UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	ORGANOKOVINSKA IN SUPRAMOLEKULARNA KEMIJA
Course Title:	ORGANOMETALLIC AND SUPRAMOLECULAR CHEMISTRY

Študijski program in stopnja Study Programme and Level	**Študijska smer Study Field**	**Letnik Academic Year**	**Semester Semester**
MAG Kemija, 2. stopnja	**/**	**2.**	**3.**
USP Chemistry, 2nd Cycle	**/**	**2nd**	**3rd**

Vrsta predmeta / Course Type: izbirni strokovni / Elective Professional

Univerzitetna koda predmeta / University Course Code: K2I06

Predavanja Lectures	**Seminar Seminar**	**Vaje Tutorial**	**Klinične vaje Work**	**Druge oblike študija**	**Samost. delo Individual Work**	**ECTS**
30	**15**	**30 LV**	**/**	**/**	**75**	**5**

Nosilec predmeta / Lecturer: prof. dr. Bogdan Štefane / Dr. Bogdan Štefane, Associate Professor
doc. dr. Andrej Pevec / Dr. Andrej Pevec, Assistant Professor

Jeziki / Languages:

Predavanja / Lectures:	**slovenski / Slovenian**
Vaje / Tutorial:	**slovenski / Slovenian**

Pogoji za vključitev v delo oz. za opravljanje študijskih obveznosti:	**Prerequisites:**
Študent oz. kandidat mora imeti predmet opredeljen kot študijsko obveznost.	The course has to be assigned to the student.

Vsebina:	**Content (Syllabus outline):**
1. Uvod 1.1. Opredelitev pojma organokovinska kemija 1.2. Opredelitev pojma supramolekularna kemija 1.3. Zgodovinski pregled in sodobni trendi 1.4. Nomenklatura organokovinskih in supramolekularnih spojin 2. Opredelitev tipa vezi in struktura organokovinskih in supramolekularnih spojin 2.1. 18-Elektronsko pravilo 2.2. Tipi vezi v organokovinskih in supramolekularnih spojinah	1. Introduction 1.1. The definition of organometallic chemistry 1.2. The definition of supramolecular chemistry 1.3. Historical survey and current trends 1.4. Nomenclature of organometallic and supramolecular compounds 2. Identifying the type of bond and the structure of organometallic and supramolecular compounds 2.1. 18-electrone rule 2.2. Types of bonds in organometallic and supramolecular compounds

2.3. Termodinamika in stabilnost vezi kovina-ogljik 2.4. Izmenjava ligandov in ravnotežja ligand-kovina 2.5. Interakcije v supramolekularnih sistemih 3. Ligandi in karakteristike ligandov 3.1. Karbonili, fosfini, hidridi 3.2. Alkili, metaloceni, karbeni, karbini, alkenilideni 3.3. Alkeni, areni, ciklopentadienili 3.4. Receptorji za vezavo kationov, anionov in nevtralnih molekul v supramolekularni kemiji 4. Sinteza najpomembnejših organokovinskih in supramolekularnih spojin 4.1. Organokovinske spojine elementov glavnih skupin 4.2. Organokovinske spojine prehodnih elemntov 4.3. Priprava supramolekularnih verig, spiral, pentelj, poligonov, rotorjev in kapsul 5. Uporaba organokovinskih spojin v organski sintezi 5.1. Mehanizmi in katalitski cikli 5.2. Homogena in heterogena kataliza in njuni posebnosti 5.3. Supramolekularna kataliza in encimska mimetika 5.4. Tvorba C–C vezi 5.5. Tvorba C–heteroatom vezi 5.6. Oksidacijske reakcije 5.7. Redukcijske reakcije 5.8. Stereokemija v organokovinski kemiji 5.9. Polimerizacije 6. Primeri praktične uporabe organokovinskih spojin in supramolekularnih sistemov v moderni kemiji.	2.3. Thermodynamics and stability of the metal-carbon bonds 2.4. The exchange of ligands and ligand-metal equilibrium 2.5. Interactions in supramolecular systems 3. Ligands and ligand characteristics 3.1. Carbonyls, phosphines, hydrides 3.2. Alkyls, metallocenes, carbenes, carbynes, alkylidenes 3.3. Alkenes, arenes, cyclopentadienyls 3.4. The receptors for binding of cations, anions and neutral molecules in the supramolecular chemistry 4. The synthesis of the most important organometallic and supramolecular compounds 4.1. Organometallic compounds of the main group elements 4.2. Organometallic compounds of the transition elements 4.3. Preparation of supramolecular chains, spirals, loops, polygons, rotors and capsules 5. The use of organometallic compounds in organic synthesis 5.1. Mechanisms and cataliytic cycles 5.2. Homogeneous and heterogeneous catalysis and their specifications 5.3. Supramolecular catalysis and enzyme mimetic 5.4. Formation of C-C bond 5.5. Formation of C-heteroatom bond 5.6. Oxidation reactions 5.7. Reduction reactions 5.8. Stereochemistry in organometallic chemistry 5.9. Polimerizacije 6. Examples of the practical application of organometallic compounds and supramolecular systems in modern chemistry.

