

UČNI NAČRT PREDMETA / COURSE SYLLABUS

Predmet: ORGANSKA KEMIJA
Course Title: ORGANIC CHEMISTRY

Študijski program in stopnja Study Programme and Level	Študijska smer Study Field	Letnik Academic Year	Semester Semester
MAG Kemija, 2. stopnja	/	1.	2.
USP Chemistry, 2 nd Cycle	/	1 st	2 nd

Vrsta predmeta / Course Type:

obvezni / Mandatory

Univerzitetna koda predmeta / University Course Code:

KE213

Predavanja Lectures	Seminar Seminar	Vaje Tutorial	Klinične vaje Work	Druge oblike študija	Samost. delo Individual Work	ECTS
45	/	30 LV	/	/	75	5

Nosilec predmeta / Lecturer:

prof. dr. Bogdan Štefane / Dr. Bogdan Štefane, Associate Professor

Jeziki / Languages:

Predavanja / Lectures: slovenski / Slovenian

Vaje / Tutorial: slovenski / Slovenian

Pogoji za vključitev v delo oz. za opravljanje študijskih obveznosti:

Študent oz. kandidat mora imeti predmet opredeljen kot študijsko obveznost.

Prerequisites:

The course has to be assigned to the student.

Vsebina:

1. Mehanizem kemijske reakcije.
Definicija, elementarne in stopenjske reakcije, tvorba in cepitev vezi, molekularnost, formuliranje mehanizma.

2. Kinetika in termodinamika organskih reakcij.
Konstanta, sprememba proste energije, entalpije in entropije, kisline, baze, pH, pK_a, uporaba podatkov o pK_a pri ravnotežjih in reakcijah. Reakcijska hitrost, red reakcije, uporaba podatkov o reakcijski kinetiki pri predlaganju mehanizma reakcije, Arrheniusova enčba, aktivacijska energija, primarni kinetski izotopski efekt.

3. Prehodno stanje.

Content (Syllabus outline):

- Mechanism of a chemical reaction: definitions, elementary and stepwise reactions, bond making and bond breaking, molecularity, formulating mechanisms.
- Kinetics and thermodynamics of organic reactions: Equilibrium and rate constants, acids, bases, pK_a, pH, kinetic order, application of kinetic data in formulating the mechanism, the dependence of rate of reaction on temperature, primary kinetic isotopic effect.
- The transition state: transition state theory, early- and late transition states,

Prehodno stanje, teorija prehodnega stanja, zgodnje in kasno prehodno stanje, Hammondov postulat, vpliv topila na ravnotežje in reakcijsko hitrost, empirične skale polarnosti topil, elektronski efekti funkcionalnih skupin, Hammettove korelacije (LFER), sigma (σ) in rho (ρ) vrednosti, sklepanje na mehanizem na osnovi Hammettovih korelacij, sterični vplivi, stereokemija reakcij, kinetska in termodinamska kontrola reakcije, kataliza (splošna ter specifična kislinska in bazna kataliza, vpliv topila)

4. Intermediat pri kemijskih reakcijah.

Nastanek, struktura, detekcija, reakcije. Anioni in nukleofilne reakcije. Kationi in elektrofilne reakcije. Radikali in karbeni.

5. Molekularne reakcije.

Simetrija molekularnih orbital pri molekularnih reakcijah, Diels-Alderjeva reakcija, periciklične in elektrociklične reakcije, sigmatropne premestitve, Woodward-Hoffmanova pravila.

Hammond postulate, solvent effects, electronic effects, linear free energy relationship (LFER; Hammett correlations), application of LFER in postulating the mechanism, steric effects, stereochemistry, kinetic and thermodynamic control, catalysis.

4. Intermediates in organic reactions: structure, detection, reactivity, anions and nucleophilic reactions, cations and electrophilic reactions, radicals, carbenes, and nitrenes.

5. Molecular reactions: molecular orbital symmetry in molecular reactions, Diels-Alder reactions, pericyclic and electrocyclic reactions, sigmatropic rearrangements, Woodward-Hoffman rules.

Temeljna literatura in viri / Readings:

- Paul H. Scudder: *Electron flow in organic chemistry*. (2nd Ed. John Wiley & Sons, Inc., 2013);
- R. A. Jackson, *Mechanisms in Organic Chemistry*, The Royal Society of Chemistry, 2004 (199 pages).

