

COURSE TITLE

Chimica Organica Fisica
Physical Organic Chemistry
(*Chemistry Bachelor*)

Prof. Vincenzo Frenna (e-mail: vincenzo.frenna@unipa.it)
Classroom site: Viale delle Scienze, Building 17, Room D

Credits (CFU) = 6

COURSE PROGRAM

face-to-face lectures (48 hrs, 8 CFU)

Molecular orbitals. Huckel method. Valence bond method. Frontier orbitals. Klopman equation. Hard and soft acids and bases. Chemical reactions and conservation of the orbitals symmetry. Correlation diagrams. Structure and mechanism. Kinetics. Transition states. Examples. Kinetics and thermodynamics. Arrhenius equation. Reaction coordinate. Zero-point energy. Activation parameters. Isotope effect and kinetics. Solvent effect. Winstein-Grunwald equation. Examples. Principles of Physical Organic Chemistry. Reactivity selectivity principle. Hammond postulate. Lefler hypothesis. Microscopic reversibility principle. Kinetic and thermodynamic control. Reaction coordinate analysis. Potential energy surface. More O'Ferrall Jencks diagrams. Marcus theory. Free energy linear relations. Reaction constant. Yukawa Tsuno equation. Hammett equation. Taft equation. Fujita Nishio equation. Brønsted acids and bases. Acids and bases strength. Acid and basic catalysis. Brønsted equation. Reaction intermediates. Carbocations. Carboanions. Radicals.

TEXTBOOKS

T. H. Lowry, K. S. Richardson-Mechanism and Theory in Organic Chemistry-III Ed.
E. V. Anslyn, D. A. Dougherty – Modern Physical Organic Chemistry.
R. Alder, R. Baker, J. M. Brown – Meccanismi di reazione della Chimica Organica.