



## CHIM2252 Chimie organique physique II

[22.5h+0h exercises] 2.5 credits

This course is not taught in 2005-2006

This course is taught in the 1st semester

Language: French

Level: Second cycle

### Aims

Quantitative interpretation of electronic structure and of physico-chemical properties of organic molecules.

### Main themes

1. Electronic structure of organic molecules; hybridisation and stereochemistry ; calculation of intra- and intermolecular perturbations ; diagrams of orbital correlation and symmetry rules ; theoretical interpretation of some physico-chemical properties.
2. The theory of activated complexes: basic principles, surface potential, activation energy, energy profile of an organic reaction, principle of Polanyi-Evans-Bell; reactivity-selectivity, principle of Curtin-Hammett.
3. Theory of chemical reactivity: static and dynamic methods; transition state in aromatic and arylaliphatic substitution ; methods of Fukui and its applications to organic reactions.
4. Hard and soft acids and bases.
5. Theoretical bases of linear free energy relationships.
6. Stereo-electronic effects. Theoretical exercises conceived and realized in a way to insure an aptitude of autonomous calculation and interpretation.

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

Prerequisites: organic chemistry, physical chemistry.

Evaluation: oral examination with written preparation.

Support: course notes written by the teacher.

### Other credits in programs

CHIM22 Deuxième licence en sciences chimiques