Dodatna literatura / Additional reading: J. Clayden, N. Greeves, S. Warren, P. Wothers, *Organic Chemistry*, Oxford University Press, Oxford, 2001.

A. Petrič, *Organska kemija* (interno študijsko gradivo), UL FKKT, Ljubljana, 2014 (197 str.).

Cilji in kompetence:

Cilji: Študent se na primerih enostavnejših kemijskih reakcij, ki jih je spoznal med študijem na prvi stopnji, nauči metod in principov določanja poteka reakcije – reakcijskega mehanizma.

Kompetence: Pridobljeno znanje študentu omogoča samostojen pristop k določanju mehanizma kemijskih reakcij, predvidevanje vplivov na potek kemijske reakcije in s tem možnost kvalificirano odločanje o spremembi reakcijskih pogojev za doseganje želenega cilja.

Objectives and Competences:

Objectives: Using selected standard transformations of organic compounds learned during the first cycle as examples the methods and principles of reaction mechanism / reaction path postulating is explained.

Competences: Ability to design, interpret, and analyze appropriate experiments required for postulating a reaction mechanism for a given organic reaction. Ability to make qualified decisions about the required changes in reaction conditions to achieve the desired effect on the reaction in question.

Predvideni študijski rezultati:

<u>Znanje in razumevanje</u> Poznavanje poteka osnovnih organskih reakcij in metod za študij oziroma dokazovanje reakcijskih mehanizmov. Razumevanje in poznavanje vplivov na potek kemijskih reakcij.
<u>Uporaba</u> Razvita sposobnost študenta, da pridobljeno znanje uporabi za raziskavo mehanizma neznane reakcije.
<u>Refleksija</u> Zavedanje, da kemijske reakcije v praksi nikoli popolnoma ne sledijo osnovnim mejnim mehanizmom ter da je za popolno razjasnitev poteka reakcije potreben natančen študij vsake reakcije posebej.
<u>Prenosljive spretnosti</u> Pri predmetu se študenti z reševanjem znanih in neznanih problemov izurijo v uporabi znanja, analitičnega mišljenja in uporabe literaturnih virov.

Intended Learning Outcomes:

<u>Knowledge and Comprehension</u> Understanding the principles and methods of postulating the reaction mechanism of an organic reaction. Understanding the influence of different parameters on reaction course.
<u>Application</u> Student will be able to apply the acquired knowledge in reaction mechanism investigation.
<u>Analysis</u> Being aware that chemical reactions never follow exclusively one elementary mechanism and that for complete analysis every reaction requires thorough investigation.
<u>Skill-transference Ability</u> Using known and unknown examples the student is trained in utilization of knowledge, analytical thinking and using literature sources.

Metode poučevanja in učenja:

- Predavanje in vaje.

Learning and Teaching Methods:

Lectures and practical laboratory work.

Načini ocenjevanja:

Pisni izpit.

Delež (v %) /

Weight (in %) **Assessment:**

Written exam.

Reference nosilca / Lecturer's references:

1. ŠTEFANE, Bogdan. Selective addition of organolithium reagents to BF₂-chelates of -ketoesters. *Organic letters*, ISSN 1523-7060, 2010, vol. 12, no. 13, str. 2900-2903, doi: 10.1021/ol100620j. [COBISS.SI-ID 34162181]
2. WANG, Jingxin, ŠTEFANE, Bogdan, JABER, Deana, SMITH, Jacqueline A. I., VICKERY, Christopher, DIOP, Mouhamed, SINTIM, Herman O. Remote C-H functionalization : using the N-O moiety as a atom-economical tether to obtain 1,5- and the rare 1,7-C-H insertions. *Angewandte Chemie*, ISSN 1433-7851. [Print ed.], 2010, vol. 49, no. 23, str. 3964-3968, doi: 10.1002/anie.201000160. [COBISS.SI-ID 34061573]
3. NAKAYAMA, Shizuka, KELSEY, Ilana, WANG, Jingxin, ROELOFS, Kevin, ŠTEFANE, Bogdan, LUO, Yiling, LEE, Vincent T., SINTIM, Herman O. Thiazole orange-induced c-di-GMP quadruplex formation facilitates a simple fluorescent detection of this ubiquitous biofilm regulating molecule. *Journal of the American Chemical Society*, ISSN 0002-7863, 2011, vol. 133, no. 13, str. 4856-4864, doi: 10.1021/ja1091062. [COBISS.SI-ID 34845957]