Systematic Physical Chemistry

List of topics and suggested materials (Spring semester)

Part 1. Electrochemistry

1. Electrochemical systems. Electrode, electrochemical cell. Measurement of the terminal voltage and electromotive force (EMF) of an electrochemical cell, determination of internal resistance. Concentration and temperature dependence of EMF. Calculation of thermodynamic data from electrochemical measurements.

Theory: Inzelt György's note., Keszei: Chapter 9.2, Atkins: Chapter 10.3-10.10.
Experimental handouts: Measurement of the terminal voltage and electromotive force (EMF), temperature dependence of EMF.

2. Thermodynamics of a single bulk phase containing charged particles. Experimental and theoretical approaches for the study of such systems. Determination of mean activity coefficients from cell measurements, transport processes in electrolyte solutions. Determination of the pH using a hydrogen electrode and a glass electrode. Determination of the ion product for water. Systems of limited solubility.

Theory: Keszei: Chapter 9.2, Atkins: Chapter 10.1-10.2
Experimental handouts: Mean activity coefficient determination, pH, ionic product for water

3. Processes at electrodes, electrochemical processes, electrolysis, fuel cells, corrosion. Theory of the kinetics of electrode processes.

Theory: Atkins: Chapter 29.

4. Kinetics of electrode processes: experimental aspects. Analysis of steady-state and potentiodynamic polarization curves. Voltammetry, the study of electrolysis mechanisms. Conductometric methods and instruments. Experimental methods for determination of transference numbers.

Experimental handouts: transport number, electrolysis,

Literature:
Atkins - P. W. Atkins, Physical Chemistry, 5th Edition, Oxford University Press
Keszei - E. Keszei. Chemical Thermodynamics, Springer, 2012.

Part 2. Colloid chemistry

1. Interfacial excess energy. Surface tension. Pressure over curved interfaces, equilibrium vapor pressure of droplets. Surface tension measurements.

2. Adsorption, Gibbs adsorption equation. Adsorption isotherms.

3. Electric properties of interfaces. Electrokinetic phenomena.

4. Association colloids. Solubilization. Wettability phenomena.

5. Dispersion colloids, colloidal stability. Thermal motion and sedimentation of particles.

6. Macromolecular colloids, conformation of polymers. Physical states of polymers. Rheology.

Literature:
Shaw, D.J.: Introduction to Colloid and Surface Chemistry (ISBN 07506 11820)

Part 3. Theoretical chemistry

1. Differential equations: categorization, boundary and initial conditions, general and particular solutions, separation of partial differential equations;

Linear algebra: vector space, Hilbert-space, properties of the scalar product, vector norm, angle of two vectors, orthonormality (ON) of vector sets, linear dependence, overlap matrix, expansion of a vector on an ON set, the Hilbert-space of square integrable functions, function resolution in L2-space, important ON sets in L2-space

Theory: Goodson: Chapters 13.2.1, 14., 16., 17., SzÁ lecture notes and recordings in Canvas

2. Linear algebra: operator, inverse operator, commutator, linear operator, matrix representation of linear operators, determinant, matrix inverse, solving linear system of equations, operator adjoint, unitary operator, Hermitian operator, eigenvalue-equation, similarity transformation

Theory: Goodson: Chapters 18.1-3, 18.5-7, 19.1-3, SzÁ lecture notes and recordings in Canvas

3. Linear algebra: properties of eigenvalues and eigenvectors of Hermitian operators, theorem on the simultaneous diagonalizability of Hermitian operators, degeneracy, variation of a function, variation of an integral, Rayleigh-quotient, variational principle, linear variation method, variational theorem

Theory: Goodson: Chapters 19.1, 19.4-5, SzÁ lecture notes and recordings in Canvas

4. Quantum mechanics: postulates of quantum mechanics, interpretation of the wavefunction, Heisenberg's commutation relation, quantization, pure/mixed state of a system, the outcome of a quantum mechanical measurement, time-dependent Schrödinger-equation (TDSE), separation of the TDSE, time-independent SE, stationary states, time derivative of a quantum mechanical expectation value, constants of motion, quantum numbers

Theory: Goodson: Chapters 20.1-3, Szalay Péter's notes: 1st part, pages 13-17, SzÁ lecture notes and recordings in Canvas

5. Quantum chemistry: atomic units, Hamiltonian of a molecular system, the Born-Oppenheimer approximation, potential energy surface, the electronic structure problem of the hydrogen atom, Pauli exclusion principle applied to many-electron wavefunctions, spin coordinate, Slater-determinant, outline of the Hartree-Fock approximation, Fock-operator, molecular orbital, Aufbau-principle, LCAO-MO, gaussian type atomic orbitals

Theory: Goodson: Chapters 20.2, 20.3.1, 20.5-6, Szabo-Ostlund: Chapter 2, pages 39-55, Szalay Péter's notes: 3rd part, pages 48-52, SzÁ lecture notes and recordings in Canvas

Suggested reading:

D. Z. Goodson: Mathematical Methods for Physical and Analytical Chemistry
A. Szabo and N. S. Ostlund: Modern Quantum Chemistry