Physical Organic Chemistry KO7008 Spring/2018

The lectures are in lecture hall A501 from 9.30-12.30

Tuesday 23 January: Introduction, registration, E1

Monday 29 January: E2

Tuesday 30 January: L1

Tuesday 6 February: L2

Monday 12 February: E3

Tuesday 13 February: L3

Monday 19 February: E4

Tuesday 20 February: L4

Tuesday 27 February: L5

Tuesday 6 March: L6

Tuesday 13 March: L7

Tuesday 27 March: L8

Wednesday 4 April: L9

Tuesday 10 April: L10

Thursday 12 April: L11

Monday 16 April: E5

Tuesday 17 April: L12

Thursday 19 April: L13

Tuesday 24 April: L14

Wednesday 2 May: L15

Tuesday 8 May: L16

Wednesday 16 May: L17

Tuesday 22 May: L18

Tuesday 29 May: L19

Thursday 31 May L20

Tuesday 5 June: Exam

Lecture teachers

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Jan-Erling Bäckvall (L14-19): jeb@organ.su.se 08-674 7178

Exercise teacher

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Lecture Contents

L1-2 (KS): Basic bonding concepts, symmetry; Perturbation MO theory. Orbital mixing, stabilization; group orbitals, geometry and electronegativity perturbation.

L3-4 (KS): Bond dissociation and stability. Construction and understanding of MO and Walsh diagrams: Carbocations, anions, carbenes and radicals; Orbital effects: aromacity, conjugation, hyperconjugation, anomeric effect, Jahn-Teller effect; Non-covalent bonding.

L5 (KS): Acid-base chemistry. Electronic and structural effects on the acidity and basicity. Pericyclic reactions based on FMO theory.

L6-7 (KS): Organometallic complexes. Metal-ligand bonding. σ,π-Bonding, carbonyl, carbene and phosphine complexes. Isolobal analogies. Basic reaction mechanisms (MO description).

L8 (FH): Transition state theory; Relationship between kinetics and potential energy surfaces; Kinetic and thermodynamic control; Hammond Postulate; Curtain-Hammett Principle.

L9-10 (FH): Chemical kinetics, first-order, second order and consecutive reactions, Michaelis Menten kinetics; Methods for solvation of kinetic equations; Kinetics simulations.

L11 (FH): Kinetic isotope effect.

L12 (FH): Linear free energy relationships; QSAR.

L13 (FH): Catalysis; Application of DFT modeling in mechanistic studies.

L14-15 (JEB): Repetition/summary of basic reaction mechanisms: nucleophilic, electrophilic, radical and redox mechanisms; Transition metal catalyzed reactions.

L16-17 (JEB): Methods for mechanistic studies. Qualitative and quantitate methods. Choice of experimental methodology. Study of asymmetric catalysis.

L18-19 (JEB): Examples for advanced mechanistic studies. Palladium catalyzed 1,4-oxidation and DKR (including the mechanism of transfer hydrogenation).

L20 (JEB) Preparation for the exam. Solving problems.

Exercises

E1: Chemical group theory
E2-E3: Construction of orbital diagrams and Walsh diagrams using pertubational MO theory and chemical group theory. Interpretation of these diagrams.
E4: Construction and interpretation of the MO diagram of transition metal complexes (e.g. ML_6 O_h symmetrical complex).
E5: Kinetics simulations

Literature

E.V. Anslyn, D. A. Dougherty: Modern Physical Organic Chemistry. ISBN: 978-1-891389-31-3.