Temeljna literatura in viri / Readings:

- J. Clayden, N. Greeves, S. Warren, P. Wothers, *Organic Chemistry*, Oxford University Press, Oxford 2001. (poglavje 48, 10 strani)
- A. F. Hill, *Organotransition Metal Chemistry*, The Royal Society of Chemistry, Cambridge, UK, 2002. (180 strani)
- J. W. Steed, D. R. Turner, K. J. Wallace, *Core Concepts in Supramolecular Chemistry and Nanotechnology*, J. Wiley & Sons, 2007. (90 strani)

Cilji in kompetence:

Objectives and Competences:

Cilji predmeta je spoznati tipične organokovinske in supramolekularne spojine, njihovo sintezo, laboratorijske tehnike, ki tako sintezo spremljajo, in metode karakterizacije. Predmet vključuje laboratorijske vaje, ki so zasnovane na principu povezave teorije in eksperimentalnega dela. Upoštevajoč, da kovine prehoda predstavljajo v organokovinski kemiji pomembno poglavje, ki ga lahko neposredno uporabimo v organski sintezi, bo vsebina tega predmeta usmerjena k spoznavanju organokovinskih transformacij, vloge kovin v katalitskih ciklih in uporabi organokovin v sintezi kompleksnih organskih spojin. Med slednje spadajo tudi »supermolekule«, ki povezujejo znanja področij anorganske in organske kemije, potrebnih za sintezo supramolekularnih sistemov, kot tudi znanja fizikalno-organske kemije za razumevanje lastnosti in njihovega kompleksnega obnašanja. Na osnovi predhodnega znanja bo študent pridobil primerjalno znanje med »klasičnim« sinteznim pristopom in »modernimi« metodami v organokovinski in supramolekularni kemiji. *Kompetence:* Z osvojenimi znanji in praktičnim delom bo študent sposoben naslednjih veščin: dela v inertni atmosferi z uporabo Schlenkove tehnike, uporabo vakuumskih tehnik, načina dela v suhi komori, sušenja inertnih plinov in organskih topil ter uporabe modernih spektroskopskih analiznih tehnik.	The aim of this course is to understand the typical organometallic and supramolecular compounds, their synthesis, laboratory techniques for preparation of these compounds and methods of characterization. The subject includes laboratory works, which are based on the principle to link the theory and experimental work. Considering that the transition metal organometallic chemistry represent an important chapter, which can be directly used in organic synthesis, the content of this course focus to learning about organometallic transformations, the role of metals in catalytic cycles and use organometallic compounds in the synthesis of complex organic compounds. Among the latter are also the "supramolecules" which linking knowledge between inorganic and organic chemistry needed for the synthesis of supramolecular systems, as well as knowledge of physical-organic chemistry for understanding the properties and their complex behavior. Based on the previous knowledge the student will informed of the correlation between the "classical" approach to the synthesis and "modern" methods of organometallic and supramolecular chemistry. With the acquired knowledge and practical work students will develop the following skills: working in an inert atmosphere using Schlenk techniques, the use of vacuum techniques, methods of work in the dry box, drying inert gases and organic solvents, and the use of modern spectroscopic analytical techniques.

Predvideni študijski rezultati:	**Intended Learning Outcomes:**
<u>Znanje in razumevanje</u> Poznavanje tematike, ki se skriva pod naslovom organokovinska kemija in supramolekularna kemija. Poznavanje strukture in reaktivnosti organokovinskih in supramolekularnih spojin. Poznavanje principov katalitskih procesov in razumevanje vloge kovine in ligandov. Pridobitev znanj s področja dela v inertni	<u>Knowledge and Comprehension</u> Acquire knowledge of the topic, which is hidden under the title organometallic chemistry and supramolecular chemistry. Acquire knowledge of the structure and reactivity of organometallic and supramolecular compounds. Acquire knowledge of the principles of catalytic processes and understanding the role of metals

