



SC

**CHIM2161 Chimie physique et calculs physico-chimiques 1ère partie: thermodynamique
2ème partie: cinétique**

[67.5h+29h exercises] 9 credits

Teacher(s): Daniel Peeters, Jacques Vandooren
Language: french
Level: 2nd cycle course

Aims

Systematic presentation of classical and statistical thermodynamics as well as bases of chemical kinetics, indispensable to the general formation of a chemist or biochemist.

Main themes

Phenomenological aspect of thermodynamics: material structure, 1st and 2nd laws of thermodynamics, changing states: pure materials, mixtures, phase diagrams, chemical reaction, thermo chemical models. Microscopic aspects of thermodynamics and kinetic theory: statistical thermodynamics: number of complexions, different distributions, partition functions, derivation of thermodynamic functions, theoretical thermo chemistry and chemical links, kinetic theories: activated complex theory, potential surface and collision dynamics. Phenomenological aspects of kinetic chemistry: speed constants, complex kinetics, reaction and diffusion, surface processes. Exercises: the exercises will allow to put in concrete form and to practice the notions of thermodynamics and chemical kinetics thought. The use of microcomputers is an important element of this course, allowing to consider the problems of a normal complexity.