UNIVERSITY OF PANNONIA

SUBJECT DATASHEET

Semester:	2009/10/2
Subject:	Physical Chemistry I.
Code:	VEMKFK2215V
Responsible department:	Department of Physical Chemistry
Responsible department code:	MKFK
Responsible lecturer:	dr. Tamás Kristóf

Educational objectives:

Teach physical chemistry via lectures and numerical examples.

Detailed content of the subject:

1. An introduction to chemical thermodynamics. Definitions (wall,system,property).Extensive and intensive properties. Temperature. Equilibrium. Thermal energy. Internal energy. Work, volumetric work, cycles. Reversible work. Heat, reduced heat as entropy. 2. The laws of thermodynamics. The first law. Chemical potential. The Gibbs-equation. Definitions of intensive properties.The second law. Irreversible processes. The 3rd law.Entropy-maximum and energy-minimum. Conditions of equilibrium.Carnot-efficiency.Refrigerators. 3.Energy functions. Enthalpy. Free energy. Gibbs free energy. Intensive properties from the derivaties of H, F and G. Planck-function, Massieu-function. Heat capacities. Thermochemistry: Hess-law, Kirchoff-equation. 4.Statistical thermodynamics. Energy distribution. Degeneracy, macrostate, microstate. The most probable distribution. Bose-Einstein, Fermi-Dirac statistics. Boltzmann-distribution. Comparison of distributions. 5.Partition functions. Translation, rotation, vibration. Molecular partition function of diatomic particles. Work, heat and entropy in statistical thermodynamics. S=klnW. Entropy and disorder. Molecular partition function and thermodynamic properties. Entropy of mixing, configurational entropy. 6.Ensembles. The ensembles. Canonical ensemble. Boltzmann-distribution. Entropy in canonical ensemble. Molecular and canonical partition functions. Fluctuations. 7.Thermodynamic relations. Maxwell-relations. Volumetric properties and heat capacities. Gibbs-Helmhotz- and Gibbs-Duhem-equations. U, H and S as functions of p, V and T. Changes in F, G, J and Y.Energy functions and cofigurational entropy. 8.Kinetic theory of gases. The pressure. Distribution of energy and velocities. Collision numbers. Average free path. Knudsen diffusion. 9.Electric properties of materials. Dielectric polarization. Debye-equation of molar polarization. Dielectric relaxation. Frequency dependent dielectric properties. Cole-Cole-plot. Frequency dependence of the displacement polarization,the origin of the spectra. Magnetic and electric properties. 10.Gases. Thermodynamic properties of perfect gases. Changes of state. The Poisson-equation. Intermolecular forces. Mie-equation, Lennard-Jones-potential. Virial equation. Equations of state for real gases. The corresponding states law. Properties of real gases. Joule-Thomson-effect. 11.Condensed states. Pair-correlation function. Crystal structures. Madelung energy of ionic crystals. Crystal energy from Born-Haber cycles. Einstein-and Debye-heat capacity. Properties of liquids:viscosity,Hagen-Poiseuille law. Special structures: water, liquid crystals,glasses. 12.Mixtures. Mixture and solution. Gaseous mixtures. Partial molar quantities. Ideal mixtures, ?G, ?S. The activity, reference states. Relationships between activities. Real mixtures, excess properties. Regular mixtures, athermic mixtures. 13.Electrolyte solutions. Ionic solvation. Real electrolyte solutions. Activity coeffitiens and Debye-

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Detailed content of the subject:

Hückel-theory. 14.Transport properties. Fourier-, Newton-, Fick-equations. Instationer diffusion. Diffusion in perfect gases. Diffusion in condensed phases. Einstein-Smoluchowski-equation. Stokes-Einstein-equation. Conductivity in electrolyte solutions, ionic mobility. Relaxation -and electrophoretic-effects. Nernst-Einstein-equation. Diffusion potential. Jones-Dole-equation. Electrochemical potential.

Requirements:

None.

Required and suggested references:

1. Liszi, J.: Fizikai kémia, Veszprém, 1993. Kézirat. 2. Liszi, J., Ruff, I., Schiller, R., Varsányi, Gy.: Bevezetés a fizikai kémiába, Muszaki Könyvkiadó, Budapest, 1993. 3. Moore, J.,W.: Chimica Fisica, Piccin, 1983. 4. Atkins,W.,P.: Physical Chemistry, Oxford University Press, 1990.