

SYLLABUS DEL CORSO

Chimica Fisica I

2122-2-E2702Q009

Aims

The aim of the course is to provide the basic concepts of classical thermodynamics for the study of macroscopic systems, in order to predict the spontaneous evolution of the processes and the achievement of the equilibrium state.

Knowledge and understanding

At the end of the course the student knows:

- the quantities used for the thermodynamic description of macroscopic systems and the definition of state variables;
- the models of perfect gas and real gases;
- the first law of thermodynamics: energy and enthalpy and their variations in physical and chemical processes;
- the second and third law of thermodynamics: entropy and its variation in physical and chemical processes;
- free energy and its variation in processes involving pure substances, simple mixtures and chemical reactivity.

Applying knowledge and understanding

At the end of the course the student is able to:

- calculate the energy and enthalpy variations in physical and chemical processes;
- calculate entropy variations in physical and chemical processes;
- calculate the variation of free energy in processes involving pure substances, simple mixtures and chemical reactivity for the prediction of the spontaneous evolution of the systems and of the final equilibrium state.

Making judgements

At the end of the course the student is able to identify, based on the considered system:

- the state variables necessary for the description of the system;
- the thermodynamic potential to be used for the study of the spontaneous evolution of the system and the characterization of the state of equilibrium.

Communication skills

The students knows how to present in a clear and correct way the reasoning and the calculations carried out for the solution of the problems in the written examination; during the oral examination, he also knows how to present the topics proposed by the teacher with language properties.

Learning skills

To be able to apply the acquired knowledge to different contexts from those presented during the course, and to understand the topics covered in the scientific literature concerning the thermodynamic aspects of the processes of interest.

Contents

Description of macroscopic systems; perfect gases and real gases; first law of thermodynamics, Energy and Enthalpy; Entropy, second and third law of thermodynamics; free energy and equilibrium; physical transformations of pure substances; simple mixtures; chemical equilibrium.

Detailed program

Description of macroscopic systems: thermodynamic representation of physical systems; work and heat definitions; mathematical description of the systems; cyclic processes. **Perfect gases and real gases:** the state equation of perfect gases; real gases; modeling of real gases. **First law of thermodynamics, Energy and Enthalpy:** molecular interpretation of energy variations; measurement of exchanged heat as a state variable; thermal capacity of gases; pure compounds: dependence of C_v , C_p , E and H from the temperature; expansion of an ideal gas; changes in Energy and Enthalpy; Thermochemistry: calculation of enthalpy variations. **Entropy, second and third law of thermodynamics:** spontaneous processes and second law; the second law of thermodynamics; criterion of spontaneous transformations in terms of Entropy; molecular interpretation of Entropy; mathematical combination of the first and second law; the third law of thermodynamics; Entropy variation in physical transformations of pure compounds; variation of Entropy in physical transformation of mixtures: mixing Entropy; reaction Entropy and its temperature dependence; heat engine; refrigeration cycle. **Free energy and equilibrium:** Gibbs free energy and Helmholtz free energy; the criterion of spontaneous transformations in terms of free energy; meaning of free energy; Gibbs free energy variation in pure compounds. **Physical transformations of pure substances:** phases and phase transformations; phase diagrams; Clausius-Clapeyron equation; changes in properties in correspondence with phase transitions. **Simple mixtures:** the partial molar quantities; the thermodynamics of mixing; the chemical potential of liquids; the thermodynamic properties of solutions; real solutions and activities; phase diagrams of binary systems. **Chemical equilibrium:** molar standard free energy of reaction; the response of equilibria to the conditions; electrochemical equilibrium.

Prerequisites

Mathematics: differential calculus for functions with one or more variables; integrals; differential equations. General Chemistry: properties of gases and solutions; stoichiometric calculations related to chemical equilibria. Physics: work and energy.

Teaching form

The course includes 5 CFU (35 hours) of lectures and 3 CFU (36 hours) of numerical exercises. During the exercises, problems are presented, with increasing complexity, to be solved using the knowledge acquired in frontal lessons. The issues addressed during the exercises will be the subject of the written tests. The performance of the problems, led by the teacher, tends to develop and strengthen the student's ability to identify the most suitable procedures to find the solution.

Textbook and teaching resource

Lecture notes of the teachers: U. Cosentino, D. Pitea *Elementi di Chimica Fisica*

P.W. Atkins, J. de Paula *Physical Chemistry*, 9a edition, 2011, Oxford University Press, or other editions

Videotaping of the lessons on the e-learning page of the course.

Semester

First semester

Assessment method

The exam consists of a written test and an oral interview.

which must be passed with a mark higher than or equal to 15/30.

The tests are divided into 2 or 3 exercises to be performed in two hours; the exercises proposed generally have the same "weight" from the point of view of evaluation. The exercises focus on the topics of the course that were the subject of the exercises carried out in class. The written test, which must be passed with a mark higher than or equal to 15/30, is valid for 6 months for the oral interview..

The oral exam includes a discussion on the outcome of the written test and questions on the topics of the course. Starting from the vote obtained in the written test, the student will be assessed on the basis of the following criteria: knowledge and understanding; ability to connect different concepts; exhibition skills; autonomy of analysis and judgment; ability to use scientific language correctly.

The final grade, expressed in thirtieths with possible praise, is given by the average of the two tests.

At the request of the student, the exam can be conducted in English.

Office hours

Every day, by appointment