atmosferi in vakuumu.	and ligands. Aquire a practical skills for working in an inert atmosphere and vacuum.
Uporaba Pridobljeno znanje in veščine se lahko uporabijo za reševanje praktičnih znanstvenih problemov in diskusijo o njih. Uporaba modernih znanj in metod organokovinske in supramolekularne kemije na drugih področjih (kemija reagentov, stereokemija, kemija materialov, nanotehnologija, biološka kemija, farmacija, medicina, …).	Application Acquired knowledge and skills can be used to solve practical scientific problems and discuss about them. Using modern knowledge and methods of organometallic and supramolecular chemistry in other areas (chemistry reagents, stereochemistry, materials chemistry, nanotechnology, biological chemistry, pharmacy, medicine...).
Refleksija Sistemi kovin prehoda kot katalizatorji ali reagenti predstavljajo kompleksno področje, ki se navezuje na anorgansko (koordinacijsko) kemijo. Obenem pa to področje od študenta zahteva znanje organske kemije in organske sinteze z osnovnim poznavanjem lastnosti kovin prehoda. Študent lahko na osnovi pridobljenih znanj kritično presoja med različnimi sinteznimi pristopi, pridobljena znanja vključuje v svoje praktično delo in načrtuje nadaljnje možnosti uporabe organokovinske kemije v organski sintezi. S pridobljenim znanjem iz supramolekularne kemije študent dobi uvid v povezanost in soodvisnost znanj anorganske, organske in fizikalne kemije za razumevanje lastnosti in obnašanja kompleksnih struktur.	Analysis Systems of transition metals as catalysts or reagents represent a complex area, which is linked to inorganic (coordination) chemistry. At the same time, this area requires knowledge of organic chemistry and organic synthesis with a basic knowledge of the properties of transition metals. A student can, based on knowledge gained, critical estimate of the various synthetic approaches, the acquired knowledge includes practical work and planning further possible use of organometallic chemistry in organic synthesis. The knowledge gained from supramolecular chemistry student gets insight into the interaction and interdependence of knowledge of inorganic, organic and physical chemistry to understand the properties and behavior of complex structures.
Prenosljive spretnosti Pridobljene veščine (delo v inertni atmosferi, čiščenje izhodnih spojin…) pri tem predmetu bodo študentu koristile tudi na drugih sinteznih področjih, kjer so predmet sinteze spojine občutljive pri atmosferskih pogojih.	Skill-transference Ability Acquired skills (work in an inert atmosphere, treatment of the starting compounds...) of the subject will also be useful to students at the other areas of the synthesis, where the compounds sensitive to atmospheric conditions are also important.

Metode poučevanja in učenja:	**Learning and Teaching Methods:**
Predavanje in vaje.	Lectures and laboratory work.

Načini ocenjevanja:	Delež (v %) / Weight (in %)	**Assessment:**

- Pisni izpit po uspešno opravljenem praktičnem delu.		-written exam -accomplished practical work

Reference nosilca / Lecturer's references:

- Hodgson, D. M.; Štefane, B.; Miles, T. J.; Witherington, J.: Unsaturated 1,2-Amino Alcohols and Ethers from Aziridines and Organolithiums, *Chem. Commun*. **2004**, 2234–2235.
- Hodgson, D. M.; Štefane, B.; Miles, T. J.; Witherington, J.: Organolithium-Induced Alkylative Ring Opening of Aziridines: Synthesis of Unsaturated Amino Alcohols and Ethers, *J. Org. Chem.* **2006**, *71*, 8510–8515.
- Štefane, B.; Polanc, S.: Aminolysis of 2,2-difluoro-4-alkoxy-1,3,2-dioxaborinanes: route to β-keto amides and β-enamino carboxamides, *Tetrahedron* **2007**, *63*, 10902–10913.

- A. Pevec, F. Perdih, J. Košmrlj, B. Modec, H. W. Roesky, A. Demšar: Lithium complexes with a $[Cp^*_2Ti_2F_7]^-$ ligand: ^{19}F NMR probe for lithium solvation.- *Dalton Trans.* **2003**, 420-425.
- A. Pevec: Syntheses and Solid-State and Solution Structures of $[Ba\{(C_5Me_5)_2Ti_2F_7\}_2(hmpa)]$ and $[Ba_8Ti_6F_{30}I_2(C_5Me_5)_6(hmpa)_6][I_3]_2$. - *Inorg. Chem.* **2004**, 43, 1250-1256.
- F. Perdih, A. Pevec, S. Petriček, A. Petrič, N. Lah, K. Kogej, A. Demšar: The Solution Structures and Dynamics and the Solid-State Structures of Substituted Cyclopentadienyltitanium(IV) Trifluorides:- *Inorg. Chem.* **2006**, 45, 7915-7921