



Study program: Pharmacy
Course title: Physical Chemistry
Teacher : Mihalj M. Poša, Zita J. Farkaš-Agatić, Kosta J. Popović
Course status: compulsory
ECTS Credits: 7
Condition: Biophysics
<p>Course aim</p> <p>Introducing the student to the system state functions, types of systems, as well as the concept of thermodynamic transformation and speed of transformation. Distinguishing between reversible and irreversible processes, nonequilibrium and equilibrium states, as well as relaxation of the system from the nonequilibrium state to the equilibrium state. As the state of the system is monitored, determining what are the functions by which spontaneous irreversible processes can be determined. Understanding of macrostates and microstates, definition of physicochemical parameters of system state based on statistical thermodynamics.</p>
<p>Expected outcome of the course:</p> <p>Knowledge of matter structure, nature of chemical bonds and state of material systems in processes of dissolution, adsorption, phase, chemical and electrochemical transformations. Practical application of knowledge in laboratory work in the field of knowledge of the structure of atoms and molecules, physical, chemical, thermal and electrochemical transformations and processes.</p>
<p>Course description</p> <p><i>Theoretical education</i></p> <p>I THERMODYNAMICS</p> <p>I.1. INTRODUCTION TO THERMODYNAMICS: Simple system; System size and system parameters; Composite system; Internal restrictions; Maximum entropy principle; Microstates.</p> <p>I.2. DIFFERENTIAL FORM OF FUNDAMENTAL THERMODYNAMIC FUNCTION: Entropy representation; Enthalpy representation; Identification of partial derivatives with T, P, μ.</p> <p>I.3. INTENSIVE AND EXTENSIVE UNITS: Homogeneous first order function; Homogeneous zero-order function; Molar sizes, partial molar sizes, example of partial molar volume; C_v, C_p, α, κ_S, κ_T; $C_p - C_v$; κ_S / κ_T; $S = S(p, T)$; $S = S(V, T)$; Substitution: $S = S(U) \rightarrow U = U(T)$; Substitution: $S = S(U) \rightarrow S = S(1/T)$.</p> <p>I.4. EULER'S RELATIONSHIP FOR U & S: Gibbs-Duhem equation.</p> <p>I.5. ENTROPY OF IDEAL GASES: Application of Euler and Gibbs-Duhem relation; The Gibbs paradox.</p> <p>I.6. CLASSICAL DEFINITION OF THE FIRST LAW OF THERMODYNAMICS: And the law of thermodynamics; Volume work; Isothermal, isochoric, isobaric, adiabatic process work.</p> <p>I.7. THERMODYNAMIC CONFIGURATION SPACE: equivalence of S_{\max} and U_{\min} for equilibrium.</p> <p>I.8. ENTROPY CHANGE IN A REVERSIBLE AND IRREVERSIBLE THERMODYNAMIC PROCESS: Reversible reservoir of work and heat; the degree of efficiency of the thermal machine; Carnot cycle; input for the degree of efficiency of the thermal machine; Thermodynamic definition of entropy (based on the Carnot cycle); Entropy change in irreversible process and Clausius inequality.</p> <p>I.9. THERMODYNAMIC POTENTIALS: Lagrangian transformation of internal energy; Helmholtz free energy; Enthalpy; Gibbs free enthalpy, Gibbs-Helmholtz energy, chemical potential, reaction equilibrium constant; Gibbs mixing energy - an ideal gas mixture; Maxwell's equality; Joule-Thomson effect .</p> <p>II KINETIC THEORY</p> <p>II.1. KINETIC THEORY OF IDEAL GAS STATE: Equipartition of thermal energy, Dalton's law; Internal energy of a two-atom ideal gas: rotational and vibrational energy; Maxwell speed distribution; Collisions between molecules, effusion.</p> <p>II.2. TRANSPORT PROCESSES: Diffusion: Fick's I and II law; Viscosity: Hagen-Poiseuille's law.</p> <p>III. QUANTUM MECHANICS</p> <p>III. 1. SCHREDINGER'S EQUATION FOR TRANSLATORY MOVEMENT: one-dimensional potential pit; two-dimensional potential pit.</p> <p>III. 2. SHREDINGER'S EQUATION FOR 2d ROTATION MOVEMENT: energy and momentum, projection of momentum on the z-axis for 3d motion.</p> <p>III. 3. SPIN</p> <p>III. 4. PAULI'S PRINCIPLE AND THE HUND RULE: A MULTIPLE PARTICLE POTENTIAL PIT.</p> <p>IV. STATISTICAL THERMODYNAMICS</p> <p>IV. 1. MICROCANONICAL ENSEMBLE: BOLZMANN'S DISTRIBUTION: microstate, statistical weight, molecular partition function; Discussion of the equilibrium constant for the $A \rightarrow B$ reaction in the gas phase; entropy in microcanonical distribution (starting from</p>

Shannon entropy).

IV. 2. THE CANON ENSEMBLE: definition of Helmholtz energy, mean energy, standard deviation of energy; canon partition function; entropy in canonical ensemble (starting from Shannon entropy); canon partition function for translational motion; Sackur–Tetrode entropy equation.

V. REAL GASES: fugidity, chemical potential in real gases.

VI. THERMODYNAMIC SYSTEM IN EQUILIBRIUM

Practical education

1. The theory of error; 2. Electromagnetic properties of molecules: - Determination of the polarization of the electron shell of a molecule by measuring the refractive index, - Testing the specific power of optical rotation; 3. Thermodynamics of open systems: - Density determination using a pycnometer, - Determination of partial molar volume of sodium chloride and potassium chloride in aqueous solution; 4. Thermodynamics of solutions and mixtures: - Colligative properties; 5. Thermodynamics of equilibrium systems: - Determination of evaporation heat based on the equilibrium of the liquid phase and the vapor phase, - Determination of osmotic coefficient by isopiezian method, - Testing of partially miscible liquids, - Determination of the partition coefficient, - Determination of the equilibrium dissociation constant of benzoic acid; 6. Occurrences in the interfacial boundary: - Freundlich adsorption isotherm, - Determination of Gibbs adsorption isotherm; 7. Association colloids: - Determination of critical micellar concentration using a pyrene test molecule, - spectrofluorimetric method; 8. Electroanalytical methods: - Conductometric titration, - Determination of the marginal molar conductivity of an electrolyte solution, - Determination of solubility of hardly soluble salts based on conductivity, - Potentiometric titration; 9. Chemical kinetics: - Determination of chemical reaction rate constant value

Literature

Compulsory

1. Peter Atkins, Julia de Paula. Physical chemistry for life science, W.H. Freeman and Copmany New York, 2006.

Additional

1. Callen, Herbert B. Thermodynamics and an Introduction to Thermostatistics, University of Pennsylvania, 1985.

Number of active classes

Theory: 60

Practice: 30

Teaching methods

Lectures, Laboratory Practice

Student activity assessment (maximally 100 points)

Pre-exam activities	points	Final exam	points
Lectures		Written	30
Practices	10	Oral	30
Colloquium	30	
Essay			