



## CHIM2251 Physical organic chemistry I

[22.5h+0h exercises] 2.5 credits

This course is taught in the 2nd semester

**Teacher(s):** Olivier Riant Language: French Level: Second cycle

#### Aims

This course aims to familiarize the students with the main methods in organic physical chemistry that allow to establish the mechanisms of reactions, to precise the structures of active complexes and to understand the molecular interactions that affect the reactivity. The course, accessible to students in their first year of licence, is a good introduction to the study techniques of enzymatic system action mechanisms.

#### Main themes

- 1. Property-structure relations: theoretical base: elements of Marcus' theory, applications to electron transfers (catalysis by electron transfer) the empiric relations of free energy: quantitative estimation of electron and steric effects (Hammett and Taft relations), applications to the establishment of reaction mechanisms Relation between alkalinity and nucleophily predictions on reactivity based on standard thermodynamic parameters.
- 2. Acid-base catalysis : definitions and experimental highlighting Broensted relations and their physico-chemical interpretations relation between acid and base structure, proton transfer speed and reaction mechanism the diagrams of reaction representation Case study.
- 3. Molecular interactions, molecular complexes, dissolving: comparison of chemistry in gaseous phase and in solution molecular forces, dissolving, ion pairs, molecular complexes Hydrophobic forces solvent effects.
- 4. Intermolecular catalysis and intramolecular catalysis.

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

Prerequisites: CHIM1270, CHIM2140. Evaluation: written examination.

Support: course notes, books from CHIM library.

### Other credits in programs

CHIM21 Première licence en sciences chimiques
CHIM22 Deuxième licence en sciences chimiques