



CHM1351 Physical chemistry and physico-chemical calculations

[45h+19h exercises] 6 credits

This course is not taught in 2005-2006

Language: French

Level: First cycle

Aims

The objective of the course is to guide students in acquiring basic knowledge in physical chemistry and to apply it to diverse concrete cases. A systematic presentation of the thermodynamic bases (classical and statistical) as well as chemical kinetics, indispensable to the general formation of a chemist or biochemist is provided.

Main themes

Phenomenological aspects of thermodynamics : structure of matter, first and second law of thermodynamics, changes of state : pure materials, phase diagrams, chemical reaction, thermochemical models.

Phenomenological aspects of chemical kinetics : rate constant and reaction orders, simple and complex kinetics, reaction and diffusion, surface processes.

Microscopic aspects of thermodynamics and kinetic theory : statistical thermodynamics : complexions, distributions, partition function, derivation of thermodynamic functions, kinetic theories : transition state theory, potential surfaces and collision dynamics.

Exercises : they aim to concretize and put into practice the thermodynamic and chemical kinetics concepts. The use of microcomputers is an important element to solve the problems of a normal complexity.