Institutionen för organisk kemi

Stockholms universitet

# Kursplan

för forskarkurs

**Physical Organic Chemistry** **15.0 Högskolepoäng**

**Physical Organic Chemistry** **15.0 ECTS credits**

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| **Kurskod:** | KO40003 |
| **Gäller från:** | VT 2020 |
| **Institution** | Institutionen för organisk kemi |

**Förkunskapskrav och andra villkor för tillträde till programmet**

Admitted to PhD studies. The course "KO7003 - Advanced Organic Synthesis (15 ECTS)", or equivalent, is not required but highly recommended.

**Lärandemål**

After the course the student should be able to:
• Build and analyze molecular orbital diagrams and Walsh diagrams. Demonstrate knowledge in the role of orbital overlap, orbital symmetry and orbital energies in the chemical bonding
• Evaluate the molecular orbital basis of the interactions in organic molecules, such as conjugation, hyperconjugation, aromaticity, anomeric effect and Jahn-Teller distortion
• Analyze organic reactions using functions and concepts of thermodynamics and thermochemistry, such as the Gibbs free energy, the Helmholtz equation, the bond dissociation energy, the heat of formation, the A-values, and the Bredt's rule
• Analyze the factors that determine the strengths non-covalent binding forces including ion-dipole, dipole-dipole interactions, dispersion forces and hydrogen bonding
• Analyze and predict the reactivity of acid-base systems in terms of the equilibrium constant (pKa) dependence on substituent effects (i.e. molecular orbital interactions), and the molecular environment (i.e. solvent effects)
• Analyze potential energy surfaces of reactions and interpret the experimental consequences by means of transition state theory
• Analyze reaction coordinate diagrams in terms of the Hammond's postulate, the Curtin-Hammett principle, and the microscopic reversibility principle
• Analyze electron transfer reactions in terms of the Marcus theory
• Deduce and analyze the basic rate laws of reaction networks using the steady state approximation and microkinetic simulation software, using basic concepts in chemical kinetics, such as equilibrium kinetics, initial-rate kinetics, and saturation kinetics
• Analyze and predict the role of organic functionality in the reactivity in terms of field, and inductive, resonance, steric, or solvation effects
• Analyze and predict the correlation between properties and reactivity of organic by using linear free energy relationships (LFER; i.e. Hammet plots), and quantitative structure-activity relationships (QSAR)
• Evaluate the origin of kinetic isotope effects (KIE; i.e. primary, secondary, and equilibrium), and interpret the results of KIE mechanistic experiments to extract the information on the rate-determining and selectivity-determining steps in the mechanism of organic reactions
• Analyze and predict the stereochemical outcome of chelated and unchelated carbonyl addition reactions (i.e.: Felkin-Anh's, Cram's, Karabatsos' and Zimmerman-Traxler models) using advanced Newman projections, molecular orbital interactions and stereoelectronic effects.
• Analyze and predict the relative rate and/or efficiency of series of related cyclization, addition and rearrangement reactions (for example, but not limited to: Baldwin rules, transannular interactions, solvent

effects, charge dispersion, non-classic carbocations).
• Design mechanistic experiments to obtain information about the stereochemical course of fundamental organometallic reactions and advanced pericyclic (for example, but not limited to: cycloadditions, sigmatropic and cheletropic) processes.
• Analyze the viability and outcome of thermal and photochemical pericyclic reactions using the concepts of molecular orbital overlap, orbital symmetry and orbital energies.
• Propose reasoned mechanisms for organic reactions involving open-shell, excited state and biocatalytic intermediates based on kinetic and stereochemical data.

**Innehåll**

Course content:

The aim of the course is to complement the education in organic synthesis and catalysis with an advanced perspective on the physical origin of chemical reactivity in organic molecules.
The main emphasis will be placed in the fundamental aspects of bonding, conformation, thermodynamics, kinetics that allow to explain and predict the behaviour of chemical systems.
The lectures are based on, but not limited to, a selection of chapters from the book "Modern Physical Organic Chemistry" by E. V. Anslyn, D. A. Dougherty (2nd Edition, Oxford University Press 2012). This base material will be complemented by printed copies of the handouts from the lecturers and the assistant(s).
In addition to the theoretical discussion, the course is complemented with embedded practice or seminar sessions that illustrate the importance of rational approaches in the solution of important problems in organic chemistry.
Formative assessment to help the student meet the learning outcomes is accomplished through assignments, oral presentations and the active participation in lectures and seminars.

**Obligatoriska moment**

Participation in lectures and seminars is compulsory. In the event of special circumstances, the examiner may, after consultation with the teacher concerned, grant a student exemption from the obligation to participate in certain compulsory instruction.

**Examinationsformer**

The course is examined as follows:
Knowledge assessment takes the form of a written exam and participation in seminars.
The course and examination language is English.
Grading (passed or failed) is related to the intended learning outcomes.
Grading criteria are handed out at the start of the course.
Students who receive a failing grade on a regular examination are allowed to retake the examination as long as the course is still given. The number of examination opportunities is not limited. Other mandatory course elements are equated with examinations. A student who has failed the examination twice is entitled to have another examiner appointed, unless there are special reasons to the contrary. Such requests should be made to the department board.
The course has at least two examination occasions per year when the course is given.
A pass grade is required in all the three parts in which the examination is divided, as well as participation in all compulsory education (see above).

**Arbetsform**

Instruction (in English) consists of lectures and seminars.