PHYS2110 Molecular statitical physics

[30h] 4 credits

This course is taught in the 1st semester

Teacher(s):	André Nauts
Language:	French
Level:	Second cycle

Aims

The objective of the course is to interpret, at a molecular level, the results of thermodynamics and molecular kinetics by means of quantum and statistical mechanics.

Main themes

Statistical thermodynamics : Boltzmann equation, statistical thermodynamics, the ideal gas in Maxwell-Boltzmann statistics, Bose-Einstein corrections, general expansion for U(T) and H(T), reaction and equilibrium constants, rate constants and Eyring theory.
Theoretical molecular physics : Hartree-Fock-Roothaan equations and configuration interactions, computation of molecular properties, electronic density, electric dipole moment, potential surfaces, physical basis of the chemical bond.

Other information (prerequisite, evaluation (assessment methods), course materials recommended readings, ...)

PREREQUISITE : Elements of quantum and statistical mechanics.
ASSESSMENT : Oral examination with written preparation.
TEACHING AIDS : Notes written by the teacher, overhead transparencies. List of recommended books.

Other credits in programs

PHYS22/A	Deuxième licence en sciences physiques (Physique appliquée)	(4 credits)	Mandatory
PHYS22/G	Deuxième licence en sciences physiques	(4 credits)	Mandatory