The course starts on October 12, 2021.
Lectures will be delivered on Tuesdays, 16:00 - 17:30, by Zoom

Thermodynamics

Andrzej Poniewierski, Institute of Physical Chemistry PAS

Lecture 1: thermodynamic equilibrium, zeroth law of thermodynamics and empirical temperature, gas laws, thermodynamic scale of temperature, perfect gas and real gases, van der Waals equation of state, thermodynamic processes, state parameters and state functions, internal energy, work and heat, first law of thermodynamics.

Lecture 2: heat capacity at constant volume and internal pressure, Joule's experiment, enthalpy and heat capacity at constant pressure, Joule-Thomson effect, inversion temperature, liquefaction of gases, entropy and second law of thermodynamics, maximum entropy principle, thermodynamic definition of entropy.

Lecture 3: entropy changes in perfect gas, heat devices, Carnot cycle, Carnot engine and its efficiency, refrigerator and heat pump, direction od spontaneous processes, Clausius inequality, free energy and free enthalpy, maximum work, fundamental equation of thermodynamics, thermodynamic potentials and natural variables.

Lecture 4: Maxwell relations, open systems, diffusive equilibrium, chemical potential, Euler relation, Gibbs-Duhem equation, fundamental equation of chemical thermodynamics, mixture of perfect gases, chemical potentials of components, free enthalpy of mixing, concept of ideal solution.

Lecture 5: phase transitions in pure substances, phase diagrams, two-phase coexistence lines, triple point and critical point, evaporation and boiling in open systems, thermodynamics of phase transitions, conditions of two-phase coexistence, first and second order phase transitions according to Ehrenfest classification, λ phase transition, Clapeyron and Clausius-Clapeyron equations.

Lecture 6: application of van der Waals equation of state to liquid-vapour coexistence, Maxwell construction, critical parameters and reduced variables, principle of corresponding states, surface phenomena, surface tension, Laplace equation, contact angle and Young equation, capillary phenomena.

Lecture 7: thermodynamics of mixtures, partial molar quantities and functions of mixing, ideal solution, phase transitions in mixtures, Gibbs phase rule, binary mxitures, liquid-vapour equilibrium, liquid and vapour composition lines, dew point and bubble point, lever rule, distillation of zeotropic mixture, Raoult's law.

Lecture 8: colligative properties of dilute solutions, vapour pressure depression, boiling point elevation, ebullioscopic constant, freezing point depression, cryoscopic constant, osmotic pressure, liquid-solid equilibrium, solubility line, simple eutectic, eutectic point, solid solutions, fractional crystallization and zone refining.

Lecture 9: liquid-vapour equilibrium in real mixtures, solubility of gases in liquids, Henry's law, deviations from Raoult's law, zeotropic and azeotropic mixtures, distillation of azeotropic mixtures, liquid solutions with miscibility gap, miscibility curve and critical temperature of solubility, simple solutions, activity coefficients and excess chemical potentials.

Lecture 10: enthalpy of mixing and stability of mixtures, liquid-vapour equilibrium in mixtures with solubility gap, positive azeotropic mixtures, heteroazeotropic and heterozeotropic mixtures, thermochemistry, standard state and standard enthalpy of reaction, Hess' law, standard enthalpy of formation, Kirchhoff's law.

Lecture 11: chemical equilibrium, extent of reaction, free enthalpy of reaction, endergonic and exergonic reactions, chemical equilibrium for mixtures of perfect gases, reaction quotient and equilibrium constant, influence of external conditions on chemical equilibrium, van't Hoff equation, Le Chatelier's principle.

Lecture 12: phase rule for systems with chemical reactions, fugacity and activity, activity of pure liquid or solvent, activity of solute, reactions in electrolyte solutions, electrochemical potential, galvanic cell, Daniell cell, work of chemical reaction, Nernst equation, standard cell potential and its relation to equilibrium constant.

Lecture 13: basic concepts of statistical mechanics, statistical ensembles, definition of probability, microstates and macrostates, statistical postulates, microcanonical ensemble and statistical definition of entropy, Nernst heat theorem and third law of thermodynamics, residual entropy.

Lecture 14: canonical ensemble and its relation to thermodynamics, equivalence of microcanonical and canonical ensembles, Boltzmann distribution, classical statistical mechanics, Maxwell distribution of velocity, equipartition theorem, heat capacity of molecular perfect gas, heat capacity of crystals, Dulong-Petit law.

Lecture 15: quantum description of monatomic perfect gas, thermal de Broglie's wavelength, indistinguishability of identical particles, entropy of monatomic perfect gas, Sackur-Tetrode equation, Gibbs paradox, molecular perfect gas, average energy of molecular rotations and vibrations, characteristic rotational and vibrational temperatures, heat capacity of diatomic perfect gas, comparison with classical statistical mechanics.

References

[1] P. W. Atkins, Physical Chemistry, 6th edn., (Oxford University Press, Oxford, 1998)

[2] R. Hołyst, A. Poniewierski, Thermodynamics for Chemists, Physicists and Engineers (Springer, Dordrecht, 2012)

[3] E. B. Smith, Basic Chemical Thermodynamics, 5th edn. (World Scientific, Singapore, 2004)

[4] F. Reif, Statistical Physics, Berkeley Physics Course - Volume 5 (Mc Graw-Hill Book Company, New York, 1967)

[5] K. Huang, Statistical Mechanics, (Wiley, New York, 1963)