. Applications of statistical thermodynamics: mean energies, heat capacities, equations of state, residual entropies, equilibrium constants
6. Diffraction techniques
 - 6.1. Lattices and unit cells
 - 6.2. X-ray diffraction: Bragg's law, powder method, single crystal X-ray diffraction, information obtained from X-ray structural analysis
7. Electric and magnetic properties of molecules
 - 7.1. Electrical properties: permanent and induced electrical dipole moments, refractive index
 - 7.2. Intermolecular forces: interactions between dipoles, repulsive and total interactions, molecular interactions in beams
 - 7.3. Magnetic properties: magnetic susceptibility, permanent magnetic moment
8. Macromolecules and colloids
 - 8.1. Size and shape: average molar masses, colligative properties, sedimentation, viscosity, light scattering
 - 8.2. Conformation and configuration: random coils, helices and sheets, higher order structures
 - 8.3. Colloids and surfactants: properties of colloids, surface films

III Change

1. Molecules in motion
 - 1.1. Molecular motions in gases: collision with walls and surfaces, rate of effusion, migration down gradients, transport properties of an ideal gas
 - 1.2. Motions of molecules and ions in liquids: liquid structure, movement of molecules in liquids, conductivity of electrolyte solutions, ion mobility, specific conductivity and interionic interactions
 - 1.3. Diffusion: thermodynamic approach, diffusion equation, probabilistic approach, statistical description
2. The rate of chemical reactions
 - 2.1. Empirical chemical kinetics: experimental methods, reaction rate, integrated rate laws, reactions approaching equilibrium, temperature dependence of reaction rates
 - 2.2. Accounting for the rate laws: elementary reactions, consecutive elementary reactions, unimolecular reactions
3. Kinetics of complex reactions
 - 3.1. Chain reactions: mechanism of chain reactions, explosion, photochemical reactions, kinetics of polymerization reactions, chain polymerization, stepwise polymerization
 - 3.2. Catalysis and oscillating reactions, homogeneous catalysis
4. Molecular reaction dynamics
 - 4.1. Reactive collisions: collision theory, diffusion-controlled reactions, material balance equation

DOCTORAL SCHOOL OF EXACT AND NATURAL SCIENCES
PHD PROGRAMME IN CHEMISTRY
TOPICS FOR QUALIFYING INTERVIEW, PHYSICAL CHEMISTRY

- 4.2. Transition state theory: reaction coordinate and transition state, Eyring equation, thermodynamic aspects
- 4.3. Molecular collision dynamics: reactive collisions, potential energy surfaces
5. Processes taking place on solid surfaces
 - 5.1. Adsorption: physical and chemical adsorption
 - 5.2. Adsorption isotherms
6. Dynamics of electrochemical processes
 - 6.1. Processes at electrodes: electric double layer, rate of charge transfer, polarization
 - 6.2. Electrochemical processes: electrolysis, working galvanic cells characterization, power production and corrosion, fuel cells and batteries