

Course description

Course Title Physical Organic Chemistry - Supramolecular Chemistry Química Físico-Orgânica – Química Supramolecular		
Type/Attendance Time Lecture: 3 hours per week Tutorial: 1 hour per week	Credit points (ECTS) 6	Type of Examination 1 written exam + 1 seminar talk
Recommended Prerequisites none		
Content <ol style="list-style-type: none"> 1. Basics: potential energy surfaces, thermodynamics and kinetics, Michaelis-Menten kinetics and catalysis, Hammond postulate, linear free enthalpy relationships, kinetic isotope effects, investigation of reaction mechanisms, elusive intermediates, short intro into symmetry and stereochemistry 2. Structure and Bonding: MO theory, aromatic, non-aromatic, antiaromatic molecules, Jahn-Teller theorem, conformation analysis 3. Pericyclic reactions: Woodward-Hoffmann rules for the different types of pericyclic reactions: cycloadditions, electrocyclic reactions, sigmatropic rearrangements, cheletropic reactions, correlation diagrams, frontier molecular orbitals, orbital coefficients and regiochemistry in cycloadditions, orbital energies and reaction rates, group transfer reactions 4. Carbenes, nitrenes, radicals, photochemistry: stable carbenes, azoketones and Wolff rearrangement, oxirene, nitrene oxide, Jablonski term scheme, radiative and non-radiative processes, excimers, exciplexes 5. Environment effects: solvatochromism, Winstein-Grunwald equation, gas-phase chemistry and solution in comparison: gas-phase acidities, gas-phase nucleophilicities 6. Non-covalent interactions: classification, physical basis 7. Fundamental concepts in supramolecular chemistry: key-lock principle and induced fit, host-guest chemistry and molecular recognition, preorganization, self-assembly, template effects, allosterics, cooperativity, multivalency 8. Methods in supramolecular chemistry: dynamic NMR spectroscopy, IR, UV/Vis, CD spectroscopy and crystal structure analysis as evidence for complex formation 9. Architectures: Metallo-supramolecular aggregates, hydrogen-bonded capsules, molecules with mechanical bonds 10. Functional molecules: molecular devices, logic gates, artificial photosynthesis Conteúdo <ol style="list-style-type: none"> 1. Fundamentos; 2. Estrutura e ligações; 3. Reações pericíclicas; 4. Carbenos, nitrenos, radicais, fotoquímica; 5. Efeitos ambientais; 6. Interações não-covalentes; 7. Conceitos fundamentais em química supramolecular; 8. Métodos em química supramolecular; 9. Arquiteturas; 10. Moléculas funcionais. 		