



KD2340 Molecular Thermodynamics 7.5 credits

Molekylär termodynamik

This is a translation of the Swedish, legally binding, course syllabus.

Establishment

Course syllabus for KD2340 valid from Autumn 2010

Grading scale

A, B, C, D, E, FX, F

Education cycle

Second cycle

Main field of study

Chemical Science and Engineering, Chemistry and Chemical Engineering

Specific prerequisites

Three years of studies in Chemical Science and Engineering at bachelor level, or equivalent.

Language of instruction

The language of instruction is specified in the course offering information in the course catalogue.

Intended learning outcomes

Principal aims

To develop the basic knowledge in statistical thermodynamics and its applications in chemistry and chemical engineering

Detailed aims

After the course the students should be able to explain and describe

- The properties of real gases in terms of intermolecular interactions
- The concept of Boltzmann distribution, microstate, molecular partition function and partition function of a system
- The principle of equipartition of energy and the difference in macroscopic properties between molecules behaving according to classical and quantum mechanics, respectively.
- The molecular interpretation of the macroscopic properties energy, entropy and temperature
- The Einstein model for simple crystals and to apply this model to calculate the heat capacity for crystalline compounds
- The molecular properties of regular mixtures and its ability to predict phase separation in liquid mixtures
- The molecular properties of liquids and the concept of radial distribution function
- The methods of Monte Carlo and Molecular Dynamics simulations of liquids
- The molecular thermodynamic properties of simple macromolecules
- The principles of experimental scattering techniques and the concepts of form factor, structure factor and radius of gyration and their relations to statistical thermodynamic properties of macromolecules in solution

The student should also be able to calculate

- The translational, rotational and vibrational partition functions for a monoatomic, diatomic and triatomic molecule
- Thermodynamic state properties and equilibrium constants for ideal gases from spectroscopic data

The student should also be able to determine

- The molecular weight and radius of gyration of macromolecules from static light scattering data

Course contents

- Molecular properties of real gases

- Boltzmann distribution and partition functions
- The theorem of equipartition of energy
- Statistical thermodynamics of ideal gases
- The Einstein model of simple crystals
- Molecular interpretation of entropy
- Regular mixtures
- Introduction to statistical thermodynamics of liquids
- Molecular simulation methods
- Molecular and thermodynamic properties of simple macromolecules in solution
- Introduction to small-angle neutron and x-ray scattering and classical light scattering

Course literature

McQuarrie and Simon, Molecular Thermodynamics, University Science Books 1999, ISBN 1-891389-05-X

Examination

- TEN1 - Examination, 6.5 credits, grading scale: A, B, C, D, E, FX, F
- LAB1 - Laborations, 1.0 credits, grading scale: P, F

Based on recommendation from KTH's coordinator for disabilities, the examiner will decide how to adapt an examination for students with documented disability.

The examiner may apply another examination format when re-examining individual students.

If the course is discontinued, students may request to be examined during the following two academic years.

Other requirements for final grade

Written examination (TEN1; 6.5 hp)

Laboratory Work, presentation of project work (LAB1; 1.0 hp)

The final grade is based on the grade of the examination when the requirements of the laborations are fulfilled.

Ethical approach

- All members of a group are responsible for the group's work.
- In any assessment, every student shall honestly disclose any help received and sources used.

- In an oral assessment, every student shall be able to present and answer questions about the entire assignment and solution.